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Conversion of 2-methyl-4-styrylquinolines into 2,4-distyrylquinolines: synthesis, and spectroscopic and structural characterization of five examples

Diana R. Vera,[a] Diana M. Ardila,[a] Alirio Palma,[a] Justo Cobo[b] and Christopher Glidewell[c]*

[a]Laboratorio de Síntesis Orgánica, Escuela de Química, Universidad Industrial de Santander, AA 678, Bucaramanga, Colombia, [b]Departamento de Química Inorgánica y Orgánica, Universidad de Jaén, 23071 Jaén, Spain, and [c]School of Chemistry, University of St Andrews, Fife, KY16 9ST, United Kingdom. *Correspondence e-mail: cg@st-andrews.ac.uk

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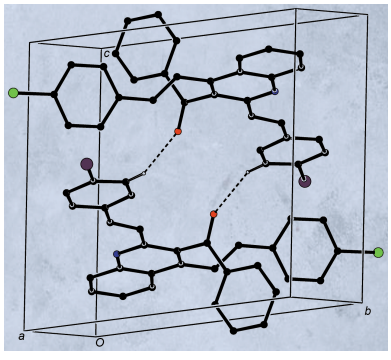
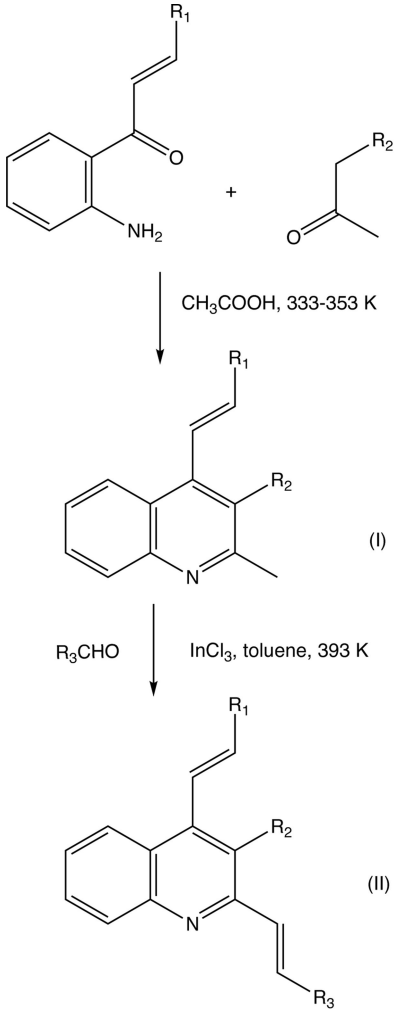
Four new 2,4-distyrylquinolines and one 2-styryl-4-[2-(thiophen-2-yl)vinyl]-quinoline have been synthesized using indium trichloride condensation reactions between aromatic aldehydes and the corresponding 2-methylquinolines, which were themselves prepared using Friedländer annulation reactions between mono- or diketones and (2-aminophenyl)chalcones: the products have all been fully characterized by spectroscopic and crystallographic methods. 2,4-Bis[(*E*)-styryl]quinoline, $C_{25}H_{19}N$, (IIa), and its dichloro analogue, 2-[(*E*)-2,4-dichlorostyryl]-4-[(*E*)-styryl]quinoline, $C_{25}H_{17}Cl_2N$, (IIb), exhibit different orientations of the 2-styryl unit relative to the quinoline nucleus. In each of the 3-benzoyl analogues {2-[(*E*)-4-bromostyryl]-4-[(*E*)-styryl]quinolin-3-yl}(phenyl)-methanone, $C_{32}H_{22}BrNO$, (IIc), {2-[(*E*)-4-bromostyryl]-4-[(*E*)-4-chlorostyryl]-quinolin-3-yl}(phenyl)methanone, $C_{32}H_{21}BrClNO$, (IId), and {2-[(*E*)-4-bromo-styryl]-4-[(*E*)-2-(thiophen-2-yl)vinyl]quinolin-3-yl}(phenyl)methanone, $C_{30}H_{20}$-BrNOS, (IIe), the orientation of the 2-styryl unit is similar to that in (IIa), but the orientation of the 4-arylvinyl units show considerable variation. The thiophene unit in (IIe) is disordered over two sets of atomic sites having occupancies of 0.926 (3) and 0.074 (3). There are no hydrogen bonds of any kind in the structure of (IIa), but in (IId), a single C—H···O hydrogen bond links the molecules into cyclic centrosymmetric $R_2^2(20)$ dimers. A combination of C—H···N and C—H···π hydrogen bonds links the molecules of (IIb) into a three-dimensional framework structure. A combination of three C—H···π hydrogen bonds links the molecules of (IIc) into sheets, and a combination of C—H···O and C—H···π hydrogen bonds forms sheets in (IIe). Comparisons are made with the structures of some related compounds.

1. Introduction

The quinoline nucleus is considered to be one of the most privileged scaffolds and to be a crucial pharmacophore in drug discovery because of its occurrence in a wide variety of natural and synthetic biologically active molecules (Solomon & Lee, 2011; Musiol *et al.*, 2017; Matada *et al.*, 2021). The outstanding therapeutic importance of quinoline derivatives is well known, particularly in the treatment of, for example, microbial (Lam *et al.*, 2014; Zhang *et al.*, 2018), malarial (Kaur *et al.*, 2010; Hu *et al.*, 2017; Okombo & Chibale, 2018; Orozco *et al.*, 2020), fungal (Musiol *et al.*, 2010; Kumar *et al.*, 2011), inflammatory (Chen *et al.*, 2006; Gilbert *et al.*, 2008), viral (Ghosh *et al.*, 2008; Matada *et al.*, 2021), protozoal (Fakhfakh *et al.*, 2003; Franck *et al.*, 2004; Kumar *et al.*, 2009), cardiovascular (Cai *et al.*, 2007; Bernotas *et al.*, 2009) and neoplastic diseases (Afzal *et al.*, 2015; Musiol, 2017; Cortes *et al.*, 2018; Lauria *et al.*, 2021; Yadav & Kamal, 2021).



Among different classes of quinoline derivatives, styrylquinolines, especially 2-styrylquinolines and to a lesser extent 4-styrylquinolines, have been studied extensively, mainly because of their potential as inhibitors of HIV-1 integrase (Leonard & Roy, 2008; Mahajan *et al.*, 2018; Mousnier *et al.*, 2004) and as antimicrobial (Kamal *et al.*, 2015), antifungal (Cieslik *et al.*, 2012; Szczepaniak *et al.*, 2017), anti-asthma (Matada *et al.*, 2021) and anticancer agents (Chang *et al.*, 2010; Mrozek-Wilczkiewicz *et al.*, 2015, 2019). The pharmacological



(a) $R_1 = C_6H_5$, R_2 = H, $R_3 = C_6H_5$
(b) $R_1 = C_6H_5$, R_2 = H, $R_3 = 2,4\text{-}C_6H_3Cl_2$
(c) $R_1 = C_6H_5$, $R_2 = COC_6H_5$, $R_3 = 4\text{-}BrC_6H_4$
(d) $R_1 = 4\text{-}ClC_6H_4$, $R_2 = COC_6H_5$, $R_3 = 4\text{-}BrC_6H_4$
(e) $R_1 = 2\text{-}C_4H_3S$, $R_2 = COC_6H_5$, $R_3 = 4\text{-}BrC_6H_4$

Scheme 1

relevance of these types of quinoline derivatives has prompted the development of different methodologies for the synthesis of drug-like compounds containing such styrylquinoline scaffolds (Staderine *et al.*, 2011; Yaragorla *et al.*, 2015; Sharma *et al.*, 2017; Musiol, 2020; Hazra *et al.*, 2020; Zhang *et al.*, 2020; Li *et al.*, 2021; Omar & Hormi, 2009; Lee *et al.*, 2009 Alacíd & Nájera, 2009; Jamal & Teo, 2014; Jamal *et al.*, 2016; Satish *et al.*, 2019; Meléndez *et al.*, 2020).

Unlike 2-styryl- and 4-styrylquinolines, the closely-related 2,4-distyrylquinolines have been scarcely investigated, with very few publications related to their synthesis and biological evaluation, and this scarcity may be due, at least in part, to the lack of satisfactory methods for their synthesis. The few reported 2,4-distyrylquinolines have been prepared by methods such as one-pot successive Arbuzov/Horner–Wadsworth–Emmons reactions using ethyl 4-(bromomethyl)-2-(chloromethyl)quinoline-3-carboxylate as the key precursor (Gao *et al.*, 2018), and the Knoevenagel-type condensation of 2-methyl-4-styrylquinoline with aromatic aldehydes, catalysed by sodium acetate (Satish *et al.*, 2019).

We have recently described an efficient and straightforward synthetic pathway, based on Friedländer annulation and starting from readily available 1-(2-aminophenyl)-3-arylprop-2-en-1-ones, to obtain several new series of polysubstituted 2-methyl-4-styrylquinolines (Meléndez *et al.*, 2020; Vera *et al.*, 2022). In an expansion of the scope of this route, in respect of both utility and flexibility, we now describe the synthesis, spectroscopic characterization, and molecular and supramolecular structures of a matched set of five closely-related 2,4-distyrylquinolines, namely, 2,4-bis[(*E*)-styryl]quinoline, (IIa), 2-[(*E*)-2,4-dichlorostyryl]-4-[(*E*)-styryl]quinoline, (IIb), {2-[(*E*)-4-bromostyryl]-4-[(*E*)-styryl]quinolin-3-yl}(phenyl)methanone, (IIc), {2-[(*E*)-4-bromostyryl]-4-[(*E*)-4-chlorostyryl]quinolin-3-yl}(phenyl)methanone, (IId), and {2-[(*E*)-4-bromostyryl]-4-[(*E*)-2-(thiophen-2-yl)vinyl]quinolin-3-yl}(phenyl)methanone, (IIe) (see Scheme 1), which differ only in the nature of the substituents at position C3 of the quinoline ring and the substituents in the 4-(arylvinyl) fragments. To the best of our knowledge, these 2,4-distyrylquinolines have not been reported previously.

The work reported here can be regarded as a continuation of an earlier crystallographic study which reported the structures of 4-styrylquinolines having different substituents at the C2 and C3 positions (Rodríguez *et al.*, 2020; Vera *et al.*, 2022; Ardila *et al.*, 2022).

2. Experimental

2.1. Synthesis and crystallization

For the synthesis of compounds (IIa)–(IIe), a mixture of the appropriate 2-methyl-4-styrylquinoline, (I) (see Scheme 1), prepared as described previously (Meléndez *et al.*, 2020; Vera *et al.*, 2022) (1.0 mmol), the appropriate aromatic aldehyde (4.0 mmol) and indium trichloride (10 mmol%) in dry toluene (1.2 ml) was stirred magnetically and heated at 393 K until the reactions were complete, shown by the complete consumption of (I), as monitored by thin-layer chromatography (TLC). The reaction times for completion were 18 h for (IIa), 16 h for (IIb), 17 h for (IIc) and 21 h for both (IId) and (IIe). Each reaction mixture was then allowed to cool to ambient temperature, washed with chloroform and the resulting suspension was removed by filtration before the filtrate was concentrated under reduced pressure. In each case, the resulting crude product was purified by silica-gel column chromato-

Table 1
Experimental details.

Experiments were carried out at 100 K with Mo $K\alpha$ radiation using a Bruker D8 Venture diffractometer. Absorption was corrected for by multi-scan methods (*SADABS*; Bruker, 2016). H-atom parameters were constrained.

	(IIa)	(IIb)	(IIc)
Crystal data			
Chemical formula	$C_{25}H_{19}N$	$C_{25}H_{17}Cl_2N$	$C_{32}H_{22}BrNO$
M_r	333.41	402.29	516.41
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$	Monoclinic, $P2_1/n$
a, b, c (Å)	12.6112 (6), 8.6352 (4), 17.3080 (8)	28.4950 (7), 9.5384 (3), 16.0520 (5)	12.287 (2), 15.528 (3), 12.844 (3)
α, β, γ (°)	90, 105.925 (2), 90	90, 118.581 (1), 90	90, 99.877 (6), 90
V (Å^3)	1812.51 (15)	3831.2 (2)	2414.2 (8)
Z	4	8	4
μ (mm^{-1})	0.07	0.35	1.73
Crystal size (mm)	0.19 × 0.14 × 0.08	0.21 × 0.10 × 0.09	0.15 × 0.12 × 0.08
Data collection			
T_{min}, T_{max}	0.924, 0.994	0.901, 0.969	0.720, 0.871
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38720, 4161, 3388	47555, 4414, 3914	5530, 5530, 4290
R_{int}	0.060	0.056	–
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.650	0.653
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.118, 1.09	0.032, 0.078, 1.09	0.064, 0.196, 1.05
No. of reflections	4161	4414	5530
No. of parameters	235	253	317
No. of restraints	0	0	0
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.24	0.35, −0.22	1.40, −0.70

	(IId)	(IIe)
Crystal data		
Chemical formula	$C_{32}H_{21}BrClNO$	$C_{30}H_{20}BrNOS$
M_r	550.86	522.44
Crystal system, space group	Triclinic, $P\overline{1}$	Orthorhombic, *Pbca*
a, b, c (Å)	9.9051 (12), 11.3936 (16), 11.8192 (16)	15.5785 (8), 16.4215 (7), 18.3126 (9)
α, β, γ (°)	77.727 (5), 76.116 (5), 86.448 (5)	90, 90, 90
V (Å^3)	1265.2 (3)	4684.8 (4)
Z	2	8
μ (mm^{-1})	1.76	1.87
Crystal size (mm)	0.19 × 0.12 × 0.10	0.20 × 0.12 × 0.08
Data collection		
T_{min}, T_{max}	0.735, 0.836	0.768, 0.861
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	61838, 5807, 5014	63672, 5363, 4456
R_{int}	0.064	0.060
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650	0.649
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.065, 1.03	0.040, 0.101, 1.02
No. of reflections	5807	5363
No. of parameters	325	320
No. of restraints	0	10
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.39	1.65, −1.18

Computer programs: *APEX3* (Bruker, 2018), *SAINT* (Bruker, 2017), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2020).

graphy using heptane–ethyl acetate mixtures as eluent (compositions ranged from 10:1 to 2:1 *v*/*v*) to give the required solid products (IIa)–(IIe). Crystallization from ethyl acetate–heptane, at ambient temperature and in the presence of air, gave crystals suitable for single-crystal X-ray diffraction.

In the NMR data listed below, unprimed ring atoms form part of the quinoline units; ring atoms carrying a single prime form part of the styryl units attached at position C2 of the quinoline system; ring atoms carrying double primes form part of the styryl units attached at position C4 for compounds (IIa) and (IIb), or part of the benzoyl units attached at position C3 for compounds (IIc)–(IIe); and ring atoms carrying triple primes form part of the styryl units attached at position C4 for compounds (IIc)–(IIe).

2,4-Bis[(*E*)-styryl]quinoline, (IIa). Yellow solid, yield 0.11 g (71%), m.p. 393–394 K, R_F = 0.40 (21% ethyl acetate–heptane). IR (ATR, cm^{-1}): 3019 [C(sp^2)H], 1723 (C═N), 1633 (C═C$_{vinyl}$), 1581 (C═C$_{arom}$), 1541 (C═C$_{arom}$), 961 (═C—H$_{trans}$). NMR ($CDCl_3$): δ(^{1}H) (400 MHz) 8.15 (*d*, *J* = 8.3 Hz, 1H, H5), 8.12 (*d*, *J* = 8.4 Hz, 1H, H8), 7.84 (*d*, *J* = 1.3 Hz, 1H, H3), 7.81 (*d*, *J* = 16.1 Hz, 1H, H$_{A''}$C═), 7.76 (*d*, *J* = 16.0 Hz, 1H, ═CH$_{B'}$), 7.72–7.68 (*m*, 1H, H7), 7.68–7.65 (*m*,

4H, H2′, H6′, H2″, H6″), 7.53 (*ddt*, *J* = 8.2, 6.9, 1.3 Hz, 1H, H6), 7.47–7.43 (*m*, 1H, $H_{A'}C$═), 7.46–7.41 (*m*, 4H, H3′, H5′, H3″, H5″), 7.40–7.32 (*m*, 2H, H4′, H4″), 7.38–7.34 (*m*, 1H, ═$CH_{B''}$); $\delta(^{13}C)$ (100 MHz) 155.7 (C2), 148.8 (C8a), 143.3 (C4), 136.7 (C1″), 136.6 (C1′), 135.0 (═$CH_{B''}$), 134.3 (═$CH_{B'}$), 129.9 (C8), 129.6 (C7), 128.9 (C3″, C5″), 128.8 (C3′, C5′, C4″, $H_{A'}C$═), 128.6 (C4′), 127.3 (C2″, C6″), 127.2 (C2′, C6′), 126.2 (C6), 125.7 (C4a), 123.4 (C5, $H_{A'}$—C═), 115.6 (C3). HRMS (ESI$^+$) *m*/*z* found for $[M + H]^+$ 334.1590, $C_{25}H_{19}N$ requires 333.1589.

2-[(*E*)-2,4-Dichlorostyryl]-4-[(*E*)-styryl]quinoline, (IIb). Yellow solid, yield 0.19 g (77%), m.p. 449–450 K, R_F = 0.41 (21% ethyl acetate–heptane). IR (ATR, cm^{-1}): 3055 [C(*sp*^{2})H], 1639 (C═N), 1580 (C═C_{vinyl}), 1541 (C═C_{arom}), 1473 (C═C_{arom}), 960 (═C—H_{trans}). NMR ($CDCl_3$): $\delta(^1H)$ (400 MHz) 8.17 (*dd*, *J* = 8.4, 1.5 Hz, 1H, 5H), 8.11 (*dd*, *J* = 8.6, 1.3 Hz, 1H, 8H), 8.03 (*d*, *J* = 16.3 Hz, 1H, ═$CH_{B'}$), 7.86 (s, 1H, 3H), 7.81 (*d*, *J* = 16.3 Hz, 1 H, $H_{A''}C$═), 7.75 (*d*, *J* = 8.4 Hz, 1H, H6′), 7.73 (*ddd*, *J* = 8.4, 6.9, 1.4 Hz, 1H, H7), 7.67–7.64 (*m*, 2H, H2″, H6″), 7.56 (*ddd*, *J* = 8.3, 6.8, 1.3 Hz, 1H, H6), 7.47–7.42 (*m*, 3H, H3′, H3″, H5″), 7.39 (*d*, *J* = 16.3 Hz, 1H, ═$CH_{B''}$), 7.39–7.35 (*m*, 1H, H4″), 7.38 (*d*, *J* = 16.3 Hz, 1H, $H_{A'}C$═), 7.29 (*dd*, *J* = 8.2, 2.0 Hz, 1H, H5′); $\delta(^{13}C)$ (100 MHz) 155.1 (C2), 148.8 (C8a), 143.5 (C4), 136.6 (C1″), 135.3 (═$CH_{B''}$), 134.6 (C2′), 134.5 (C4′), 133.4 (C1′), 132.3 ($H_{A'}C$═), 130.1 (C8), 129.8 (C7, C3′), 129.0 (C3″, C5″), 128.9 (═$CH_{B'}$), 128.8 (C4″), 127.7 (C6′), 127.5 (C5′), 127.2 (C2″, C6″), 126.5 (C6), 125.8 (C4a), 123.5 (C5), 123.2 ($H_{A''}C$═), 115.4 (C3). HRMS (ESI$^+$) *m*/*z* found for $[M + H]^+$ 402.0812, $C_{25}H_{17}{}^{35}Cl_2N$ requires 402.0811.

