N-(4-Bromobenzyl)-2-(5,6-dimethyl-1*H*-benzo[*d*]imidazol-2-yl)benzeneamine

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SUPPLEMENTARY MATERIAL

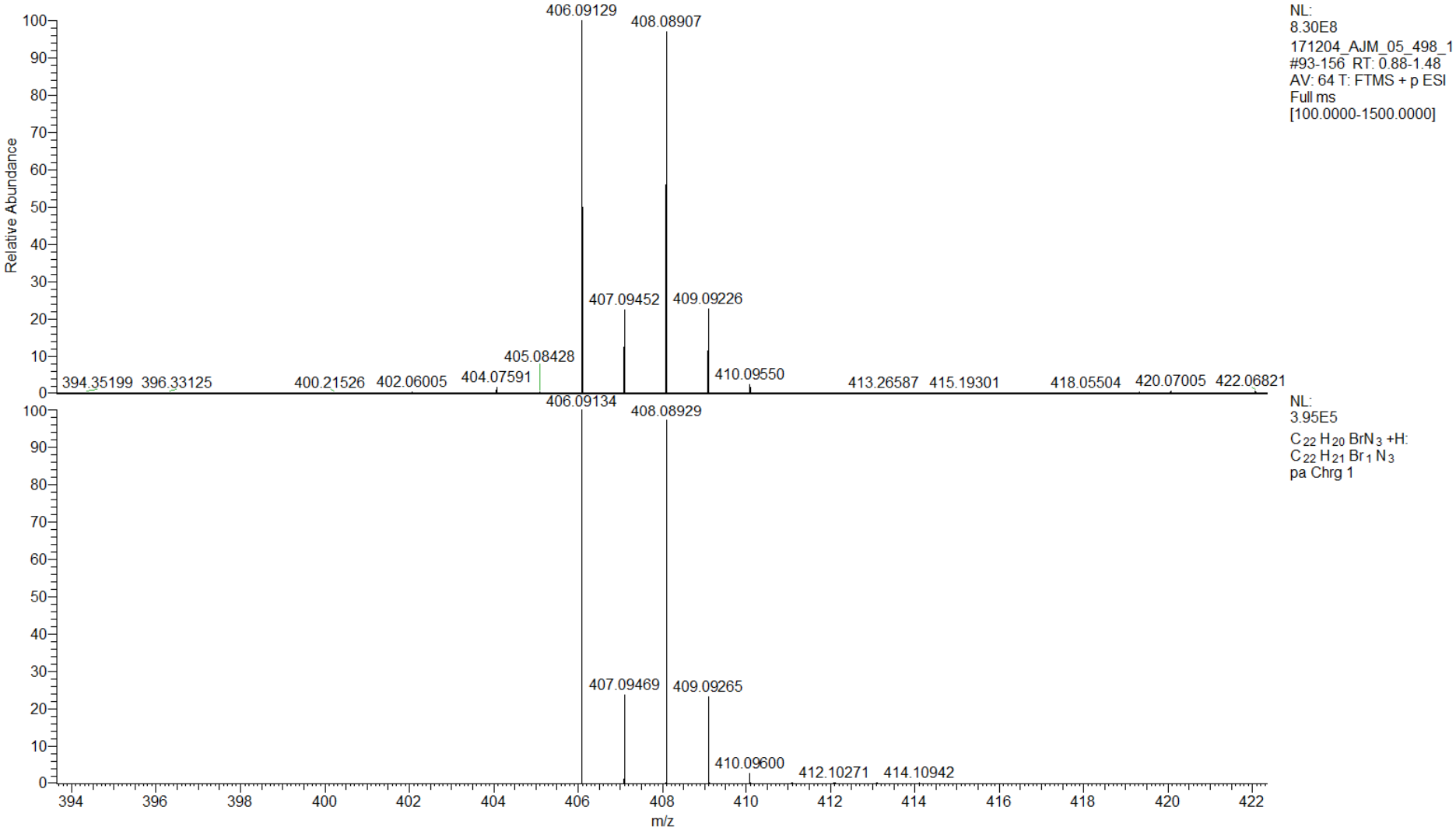

Fig. S1 HRMS spectrum for **15**

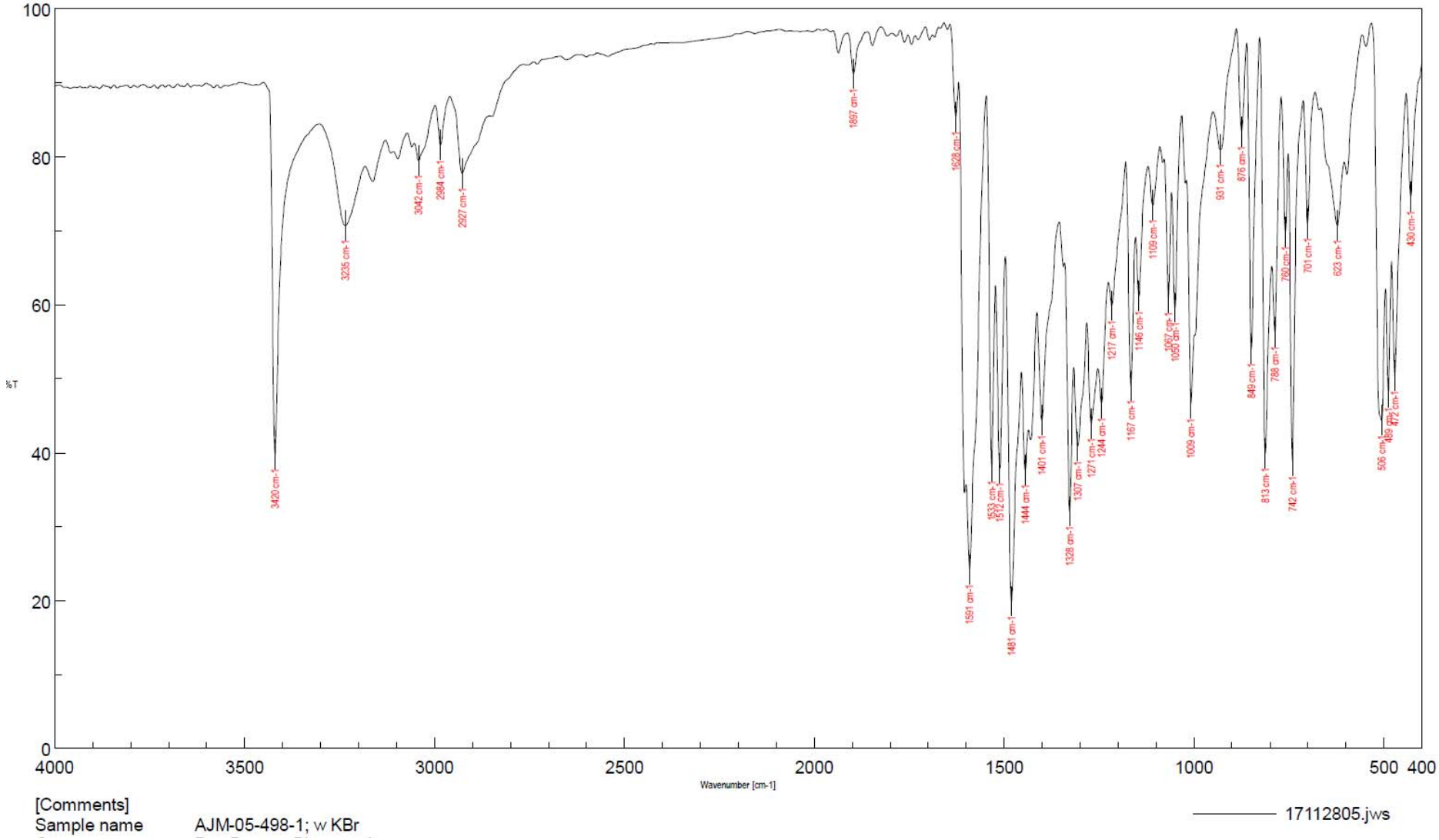

Fig. 2S IR spectrum for **15**

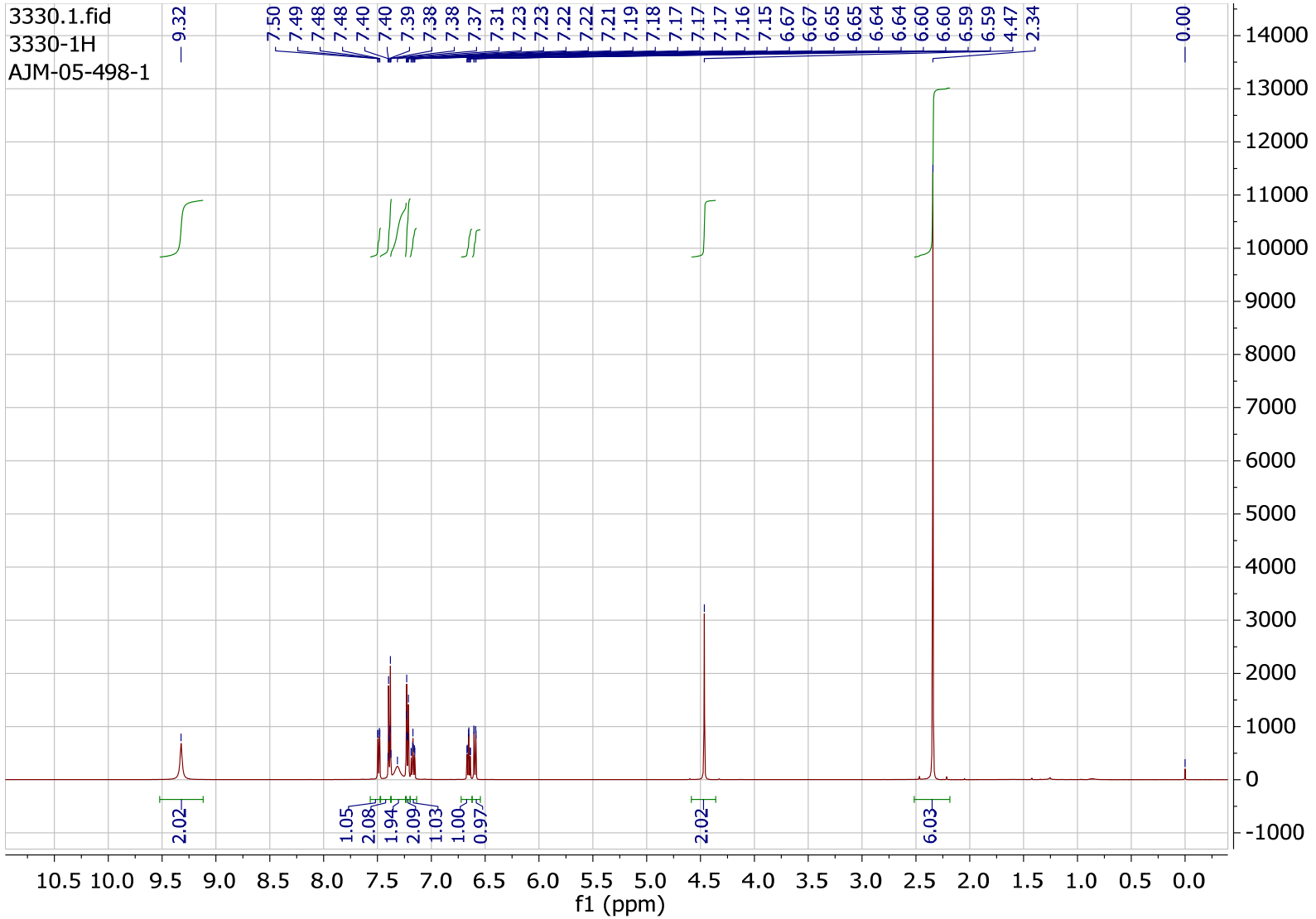

Fig. 3S 1H-NMR for **15**

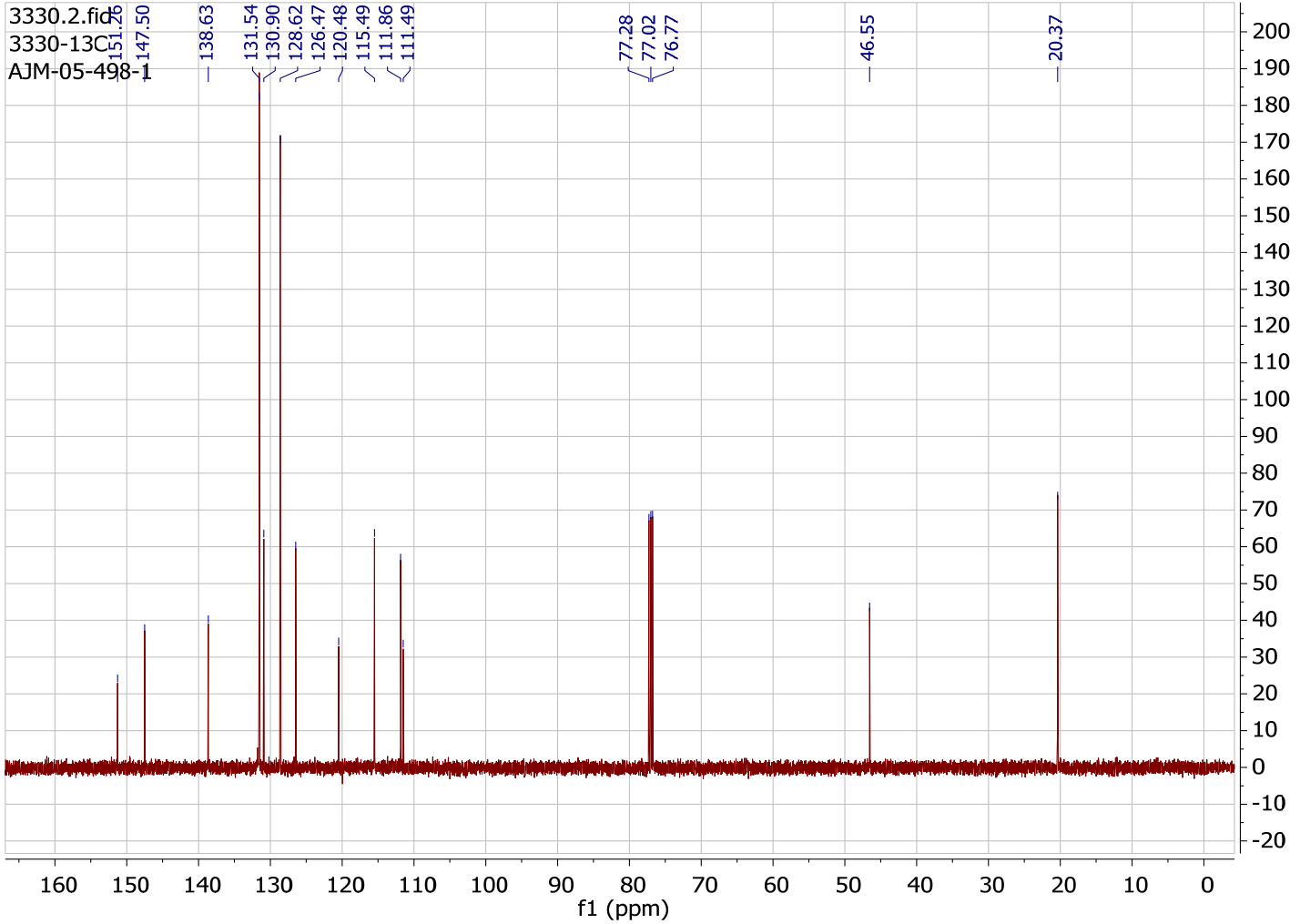

Fig. 4S 13C-NMR for **15**

Table 1S. Crystal data and structure refinement details for **15**

Empirical formula	$C_{22}H_{20}BrN_3$
Formula weight	406.32
Temperature/K	100(2)
