Supplementary material

Synthesis and crystal structures of halogen-substituted 2-aryl-*N*-phenylbenzimidazoles

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Part 1. NMR spectroscopy data: Figures S1–S14;

Part 2. X-ray crystallography: Table S1, Figure S15-S17;

Part 3. Optical data: Figure S18.

1. *NMR spectroscopy data*

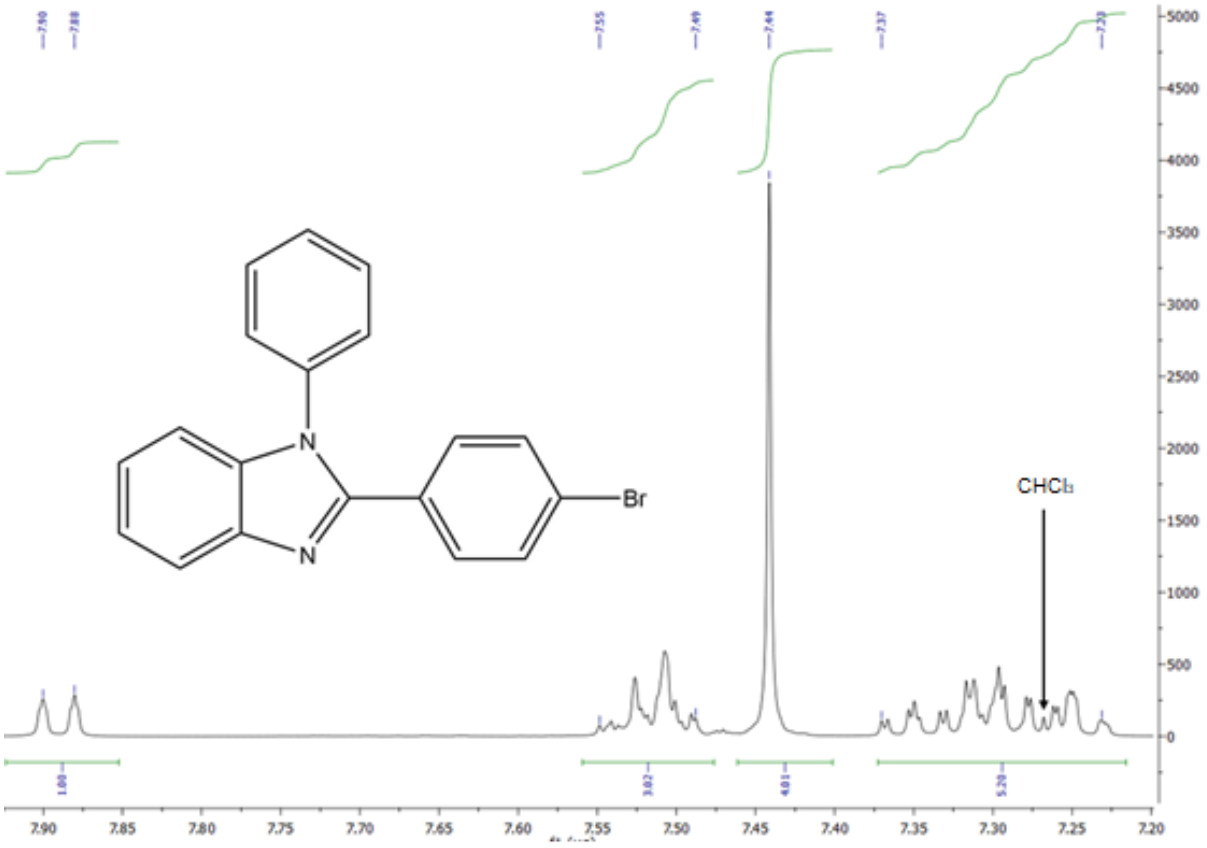

Figure S1. ^{1}H NMR spectrum of the **1** ($CDCl_3$, 400 MHz, 25°C).