{2-[(*E*)-4-Bromostyryl]-4-[(*E*)-styryl]quinolin-3-yl}(phenyl)-methanone, (IIc). Orange solid. yield 0.20 g (86%), m.p. 471–472 K, R_F = 0.38 (9.1% ethyl acetate–heptane). IR (ATR, cm^{-1}): 3025 [C(*sp*^{2})H], 1666 (C═O), 1627 (C═N), 1595 (C═C_{vinyl}), 1535 (C═C_{arom}), 1483 (C═C_{arom}), 957 (═C—H_{trans}). NMR ($CDCl_3$): $\delta(^1H)$ (400 MHz) 8.20 (*dd*, *J* = 8.5, 1.2 Hz, 1H, H8), 8.12 (*dd*, *J* = 8.4, 1.4 Hz, 1H, H5), 8.00 (*d*, *J* = 15.5 Hz, 1H, ═$CH_{B'}$), 7.80 (*ddd*, *J* = 8.6, 6.9, 1.3 Hz 1H, H7), 7.78–7.76 (*m*, 2H, H2″, H6″), 7.57 (*ddd*, *J* = 8.3, 6.9, 1.2 Hz, 1H, H6), 7.56–7.52 (*m*, 1H, H4″), 7.44–7.42 (*m*, 2H, H3′, H5′), 7.39 (*t*, *J* = 7.8 Hz, 2H, H3″, H5″), 7.35–7.32 (*m*, 2H, H2′, H6′), 7.30–7.26 (*m*, 5H, H2‴, H6‴, H3‴, H5‴, H4‴), 7.23 (*dd*, *J* = 16.4, 0.8 Hz, 1H, $H_{A''}C$═), 7.09 (*dd*, *J* = 15.5, 0.8 Hz, 1H, $H_{a'}C$═), 6.87 (*d*, *J* = 16.4 Hz, 1H, ═$CH_{B'''}$); $\delta(^{13}C)$ (100 MHz) 198.4 (C═O), 151.4 (C2), 148.1 (C8a), 142.4 (C4), 139.5 (═$CH_{B'''}$), 137.9 (C1″), 136.3 (C1‴), 135.4 (C1′), 135.0 (═$CH_{B'}$), 134.0 (C4″), 131.8 (C3′, C5′), 131.1 (C3), 130.6 (C7), 130.0 (C8), 129.5 (C2″, C6″), 129.0 (C2′, C6′), 128.9 (C3″, C5″), 128.8 (C4‴), 128.7 (C3‴, C5‴), 126.9 (C6), 126.8 (C2‴, C6‴), 125.4 (C4a), 125.2 (C5), 125.0 ($H_{A'}C$═), 122.7 (C4′), 122.1 ($H_{A''}C$═). HRMS (ESI$^+$) *m*/*z* found for $[M + H]^+$ 516.09656, $C_{32}H_{22}{}^{79}BrNO$ requires 516.09575.

{2-[(*E*)-4-Bromostyryl]-4-[(*E*)-4-chlorostyryl]quinolin-3-yl}-(phenyl)methanone, (IId). Orange solid, yield 0.19 g (80%), m.p. 476–477 K, R_F = 0.35 (9.1% ethyl acetate–heptane). IR (ATR, cm^{-1}): 3046 [C(*sp*^{2})H], 1661 (C═O), 1630 (C═N), 1590, 1595 (C═C_{vinyl}), 1540 (C═C_{arom}), 1487 (C═C_{arom}), 978 (═C—H_{trans}). NMR ($CDCl_3$): $\delta(^1H)$ 8.20 (400 MHz) (*dd*, *J* = 8.4, 1.4 Hz, 1H, H8), 8.08 (*ddd*, *J* = 8.4, 1.4, 0.7 Hz, 1H, H5), 8.00 (*d*, *J* = 15.5 Hz, 1H, ═$CH_{B'}$), 7.80 (*ddd*, *J* = 8.4, 6.8, 1.3 Hz, 1H, H7), 7.76–7.74 (*m*, 2H, H2″, H6″), 7.57 (*ddd*, *J* = 8.3, 6.8, 1.3 Hz, 1H, H6), 7.56–7.52 (*m*, 1H, H4″), 7.44–7.42 (*m*, 2H, H3′, H5′), 7.39 (*t*, *J* = 7.8 Hz, 2H, H3″, H5″), 7.34–7.31 (*m*, 2H, H2′, H6′), 7.27–7.25 (*m*, 2H, H3‴, H5‴), 7.22–7.18 (*m*, 2H, H2‴, H6‴), 7.20 (*d*, *J* = 16.4 Hz, 1H, $H_{A''}C$═), 7.08 (*d*, *J* = 15.5 Hz, 1H, $H_{A'}C$═), 6.81 (*d*, *J* = 16.4 Hz, 1H, ═$CH_{B'''}$); $\delta(^{13}C)$ (100 MHz) 198.4 (C═O), 151.4 (C2), 148.1 (C8a), 142.0 (C4), 138.1 (═$CH_{B'''}$), 137.9 (C1″), 135.4 (C1′), 135.1 (═$CH_{B'}$), 134.7 (C4‴), 134.6 (C1‴), 134.1 (C4″), 131.8 (C3′, C5′), 131.1 (C3), 130.7 (C7), 130.0 (C8), 129.5 (C2″, C6″), 129.0 (C2′, C6′, C3‴, C5‴), 128.9 (C3″, C5″), 128.0 (C2‴, C6‴), 127.0 (C6), 125.2 (C4a), 125.1 ($HH_{A'}C$═), 124.9 (C5), 122.7 (C4′, $H_{A''}C$═). HRMS (ESI$^+$) *m*/*z* found for $[M + H]^+$ 550.05750, $C_{32}H_{21}{}^{79}Br^{35}ClNO$ requires 550.05678.

{2-[(*E*)-4-Bromostyryl]-4-[(*E*)-2-(thiophen-2-yl)vinyl]quinolin-3-yl}(phenyl)methanone, (IIe). Yellow solid, yield 0.24 g (93%), m.p. 472–473 K, R_F = 0.38 (9.1% ethyl acetate–heptane). IR (ATR, cm^{-1}): 3026 [C(*sp*^{2})H], 1663 (C═O), 1627 (C═N), 1589 (C═C_{vinyl}), 1537 (C═C_{arom}), 1483 (C═C_{arom}), 957 (═C—H_{trans}). NMR ($CDCl_3$): $\delta(^1H)$ (400 MHz) 8.18 (*d*, *J* = 8.3 Hz, 1H, H8), 8.11 (*d*, *J* = 8.3 Hz, 1H, H5), 7.99 (*d*, *J* = 15.5 Hz, 1H, ═$CH_{B'}$), 7.82–7.78 (*m*, 1H, H7), 7.77–7.75 (*m*, 2H, H2″, H6″), 7.58 (*ddd*, *J* = 8.3, 6.8, 1.2 Hz, 1H, H6), 7.56–7.52 (*m*, 1H, H4″), 7.43 (*d*, *J* = 8.4 Hz, 2H, H3′, H5′), 7.38 (*t*, *J* = 7.8 Hz, 2H, H3″, H5″), 7.33 (*d*, *J* = 8.4 Hz, 2H, H2′, H6′), 7.21 (*d*, *J* = 4.9 Hz, 1H, H3‴), 7.08 (*d*, *J* = 15.5 Hz, 1H, $H_{A'}C$═), 7.08 (*d*, *J* = 16.2 Hz, 1H, $H_{a''}C$═), 6.99 (*d*, *J* = 16.2 Hz, 1H, ═$CH_{B'''}$), 6.98–6.95 (*m*, 2H, H4‴, H5‴); $\delta(^{13}C)$ (100 MHz) 198.5 (C═O), 151.4 (C2), 148.1 (C8a), 141.7 (C4), 141.3 (C2‴), 137.8 (C1″), 135.4 (C1′), 135.0 (═$CH_{B'}$), 134.0 (C4″), 132.3 (═$CH_{B'''}$), 131.8 (C3′, C5′), 130.9 (C3), 130.6 (C7), 130.0 (C8), 129.5 (C2″, C6″), 129.0 (C2′, C6′), 128.9 (C3″, C5″), 128.0 (C5‴), 127.7 (C4‴), 127.0 (C6), 126.1 (C3‴), 125.2 (C4a), 125.1 ($H_{A'}C$═), 124.9 (C5), 122.7 (C4′), 121.1 ($H_{A''}C$═). HRMS (ESI$^+$) *m*/*z* found for $[M + H]^+$ 522.05249, $C_{30}H_{20}{}^{79}BrNOS$ = requires 522.05217.

2.2. Refinement

Crystal data, data collection and refinement details for compounds (IIa)–(IIe) are summarized in Table 1. For compound (IId), the reflection 100, which had been attenuated by the beam stop, was removed from the data set. In addition, a small number of bad outlier reflections [$\bar{1}$04 for (IIa) and 141, 231, 241, 033 and $\bar{3}$03 for (IIc)] were also removed. Compound (IIc) was handled as a nonmerohedral twin, with twin matrix (−0.053, 0.000, 0.947/0.000, −1.000, 0.000/1.053, 0.000, 0.053) and with refined twin fractions of 0.865 (2) and 0.135 (2). In compound (IIe), the thienyl unit was disordered over two sets of atomic sites having unequal occupancies. For the minor-disorder component, the bonded distances and the 1,3 nonbonded distances were restrained to be the same as the corresponding distances in the major-disorder component, subject to s.u. values of 0.01 and 0.02 Å,

Table 2
Selected torsion angles (°) for compounds (IIa)–(IIe).

Parameter	(IIa)	(IIb)	(IIc)	(IId)	(IIe)
C3—C2—C21—C22	−178.77 (14)	−12.9 (2)	−171.8 (4)	179.16 (16)	178.5 (2)
C21—C22—C221—*C222*	−173.99 (15)	−161.58 (14)	171.4 (4)	−171.95 (17)	−174.5 (3)
C2—C3—C31—C311			87.2 (5)	109.43 (17)	85.9 (3)
C3—C31—C311—C312			−15.6 (6)	−12.3 (2)	−10.9 (3)
C3—C4—C41—C42	19.8 (2)	23.4 (2)	−131.9 (4)	−44.4 (2)	37.6 (4)
C41—C42—C421—C422	8.3 (2)	−6.1 (2)	−4.5 (6)	−21.4 (3)	
C41—C42—C422—S421					0.8 (4)
C41—C42—C522—S521					−175.9 (7)

respectively. In addition, the anisotropic displacement parameters for pairs of partial-occupancy atoms occupying essentially the same physical space were constrained to be identical. All H atoms, apart from those in the minor-disorder component of compound (IIe), were located in difference maps and then treated as riding atoms in geometrically idealized positions, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C); the H atoms in the minor-disorder component of compound (IIe) were included in the refinement in exactly the same manner. Subject to these conditions, the refined occupancy values for the disorder components of (IIe) were 0.926 (3) and 0.074 (3). In the final difference map, the largest maximum of 1.65 e Å^{-3} was 0.86 Å from atom Br24, while the largest minimum of −1.18 e Å^{-3} was 0.66 Å from Br24. While these features might indicate some further minor disorder, the anisotropic displacement parameters provided no support for this possibility, which was therefore not pursued further.

3. Results and discussion

The 2-methyl-4-styrylquinoline precursors of type (I) (see Scheme 1) were prepared in high yields using Friedländer annulation reactions (Meléndez *et al.*, 2020; Vera *et al.*, 2022) between (2-aminophenyl)chalcones and either acetone, for compounds (Ia) and (Ib), or 1-phenylbutane-l-1,3-dione, for compounds (Ic)–(Ie). These precursors of type (I) were then converted successfully into the target 2,4-distyrylquinolines (IIa)–(IIe) in yields of 71–93% by means of indium trichloride-catalyzed Knoevenagel-type condensation reactions with the appropriate aromatic aldehydes (see Scheme 1). Compounds (IIa)–(IIe) were all fully characterized by standard spectroscopic means (FT–IR, ^{1}H and ^{13}C NMR spectroscopy, and high-resolution mass spectrometry) and full details of the spectroscopic characterization are provided in Section 2.1.

The formation of the second styryl fragment in products (IIa)–(IIe) was established by the disappearance from both the ^{1}H and ^{13}C NMR spectra of the signals from the methyl group at position C2, and their replacement by new sets of signals corresponding to the newly-introduced C and H atoms; thus, eight new C atoms in each case and seven new H atoms in (IIa), five in (IIb) and six in each of (IIc)–(IIe). In each case, the Knoevenagel-type condensation proceeded in a highly stereoselective manner giving exclusively the *E* stereoisomers, as indicated by the ^{1}H NMR spectra. The *E* configuration of the newly-formed styryl fragment was deduced on the basis of the coupling constant values ($^3J_{HA',HB'}$ *ca* 16.0 Hz) between HA′ and HB′. The constitutions of compounds (IIa)–(IIe), which were deduced from the spectroscopic data, were then fully confirmed by the results of single-crystal X-ray diffraction, which additionally provided information on the molecular conformations and the intermolecular interactions in the solid state.

The versatility of this synthetic route to 2,4-distyrylquinolines and their analogues is underpinned by the possibility of incorporating a wide variety of substituents into the initial chalcone precursor, into the ketone employed in the annulation step and into the aldehyde used in the final condensation step.

In compound (IIe), the thiophene unit is disordered over two sets of atomic sites having occupancies of 0.926 (3) and 0.074 (3), such that the two disorder forms are related by a rotation of approximately 180° around the exocyclic C—C bond; the dihedral angle between the mean planes of the two disorder components is only 4(2)°.

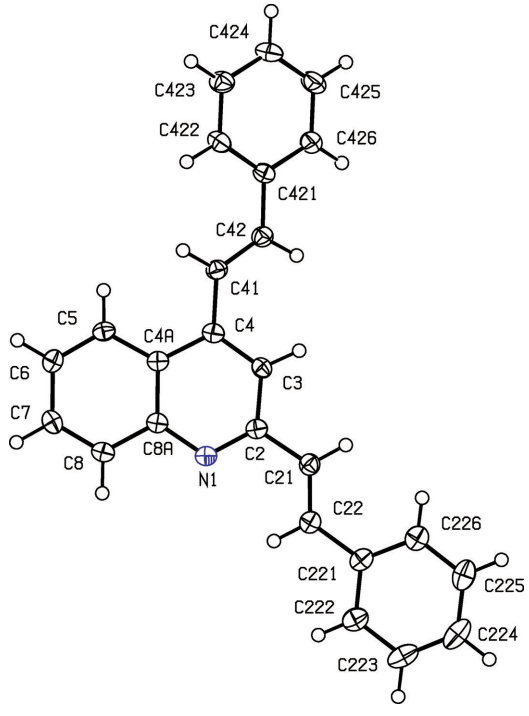


Figure 1
The molecular structure of compound (IIa), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Table 3
Hydrogen bonds and short intermolecular contacts (Å, °) for compounds (IIb)–(IIe).

*Cg*1–*Cg*4 represent the centroids of rings C421–C426, C4*A*/C5–C8/C8*A*, C311–C316 and C221–C216, respectively.

Compound	*D*—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
(IIb)	C225—H225···N1^{i}	0.95	2.62	3.522 (2)	158
	C6—H6···*Cg*1^{ii}	0.95	2.65	3.4152 (16)	138
	C422—H422···*Cg*2^{iii}	0.95	2.88	3.5843 (17)	132
(IIc)	C8—H8···O31^{iv}	0.95	2.51	3.164 (6)	126
	C5—H5···*Cg*3^{v}	0.95	2.96	3.728 (4)	138
	C42—H42···*Cg*4^{vi}	0.95	2.88	3.766 (5)	155
	C223—H223···*Cg*2^{vii}	0.95	2.84	3.429 (3)	122
(IId)	C225—H225···O31^{v}	0.95	2.37	3.266 (2)	156
(IIe)	C8—H8···O31^{viii}	0.95	2.58	3.122 (3)	116
	C425—H425···O31^{ix}	0.95	2.45	3.361 (4)	161
	C5—H5···*Cg*3^{v}	0.95	2.90	3.647 (3)	136
	C423—H423···*Cg*3^{v}	0.95	2.76	3.449 (3)	130

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+2, z+\frac{1}{2}$; (iii) $-x+1, y, -z+\frac{3}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $-x+1, -y+1, -z+1$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (vii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (viii) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (ix) $x, -y+2, z-\frac{1}{2}$.

The molecules of compounds (IIa)–(IIe) exhibit no internal symmetry and hence these compounds are all conformationally chiral (Moss, 1996; Flack & Bernardinelli, 1999), but the centrosymmetric space groups (Table 1) confirm that equal numbers of the two conformational enantiomers are present in each of (IIa)–(IIe).