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a/Å	5.70329(14)
b/Å	8.37203(17)
c/Å	37.9019(9)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1809.75(7)
Z	4
ρ_{calc}g/cm^3	1.491
μ/mm^{-1}	3.163
F(000)	832.0
Crystal size/mm	0.35 × 0.22 × 0.10
Radiation	Cu$K\alpha$ (λ = 1.54184)
2Θ range for data collection/°	4.662 to 134.094
Index Ganges	$-6 \le h \le 4$, $-10 \le k \le 9$, $-45 \le l \le 43$
Reflections collected	5443
Independent reflections	3199 [R_{int} = 0.0228, R_{sigma} = 0.0291]
Data/restraints/parameters	3199/0/243
Goodness-of-fit on F^2	1.165
Final R indexes [I>=2σ (I)]	R_1 = 0.0293, wR_2 = 0.0766
Final R indexes [all data]	R_1 = 0.0309, wR_2 = 0.0768
Largest diff. peak/hole / e Å^{-3}	0.37/-0.86
Flack parametr	-0.029(13)

Table 2S. Bond lengths for **15**.

Atom	Atom	Length/Å
Br(1)	C(20)	1.896(4)
C(1)	C(10)	1.465(6)
C(1)	N(1)	1.386(5)
C(1)	N(2)	1.318(5)
C(2)	C(3)	1.390(6)
C(2)	C(7)	1.406(6)
C(2)	N(1)	1.382(5)
C(3)	C(4)	1.384(6)
C(4)	C(5)	1.425(6)
C(4)	C(8)	1.512(6)
C(5)	C(6)	1.394(6)
C(5)	C(9)	1.508(6)
C(6)	C(7)	1.393(6)
C(7)	N(2)	1.392(5)
-C(10)	C(11)	1.434(6)
C(10)	C(15)	1.396(6)
C(11)	C(12)	1.406(6)
C(11)	N(3)	1.363(6)
C(12)	C(13)	1.382(7)
C(13)	C(14)	1.395(6)
C(14)	C(15)	1.386(6)
C(16)	C(17)	1.516(6)
C(16)	N(3)	1.444(5)
C(17)	C(18)	1.398(6)