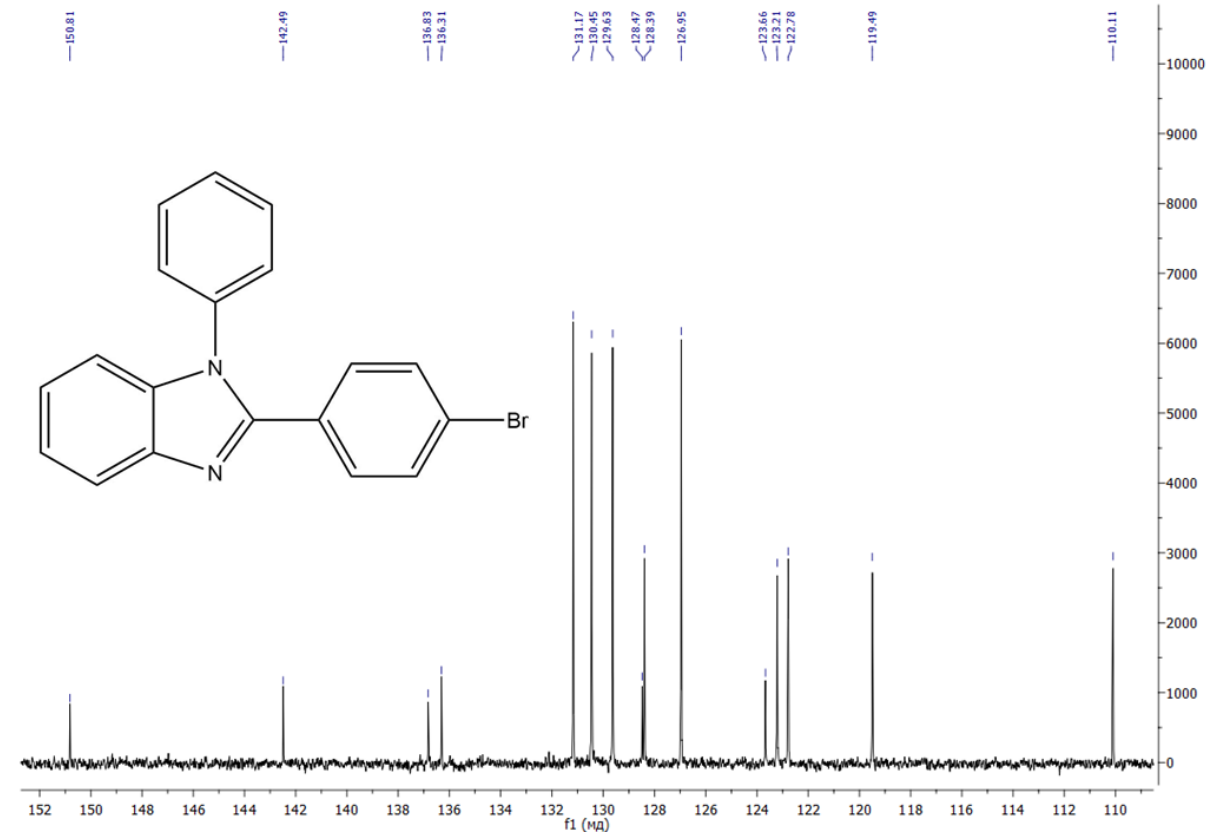

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of the **1** ($CDCl_3$, 101 MHz, 25°C).