For the 3-benzoyl products (IIc)–(IIe), the reference molecules are all such that the torsion angle C2—C3—C31—C311 has a positive sign (Table 2), while the value of the torsion angle C3—C4—C41—C42 in (IIc) is markedly different from those in the other four compound reported here (Table 2 and Figs. 1–5). In each of (IIa)–(IIe), the 2-styryl unit is close to being coplanar with the quinoline unit, while the 4-substituent

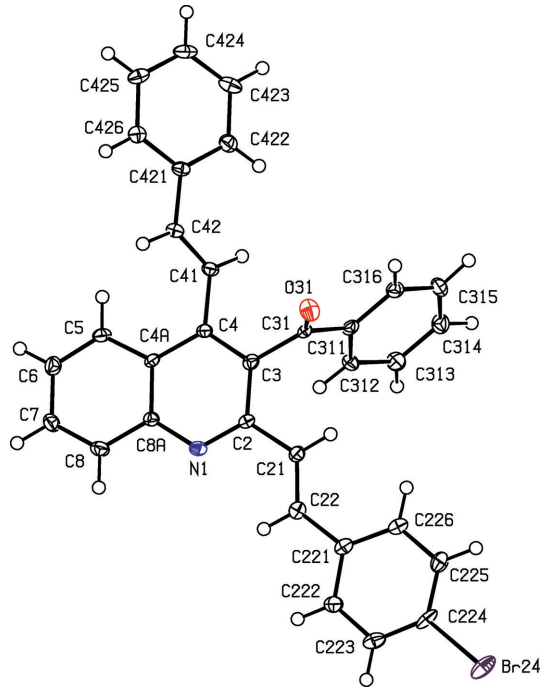


Figure 3
The molecular structure of compound (IIc), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

is twisted well out of the plane of the quinoline unit. These observations thus complement the general pattern in styrylquinolines that we have noted previously (Vera *et al.*, 2022; Ardila *et al.*, 2022). Amongst the styrylquinolines whose structures are recorded in the Cambridge Structural Database (Groom *et al.*, 2016), 2-styryl- and 8-styrylquinolines all have

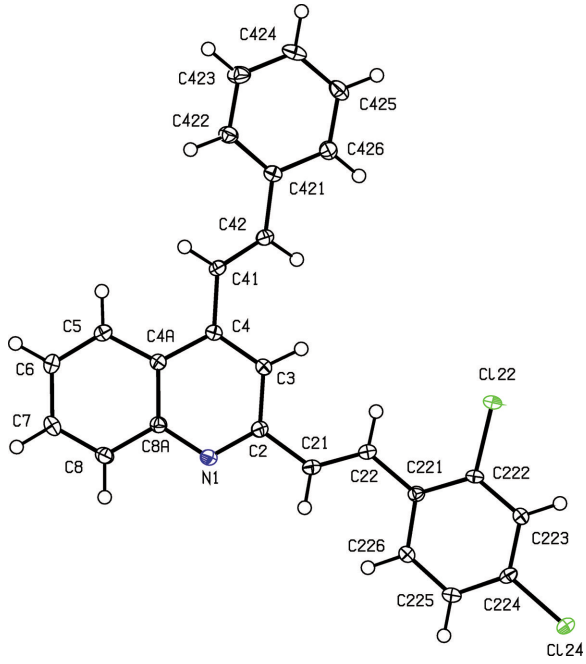


Figure 2
The molecular structure of compound (IIb), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

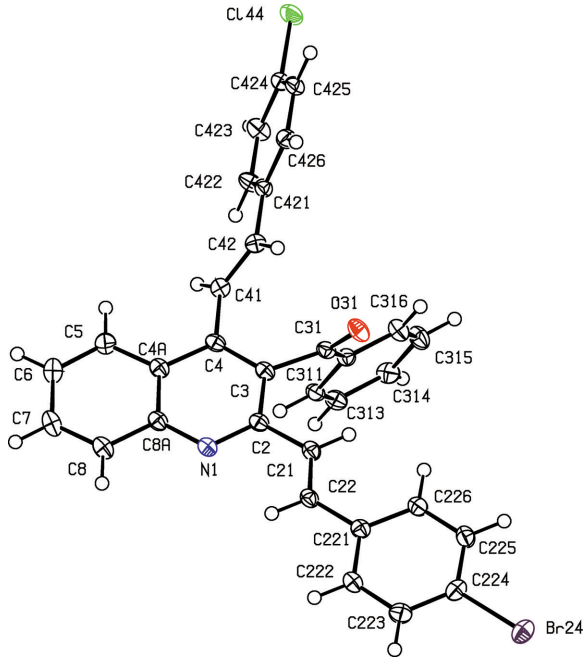


Figure 4
The molecular structure of compound (IId), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

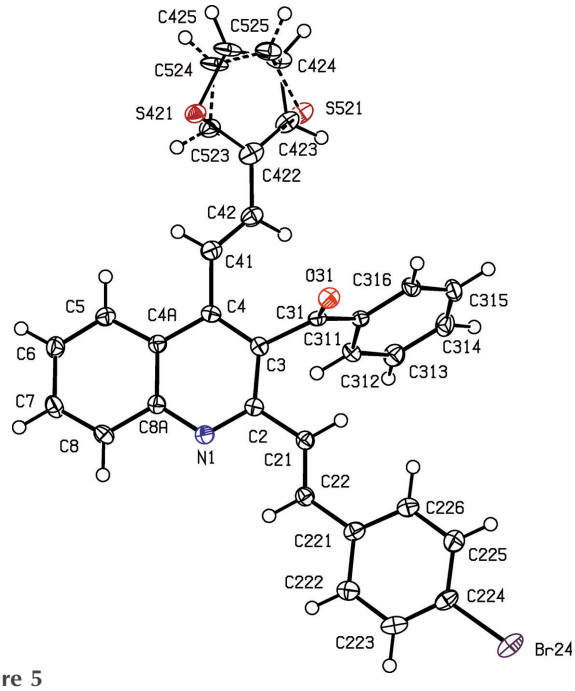


Figure 5
The molecular structure of compound (IIe), showing the conformational disorder and the atom-labelling scheme. The major-disorder component is drawn with full lines and the minor-disorder component is drawn using broken lines. Displacement ellipsoids are drawn at the 50% probability level.

molecular skeletons which are effectively planar, while in 4-styrylquinolines, the styryl unit is always markedly twisted

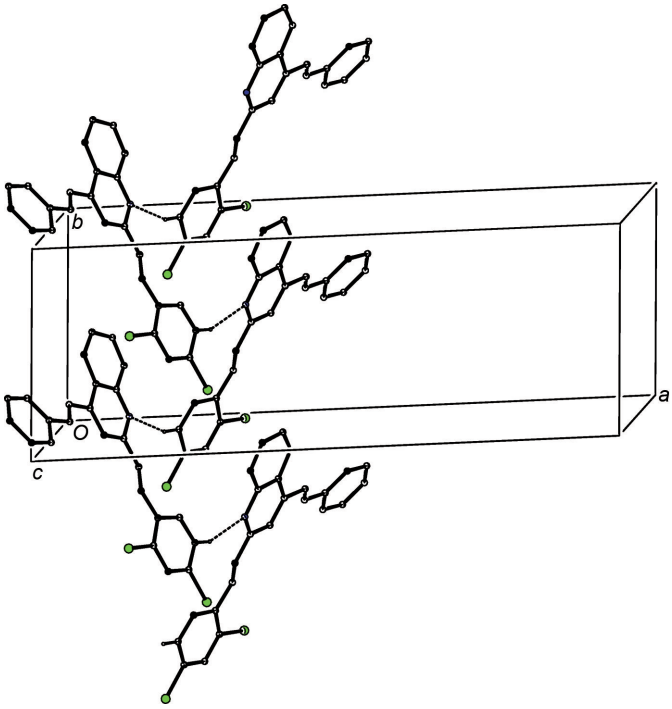


Figure 6
Part of the crystal structure of compound (IIb), showing the formation of a $C(8)$ chain parallel to [010], built from C—H···N hydrogen bonds, which are drawn as dashed lines. For the sake of clarity, H atoms which are not involved in the motif shown have been omitted.

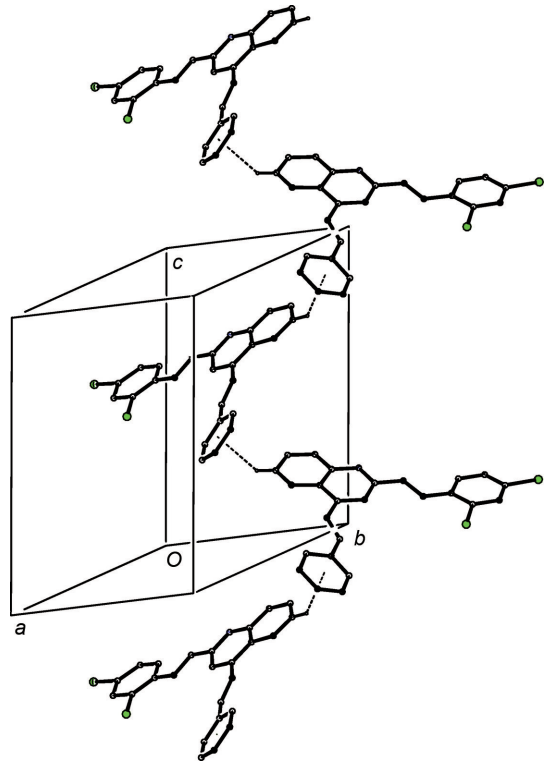


Figure 7
Part of the crystal structure of compound (IIb), showing the formation of a chain parallel to [001], built from C—H···π(arene) hydrogen bonds, which are drawn as dashed lines. For the sake of clarity, H atoms which are not involved in the motif shown have been omitted.

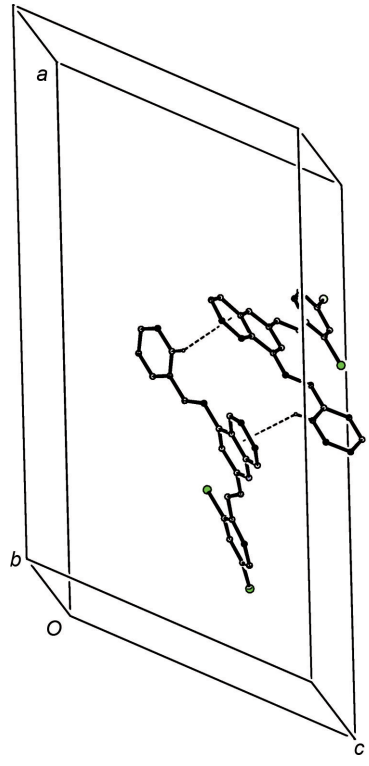


Figure 8
Part of the crystal structure of compound (IIb), showing the formation of a centrosymmetric dimer built from C—H···π(arene) hydrogen bonds, which are drawn as dashed lines. For the sake of clarity, H atoms which are not involved in the motif shown have been omitted.

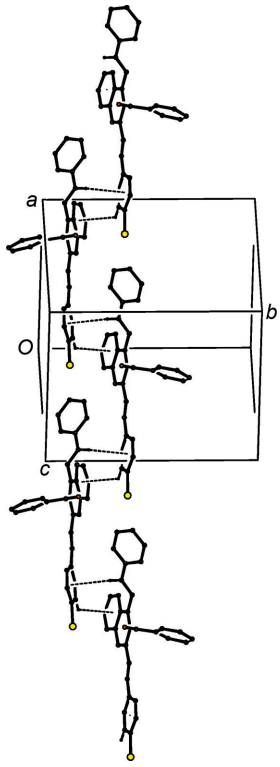


Figure 9
Part of the crystal structure of compound (IIc), showing the formation of a chain of rings running parallel to the [10$\bar{1}$] direction and built from two independent C—H···π(arene) hydrogen bonds, which are drawn as dashed lines. For the sake of clarity, H atoms which are not involved in the motif shown have been omitted.

out of the plane of the quinoline unit by a rotation about the exocyclic bond corresponding to C4—C41 in the numbering system used here.

Despite this, there are some unexpected differences in the molecular orientations of the two arylvinyl units (Figs. 1–5 and Table 2). Thus, the orientation of the 2-styryl substituent in (IIb) differs from that in each of (IIa) and (IIc)–(IIe) by a rotation about the C2—C21 bond of approximately 180°. In addition, the orientation of the 4-styryl unit in (IIc) differs markedly from that in each of the other examples, but the torsion angle C3—C4—C41—C42 shows quite a wide range of variation (Table 2). These differences in conformation cannot reasonably be explained in terms of the patterns of hydrogen bonding discussed below (*cf.* Table 3).

The patterns of supramolecular assembly in compounds (IIa)–(IIe) show some wide variations. Despite the large numbers of aromatic rings and C—H bonds in the molecules of (IIa), the crystal structure contains no significant direction-specific intermolecular interactions of any sort. By contrast, in the dichloro analogue (IIb), a combination of one C—H···N hydrogen bond and two independent C—H···π(arene) hydrogen bonds (Table 3) links the molecules into a three-dimensional framework structure, whose formation is readily analysed in terms of three simple substructures (Ferguson *et al.*, 1998*a*,*b*; Gregson *et al.*, 2000). The C—H···N hydrogen bonds link molecules of (IIb) which are related by the 2_1 screw

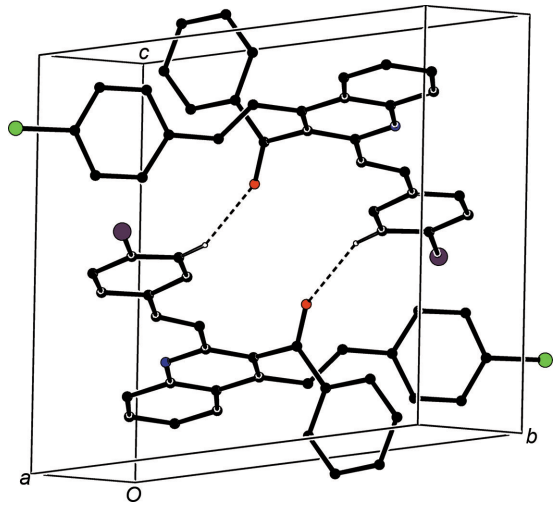


Figure 10
Part of the crystal structure of compound (IId), showing the formation of a cyclic $R_2^2(20)$ dimer built from C—H···O hydrogen bonds, which are drawn as dashed lines. For the sake of clarity, H atoms which are not involved in the motif shown have been omitted.

axis along ($\frac{1}{4}$, y, $\frac{3}{4}$) to form a $C(8)$ (Etter, 1990; Etter *et al.*, 1990; Bernstein *et al.*, 1995) chain running parallel to the [010] direction (Fig. 6). In the second substructure, the C—H···π(arene) hydrogen bond having atom C6 as the donor links molecules which are related by the *c*-glide plane at y = 1 to form a chain running parallel to the [001] direction (Fig. 7).

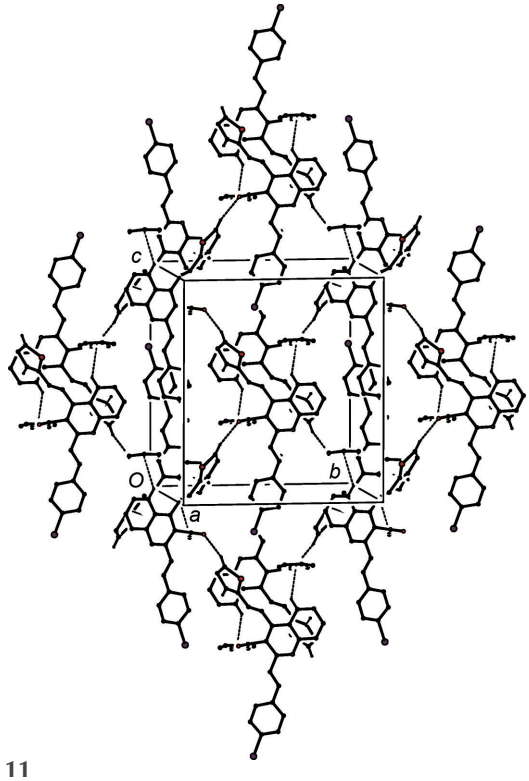
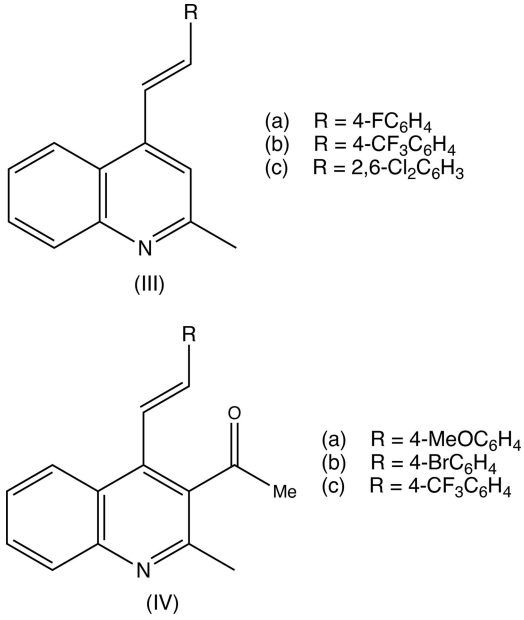


Figure 11
Part of the crystal structure of compound (IIe), showing the formation of a sheet lying parallel to {100} and built from a combination of C—H···O and C—H···π(arene) hydrogen bonds, which are drawn as dashed lines. For the sake of clarity, the minor-disorder component and H atoms which are not involved in the motif shown have been omitted.

The combination of the chains along [010] and [001] generates a sheet lying parallel to (100) in the domain $0 < x < \frac{1}{2}$. A second sheet, related to the first by inversion, lies in the domain $\frac{1}{2} < x < 1.0$, and adjacent sheets are linked by the third substructure which takes the form of a cyclic centrosymmetric dimer built from C—H···π(arene) hydrogen bonds having atom C422 as the donor (Fig. 8).

The short intermolecular C—H···O contact in compound (IIc) has a very small C—H···O angle (Table 3), and so cannot be regarded as structurally significant (Wood *et al.*, 2009). However, the co-operative action of two C—H···π(arene) hydrogen bonds links molecules which are related by the *n*-glide plane at $y = \frac{1}{4}$ into a chain of rings running parallel to the [10$\bar{1}$] direction (Fig. 9). The structure also contains a third C—H···π(arene) contact, involving atom C5, but here the H···*A* distance is quite long; if this were regarded as structurally significant, its action would be to link the chains of rings into a sheet parallel to (101).



Scheme 2

A single C—H···O hydrogen bond links inversion-related molecules of compound (IId) into a cyclic centrosymmetric $R_2^2(20)$ dimer (Fig. 10), but there are no direction-specific interactions between adjacent dimers.

In the crystal structure of compound (IIe), the C—H···O contact involving atom C8 is not structurally significant (Wood *et al.*, 2009), but the combination of the C—H···O hydrogen bond involving atom C425 with the two C—H···π(arene) hydrogen bonds links the molecules into a complex sheet lying parallel to (100) in the domain $\frac{1}{4} < x < \frac{3}{4}$ (Fig. 11). A second sheet, related to the first by the action of the 2_1 screw axes, lies in the domain $\frac{3}{4} < x < 1.35$, but there are no direction-specific interactions between adjacent sheets.

It is of interest briefly to compare the supramolecular assembly in compounds (IIa)–(IIe) reported here with those of some simpler 2-methyl-4-styrylquinoline analogues. Crystal structures have been reported (Vera *et al.*, 2022) for compounds (IIIa)–(IIIc) (see Scheme 2), which have no substituent at position C3 of the quinoline unit, and are thus related to compounds (IIa) and (IIb) reported here. In the crystal structure of (IIIa), the molecules are linked into sheets by a combination of C—H···N hydrogen bonds and π–π stacking interactions, while a similar combination of interactions links the molecules of (IIIb) into chains of rings. There are no hydrogen bonds in the structure of (IIIc), but a π–π stacking interaction links the molecules into stacks.

Compounds of the type (IV) (see Scheme 2), carrying a 3-acetyl substituent, are thus analogous to compounds (IIc)–(IIe). Compounds (IVa)–(IVc) are isomorphous (Rodríguez *et al.*, 2020); in each, the molecules are linked into chains by a C—H···O hydrogen bond, but only in (IVa) is this augmented by a C—H···π hydrogen bonds to form a chain of rings. Thus, although (IVa)–(IVc) are isomorphous, they are not strictly isostructural.