C(17)	C(22)	1.386(6)
C(18)	C(19)	1.385(6)
C(19)	C(20)	1.382(6)
C(20)	C(21)	1.390(6)
C(21)	C(22)	1.393(6)

Table 3S. Valence angles for **15**.

Atom	Atom	Atom	Angle/˚
N(1)	C(1)	C(10)	122.0(4)
N(2)	C(1)	C(10)	126.3(4)
N(2)	C(1)	N(1)	111.6(4)
C(3)	C(2)	C(7)	121.9(4)
N(1)	C(2)	C(3)	132.7(4)
N(1)	C(2)	C(7)	105.4(4)
C(4)	C(3)	C(2)	118.2(4)
C(3)	C(4)	C(5)	120.6(4)
C(3)	C(4)	C(8)	120.3(4)
C(5)	C(4)	C(8)	119.1(4)
C(4)	C(5)	C(9)	119.9(4)
C(6)	C(5)	C(4)	120.4(4)
C(6)	C(5)	C(9)	119.6(4)
C(7)	C(6)	C(5)	118.8(4)
C(6)	C(7)	C(2)	119.9(4)
N(2)	C(7)	C(2)	109.5(4)
N(2)	C(7)	C(6)	130.4(4)
C(11)	C(10)	C(1)	120.4(4)
C(15)	C(10)	C(1)	120.5(4)
C(15)	C(10)	C(11)	119.1(4)
C(12)	C(11)	C(10)	117.6(4)
N(3)	C(11)	C(10)	121.0(4)
N(3)	C(11)	C(12)	121.4(4)
C(13)	C(12)	C(11)	121.5(4)
C(12)	C(13)	C(14)	121.1(4)
C(15)	C(14)	C(13)	118.2(4)
C(14)	C(15)	C(10)	122.4(4)
N(3)	C(16)	C(17)	115.8(4)
C(18)	C(17)	C(16)	118.6(4)
C(22)	C(17)	C(16)	122.8(4)
C(22)	C(17)	C(18)	118.6(4)

C(19)	C(18)	C(17)	121.5(4)
C(20)	C(19)	C(18)	118.7(4)
C(19)	C(20)	Br(1)	119.9(3)
C(19)	C(20)	C(21)	121.3(4)
C(21)	C(20)	Br(1)	118.8(3)
C(20)	C(21)	C(22)	119.1(4)
C(17)	C(22)	C(21)	120.8(4)
C(2)	N(1)	C(1)	107.3(4)
C(1)	N(2)	C(7)	106.2(3)
C(11)	N(3)	C(16)	123.5(4)

Table 4S. Torsion angles for **15**.