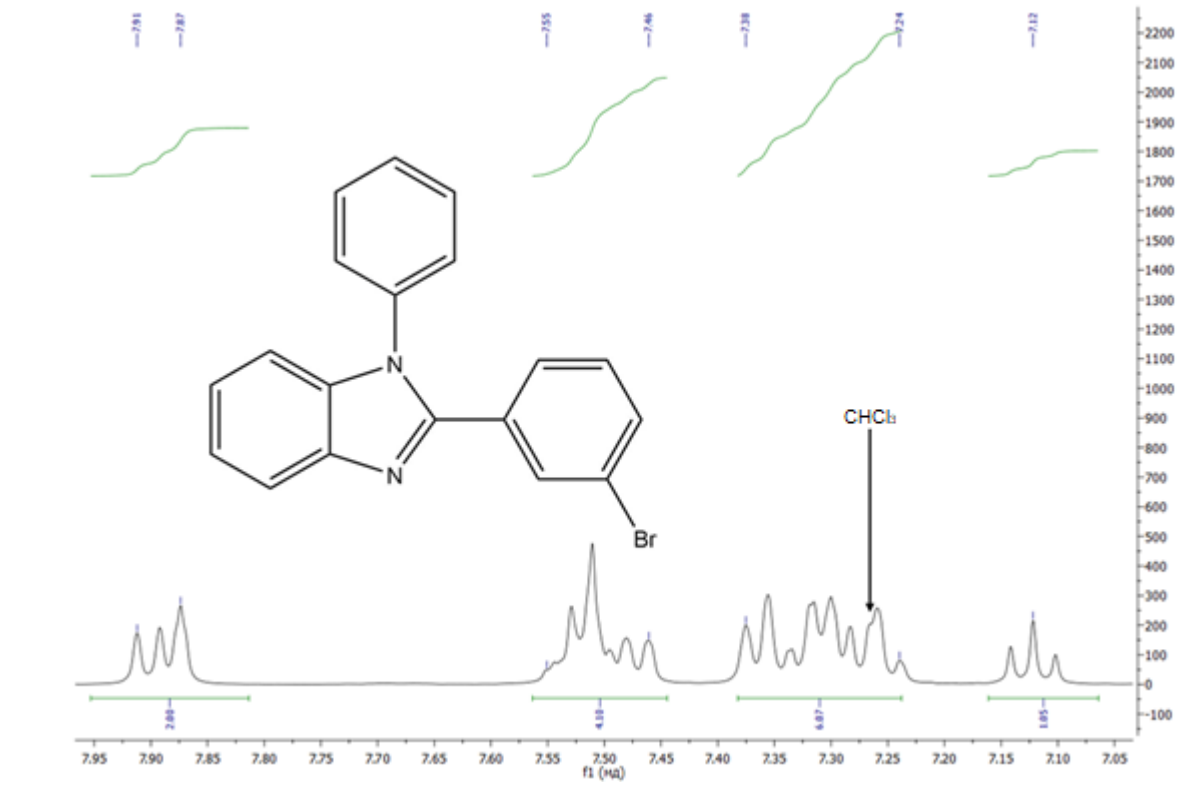

Figure S3. ^{1}H NMR spectrum of the **2** ($CDCl_3$, 400 MHz, 25°C).