4. Summary

We have developed an efficient and highly versatile route to 2,4-distyrylquinolines and to their 2-arylvinyl analogues, using only simple and readily accessible building blocks such as simple aldehydes and ketone. We have characterized by spectroscopic means (IR, ^{1}H and ^{13}C NMR spectroscopy, and HRMS) five representative examples and we have determined their molecular and crystal structures, which fully confirm the molecular constitutions deduced from the spectroscopic data, as well as providing further information on their molecular conformations in the solid state, and on their supramolecular assemblies.

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supporting information

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Conversion of 2-methyl-4-styrylquinolines into 2,4-distyrylquinolines: synthesis, and spectroscopic and structural characterization of five examples

Diana R. Vera, Diana M. Ardila, Alirio Palma, Justo Cobo and Christopher Glidewell

Computing details

For all structures, data collection: *APEX3* (Bruker, 2018); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2020); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015b) and *PLATON* (Spek, 2020).

2,4-Bis[(*E*)-2-phenylethenyl]quinoline (IIa)

Crystal data

$C_{25}H_{19}N$
$M_r = 333.41$
Monoclinic, $P2_1/c$
$a = 12.6112$ (6) Å
$b = 8.6352$ (4) Å
$c = 17.3080$ (8) Å
$\beta = 105.925$ (2)°
$V = 1812.51$ (15) Å^3
$Z = 4$
$F(000) = 704$
$D_x = 1.222$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4167 reflections
$\theta = 2.5$–27.5°
$\mu = 0.07$ mm^{-1}
$T = 100$ K
Block, yellow
0.19 × 0.14 × 0.08 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: INCOATEC high brilliance microfocus sealed tube
Multilayer mirror monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.924$, $T_{max} = 0.994$
38720 measured reflections
4161 independent reflections
3388 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.5°$
$h = -16\rightarrow16$
$k = -10\rightarrow11$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.118$
$S = 1.09$
4161 reflections
235 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.9448P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.30510 (10)	0.54242 (14)	0.21630 (7)	0.0228 (3)
C2	0.39111 (12)	0.48035 (16)	0.26929 (8)	0.0217 (3)
C3	0.49565 (12)	0.46407 (16)	0.25495 (9)	0.0224 (3)
H3	0.5541	0.4169	0.2946	0.027*
C4	0.51400 (11)	0.51553 (16)	0.18435 (9)	0.0212 (3)
C4A	0.42226 (11)	0.58233 (15)	0.12564 (8)	0.0203 (3)
C5	0.42744 (12)	0.63945 (16)	0.04991 (8)	0.0227 (3)
H5	0.4943	0.6307	0.0350	0.027*
C6	0.33789 (12)	0.70684 (17)	−0.00194 (9)	0.0251 (3)
H6	0.3435	0.7459	−0.0520	0.030*
C7	0.23722 (12)	0.71894 (17)	0.01804 (9)	0.0264 (3)
H7	0.1754	0.7664	−0.0184	0.032*
C8	0.22845 (12)	0.66260 (17)	0.08957 (9)	0.0257 (3)
H8	0.1600	0.6701	0.1023	0.031*
C8A	0.31991 (11)	0.59285 (16)	0.14540 (8)	0.0207 (3)
C21	0.37736 (12)	0.43385 (16)	0.34781 (9)	0.0241 (3)
H21	0.4403	0.3959	0.3870	0.029*
C22	0.28261 (12)	0.44134 (16)	0.36762 (9)	0.0240 (3)
H22	0.2198	0.4754	0.3271	0.029*
C221	0.26566 (13)	0.40205 (16)	0.44600 (9)	0.0248 (3)
C222	0.15863 (14)	0.40227 (18)	0.45468 (10)	0.0310 (3)
H222	0.0981	0.4265	0.4099	0.037*
C223	0.13992 (15)	0.3673 (2)	0.52835 (11)	0.0383 (4)
H223	0.0669	0.3684	0.5335	0.046*
C224	0.22673 (16)	0.3313 (2)	0.59377 (10)	0.0401 (4)
H224	0.2136	0.3083	0.6440	0.048*
C225	0.33301 (15)	0.32869 (19)	0.58609 (10)	0.0352 (4)
H225	0.3927	0.3017	0.6309	0.042*
C226	0.35281 (14)	0.36517 (18)	0.51339 (9)	0.0288 (3)
H226	0.4263	0.3652	0.5091	0.035*
C41	0.62282 (12)	0.50961 (17)	0.16929 (9)	0.0238 (3)
H41	0.6340	0.5758	0.1284	0.029*
C42	0.70752 (12)	0.42098 (17)	0.20709 (9)	0.0243 (3)
H42	0.6975	0.3542	0.2481	0.029*
C421	0.81585 (11)	0.41880 (17)	0.19004 (9)	0.0229 (3)
C422	0.84436 (12)	0.52532 (18)	0.13856 (10)	0.0273 (3)
H422	0.7932	0.6033	0.1138	0.033*
C423	0.94624 (12)	0.51886 (18)	0.12314 (10)	0.0297 (3)
H423	0.9643	0.5921	0.0878	0.036*

C424	1.02212 (12)	0.40646 (19)	0.15887 (10)	0.0318 (4)
H424	1.0925	0.4033	0.1489	0.038*
C425	0.99439 (13)	0.2989 (2)	0.20920 (11)	0.0365 (4)
H425	1.0457	0.2204	0.2333	0.044*
C426	0.89210 (13)	0.30456 (19)	0.22480 (10)	0.0304 (3)
H426	0.8740	0.2299	0.2595	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0218 (6)	0.0222 (6)	0.0253 (6)	−0.0004 (5)	0.0082 (5)	−0.0011 (5)
C2	0.0230 (7)	0.0179 (6)	0.0253 (7)	−0.0007 (5)	0.0086 (6)	−0.0015 (5)
C3	0.0213 (7)	0.0209 (7)	0.0241 (7)	0.0021 (5)	0.0050 (5)	0.0010 (6)
C4	0.0211 (7)	0.0161 (6)	0.0270 (7)	−0.0009 (5)	0.0076 (6)	−0.0023 (5)
C4A	0.0219 (7)	0.0155 (6)	0.0239 (7)	−0.0019 (5)	0.0072 (5)	−0.0034 (5)
C5	0.0232 (7)	0.0209 (7)	0.0263 (7)	−0.0009 (6)	0.0104 (6)	−0.0022 (6)
C6	0.0306 (8)	0.0228 (7)	0.0225 (7)	−0.0009 (6)	0.0080 (6)	0.0007 (6)
C7	0.0248 (7)	0.0244 (7)	0.0273 (7)	0.0027 (6)	0.0026 (6)	0.0019 (6)
C8	0.0210 (7)	0.0268 (7)	0.0299 (8)	0.0006 (6)	0.0080 (6)	−0.0009 (6)
C8A	0.0215 (7)	0.0172 (6)	0.0235 (7)	−0.0013 (5)	0.0064 (5)	−0.0032 (5)
C21	0.0269 (7)	0.0207 (7)	0.0250 (7)	0.0020 (6)	0.0077 (6)	0.0015 (6)
C22	0.0283 (7)	0.0206 (7)	0.0238 (7)	−0.0001 (6)	0.0080 (6)	−0.0014 (6)
C221	0.0334 (8)	0.0171 (7)	0.0267 (7)	−0.0015 (6)	0.0132 (6)	−0.0031 (6)
C222	0.0354 (8)	0.0275 (8)	0.0331 (8)	−0.0025 (7)	0.0143 (7)	−0.0034 (7)
C223	0.0458 (10)	0.0361 (9)	0.0418 (10)	−0.0111 (8)	0.0270 (8)	−0.0055 (8)
C224	0.0637 (12)	0.0323 (9)	0.0305 (9)	−0.0137 (8)	0.0233 (8)	−0.0029 (7)
C225	0.0529 (11)	0.0247 (8)	0.0275 (8)	−0.0045 (7)	0.0102 (7)	−0.0005 (6)
C226	0.0363 (8)	0.0232 (7)	0.0280 (8)	−0.0006 (6)	0.0105 (6)	−0.0031 (6)
C41	0.0228 (7)	0.0243 (7)	0.0262 (7)	0.0000 (6)	0.0097 (6)	0.0017 (6)
C42	0.0235 (7)	0.0235 (7)	0.0266 (7)	−0.0014 (6)	0.0083 (6)	0.0017 (6)
C421	0.0194 (7)	0.0231 (7)	0.0256 (7)	−0.0002 (5)	0.0050 (5)	−0.0029 (6)
C422	0.0206 (7)	0.0230 (7)	0.0372 (8)	0.0010 (6)	0.0063 (6)	0.0030 (6)
C423	0.0251 (7)	0.0265 (8)	0.0387 (9)	−0.0036 (6)	0.0109 (6)	0.0021 (7)
C424	0.0204 (7)	0.0335 (8)	0.0437 (9)	0.0009 (6)	0.0126 (6)	−0.0020 (7)
C425	0.0260 (8)	0.0373 (9)	0.0472 (10)	0.0109 (7)	0.0115 (7)	0.0118 (8)
C426	0.0264 (8)	0.0332 (8)	0.0325 (8)	0.0044 (6)	0.0097 (6)	0.0077 (7)

Geometric parameters (Å, º)

N1—C2	1.3263 (18)	C222—C223	1.392 (2)
N1—C8A	1.3624 (18)	C222—H222	0.9500
C2—C3	1.414 (2)	C223—C224	1.378 (3)
C2—C21	1.472 (2)	C223—H223	0.9500
C3—C4	1.378 (2)	C224—C225	1.383 (3)
C3—H3	0.9500	C224—H224	0.9500
C4—C4A	1.4348 (19)	C225—C226	1.385 (2)
C4—C41	1.4663 (19)	C225—H225	0.9500
C4A—C5	1.4185 (19)	C226—H226	0.9500

C4A—C8A	1.4261 (19)	C41—C42	1.331 (2)
C5—C6	1.365 (2)	C41—H41	0.9500
C5—H5	0.9500	C42—C421	1.475 (2)
C6—C7	1.408 (2)	C42—H42	0.9500
C6—H6	0.9500	C421—C426	1.394 (2)
C7—C8	1.363 (2)	C421—C422	1.395 (2)
C7—H7	0.9500	C422—C423	1.383 (2)
C8—C8A	1.4195 (19)	C422—H422	0.9500
C8—H8	0.9500	C423—C424	1.384 (2)
C21—C22	1.332 (2)	C423—H423	0.9500
C21—H21	0.9500	C424—C425	1.383 (2)
C22—C221	1.470 (2)	C424—H424	0.9500
C22—H22	0.9500	C425—C426	1.389 (2)
C221—C222	1.399 (2)	C425—H425	0.9500
C221—C226	1.402 (2)	C426—H426	0.9500

C2—N1—C8A	117.65 (12)	C223—C222—H222	119.7
N1—C2—C3	122.94 (13)	C221—C222—H222	119.7
N1—C2—C21	117.88 (13)	C224—C223—C222	120.38 (16)
C3—C2—C21	119.12 (13)	C224—C223—H223	119.8
C4—C3—C2	121.01 (13)	C222—C223—H223	119.8
C4—C3—H3	119.5	C223—C224—C225	119.83 (15)
C2—C3—H3	119.5	C223—C224—H224	120.1
C3—C4—C4A	117.29 (13)	C225—C224—H224	120.1
C3—C4—C41	122.64 (13)	C224—C225—C226	120.32 (16)
C4A—C4—C41	120.02 (13)	C224—C225—H225	119.8
C5—C4A—C8A	118.27 (13)	C226—C225—H225	119.8
C5—C4A—C4	124.16 (13)	C225—C226—C221	120.80 (16)
C8A—C4A—C4	117.57 (12)	C225—C226—H226	119.6
C6—C5—C4A	121.08 (13)	C221—C226—H226	119.6
C6—C5—H5	119.5	C42—C41—C4	126.64 (14)
C4A—C5—H5	119.5	C42—C41—H41	116.7
C5—C6—C7	120.60 (13)	C4—C41—H41	116.7
C5—C6—H6	119.7	C41—C42—C421	124.87 (14)
C7—C6—H6	119.7	C41—C42—H42	117.6
C8—C7—C6	120.00 (13)	C421—C42—H42	117.6
C8—C7—H7	120.0	C426—C421—C422	118.31 (13)
C6—C7—H7	120.0	C426—C421—C42	119.34 (14)
C7—C8—C8A	121.10 (13)	C422—C421—C42	122.33 (13)
C7—C8—H8	119.4	C423—C422—C421	120.84 (14)
C8A—C8—H8	119.5	C423—C422—H422	119.6
N1—C8A—C8	117.53 (12)	C421—C422—H422	119.6
N1—C8A—C4A	123.53 (13)	C422—C423—C424	120.47 (15)
C8—C8A—C4A	118.93 (13)	C422—C423—H423	119.8
C22—C21—C2	124.43 (14)	C424—C423—H423	119.8
C22—C21—H21	117.8	C425—C424—C423	119.30 (14)
C2—C21—H21	117.8	C425—C424—H424	120.3
C21—C22—C221	126.46 (14)	C423—C424—H424	120.3

C21—C22—H22	116.8	C424—C425—C426	120.49 (15)
C221—C22—H22	116.8	C424—C425—H425	119.8
C222—C221—C226	118.04 (14)	C426—C425—H425	119.8
C222—C221—C22	119.21 (14)	C425—C426—C421	120.57 (15)
C226—C221—C22	122.74 (14)	C425—C426—H426	119.7
C223—C222—C221	120.62 (16)	C421—C426—H426	119.7

C8A—N1—C2—C3	−0.4 (2)	C2—C21—C22—C221	−177.49 (14)
C8A—N1—C2—C21	176.56 (12)	C21—C22—C221—C222	−173.99 (15)
N1—C2—C3—C4	1.2 (2)	C21—C22—C221—C226	6.5 (2)
C21—C2—C3—C4	−175.69 (13)	C226—C221—C222—C223	0.2 (2)
C2—C3—C4—C4A	−1.5 (2)	C22—C221—C222—C223	−179.25 (15)
C2—C3—C4—C41	176.08 (13)	C221—C222—C223—C224	−0.3 (3)
C3—C4—C4A—C5	−179.49 (13)	C222—C223—C224—C225	−0.5 (3)
C41—C4—C4A—C5	2.8 (2)	C223—C224—C225—C226	1.3 (3)
C3—C4—C4A—C8A	1.10 (19)	C224—C225—C226—C221	−1.4 (2)
C41—C4—C4A—C8A	−176.57 (12)	C222—C221—C226—C225	0.6 (2)
C8A—C4A—C5—C6	1.8 (2)	C22—C221—C226—C225	−179.93 (14)
C4—C4A—C5—C6	−177.56 (13)	C3—C4—C41—C42	19.8 (2)
C4A—C5—C6—C7	−1.1 (2)	C4A—C4—C41—C42	−162.67 (14)
C5—C6—C7—C8	−0.2 (2)	C4—C41—C42—C421	−179.93 (14)
C6—C7—C8—C8A	0.7 (2)	C41—C42—C421—C426	−170.19 (15)
C2—N1—C8A—C8	−178.53 (13)	C41—C42—C421—C422	8.3 (2)
C2—N1—C8A—C4A	0.0 (2)	C426—C421—C422—C423	−0.7 (2)
C7—C8—C8A—N1	178.61 (14)	C42—C421—C422—C423	−179.23 (14)
C7—C8—C8A—C4A	0.0 (2)	C421—C422—C423—C424	−0.2 (2)
C5—C4A—C8A—N1	−179.79 (13)	C422—C423—C424—C425	1.1 (3)
C4—C4A—C8A—N1	−0.3 (2)	C423—C424—C425—C426	−0.9 (3)
C5—C4A—C8A—C8	−1.31 (19)	C424—C425—C426—C421	0.0 (3)
C4—C4A—C8A—C8	178.13 (12)	C422—C421—C426—C425	0.9 (2)
N1—C2—C21—C22	4.2 (2)	C42—C421—C426—C425	179.40 (15)
C3—C2—C21—C22	−178.77 (14)		

2-[(*E*)-2-(2,4-Dichlorophenyl)ethenyl]-4-[(*E*)-2-phenylethenyl]quinoline (IIb)

Crystal data

$C_{25}H_{17}Cl_2N$	$F(000) = 1664$
$M_r = 402.29$	$D_x = 1.395$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *Kα* radiation, $\lambda = 0.71073$ Å
$a = 28.4950$ (7) Å	Cell parameters from 4414 reflections
$b = 9.5384$ (3) Å	$\theta = 2.3$–$27.5°$
$c = 16.0520$ (5) Å	$\mu = 0.35$ mm^{-1}
$\beta = 118.581$ (1)°	$T = 100$ K
$V = 3831.2$ (2) Å^3	Needle, yellow
$Z = 8$	0.21 × 0.10 × 0.09 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: INCOATEC high brilliance microfocus sealed tube
Multilayer mirror monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.901, T_{max} = 0.969
47555 measured reflections
4414 independent reflections
3914 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 27.5°, θ_{min} = 2.3°
h = −36→36
k = −12→12
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.078
S = 1.09
4414 reflections
253 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2 + 5.0618P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.34810 (5)	0.64678 (13)	0.74277 (9)	0.0163 (2)
C2	0.35420 (6)	0.55453 (15)	0.68669 (10)	0.0156 (3)
C3	0.38455 (6)	0.58355 (15)	0.63990 (10)	0.0154 (3)
H3	0.3877	0.5141	0.6005	0.018*
C4	0.40950 (5)	0.71125 (15)	0.65081 (10)	0.0137 (3)
C4A	0.40294 (5)	0.81360 (14)	0.71004 (10)	0.0129 (3)
C5	0.42460 (5)	0.95117 (15)	0.72584 (10)	0.0154 (3)
H5	0.4465	0.9781	0.6988	0.018*
C6	0.41446 (6)	1.04583 (15)	0.77956 (10)	0.0169 (3)
H6	0.4292	1.1375	0.7890	0.020*
C7	0.38231 (6)	1.00820 (16)	0.82102 (10)	0.0179 (3)
H7	0.3751	1.0748	0.8575	0.021*
C8	0.36151 (6)	0.87583 (16)	0.80862 (10)	0.0169 (3)
H8	0.3403	0.8507	0.8374	0.020*
C8A	0.37117 (5)	0.77557 (15)	0.75332 (10)	0.0141 (3)
C21	0.32776 (6)	0.41923 (16)	0.67809 (11)	0.0187 (3)
H21	0.3149	0.4024	0.7219	0.022*
C22	0.31970 (5)	0.31729 (15)	0.61607 (10)	0.0146 (3)
H22	0.3335	0.3292	0.5731	0.018*
C221	0.29064 (5)	0.18744 (14)	0.61034 (10)	0.0133 (3)