A	B	C	D	Angle/˚
Br(1)	C(20)	C(21)	C(22)	178.7(3)
C(1)	C(10)	C(11)	C(12)	-175.4(4)
C(1)	C(10)	C(11)	N(3)	3.2(6)
C(1)	C(10)	C(15)	C(14)	177.1(4)
C(2)	C(3)	C(4)	C(5)	-0.8(6)
C(2)	C(3)	C(4)	C(8)	176.7(4)
C(2)	C(7)	N(2)	C(1)	0.8(4)
C(3)	C(2)	C(7)	C(6)	-1.9(6)
C(3)	C(2)	C(7)	N(2)	-177.5(4)
C(3)	C(2)	N(1)	C(1)	176.4(4)
C(3)	C(4)	C(5)	C(6)	-1.4(6)
C(3)	C(4)	C(5)	C(9)	175.5(4)
C(4)	C(5)	C(6)	C(7)	2.0(6)
C(5)	C(6)	C(7)	C(2)	-0.4(6)
C(5)	C(6)	C(7)	N(2)	174.3(4)
C(6)	C(7)	N(2)	C(1)	-174.3(4)
C(7)	C(2)	C(3)	C(4)	2.4(6)
C(7)	C(2)	N(1)	C(1)	-0.9(4)
C(8)	C(4)	C(5)	C(6)	-178.9(4)
C(8)	C(4)	C(5)	C(9)	-2.0(6)
C(9)	C(5)	C(6)	C(7)	-175.0(4)

C(10)	C(1)	N(1)	C(2)	-176.6(4)
C(10)	C(1)	N(2)	C(7)	176.6(4)
C(10)	C(11)	C(12)	C(13)	-2.9(6)
C(10)	C(11)	N(3)	C(16)	166.2(4)
C(11)	C(10)	C(15)	C(14)	-2.2(6)
C(11)	C(12)	C(13)	C(14)	0.1(6)
C(12)	C(11)	N(3)	C(16)	-15.2(6)
C(12)	C(13)	C(14)	C(15)	1.8(6)
C(13)	C(14)	C(15)	C(10)	-0.6(7)
C(15)	C(10)	C(11)	C(12)	3.9(6)
C(15)	C(10)	C(11)	N(3)	-177.5(4)
C(16)	C(17)	C(18)	C(19)	-179.8(4)
C(16)	C(17)	C(22)	C(21)	-179.9(4)
C(17)	C(16)	N(3)	C(11)	91.4(5)
C(17)	C(18)	C(19)	C(20)	-0.3(6)
C(18)	C(17)	C(22)	C(21)	-0.5(6)
C(18)	C(19)	C(20)	Br(1)	-178.5(3)
C(18)	C(19)	C(20)	C(21)	-0.3(6)
C(19)	C(20)	C(21)	C(22)	0.5(6)
C(20)	C(21)	C(22)	C(17)	-0.1(6)
C(22)	C(17)	C(18)	C(19)	0.7(6)
N(1)	C(1)	C(10)	C(11)	168.2(4)
N(1)	C(1)	C(10)	C(15)	-11.1(6)
N(1)	C(1)	N(2)	C(7)	-1.4(5)
N(1)	C(2)	C(3)	C(4)	-174.5(4)
N(1)	C(2)	C(7)	C(6)	175.8(4)
N(1)	C(2)	C(7)	N(2)	0.1(4)
N(2)	C(1)	C(10)	C(11)	-9.5(6)
N(2)	C(1)	C(10)	C(15)	171.2(4)
N(2)	C(1)	N(1)	C(2)	1.5(5)
N(3)	C(11)	C(12)	C(13)	178.5(4)
N(3)	C(16)	C(17)	C(18)	-179.4(4)
N(3)	C(16)	C(17)	C(22)	0.0(6)