C222	0.29510 (5)	0.06659 (15)	0.56496 (10)	0.0132 (3)
Cl22	0.33362 (2)	0.06845 (4)	0.50727 (2)	0.01717 (9)
C223	0.26987 (5)	−0.05849 (15)	0.56351 (10)	0.0147 (3)
H223	0.2746	−0.1396	0.5340	0.018*
C224	0.23759 (5)	−0.06212 (15)	0.60632 (10)	0.0149 (3)
Cl24	0.20662 (2)	−0.21921 (4)	0.60666 (3)	0.01962 (9)
C225	0.22975 (6)	0.05596 (15)	0.64870 (10)	0.0158 (3)
H225	0.2066	0.0530	0.6760	0.019*
C226	0.25633 (5)	0.17802 (15)	0.65033 (10)	0.0150 (3)
H226	0.2512	0.2588	0.6797	0.018*
C41	0.44200 (6)	0.74136 (15)	0.60404 (10)	0.0154 (3)
H41	0.4686	0.8120	0.6306	0.018*
C42	0.43613 (6)	0.67480 (15)	0.52616 (10)	0.0153 (3)
H42	0.4082	0.6076	0.4993	0.018*
C421	0.46824 (5)	0.69448 (15)	0.47787 (10)	0.0145 (3)
C422	0.50747 (6)	0.79820 (16)	0.50348 (11)	0.0186 (3)
H422	0.5137	0.8613	0.5535	0.022*
C423	0.53739 (6)	0.80969 (18)	0.45648 (11)	0.0223 (3)
H423	0.5637	0.8811	0.4742	0.027*
C424	0.52924 (6)	0.71746 (17)	0.38357 (11)	0.0214 (3)
H424	0.5501	0.7251	0.3520	0.026*
C425	0.49045 (6)	0.61427 (16)	0.35741 (11)	0.0207 (3)
H425	0.4847	0.5509	0.3078	0.025*
C426	0.45998 (6)	0.60331 (15)	0.40360 (10)	0.0177 (3)
H426	0.4332	0.5331	0.3846	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0176 (6)	0.0181 (6)	0.0158 (6)	−0.0030 (5)	0.0101 (5)	−0.0026 (5)
C2	0.0170 (6)	0.0156 (7)	0.0154 (7)	−0.0022 (5)	0.0087 (6)	−0.0009 (5)
C3	0.0180 (6)	0.0152 (7)	0.0151 (7)	−0.0009 (5)	0.0096 (6)	−0.0016 (5)
C4	0.0137 (6)	0.0147 (6)	0.0137 (6)	0.0005 (5)	0.0073 (5)	0.0004 (5)
C4A	0.0114 (6)	0.0142 (6)	0.0122 (6)	0.0004 (5)	0.0048 (5)	0.0001 (5)
C5	0.0143 (6)	0.0163 (7)	0.0149 (7)	−0.0014 (5)	0.0065 (5)	0.0012 (5)
C6	0.0176 (7)	0.0137 (7)	0.0175 (7)	−0.0014 (5)	0.0069 (6)	−0.0011 (5)
C7	0.0191 (7)	0.0185 (7)	0.0162 (7)	0.0021 (6)	0.0085 (6)	−0.0032 (6)
C8	0.0162 (6)	0.0206 (7)	0.0160 (7)	−0.0005 (6)	0.0093 (6)	−0.0017 (6)
C8A	0.0135 (6)	0.0158 (7)	0.0129 (6)	−0.0005 (5)	0.0061 (5)	−0.0004 (5)
C21	0.0236 (7)	0.0186 (7)	0.0198 (7)	−0.0048 (6)	0.0150 (6)	−0.0011 (6)
C22	0.0143 (6)	0.0159 (7)	0.0152 (7)	−0.0007 (5)	0.0083 (5)	0.0017 (5)
C221	0.0132 (6)	0.0144 (6)	0.0120 (6)	−0.0004 (5)	0.0059 (5)	0.0007 (5)
C222	0.0123 (6)	0.0173 (7)	0.0123 (6)	0.0001 (5)	0.0077 (5)	0.0013 (5)
Cl22	0.01978 (17)	0.01936 (17)	0.01910 (17)	−0.00169 (13)	0.01472 (14)	−0.00115 (13)
C223	0.0163 (6)	0.0148 (6)	0.0142 (6)	−0.0003 (5)	0.0082 (5)	−0.0015 (5)
C224	0.0147 (6)	0.0146 (6)	0.0151 (6)	−0.0027 (5)	0.0070 (5)	0.0021 (5)
Cl24	0.02385 (18)	0.01647 (17)	0.02334 (18)	−0.00653 (13)	0.01515 (15)	−0.00166 (14)
C225	0.0157 (6)	0.0194 (7)	0.0156 (7)	0.0002 (5)	0.0100 (6)	0.0011 (6)

C226	0.0165 (6)	0.0154 (7)	0.0150 (7)	−0.0002 (5)	0.0090 (5)	−0.0016 (5)
C41	0.0157 (6)	0.0139 (6)	0.0187 (7)	−0.0020 (5)	0.0101 (6)	0.0000 (5)
C42	0.0149 (6)	0.0154 (6)	0.0168 (7)	−0.0008 (5)	0.0086 (5)	0.0010 (5)
C421	0.0143 (6)	0.0162 (7)	0.0135 (6)	0.0026 (5)	0.0070 (5)	0.0023 (5)
C422	0.0177 (7)	0.0239 (8)	0.0157 (7)	−0.0028 (6)	0.0092 (6)	−0.0024 (6)
C423	0.0169 (7)	0.0304 (8)	0.0210 (8)	−0.0037 (6)	0.0102 (6)	0.0000 (6)
C424	0.0204 (7)	0.0300 (8)	0.0198 (7)	0.0067 (6)	0.0145 (6)	0.0052 (6)
C425	0.0281 (8)	0.0203 (7)	0.0169 (7)	0.0059 (6)	0.0134 (6)	0.0014 (6)
C426	0.0220 (7)	0.0155 (7)	0.0161 (7)	0.0015 (6)	0.0096 (6)	0.0014 (5)

Geometric parameters (Å, º)

N1—C2	1.3285 (18)	C222—C223	1.3874 (19)
N1—C8A	1.3650 (18)	C222—Cl22	1.7421 (14)
C2—C3	1.4178 (19)	C223—C224	1.3872 (19)
C2—C21	1.4672 (19)	C223—H223	0.9500
C3—C4	1.3785 (19)	C224—C225	1.388 (2)
C3—H3	0.9500	C224—Cl24	1.7403 (14)
C4—C4A	1.4360 (19)	C225—C226	1.382 (2)
C4—C41	1.4728 (19)	C225—H225	0.9500
C4A—C5	1.4204 (19)	C226—H226	0.9500
C4A—C8A	1.4268 (19)	C41—C42	1.339 (2)
C5—C6	1.371 (2)	C41—H41	0.9500
C5—H5	0.9500	C42—C421	1.4671 (19)
C6—C7	1.412 (2)	C42—H42	0.9500
C6—H6	0.9500	C421—C422	1.399 (2)
C7—C8	1.368 (2)	C421—C426	1.401 (2)
C7—H7	0.9500	C422—C423	1.387 (2)
C8—C8A	1.418 (2)	C422—H422	0.9500
C8—H8	0.9500	C423—C424	1.392 (2)
C21—C22	1.331 (2)	C423—H423	0.9500
C21—H21	0.9500	C424—C425	1.387 (2)
C22—C221	1.4681 (19)	C424—H424	0.9500
C22—H22	0.9500	C425—C426	1.389 (2)
C221—C222	1.4015 (19)	C425—H425	0.9500
C221—C226	1.4061 (19)	C426—H426	0.9500
C2—N1—C8A	117.96 (12)	C223—C222—Cl22	116.95 (11)
N1—C2—C3	122.71 (13)	C221—C222—Cl22	120.32 (10)
N1—C2—C21	114.75 (13)	C224—C223—C222	118.32 (13)
C3—C2—C21	122.54 (13)	C224—C223—H223	120.8
C4—C3—C2	120.89 (13)	C222—C223—H223	120.8
C4—C3—H3	119.6	C223—C224—C225	121.52 (13)
C2—C3—H3	119.6	C223—C224—Cl24	118.71 (11)
C3—C4—C4A	117.53 (12)	C225—C224—Cl24	119.76 (11)
C3—C4—C41	121.29 (13)	C226—C225—C224	118.53 (13)
C4A—C4—C41	121.18 (12)	C226—C225—H225	120.7
C5—C4A—C8A	118.08 (12)	C224—C225—H225	120.7

C5—C4A—C4	124.28 (13)	C225—C226—C221	122.65 (13)
C8A—C4A—C4	117.61 (12)	C225—C226—H226	118.7
C6—C5—C4A	121.07 (13)	C221—C226—H226	118.7
C6—C5—H5	119.5	C42—C41—C4	123.72 (13)
C4A—C5—H5	119.5	C42—C41—H41	118.1
C5—C6—C7	120.56 (13)	C4—C41—H41	118.1
C5—C6—H6	119.7	C41—C42—C421	126.98 (13)
C7—C6—H6	119.7	C41—C42—H42	116.5
C8—C7—C6	119.97 (13)	C421—C42—H42	116.5
C8—C7—H7	120.0	C422—C421—C426	118.31 (13)
C6—C7—H7	120.0	C422—C421—C42	123.22 (13)
C7—C8—C8A	120.86 (13)	C426—C421—C42	118.46 (13)
C7—C8—H8	119.6	C423—C422—C421	120.57 (14)
C8A—C8—H8	119.6	C423—C422—H422	119.7
N1—C8A—C8	117.28 (12)	C421—C422—H422	119.7
N1—C8A—C4A	123.26 (13)	C422—C423—C424	120.58 (15)
C8—C8A—C4A	119.44 (13)	C422—C423—H423	119.7
C22—C21—C2	127.60 (13)	C424—C423—H423	119.7
C22—C21—H21	116.2	C425—C424—C423	119.43 (14)
C2—C21—H21	116.2	C425—C424—H424	120.3
C21—C22—C221	123.61 (13)	C423—C424—H424	120.3
C21—C22—H22	118.2	C424—C425—C426	120.19 (14)
C221—C22—H22	118.2	C424—C425—H425	119.9
C222—C221—C226	116.14 (12)	C426—C425—H425	119.9
C222—C221—C22	122.53 (12)	C425—C426—C421	120.91 (14)
C226—C221—C22	121.33 (13)	C425—C426—H426	119.5
C223—C222—C221	122.74 (12)	C421—C426—H426	119.5

C8A—N1—C2—C3	1.6 (2)	C21—C22—C221—C226	18.6 (2)
C8A—N1—C2—C21	−179.32 (12)	C226—C221—C222—C223	−3.6 (2)
N1—C2—C3—C4	0.0 (2)	C22—C221—C222—C223	176.63 (13)
C21—C2—C3—C4	−179.02 (13)	C226—C221—C222—Cl22	176.57 (10)
C2—C3—C4—C4A	−0.8 (2)	C22—C221—C222—Cl22	−3.22 (19)
C2—C3—C4—C41	178.76 (13)	C221—C222—C223—C224	2.1 (2)
C3—C4—C4A—C5	−177.89 (13)	Cl22—C222—C223—C224	−178.06 (11)
C41—C4—C4A—C5	2.5 (2)	C222—C223—C224—C225	0.9 (2)
C3—C4—C4A—C8A	0.08 (19)	C222—C223—C224—Cl24	−178.95 (10)
C41—C4—C4A—C8A	−179.49 (12)	C223—C224—C225—C226	−2.1 (2)
C8A—C4A—C5—C6	−1.3 (2)	Cl24—C224—C225—C226	177.75 (11)
C4—C4A—C5—C6	176.68 (14)	C224—C225—C226—C221	0.4 (2)
C4A—C5—C6—C7	0.3 (2)	C222—C221—C226—C225	2.3 (2)
C5—C6—C7—C8	0.8 (2)	C22—C221—C226—C225	−177.90 (13)
C6—C7—C8—C8A	−0.9 (2)	C3—C4—C41—C42	23.4 (2)
C2—N1—C8A—C8	176.15 (13)	C4A—C4—C41—C42	−157.03 (14)
C2—N1—C8A—C4A	−2.4 (2)	C4—C41—C42—C421	−177.25 (13)
C7—C8—C8A—N1	−178.68 (13)	C41—C42—C421—C422	−6.1 (2)
C7—C8—C8A—C4A	−0.1 (2)	C41—C42—C421—C426	172.66 (14)
C5—C4A—C8A—N1	179.65 (13)	C426—C421—C422—C423	−0.2 (2)

C4—C4A—C8A—N1	1.6 (2)	C42—C421—C422—C423	178.56 (14)
C5—C4A—C8A—C8	1.14 (19)	C421—C422—C423—C424	−0.6 (2)
C4—C4A—C8A—C8	−176.96 (13)	C422—C423—C424—C425	0.6 (2)
N1—C2—C21—C22	168.07 (15)	C423—C424—C425—C426	0.1 (2)
C3—C2—C21—C22	−12.9 (2)	C424—C425—C426—C421	−0.8 (2)
C2—C21—C22—C221	−177.26 (14)	C422—C421—C426—C425	0.9 (2)
C21—C22—C221—C222	−161.58 (14)	C42—C421—C426—C425	−177.92 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C225—H225···N1^{i}	0.95	2.62	3.522 (2)	158
C6—H6···*Cg*1^{ii}	0.95	2.65	3.4152 (16)	138
C422—H422···*Cg*2^{iii}	0.95	2.88	3.5843 (17)	132

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+3/2; (ii) *x*, −*y*+2, *z*+1/2; (iii) −*x*+1, *y*, −*z*+3/2.

{2-[(*E*)-2-(4-Bromophenyl)ethenyl]-4-[(*E*)-2-phenylethenyl]quinolin-3-yl}(phenyl)methanone (IIc)

Crystal data

$C_{32}H_{22}BrNO$
M_r = 516.41
Monoclinic, $P2_1/n$
a = 12.287 (2) Å
b = 15.528 (3) Å
c = 12.844 (3) Å
β = 99.877 (6)°
V = 2414.2 (8) Å^3
Z = 4
$F(000)$ = 1056
D_x = 1.421 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5610 reflections
θ = 2.1–27.6°
μ = 1.73 mm^{-1}
T = 100 K
Block, orange
0.15 × 0.12 × 0.08 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: INCOATEC high brilliance microfocus sealed tube
Multilayer mirror monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.720, T_{max} = 0.871
5530 measured reflections
5530 independent reflections
4290 reflections with $I > 2\sigma(I)$
θ_{max} = 27.7°, θ_{min} = 2.1°
h = −15→15
k = −20→20
l = −13→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.196
S = 1.05
5530 reflections
317 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1201P)^2 + 3.4939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.4215 (3)	0.3390 (2)	0.8002 (3)	0.0148 (7)
C2	0.3349 (3)	0.3701 (2)	0.7353 (3)	0.0128 (8)
C3	0.3391 (3)	0.3892 (2)	0.6276 (3)	0.0141 (8)
C4	0.4366 (3)	0.3801 (2)	0.5881 (3)	0.0126 (7)
C4A	0.5332 (3)	0.3511 (3)	0.6594 (3)	0.0131 (7)
C5	0.6411 (3)	0.3442 (3)	0.6328 (3)	0.0157 (8)
H5	0.6538	0.3631	0.5656	0.019*
C6	0.7264 (3)	0.3106 (3)	0.7039 (3)	0.0190 (9)
H6	0.7977	0.3061	0.6852	0.023*
C7	0.7098 (3)	0.2828 (3)	0.8042 (3)	0.0184 (8)
H7	0.7688	0.2572	0.8515	0.022*
C8	0.6083 (3)	0.2925 (3)	0.8338 (3)	0.0182 (8)
H8	0.5981	0.2749	0.9023	0.022*
C8A	0.5189 (3)	0.3285 (3)	0.7637 (3)	0.0128 (8)
C21	0.2315 (3)	0.3833 (3)	0.7768 (3)	0.0154 (8)
H21	0.1662	0.3971	0.7286	0.018*
C22	0.2255 (3)	0.3765 (3)	0.8796 (3)	0.0157 (8)
H22	0.2930	0.3658	0.9261	0.019*
C221	0.1265 (3)	0.3837 (3)	0.9281 (3)	0.0164 (8)
C222	0.1348 (4)	0.3630 (3)	1.0353 (3)	0.0181 (8)
H222	0.2050	0.3487	1.0750	0.022*
C223	0.0431 (4)	0.3628 (3)	1.0853 (4)	0.0209 (9)
H223	0.0500	0.3477	1.1578	0.025*
C224	−0.0587 (4)	0.3850 (3)	1.0271 (4)	0.0195 (9)
Br24	−0.18670 (4)	0.38279 (3)	1.09166 (4)	0.02932 (18)
C225	−0.0702 (3)	0.4086 (3)	0.9209 (4)	0.0199 (9)
H225	−0.1403	0.4247	0.8824	0.024*
C226	0.0224 (3)	0.4081 (3)	0.8724 (3)	0.0178 (8)
H226	0.0154	0.4245	0.8003	0.021*
C31	0.2347 (3)	0.4121 (3)	0.5521 (3)	0.0138 (8)
O31	0.1835 (3)	0.3554 (2)	0.5000 (3)	0.0226 (7)
C311	0.1978 (3)	0.5040 (3)	0.5436 (3)	0.0145 (8)
C312	0.2408 (3)	0.5642 (3)	0.6201 (3)	0.0161 (8)
H312	0.2989	0.5484	0.6756	0.019*
C313	0.1985 (4)	0.6477 (3)	0.6148 (3)	0.0199 (9)
H313	0.2256	0.6884	0.6682	0.024*
C314	0.1159 (4)	0.6713 (3)	0.5308 (4)	0.0200 (9)
H314	0.0868	0.7280	0.5273	0.024*

C315	0.0762 (4)	0.6118 (3)	0.4521 (4)	0.0194 (9)
H315	0.0223	0.6287	0.3935	0.023*
C316	0.1154 (3)	0.5281 (3)	0.4594 (3)	0.0164 (8)
H316	0.0863	0.4870	0.4072	0.020*
C41	0.4372 (3)	0.3989 (3)	0.4752 (3)	0.0143 (8)
H41	0.4039	0.4513	0.4478	0.017*
C42	0.4805 (3)	0.3485 (3)	0.4088 (3)	0.0145 (8)
H42	0.5158	0.2972	0.4372	0.017*
C421	0.4788 (3)	0.3649 (3)	0.2956 (3)	0.0142 (8)
C422	0.4231 (3)	0.4349 (3)	0.2418 (3)	0.0195 (9)
H422	0.3809	0.4724	0.2777	0.023*
C423	0.4292 (4)	0.4499 (3)	0.1362 (3)	0.0236 (9)
H423	0.3914	0.4975	0.1003	0.028*
C424	0.4910 (4)	0.3950 (3)	0.0828 (3)	0.0222 (9)
H424	0.4960	0.4059	0.0110	0.027*
C425	0.5451 (3)	0.3243 (3)	0.1344 (3)	0.0186 (9)
H425	0.5867	0.2866	0.0981	0.022*
C426	0.5376 (3)	0.3094 (3)	0.2400 (3)	0.0162 (8)
H426	0.5732	0.2605	0.2748	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0167 (16)	0.0156 (17)	0.0127 (16)	−0.0016 (13)	0.0040 (13)	0.0026 (13)
C2	0.0146 (18)	0.0130 (18)	0.0117 (18)	−0.0005 (14)	0.0045 (14)	−0.0014 (14)
C3	0.0177 (18)	0.0105 (18)	0.0147 (19)	0.0015 (14)	0.0047 (15)	−0.0016 (15)
C4	0.0155 (18)	0.0125 (18)	0.0101 (18)	0.0005 (14)	0.0033 (14)	0.0004 (14)
C4A	0.0127 (17)	0.0166 (19)	0.0111 (18)	0.0009 (14)	0.0049 (14)	−0.0015 (15)
C5	0.0166 (19)	0.021 (2)	0.0105 (18)	−0.0027 (16)	0.0037 (15)	−0.0021 (16)
C6	0.0134 (18)	0.022 (2)	0.021 (2)	0.0005 (16)	0.0031 (16)	−0.0010 (17)
C7	0.0149 (18)	0.022 (2)	0.017 (2)	0.0010 (16)	−0.0009 (16)	0.0023 (17)
C8	0.020 (2)	0.022 (2)	0.0131 (19)	−0.0001 (16)	0.0031 (16)	0.0040 (16)
C8A	0.0143 (18)	0.0128 (18)	0.0113 (18)	−0.0001 (14)	0.0023 (14)	−0.0006 (14)
C21	0.0137 (18)	0.0181 (19)	0.0147 (19)	0.0006 (15)	0.0037 (15)	−0.0013 (15)
C22	0.0152 (19)	0.0143 (19)	0.018 (2)	−0.0016 (14)	0.0037 (16)	−0.0005 (15)
C221	0.020 (2)	0.0140 (19)	0.017 (2)	−0.0008 (15)	0.0080 (16)	−0.0010 (16)
C222	0.022 (2)	0.018 (2)	0.015 (2)	0.0004 (16)	0.0044 (17)	0.0004 (16)
C223	0.029 (2)	0.018 (2)	0.018 (2)	−0.0036 (17)	0.0112 (18)	−0.0006 (17)
C224	0.023 (2)	0.015 (2)	0.026 (2)	−0.0047 (16)	0.0182 (18)	−0.0063 (17)
Br24	0.0283 (3)	0.0292 (3)	0.0366 (3)	−0.00666 (19)	0.0230 (2)	−0.0062 (2)
C225	0.0143 (19)	0.021 (2)	0.025 (2)	−0.0026 (16)	0.0063 (17)	−0.0024 (18)
C226	0.021 (2)	0.018 (2)	0.016 (2)	−0.0017 (16)	0.0075 (16)	−0.0026 (16)
C31	0.0116 (17)	0.0198 (19)	0.0109 (18)	0.0023 (15)	0.0043 (14)	−0.0007 (15)
O31	0.0221 (15)	0.0184 (15)	0.0245 (17)	−0.0016 (12)	−0.0035 (13)	−0.0064 (13)
C311	0.0133 (18)	0.017 (2)	0.0148 (19)	−0.0010 (15)	0.0073 (15)	0.0015 (15)
C312	0.0149 (18)	0.019 (2)	0.0132 (19)	0.0003 (15)	−0.0004 (15)	0.0003 (15)
C313	0.023 (2)	0.017 (2)	0.019 (2)	0.0012 (16)	0.0021 (17)	−0.0027 (17)
C314	0.021 (2)	0.017 (2)	0.023 (2)	0.0033 (16)	0.0041 (17)	0.0006 (17)

C315	0.0156 (19)	0.022 (2)	0.019 (2)	0.0018 (16)	−0.0001 (16)	0.0054 (17)
C316	0.0140 (18)	0.021 (2)	0.015 (2)	−0.0023 (15)	0.0032 (15)	−0.0009 (16)
C41	0.0135 (18)	0.019 (2)	0.0105 (18)	−0.0016 (14)	0.0016 (14)	0.0023 (15)
C42	0.0180 (19)	0.0143 (18)	0.0108 (18)	−0.0010 (15)	0.0013 (15)	0.0009 (15)
C421	0.0151 (18)	0.016 (2)	0.0112 (19)	−0.0044 (14)	0.0016 (15)	0.0004 (15)
C422	0.020 (2)	0.021 (2)	0.017 (2)	0.0020 (16)	0.0006 (16)	−0.0005 (17)
C423	0.031 (2)	0.025 (2)	0.014 (2)	−0.0016 (19)	0.0002 (17)	0.0059 (17)
C424	0.024 (2)	0.033 (3)	0.0100 (19)	−0.0086 (18)	0.0036 (16)	−0.0005 (17)
C425	0.021 (2)	0.021 (2)	0.014 (2)	−0.0068 (16)	0.0069 (16)	−0.0052 (16)
C426	0.0155 (18)	0.017 (2)	0.0158 (19)	−0.0034 (15)	0.0022 (15)	−0.0011 (16)

Geometric parameters (Å, º)

N1—C2	1.325 (5)	C225—H225	0.9500
N1—C8A	1.368 (5)	C226—H226	0.9500
C2—C3	1.424 (6)	C31—O31	1.214 (5)
C2—C21	1.474 (5)	C31—C311	1.496 (6)
C3—C4	1.387 (6)	C311—C312	1.393 (6)
C3—C31	1.512 (5)	C311—C316	1.399 (6)
C4—C4A	1.441 (5)	C312—C313	1.395 (6)
C4—C41	1.480 (5)	C312—H312	0.9500
C4A—C8A	1.425 (5)	C313—C314	1.397 (6)
C4A—C5	1.429 (5)	C313—H313	0.9500
C5—C6	1.370 (6)	C314—C315	1.395 (6)
C5—H5	0.9500	C314—H314	0.9500
C6—C7	1.406 (6)	C315—C316	1.382 (6)
C6—H6	0.9500	C315—H315	0.9500
C7—C8	1.374 (6)	C316—H316	0.9500
C7—H7	0.9500	C41—C42	1.334 (6)
C8—C8A	1.410 (6)	C41—H41	0.9500
C8—H8	0.9500	C42—C421	1.474 (5)
C21—C22	1.338 (6)	C42—H42	0.9500
C21—H21	0.9500	C421—C426	1.397 (6)
C22—C221	1.463 (6)	C421—C422	1.401 (6)
C22—H22	0.9500	C422—C423	1.391 (6)
C221—C222	1.400 (6)	C422—H422	0.9500
C221—C226	1.406 (6)	C423—C424	1.396 (7)
C222—C223	1.388 (6)	C423—H423	0.9500
C222—H222	0.9500	C424—C425	1.391 (7)
C223—C224	1.387 (7)	C424—H424	0.9500
C223—H223	0.9500	C425—C426	1.394 (6)
C224—C225	1.396 (6)	C425—H425	0.9500
C224—Br24	1.899 (4)	C426—H426	0.9500
C225—C226	1.388 (6)		

C2—N1—C8A	118.9 (3)	C225—C226—C221	121.1 (4)
N1—C2—C3	121.9 (4)	C225—C226—H226	119.4
N1—C2—C21	118.1 (4)	C221—C226—H226	119.4

C3—C2—C21	120.0 (4)	O31—C31—C311	122.0 (4)
C4—C3—C2	120.8 (4)	O31—C31—C3	119.0 (4)
C4—C3—C31	118.7 (4)	C311—C31—C3	119.0 (3)
C2—C3—C31	120.3 (4)	C312—C311—C316	120.1 (4)
C3—C4—C4A	117.9 (3)	C312—C311—C31	121.0 (4)
C3—C4—C41	119.2 (3)	C316—C311—C31	118.8 (4)
C4A—C4—C41	122.9 (3)	C311—C312—C313	119.8 (4)
C8A—C4A—C5	118.4 (4)	C311—C312—H312	120.1
C8A—C4A—C4	117.0 (3)	C313—C312—H312	120.1
C5—C4A—C4	124.6 (4)	C312—C313—C314	119.7 (4)
C6—C5—C4A	120.3 (4)	C312—C313—H313	120.1
C6—C5—H5	119.8	C314—C313—H313	120.1
C4A—C5—H5	119.8	C315—C314—C313	120.3 (4)
C5—C6—C7	120.9 (4)	C315—C314—H314	119.9
C5—C6—H6	119.6	C313—C314—H314	119.9
C7—C6—H6	119.6	C316—C315—C314	119.9 (4)
C8—C7—C6	120.1 (4)	C316—C315—H315	120.1
C8—C7—H7	120.0	C314—C315—H315	120.1
C6—C7—H7	120.0	C315—C316—C311	120.1 (4)
C7—C8—C8A	120.8 (4)	C315—C316—H316	120.0
C7—C8—H8	119.6	C311—C316—H316	120.0
C8A—C8—H8	119.6	C42—C41—C4	125.4 (4)
N1—C8A—C8	117.4 (4)	C42—C41—H41	117.3
N1—C8A—C4A	123.3 (3)	C4—C41—H41	117.3
C8—C8A—C4A	119.3 (4)	C41—C42—C421	126.1 (4)
C22—C21—C2	122.8 (4)	C41—C42—H42	116.9
C22—C21—H21	118.6	C421—C42—H42	116.9
C2—C21—H21	118.6	C426—C421—C422	118.6 (4)
C21—C22—C221	127.2 (4)	C426—C421—C42	118.4 (4)
C21—C22—H22	116.4	C422—C421—C42	123.0 (4)
C221—C22—H22	116.4	C423—C422—C421	120.4 (4)
C222—C221—C226	117.9 (4)	C423—C422—H422	119.8
C222—C221—C22	118.4 (4)	C421—C422—H422	119.8
C226—C221—C22	123.6 (4)	C422—C423—C424	120.1 (4)
C223—C222—C221	121.8 (4)	C422—C423—H423	120.0
C223—C222—H222	119.1	C424—C423—H423	120.0
C221—C222—H222	119.1	C425—C424—C423	120.3 (4)
C224—C223—C222	118.7 (4)	C425—C424—H424	119.9
C224—C223—H223	120.7	C423—C424—H424	119.9
C222—C223—H223	120.7	C424—C425—C426	119.2 (4)
C223—C224—C225	121.5 (4)	C424—C425—H425	120.4
C223—C224—Br24	119.9 (3)	C426—C425—H425	120.4
C225—C224—Br24	118.6 (3)	C425—C426—C421	121.4 (4)
C226—C225—C224	119.0 (4)	C425—C426—H426	119.3
C226—C225—H225	120.5	C421—C426—H426	119.3
C224—C225—H225	120.5		
C8A—N1—C2—C3	2.9 (6)	C222—C223—C224—Br24	178.5 (3)

C8A—N1—C2—C21	−178.4 (4)	C223—C224—C225—C226	1.2 (7)
N1—C2—C3—C4	−3.6 (6)	Br24—C224—C225—C226	−178.2 (3)
C21—C2—C3—C4	177.7 (4)	C224—C225—C226—C221	0.5 (6)
N1—C2—C3—C31	171.0 (4)	C222—C221—C226—C225	−2.4 (6)
C21—C2—C3—C31	−7.7 (6)	C22—C221—C226—C225	175.9 (4)
C2—C3—C4—C4A	−0.1 (6)	C4—C3—C31—O31	81.8 (5)
C31—C3—C4—C4A	−174.8 (4)	C2—C3—C31—O31	−92.8 (5)
C2—C3—C4—C41	178.8 (3)	C4—C3—C31—C311	−98.1 (4)
C31—C3—C4—C41	4.2 (6)	C2—C3—C31—C311	87.2 (5)
C3—C4—C4A—C8A	4.0 (5)	O31—C31—C311—C312	164.5 (4)
C41—C4—C4A—C8A	−174.9 (4)	C3—C31—C311—C312	−15.6 (6)
C3—C4—C4A—C5	−175.5 (4)	O31—C31—C311—C316	−12.9 (6)
C41—C4—C4A—C5	5.6 (6)	C3—C31—C311—C316	167.0 (4)
C8A—C4A—C5—C6	4.8 (6)	C316—C311—C312—C313	2.6 (6)
C4—C4A—C5—C6	−175.7 (4)	C31—C311—C312—C313	−174.8 (4)
C4A—C5—C6—C7	−0.4 (6)	C311—C312—C313—C314	−2.4 (7)
C5—C6—C7—C8	−2.9 (7)	C312—C313—C314—C315	−0.2 (7)
C6—C7—C8—C8A	1.5 (7)	C313—C314—C315—C316	2.6 (7)
C2—N1—C8A—C8	−178.0 (4)	C314—C315—C316—C311	−2.4 (6)
C2—N1—C8A—C4A	1.4 (6)	C312—C311—C316—C315	−0.2 (6)
C7—C8—C8A—N1	−177.7 (4)	C31—C311—C316—C315	177.2 (4)
C7—C8—C8A—C4A	2.9 (6)	C3—C4—C41—C42	−131.9 (4)
C5—C4A—C8A—N1	174.7 (4)	C4A—C4—C41—C42	46.9 (6)
C4—C4A—C8A—N1	−4.9 (6)	C4—C41—C42—C421	178.0 (4)
C5—C4A—C8A—C8	−6.0 (6)	C41—C42—C421—C426	173.9 (4)
C4—C4A—C8A—C8	174.5 (4)	C41—C42—C421—C422	−4.5 (6)
N1—C2—C21—C22	9.4 (6)	C426—C421—C422—C423	−1.8 (6)
C3—C2—C21—C22	−171.8 (4)	C42—C421—C422—C423	176.5 (4)
C2—C21—C22—C221	−176.5 (4)	C421—C422—C423—C424	0.1 (7)
C21—C22—C221—C222	171.4 (4)	C422—C423—C424—C425	1.1 (7)
C21—C22—C221—C226	−6.8 (7)	C423—C424—C425—C426	−0.4 (6)
C226—C221—C222—C223	2.6 (6)	C424—C425—C426—C421	−1.4 (6)
C22—C221—C222—C223	−175.7 (4)	C422—C421—C426—C425	2.5 (6)
C221—C222—C223—C224	−1.0 (6)	C42—C421—C426—C425	−175.9 (4)
C222—C223—C224—C225	−1.0 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O31^{i}	0.95	2.51	3.164 (6)	126
C5—H5···*Cg*3^{ii}	0.95	2.96	3.728 (4)	138
C42—H42···*Cg*4^{iii}	0.95	2.88	3.766 (5)	155
C223—H223···*Cg*2^{iv}	0.95	2.84	3.429 (3)	122

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1/2, −*y*+1/2, *z*−1/2; (iv) *x*−1/2, −*y*+1/2, *z*+1/2.

{2-[(*E*)-2-(4-Bromophenyl)ethenyl]-4-[(*E*)-2-(4-chlorophenyl)ethenyl]quinolin-3-yl}(phenyl)methanone (IId)

Crystal data

$C_{32}H_{21}BrClNO$
$M_r = 550.86$
Triclinic, $P\overline{1}$
$a = 9.9051$ (12) Å
$b = 11.3936$ (16) Å
$c = 11.8192$ (16) Å
$\alpha = 77.727$ (5)°
$\beta = 76.116$ (5)°
$\gamma = 86.448$ (5)°
$V = 1265.2$ (3) Å^3
$Z = 2$
$F(000) = 560$
$D_x = 1.446$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5808 reflections
$\theta = 2.1$–27.5°
$\mu = 1.76$ mm^{-1}
$T = 100$ K
Needle, orange
0.19 × 0.12 × 0.10 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: INCOATEC high brilliance microfocus sealed tube
Multilayer mirror monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.735$, $T_{max} = 0.836$
61838 measured reflections
5807 independent reflections
5014 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -12\rightarrow12$
$k = -14\rightarrow14$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.065$
$S = 1.03$
5807 reflections
325 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0211P)^2 + 0.9058P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.25739 (15)	0.14281 (12)	0.26486 (12)	0.0186 (3)
C2	0.27568 (17)	0.25070 (15)	0.28341 (14)	0.0177 (3)
C3	0.18801 (17)	0.35119 (15)	0.25316 (14)	0.0174 (3)
C4	0.07281 (17)	0.33605 (15)	0.21049 (14)	0.0178 (3)
C4A	0.04978 (18)	0.21906 (15)	0.19294 (14)	0.0186 (3)
C5	−0.06396 (19)	0.19160 (16)	0.15045 (16)	0.0229 (4)
H5	−0.1308	0.2522	0.1338	0.027*
C6	−0.0786 (2)	0.07815 (17)	0.13304 (17)	0.0259 (4)

H6	−0.1550	0.0612	0.1037	0.031*
C7	0.0187 (2)	−0.01340 (17)	0.15836 (16)	0.0268 (4)
H7	0.0077	−0.0915	0.1458	0.032*
C8	0.1287 (2)	0.00997 (16)	0.20101 (16)	0.0239 (4)
H8	0.1936	−0.0523	0.2182	0.029*
C8A	0.14692 (18)	0.12607 (15)	0.21983 (14)	0.0189 (3)
C21	0.39417 (17)	0.26536 (15)	0.33401 (15)	0.0189 (3)
H21	0.4107	0.3431	0.3446	0.023*
C22	0.47975 (17)	0.17587 (15)	0.36585 (14)	0.0187 (3)
H22	0.4604	0.0981	0.3572	0.022*
C221	0.60111 (17)	0.18767 (15)	0.41304 (14)	0.0184 (3)
C222	0.69215 (19)	0.09039 (16)	0.42888 (16)	0.0222 (4)
H222	0.6732	0.0169	0.4104	0.027*
C223	0.81012 (19)	0.09851 (17)	0.47115 (16)	0.0248 (4)
H223	0.8715	0.0317	0.4812	0.030*
C224	0.83589 (18)	0.20575 (17)	0.49815 (15)	0.0217 (4)
Br24	0.99791 (2)	0.22361 (2)	0.55228 (2)	0.02713 (6)
C225	0.74666 (19)	0.30359 (16)	0.48620 (16)	0.0231 (4)
H225	0.7650	0.3760	0.5071	0.028*
C226	0.63015 (18)	0.29440 (16)	0.44326 (16)	0.0218 (4)
H226	0.5689	0.3615	0.4341	0.026*
C31	0.22620 (17)	0.47358 (15)	0.26497 (15)	0.0179 (3)
O31	0.22130 (14)	0.49477 (11)	0.36281 (11)	0.0243 (3)
C311	0.27711 (17)	0.56428 (15)	0.15343 (15)	0.0177 (3)
C312	0.31444 (17)	0.53198 (15)	0.04237 (15)	0.0188 (3)
H312	0.3043	0.4512	0.0366	0.023*
C313	0.36616 (19)	0.61701 (16)	−0.05946 (16)	0.0228 (4)
H313	0.3914	0.5944	−0.1347	0.027*
C314	0.38126 (19)	0.73545 (16)	−0.05168 (16)	0.0243 (4)
H314	0.4170	0.7936	−0.1215	0.029*
C315	0.3439 (2)	0.76857 (16)	0.05844 (17)	0.0264 (4)
H315	0.3534	0.8496	0.0637	0.032*
C316	0.29282 (19)	0.68348 (16)	0.16068 (16)	0.0240 (4)
H316	0.2684	0.7062	0.2359	0.029*
C41	−0.02388 (17)	0.43635 (15)	0.18546 (15)	0.0188 (3)
H41	−0.0546	0.4478	0.1136	0.023*
C42	−0.07061 (17)	0.51205 (15)	0.25875 (15)	0.0191 (3)
H42	−0.0399	0.4977	0.3308	0.023*
C421	−0.16475 (17)	0.61522 (15)	0.23908 (15)	0.0176 (3)
C422	−0.18229 (19)	0.67061 (16)	0.12605 (16)	0.0236 (4)
H422	−0.1320	0.6407	0.0587	0.028*
C423	−0.2715 (2)	0.76825 (16)	0.11010 (16)	0.0252 (4)
H423	−0.2825	0.8052	0.0328	0.030*
C424	−0.34445 (18)	0.81098 (15)	0.20919 (16)	0.0214 (4)
Cl44	−0.45721 (5)	0.93371 (4)	0.19179 (5)	0.03007 (11)
C425	−0.32830 (18)	0.75949 (16)	0.32232 (16)	0.0215 (4)
H425	−0.3780	0.7905	0.3892	0.026*
C426	−0.23864 (18)	0.66202 (16)	0.33677 (15)	0.0206 (3)