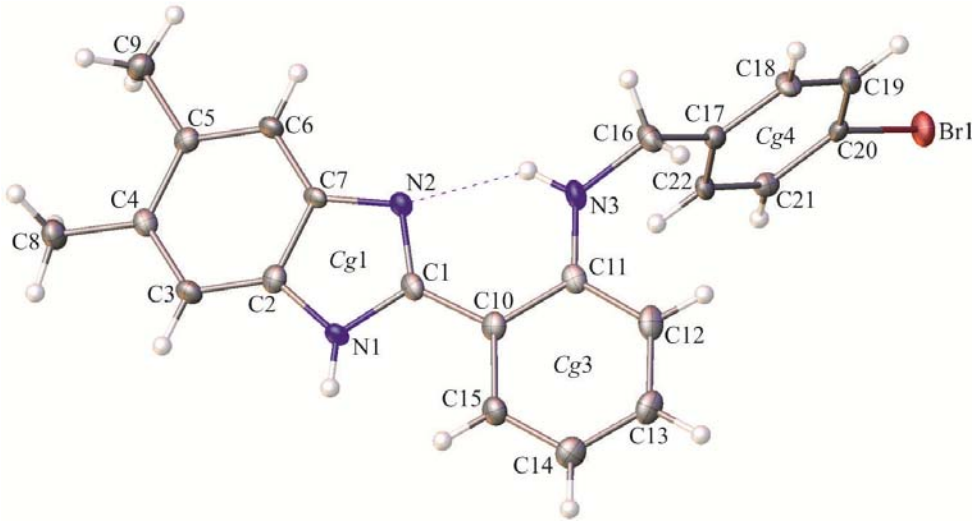

Figure 1S. Asymmetric unit of the crystal lattice of **15** with crystallographic numbering. Displacement ellipsoids are drawn at the 50% probability level and the H-atoms are shown as small spheres of arbitrary radius. The intramolecular N–H···N hydrogen bond is represented by dashed line. *Cg*1, *Cg*3 and *Cg*4 denote the geometric centres of gravity of the aromatic rings delineated by the N1/C1/N2/C7/C2, C10–C15 and C17–C22 atoms respectively.

Table 5S. The geometry of hydrogen bonds in the crystal of **15**.

D–H	**A**	**d(D···A) (Å)**	**< D–H···A (°)**
N3–H3A	N2*	2.705(5)	138(5)
C15–H15	N1*	2.918(5)	101
C22–H22	N3*	2.897(5)	102

Symmetry codes: (*) intramolecular interaction.

Table 6S. The geometry of C–H···π contacts in the crystal of **15**.

D–H	***Cg*I**	**d(D···*Cg*I) (Å)**	**< D–X···*Cg*I (°)**
C3–H3	1^{i}	3.489(4)	139
C9–H9B	1^{ii}	3.511(5)	126
C16–H16A	3^{iii}	3.296(5)	108
C16–H16B	3^{iii}	3.296(5)	111

Symmetry codes: (i) $x - 1/2, -y + 3/2, -z + 1$; (ii) $x + 1/2, -y + 1/2, -z + 1$; (iii) $x + 1, y, z$.
*Cg*1 and *Cg*3 denote the geometric centres of gravity of the aromatic rings delineated by the N1/C1/N2/C7/C2 and C10–C15 atoms respectively (Fig. 1S).

Table 7S. The geometry of C–Br···π contacts in the crystal of **15**.

Y–X	***Cg*I**	**d(X···*Cg*I) (Å)**	**< Y–X···*Cg*I (°)**
C20–Br1	4^{iv}	3.393(2)	151.53(13)

Symmetry code: (iv) $-x + 1, y - 1/2, -z + 3/2$.
*Cg*4 denotes the geometric centre of gravity of the aromatic ring defined by the C17–C22 atoms (Fig. 1S).