H426	−0.2271	0.6264	0.4142	0.025*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0214 (7)	0.0165 (7)	0.0177 (7)	0.0009 (6)	−0.0040 (6)	−0.0039 (6)
C2	0.0202 (8)	0.0173 (8)	0.0143 (8)	0.0006 (6)	−0.0016 (6)	−0.0031 (6)
C3	0.0218 (8)	0.0157 (8)	0.0133 (7)	0.0001 (6)	−0.0017 (6)	−0.0029 (6)
C4	0.0208 (8)	0.0170 (8)	0.0140 (8)	0.0015 (6)	−0.0014 (6)	−0.0033 (6)
C4A	0.0227 (8)	0.0176 (8)	0.0145 (8)	−0.0008 (7)	−0.0022 (6)	−0.0032 (6)
C5	0.0240 (9)	0.0220 (9)	0.0228 (9)	0.0000 (7)	−0.0066 (7)	−0.0036 (7)
C6	0.0290 (9)	0.0249 (9)	0.0255 (9)	−0.0060 (8)	−0.0088 (8)	−0.0048 (7)
C7	0.0381 (11)	0.0198 (9)	0.0244 (9)	−0.0043 (8)	−0.0081 (8)	−0.0067 (7)
C8	0.0316 (10)	0.0178 (9)	0.0225 (9)	0.0001 (7)	−0.0058 (7)	−0.0052 (7)
C8A	0.0230 (8)	0.0178 (8)	0.0151 (8)	−0.0004 (7)	−0.0023 (6)	−0.0038 (6)
C21	0.0217 (8)	0.0178 (8)	0.0173 (8)	−0.0012 (6)	−0.0029 (6)	−0.0052 (6)
C22	0.0212 (8)	0.0183 (8)	0.0164 (8)	−0.0009 (6)	−0.0014 (6)	−0.0065 (6)
C221	0.0200 (8)	0.0201 (8)	0.0137 (8)	−0.0007 (6)	−0.0012 (6)	−0.0039 (6)
C222	0.0259 (9)	0.0179 (8)	0.0234 (9)	0.0003 (7)	−0.0055 (7)	−0.0060 (7)
C223	0.0251 (9)	0.0229 (9)	0.0260 (9)	0.0037 (7)	−0.0068 (7)	−0.0044 (7)
C224	0.0187 (8)	0.0288 (10)	0.0167 (8)	−0.0023 (7)	−0.0039 (6)	−0.0028 (7)
Br24	0.02189 (9)	0.03552 (11)	0.02435 (10)	−0.00343 (7)	−0.00719 (7)	−0.00397 (7)
C225	0.0263 (9)	0.0215 (9)	0.0229 (9)	−0.0026 (7)	−0.0046 (7)	−0.0082 (7)
C226	0.0226 (8)	0.0198 (9)	0.0243 (9)	0.0024 (7)	−0.0060 (7)	−0.0077 (7)
C31	0.0191 (8)	0.0168 (8)	0.0187 (8)	0.0039 (6)	−0.0060 (6)	−0.0052 (6)
O31	0.0362 (7)	0.0207 (6)	0.0183 (6)	0.0028 (5)	−0.0089 (5)	−0.0073 (5)
C311	0.0173 (8)	0.0180 (8)	0.0187 (8)	0.0016 (6)	−0.0054 (6)	−0.0049 (6)
C312	0.0198 (8)	0.0174 (8)	0.0203 (8)	0.0031 (6)	−0.0046 (7)	−0.0072 (7)
C313	0.0247 (9)	0.0238 (9)	0.0192 (8)	0.0017 (7)	−0.0021 (7)	−0.0065 (7)
C314	0.0247 (9)	0.0215 (9)	0.0227 (9)	−0.0005 (7)	−0.0009 (7)	−0.0005 (7)
C315	0.0333 (10)	0.0164 (9)	0.0288 (10)	−0.0027 (7)	−0.0048 (8)	−0.0051 (7)
C316	0.0300 (9)	0.0209 (9)	0.0223 (9)	0.0004 (7)	−0.0058 (7)	−0.0073 (7)
C41	0.0202 (8)	0.0187 (8)	0.0168 (8)	−0.0003 (6)	−0.0046 (6)	−0.0019 (6)
C42	0.0189 (8)	0.0211 (9)	0.0159 (8)	0.0004 (7)	−0.0029 (6)	−0.0021 (7)
C421	0.0183 (8)	0.0178 (8)	0.0171 (8)	−0.0009 (6)	−0.0029 (6)	−0.0055 (6)
C422	0.0298 (9)	0.0226 (9)	0.0180 (8)	0.0051 (7)	−0.0029 (7)	−0.0079 (7)
C423	0.0341 (10)	0.0220 (9)	0.0206 (9)	0.0048 (8)	−0.0093 (8)	−0.0046 (7)
C424	0.0200 (8)	0.0166 (8)	0.0296 (9)	0.0027 (7)	−0.0072 (7)	−0.0083 (7)
Cl44	0.0321 (2)	0.0214 (2)	0.0424 (3)	0.01031 (18)	−0.0158 (2)	−0.0138 (2)
C425	0.0217 (8)	0.0220 (9)	0.0220 (9)	0.0002 (7)	−0.0014 (7)	−0.0110 (7)
C426	0.0208 (8)	0.0231 (9)	0.0179 (8)	0.0002 (7)	−0.0033 (7)	−0.0059 (7)

Geometric parameters (Å, º)

N1—C2	1.324 (2)	C225—H225	0.9500
N1—C8A	1.366 (2)	C226—H226	0.9500
C2—C3	1.430 (2)	C31—O31	1.220 (2)
C2—C21	1.472 (2)	C31—C311	1.492 (2)

C3—C4	1.387 (2)	C311—C312	1.397 (2)
C3—C31	1.510 (2)	C311—C316	1.399 (2)
C4—C4A	1.432 (2)	C312—C313	1.385 (2)
C4—C41	1.472 (2)	C312—H312	0.9500
C4A—C5	1.415 (2)	C313—C314	1.391 (3)
C4A—C8A	1.424 (2)	C313—H313	0.9500
C5—C6	1.373 (3)	C314—C315	1.391 (3)
C5—H5	0.9500	C314—H314	0.9500
C6—C7	1.410 (3)	C315—C316	1.388 (3)
C6—H6	0.9500	C315—H315	0.9500
C7—C8	1.368 (3)	C316—H316	0.9500
C7—H7	0.9500	C41—C42	1.336 (2)
C8—C8A	1.416 (2)	C41—H41	0.9500
C8—H8	0.9500	C42—C421	1.469 (2)
C21—C22	1.335 (2)	C42—H42	0.9500
C21—H21	0.9500	C421—C422	1.397 (2)
C22—C221	1.465 (2)	C421—C426	1.400 (2)
C22—H22	0.9500	C422—C423	1.387 (2)
C221—C222	1.395 (2)	C422—H422	0.9500
C221—C226	1.402 (2)	C423—C424	1.387 (3)
C222—C223	1.392 (2)	C423—H423	0.9500
C222—H222	0.9500	C424—C425	1.384 (3)
C223—C224	1.380 (3)	C424—Cl44	1.7434 (17)
C223—H223	0.9500	C425—C426	1.386 (2)
C224—C225	1.384 (3)	C425—H425	0.9500
C224—Br24	1.9012 (17)	C426—H426	0.9500
C225—C226	1.385 (2)		

C2—N1—C8A	118.52 (14)	C225—C226—C221	121.07 (16)
N1—C2—C3	122.50 (15)	C225—C226—H226	119.5
N1—C2—C21	117.24 (15)	C221—C226—H226	119.5
C3—C2—C21	120.24 (15)	O31—C31—C311	121.58 (15)
C4—C3—C2	120.13 (15)	O31—C31—C3	120.48 (15)
C4—C3—C31	121.16 (15)	C311—C31—C3	117.85 (14)
C2—C3—C31	118.69 (14)	C312—C311—C316	119.22 (16)
C3—C4—C4A	117.81 (15)	C312—C311—C31	121.46 (15)
C3—C4—C41	121.26 (15)	C316—C311—C31	119.27 (15)
C4A—C4—C41	120.93 (15)	C313—C312—C311	120.39 (16)
C5—C4A—C8A	118.69 (15)	C313—C312—H312	119.8
C5—C4A—C4	123.41 (16)	C311—C312—H312	119.8
C8A—C4A—C4	117.90 (15)	C312—C313—C314	120.10 (16)
C6—C5—C4A	120.61 (17)	C312—C313—H313	119.9
C6—C5—H5	119.7	C314—C313—H313	119.9
C4A—C5—H5	119.7	C315—C314—C313	119.93 (17)
C5—C6—C7	120.58 (17)	C315—C314—H314	120.0
C5—C6—H6	119.7	C313—C314—H314	120.0
C7—C6—H6	119.7	C316—C315—C314	120.11 (17)
C8—C7—C6	120.17 (17)	C316—C315—H315	119.9

C8—C7—H7	119.9	C314—C315—H315	119.9
C6—C7—H7	119.9	C315—C316—C311	120.24 (16)
C7—C8—C8A	120.65 (17)	C315—C316—H316	119.9
C7—C8—H8	119.7	C311—C316—H316	119.9
C8A—C8—H8	119.7	C42—C41—C4	123.27 (15)
N1—C8A—C8	117.71 (15)	C42—C41—H41	118.4
N1—C8A—C4A	122.99 (15)	C4—C41—H41	118.4
C8—C8A—C4A	119.29 (16)	C41—C42—C421	126.48 (16)
C22—C21—C2	123.88 (16)	C41—C42—H42	116.8
C22—C21—H21	118.1	C421—C42—H42	116.8
C2—C21—H21	118.1	C422—C421—C426	118.16 (16)
C21—C22—C221	125.45 (16)	C422—C421—C42	122.70 (15)
C21—C22—H22	117.3	C426—C421—C42	119.14 (15)
C221—C22—H22	117.3	C423—C422—C421	121.44 (16)
C222—C221—C226	118.02 (16)	C423—C422—H422	119.3
C222—C221—C22	119.70 (15)	C421—C422—H422	119.3
C226—C221—C22	122.27 (15)	C424—C423—C422	118.73 (16)
C223—C222—C221	121.57 (16)	C424—C423—H423	120.6
C223—C222—H222	119.2	C422—C423—H423	120.6
C221—C222—H222	119.2	C425—C424—C423	121.45 (16)
C224—C223—C222	118.52 (17)	C425—C424—Cl44	118.81 (14)
C224—C223—H223	120.7	C423—C424—Cl44	119.73 (14)
C222—C223—H223	120.7	C424—C425—C426	119.11 (16)
C223—C224—C225	121.76 (16)	C424—C425—H425	120.4
C223—C224—Br24	120.44 (14)	C426—C425—H425	120.4
C225—C224—Br24	117.80 (13)	C425—C426—C421	121.10 (16)
C224—C225—C226	119.04 (16)	C425—C426—H426	119.5
C224—C225—H225	120.5	C421—C426—H426	119.5
C226—C225—H225	120.5		

C8A—N1—C2—C3	−2.9 (2)	C223—C224—C225—C226	−1.6 (3)
C8A—N1—C2—C21	178.93 (14)	Br24—C224—C225—C226	177.93 (13)
N1—C2—C3—C4	4.7 (2)	C224—C225—C226—C221	0.6 (3)
C21—C2—C3—C4	−177.11 (15)	C222—C221—C226—C225	0.8 (3)
N1—C2—C3—C31	−173.35 (15)	C22—C221—C226—C225	−179.12 (16)
C21—C2—C3—C31	4.8 (2)	C4—C3—C31—O31	114.68 (19)
C2—C3—C4—C4A	−2.9 (2)	C2—C3—C31—O31	−67.3 (2)
C31—C3—C4—C4A	175.12 (15)	C4—C3—C31—C311	−68.6 (2)
C2—C3—C4—C41	176.29 (15)	C2—C3—C31—C311	109.43 (17)
C31—C3—C4—C41	−5.7 (2)	O31—C31—C311—C312	164.36 (16)
C3—C4—C4A—C5	179.71 (16)	C3—C31—C311—C312	−12.3 (2)
C41—C4—C4A—C5	0.5 (3)	O31—C31—C311—C316	−13.2 (2)
C3—C4—C4A—C8A	−0.3 (2)	C3—C31—C311—C316	170.18 (15)
C41—C4—C4A—C8A	−179.52 (15)	C316—C311—C312—C313	−0.1 (2)
C8A—C4A—C5—C6	−1.4 (3)	C31—C311—C312—C313	−177.67 (15)
C4—C4A—C5—C6	178.57 (16)	C311—C312—C313—C314	0.0 (3)
C4A—C5—C6—C7	0.7 (3)	C312—C313—C314—C315	−0.2 (3)
C5—C6—C7—C8	0.2 (3)	C313—C314—C315—C316	0.6 (3)

C6—C7—C8—C8A	−0.3 (3)	C314—C315—C316—C311	−0.7 (3)
C2—N1—C8A—C8	−179.77 (15)	C312—C311—C316—C315	0.5 (3)
C2—N1—C8A—C4A	−0.6 (2)	C31—C311—C316—C315	178.07 (16)
C7—C8—C8A—N1	178.69 (16)	C3—C4—C41—C42	−44.4 (2)
C7—C8—C8A—C4A	−0.5 (3)	C4A—C4—C41—C42	134.79 (18)
C5—C4A—C8A—N1	−177.83 (16)	C4—C41—C42—C421	178.76 (16)
C4—C4A—C8A—N1	2.2 (2)	C41—C42—C421—C422	−21.4 (3)
C5—C4A—C8A—C8	1.3 (2)	C41—C42—C421—C426	159.74 (17)
C4—C4A—C8A—C8	−178.65 (15)	C426—C421—C422—C423	−0.9 (3)
N1—C2—C21—C22	−2.6 (2)	C42—C421—C422—C423	−179.73 (17)
C3—C2—C21—C22	179.16 (16)	C421—C422—C423—C424	−0.1 (3)
C2—C21—C22—C221	178.02 (15)	C422—C423—C424—C425	1.0 (3)
C21—C22—C221—C222	−171.95 (17)	C422—C423—C424—Cl44	179.93 (14)
C21—C22—C221—C226	7.9 (3)	C423—C424—C425—C426	−0.9 (3)
C226—C221—C222—C223	−1.2 (3)	Cl44—C424—C425—C426	−179.89 (13)
C22—C221—C222—C223	178.68 (16)	C424—C425—C426—C421	0.0 (3)
C221—C222—C223—C224	0.3 (3)	C422—C421—C426—C425	0.9 (3)
C222—C223—C224—C225	1.1 (3)	C42—C421—C426—C425	179.82 (16)
C222—C223—C224—Br24	−178.35 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C225—H225···O31^{i}	0.95	2.37	3.266 (2)	156

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

{2-[(*E*)-2-(4-Bromophenyl)ethenyl]-4-[(*E*)-2-(thiophen-2-yl)ethenyl]quinolin-3-yl}(phenyl)methanone (IIe)

Crystal data

$C_{30}H_{20}BrNOS$
M_r = 522.44
Orthorhombic, *Pbca*
a = 15.5785 (8) Å
b = 16.4215 (7) Å
c = 18.3126 (9) Å
V = 4684.8 (4) Å^3
Z = 8
F(000) = 2128

D_x = 1.481 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5363 reflections
θ = 2.1–27.5°
μ = 1.87 mm^{-1}
T = 100 K
Needle, yellow
0.20 × 0.12 × 0.08 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: INCOATEC high brilliance microfocus sealed tube
Multilayer mirror monochromator
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.768, T_{max} = 0.861

63672 measured reflections
5363 independent reflections
4456 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −20→19
k = −21→19
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.101$
$S = 1.01$
5363 reflections
320 parameters
10 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 11.0155P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.65$ e Å^{-3}
$\Delta\rho_{min} = -1.17$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.32950 (13)	0.39696 (13)	0.69963 (11)	0.0180 (4)	
C2	0.36313 (14)	0.47051 (14)	0.70599 (13)	0.0158 (5)	
C3	0.38281 (14)	0.52091 (14)	0.64445 (13)	0.0160 (5)	
C4	0.36504 (15)	0.49389 (14)	0.57424 (13)	0.0163 (5)	
C4A	0.33141 (15)	0.41306 (14)	0.56663 (13)	0.0170 (5)	
C5	0.31541 (16)	0.37594 (16)	0.49792 (14)	0.0214 (5)	
H5	0.3277	0.4050	0.4543	0.026*	
C6	0.28259 (17)	0.29886 (16)	0.49372 (14)	0.0236 (5)	
H6	0.2730	0.2746	0.4473	0.028*	
C7	0.26283 (17)	0.25507 (16)	0.55779 (14)	0.0236 (5)	
H7	0.2379	0.2024	0.5543	0.028*	
C8	0.27928 (16)	0.28802 (15)	0.62478 (14)	0.0210 (5)	
H8	0.2671	0.2575	0.6676	0.025*	
C8A	0.31445 (15)	0.36752 (15)	0.63117 (13)	0.0171 (5)	
C21	0.37733 (15)	0.50202 (15)	0.78042 (13)	0.0179 (5)	
H21	0.4008	0.5552	0.7852	0.021*	
C22	0.35954 (16)	0.46108 (15)	0.84131 (13)	0.0194 (5)	
H22	0.3366	0.4079	0.8356	0.023*	
C221	0.37195 (16)	0.49021 (16)	0.91640 (13)	0.0204 (5)	
C222	0.35708 (19)	0.43739 (17)	0.97459 (15)	0.0274 (6)	
H222	0.3391	0.3832	0.9650	0.033*	
C223	0.36818 (19)	0.46261 (18)	1.04677 (15)	0.0299 (6)	
H223	0.3579	0.4261	1.0860	0.036*	
C224	0.39418 (16)	0.54118 (17)	1.06010 (14)	0.0234 (5)	
Br24	0.40941 (2)	0.57825 (2)	1.15760 (2)	0.03048 (10)	
C225	0.40920 (19)	0.59520 (18)	1.00377 (15)	0.0284 (6)	
H225	0.4273	0.6493	1.0137	0.034*	
C226	0.39754 (18)	0.56930 (17)	0.93253 (15)	0.0269 (6)	
H226	0.4073	0.6065	0.8937	0.032*	
C31	0.41532 (15)	0.60611 (14)	0.65844 (12)	0.0159 (4)	

O31	0.36482 (12)	0.66263 (11)	0.66219 (10)	0.0226 (4)	
C311	0.50923 (15)	0.61866 (14)	0.67052 (12)	0.0161 (5)	
C312	0.56445 (16)	0.55250 (15)	0.68127 (14)	0.0186 (5)	
H312	0.5431	0.4985	0.6773	0.022*	
C313	0.65043 (17)	0.56566 (17)	0.69773 (15)	0.0245 (5)	
H313	0.6877	0.5207	0.7054	0.029*	
C314	0.68187 (17)	0.64456 (17)	0.70291 (15)	0.0266 (6)	
H314	0.7405	0.6534	0.7147	0.032*	
C315	0.62798 (18)	0.71048 (16)	0.69097 (15)	0.0257 (6)	
H315	0.6500	0.7643	0.6941	0.031*	
C316	0.54200 (17)	0.69794 (15)	0.67447 (14)	0.0213 (5)	
H316	0.5054	0.7432	0.6659	0.026*	
C41	0.37274 (17)	0.54578 (15)	0.50877 (14)	0.0220 (5)	
H41	0.3302	0.5378	0.4723	0.026*	
C42	0.43069 (17)	0.60160 (17)	0.49439 (14)	0.0234 (5)	
H42	0.4758	0.6081	0.5288	0.028*	
S421	0.35458 (5)	0.65236 (4)	0.36256 (4)	0.0220 (2)	0.926 (3)
C422	0.43224 (18)	0.65476 (17)	0.43028 (15)	0.0260 (6)	0.926 (3)
C423	0.4861 (3)	0.7044 (3)	0.4156 (3)	0.0241 (8)	0.926 (3)
H423	0.5325	0.7140	0.4481	0.029*	0.926 (3)
C424	0.4798 (2)	0.7505 (2)	0.3465 (2)	0.0254 (7)	0.926 (3)
H424	0.5194	0.7901	0.3294	0.031*	0.926 (3)
C425	0.4069 (2)	0.72597 (18)	0.31194 (17)	0.0252 (7)	0.926 (3)
H425	0.3875	0.7465	0.2663	0.030*	0.926 (3)
S521	0.5097 (9)	0.7195 (10)	0.4125 (10)	0.0241 (8)	0.074 (3)
C522	0.43224 (18)	0.65476 (17)	0.43028 (15)	0.0260 (6)	0.074 (3)
C523	0.3793 (18)	0.647 (2)	0.3830 (13)	0.0220 (2)	0.074 (3)
H523	0.3346	0.6079	0.3856	0.026*	0.074 (3)
C524	0.389 (2)	0.704 (2)	0.3200 (15)	0.0252 (7)	0.074 (3)
H524	0.3551	0.7046	0.2770	0.030*	0.074 (3)
C525	0.456 (2)	0.755 (3)	0.336 (2)	0.0254 (7)	0.074 (3)
H525	0.4707	0.8023	0.3087	0.031*	0.074 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0142 (9)	0.0210 (10)	0.0189 (10)	0.0000 (8)	0.0003 (8)	0.0015 (8)
C2	0.0106 (10)	0.0179 (11)	0.0189 (11)	0.0024 (8)	0.0007 (8)	0.0014 (9)
C3	0.0114 (10)	0.0162 (11)	0.0203 (11)	0.0018 (9)	0.0007 (9)	−0.0005 (9)
C4	0.0133 (11)	0.0166 (11)	0.0191 (11)	0.0030 (9)	0.0012 (9)	0.0029 (9)
C4A	0.0147 (11)	0.0185 (11)	0.0177 (11)	0.0005 (9)	−0.0006 (9)	0.0005 (9)
C5	0.0230 (12)	0.0235 (12)	0.0177 (12)	−0.0020 (10)	0.0007 (10)	0.0010 (10)
C6	0.0263 (13)	0.0243 (13)	0.0202 (12)	−0.0045 (11)	0.0012 (10)	−0.0044 (10)
C7	0.0239 (13)	0.0200 (12)	0.0271 (13)	−0.0064 (10)	0.0039 (10)	−0.0033 (10)
C8	0.0184 (12)	0.0207 (12)	0.0240 (13)	−0.0037 (10)	0.0040 (10)	0.0022 (10)
C8A	0.0136 (11)	0.0190 (11)	0.0187 (11)	−0.0004 (9)	0.0012 (9)	−0.0004 (9)
C21	0.0148 (11)	0.0185 (11)	0.0203 (12)	−0.0002 (9)	−0.0007 (9)	0.0005 (9)
C22	0.0192 (12)	0.0188 (11)	0.0202 (12)	−0.0002 (9)	0.0008 (9)	−0.0004 (9)

C221	0.0161 (11)	0.0269 (13)	0.0181 (12)	0.0009 (10)	0.0013 (9)	0.0025 (10)
C222	0.0331 (15)	0.0254 (13)	0.0237 (13)	−0.0021 (11)	0.0009 (11)	0.0039 (11)
C223	0.0342 (15)	0.0340 (15)	0.0214 (13)	0.0036 (12)	0.0008 (11)	0.0091 (11)
C224	0.0185 (12)	0.0344 (14)	0.0174 (12)	0.0052 (10)	−0.0011 (9)	0.0009 (10)
Br24	0.02658 (15)	0.04757 (19)	0.01730 (14)	0.00720 (12)	−0.00317 (10)	−0.00200 (11)
C225	0.0321 (15)	0.0297 (14)	0.0234 (13)	−0.0051 (12)	−0.0009 (11)	−0.0013 (11)
C226	0.0343 (15)	0.0280 (14)	0.0184 (12)	−0.0048 (11)	0.0020 (11)	0.0024 (10)
C31	0.0193 (11)	0.0155 (11)	0.0128 (10)	0.0016 (9)	0.0012 (9)	0.0018 (8)
O31	0.0252 (9)	0.0189 (9)	0.0236 (9)	0.0081 (7)	−0.0018 (7)	−0.0016 (7)
C311	0.0181 (11)	0.0170 (11)	0.0131 (11)	−0.0015 (9)	0.0019 (9)	0.0004 (9)
C312	0.0188 (11)	0.0153 (11)	0.0217 (12)	−0.0006 (9)	0.0013 (9)	0.0002 (9)
C313	0.0187 (12)	0.0285 (14)	0.0263 (13)	0.0007 (10)	−0.0022 (10)	−0.0001 (11)
C314	0.0207 (13)	0.0358 (15)	0.0233 (13)	−0.0094 (11)	−0.0002 (10)	−0.0038 (11)
C315	0.0313 (14)	0.0232 (13)	0.0227 (13)	−0.0119 (11)	0.0036 (11)	−0.0042 (10)
C316	0.0299 (13)	0.0149 (11)	0.0190 (12)	−0.0014 (10)	0.0042 (10)	−0.0024 (9)
C41	0.0274 (13)	0.0191 (12)	0.0195 (12)	0.0049 (10)	0.0005 (10)	−0.0006 (10)
C42	0.0255 (13)	0.0256 (13)	0.0191 (12)	0.0045 (10)	0.0004 (10)	−0.0006 (10)
S421	0.0248 (4)	0.0210 (3)	0.0200 (4)	0.0039 (3)	−0.0026 (3)	0.0021 (3)
C422	0.0310 (15)	0.0255 (13)	0.0214 (13)	0.0130 (12)	0.0010 (11)	−0.0028 (11)
C423	0.021 (2)	0.031 (2)	0.0194 (12)	0.0092 (17)	−0.0008 (18)	−0.0012 (14)
C424	0.0302 (18)	0.0221 (13)	0.0240 (16)	0.0075 (14)	0.0074 (13)	0.0057 (11)
C425	0.0382 (18)	0.0166 (16)	0.0209 (13)	0.0095 (13)	0.0112 (13)	0.0099 (11)
S521	0.021 (2)	0.031 (2)	0.0194 (12)	0.0092 (17)	−0.0008 (18)	−0.0012 (14)
C522	0.0310 (15)	0.0255 (13)	0.0214 (13)	0.0130 (12)	0.0010 (11)	−0.0028 (11)
C523	0.0248 (4)	0.0210 (3)	0.0200 (4)	0.0039 (3)	−0.0026 (3)	0.0021 (3)
C524	0.0382 (18)	0.0166 (16)	0.0209 (13)	0.0095 (13)	0.0112 (13)	0.0099 (11)
C525	0.0302 (18)	0.0221 (13)	0.0240 (16)	0.0075 (14)	0.0074 (13)	0.0057 (11)

Geometric parameters (Å, º)

N1—C2	1.322 (3)	C226—H226	0.9500
N1—C8A	1.364 (3)	C31—O31	1.219 (3)
C2—C3	1.431 (3)	C31—C311	1.494 (3)
C2—C21	1.475 (3)	C311—C312	1.400 (3)
C3—C4	1.388 (3)	C311—C316	1.400 (3)
C3—C31	1.510 (3)	C312—C313	1.390 (4)
C4—C4A	1.434 (3)	C312—H312	0.9500
C4—C41	1.476 (3)	C313—C314	1.388 (4)
C4A—C5	1.420 (3)	C313—H313	0.9500
C4A—C8A	1.423 (3)	C314—C315	1.387 (4)
C5—C6	1.367 (4)	C314—H314	0.9500
C5—H5	0.9500	C315—C316	1.388 (4)
C6—C7	1.410 (4)	C315—H315	0.9500
C6—H6	0.9500	C316—H316	0.9500
C7—C8	1.365 (4)	C41—C42	1.313 (4)
C7—H7	0.9500	C41—H41	0.9500
C8—C8A	1.421 (3)	C42—C422	1.463 (4)
C8—H8	0.9500	C42—H42	0.9500

C21—C22	1.331 (3)	S421—C425	1.728 (3)
C21—H21	0.9500	S421—C422	1.733 (3)
C22—C221	1.469 (3)	C422—C423	1.201 (5)
C22—H22	0.9500	C423—C424	1.476 (5)
C221—C226	1.390 (4)	C423—H423	0.9500
C221—C222	1.393 (4)	C424—C425	1.361 (5)
C222—C223	1.396 (4)	C424—H424	0.9500
C222—H222	0.9500	C425—H425	0.9500
C223—C224	1.374 (4)	S521—C525	1.738 (10)
C223—H223	0.9500	C523—C524	1.492 (11)
C224—C225	1.381 (4)	C523—H523	0.9500
C224—Br24	1.901 (3)	C524—C525	1.366 (11)
C225—C226	1.384 (4)	C524—H524	0.9500
C225—H225	0.9500	C525—H525	0.9500

C2—N1—C8A	118.2 (2)	C225—C226—H226	119.2
N1—C2—C3	122.9 (2)	C221—C226—H226	119.2
N1—C2—C21	117.5 (2)	O31—C31—C311	121.3 (2)
C3—C2—C21	119.5 (2)	O31—C31—C3	119.9 (2)
C4—C3—C2	120.1 (2)	C311—C31—C3	118.8 (2)
C4—C3—C31	121.4 (2)	C312—C311—C316	119.4 (2)
C2—C3—C31	118.3 (2)	C312—C311—C31	121.0 (2)
C3—C4—C4A	117.3 (2)	C316—C311—C31	119.5 (2)
C3—C4—C41	123.5 (2)	C313—C312—C311	120.1 (2)
C4A—C4—C41	119.0 (2)	C313—C312—H312	119.9
C5—C4A—C8A	118.5 (2)	C311—C312—H312	119.9
C5—C4A—C4	123.2 (2)	C314—C313—C312	120.0 (3)
C8A—C4A—C4	118.3 (2)	C314—C313—H313	120.0
C6—C5—C4A	120.9 (2)	C312—C313—H313	120.0
C6—C5—H5	119.6	C315—C314—C313	120.3 (2)
C4A—C5—H5	119.6	C315—C314—H314	119.9
C5—C6—C7	120.4 (2)	C313—C314—H314	119.9
C5—C6—H6	119.8	C314—C315—C316	120.2 (2)
C7—C6—H6	119.8	C314—C315—H315	119.9
C8—C7—C6	120.3 (2)	C316—C315—H315	119.9
C8—C7—H7	119.8	C315—C316—C311	120.1 (2)
C6—C7—H7	119.8	C315—C316—H316	120.0
C7—C8—C8A	120.7 (2)	C311—C316—H316	120.0
C7—C8—H8	119.6	C42—C41—C4	128.5 (2)
C8A—C8—H8	119.6	C42—C41—H41	115.8
N1—C8A—C8	117.9 (2)	C4—C41—H41	115.8
N1—C8A—C4A	123.0 (2)	C41—C42—C422	126.1 (3)
C8—C8A—C4A	119.1 (2)	C41—C42—H42	117.0
C22—C21—C2	124.5 (2)	C422—C42—H42	117.0
C22—C21—H21	117.8	C425—S421—C422	92.22 (15)
C2—C21—H21	117.8	C423—C422—C42	126.6 (3)
C21—C22—C221	126.3 (2)	C423—C422—S421	110.1 (3)
C21—C22—H22	116.8	C42—C422—S421	123.3 (2)

C221—C22—H22	116.8	C422—C423—C424	119.5 (4)
C226—C221—C222	117.8 (2)	C422—C423—H423	120.2
C226—C221—C22	122.7 (2)	C424—C423—H423	120.2
C222—C221—C22	119.4 (2)	C425—C424—C423	107.7 (3)
C221—C222—C223	121.3 (3)	C425—C424—H424	126.2
C221—C222—H222	119.4	C423—C424—H424	126.2
C223—C222—H222	119.4	C424—C425—S421	110.5 (2)
C224—C223—C222	118.9 (3)	C424—C425—H425	124.7
C224—C223—H223	120.6	S421—C425—H425	124.7
C222—C223—H223	120.6	C524—C523—H523	122.5
C223—C224—C225	121.4 (3)	C525—C524—C523	107.4 (11)
C223—C224—Br24	120.3 (2)	C525—C524—H524	126.3
C225—C224—Br24	118.3 (2)	C523—C524—H524	126.3
C224—C225—C226	119.0 (3)	C524—C525—S521	109.4 (10)
C224—C225—H225	120.5	C524—C525—H525	125.3
C226—C225—H225	120.5	S521—C525—H525	125.3
C225—C226—C221	121.7 (3)		

C8A—N1—C2—C3	1.2 (3)	C222—C223—C224—Br24	179.6 (2)
C8A—N1—C2—C21	178.8 (2)	C223—C224—C225—C226	0.1 (4)
N1—C2—C3—C4	1.3 (3)	Br24—C224—C225—C226	−179.4 (2)
C21—C2—C3—C4	−176.2 (2)	C224—C225—C226—C221	−0.6 (4)
N1—C2—C3—C31	175.8 (2)	C222—C221—C226—C225	0.8 (4)
C21—C2—C3—C31	−1.7 (3)	C22—C221—C226—C225	−179.7 (3)
C2—C3—C4—C4A	−3.4 (3)	C4—C3—C31—O31	82.8 (3)
C31—C3—C4—C4A	−177.7 (2)	C2—C3—C31—O31	−91.6 (3)
C2—C3—C4—C41	171.8 (2)	C4—C3—C31—C311	−99.7 (3)
C31—C3—C4—C41	−2.5 (4)	C2—C3—C31—C311	85.9 (3)
C3—C4—C4A—C5	−176.0 (2)	O31—C31—C311—C312	166.6 (2)
C41—C4—C4A—C5	8.6 (4)	C3—C31—C311—C312	−10.9 (3)
C3—C4—C4A—C8A	3.1 (3)	O31—C31—C311—C316	−10.5 (3)
C41—C4—C4A—C8A	−172.3 (2)	C3—C31—C311—C316	172.1 (2)
C8A—C4A—C5—C6	1.5 (4)	C316—C311—C312—C313	1.8 (4)
C4—C4A—C5—C6	−179.5 (2)	C31—C311—C312—C313	−175.3 (2)
C4A—C5—C6—C7	0.9 (4)	C311—C312—C313—C314	−0.6 (4)
C5—C6—C7—C8	−2.5 (4)	C312—C313—C314—C315	−0.7 (4)
C6—C7—C8—C8A	1.6 (4)	C313—C314—C315—C316	0.6 (4)
C2—N1—C8A—C8	179.2 (2)	C314—C315—C316—C311	0.6 (4)
C2—N1—C8A—C4A	−1.5 (3)	C312—C311—C316—C315	−1.8 (4)
C7—C8—C8A—N1	−179.9 (2)	C31—C311—C316—C315	175.3 (2)
C7—C8—C8A—C4A	0.8 (4)	C3—C4—C41—C42	37.6 (4)
C5—C4A—C8A—N1	178.5 (2)	C4A—C4—C41—C42	−147.3 (3)
C4—C4A—C8A—N1	−0.7 (3)	C4—C41—C42—C422	−176.1 (2)
C5—C4A—C8A—C8	−2.3 (3)	C41—C42—C422—C423	−177.8 (4)
C4—C4A—C8A—C8	178.6 (2)	C41—C42—C422—S421	0.8 (4)
N1—C2—C21—C22	0.8 (4)	C425—S421—C422—C423	1.1 (3)
C3—C2—C21—C22	178.5 (2)	C425—S421—C422—C42	−177.7 (2)
C2—C21—C22—C221	−179.5 (2)	C42—C422—C423—C424	177.2 (3)

C21—C22—C221—C226	6.0 (4)	S421—C422—C423—C424	−1.6 (5)
C21—C22—C221—C222	−174.5 (3)	C422—C423—C424—C425	1.4 (6)
C226—C221—C222—C223	−0.5 (4)	C423—C424—C425—S421	−0.4 (4)
C22—C221—C222—C223	180.0 (3)	C422—S421—C425—C424	−0.3 (3)
C221—C222—C223—C224	0.1 (4)	C523—C524—C525—S521	10 (6)
C222—C223—C224—C225	0.1 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O31^{i}	0.95	2.58	3.122 (3)	116
C425—H425···O31^{ii}	0.95	2.45	3.361 (4)	161
C5—H5···*Cg*3^{iii}	0.95	2.90	3.647 (3)	136
C423—H423···*Cg*2^{iv}	0.95	2.76	3.449 (3)	130

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*; (ii) *x*, −*y*+3/2, *z*−1/2; (iii) −*x*+1, *y*+3/2, −*z*+3/2; (iv) −*x*+1, −*y*+1, −*z*+1.