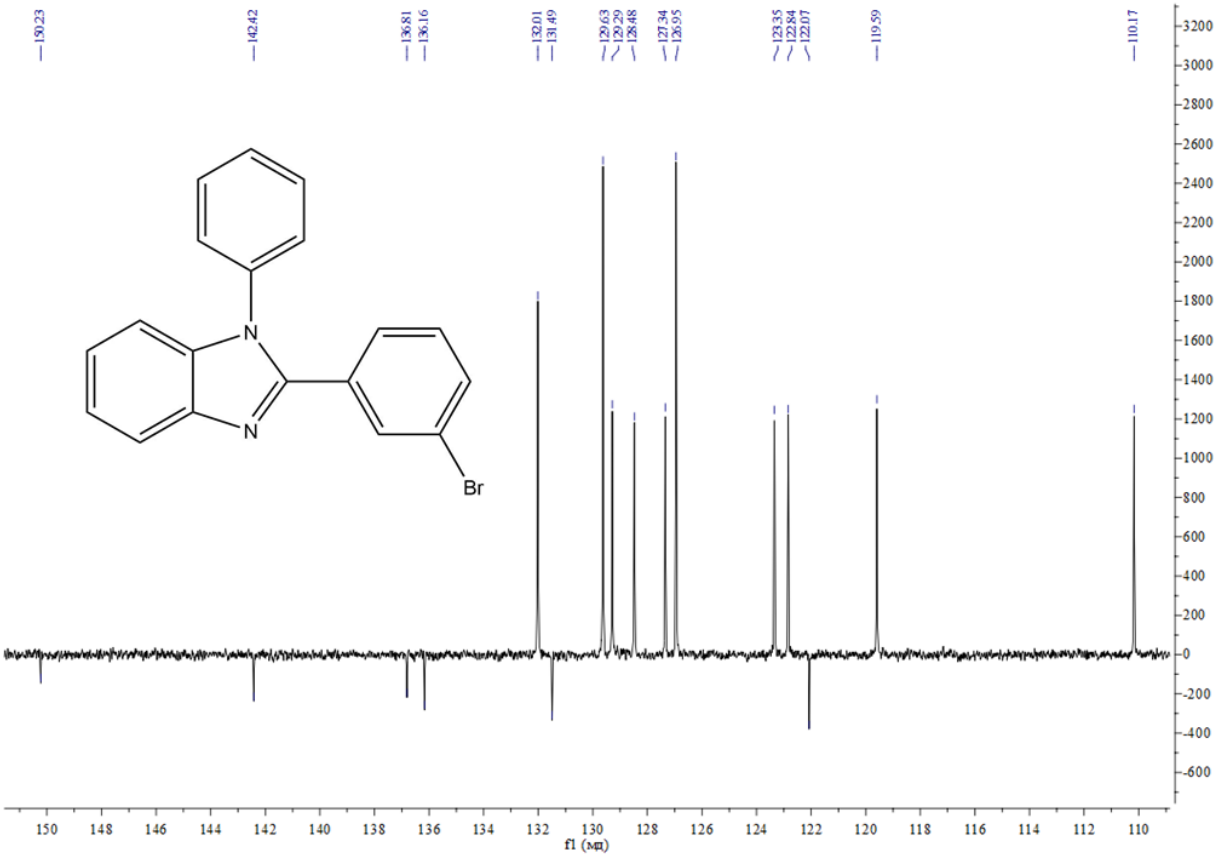

Figure S4. $^{13}C\{^{1}H\}$ apt NMR spectrum of the **2** ($CDCl_3$, 101 MHz, 25°C).

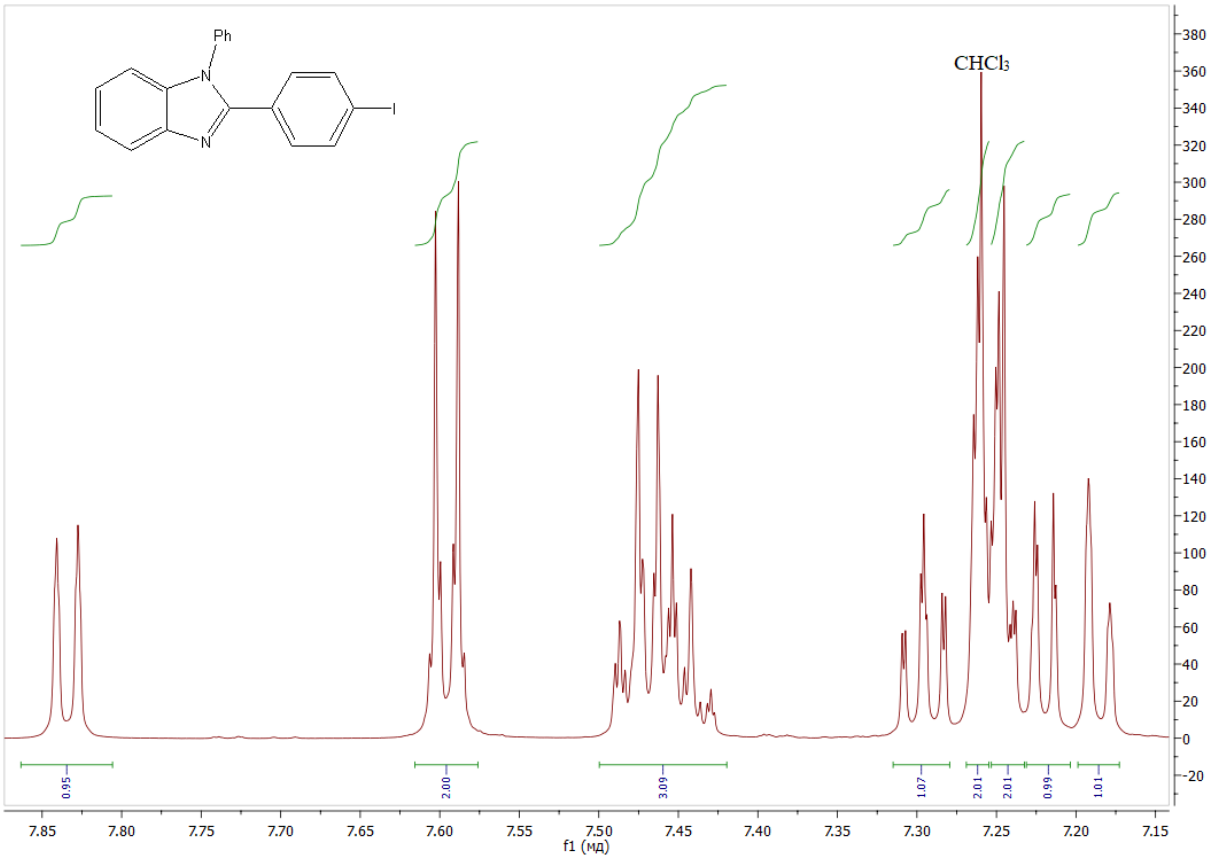

Figure S5. ^{1}H NMR spectrum of the **3** ($CDCl_3$, 600 MHz, 25°C).

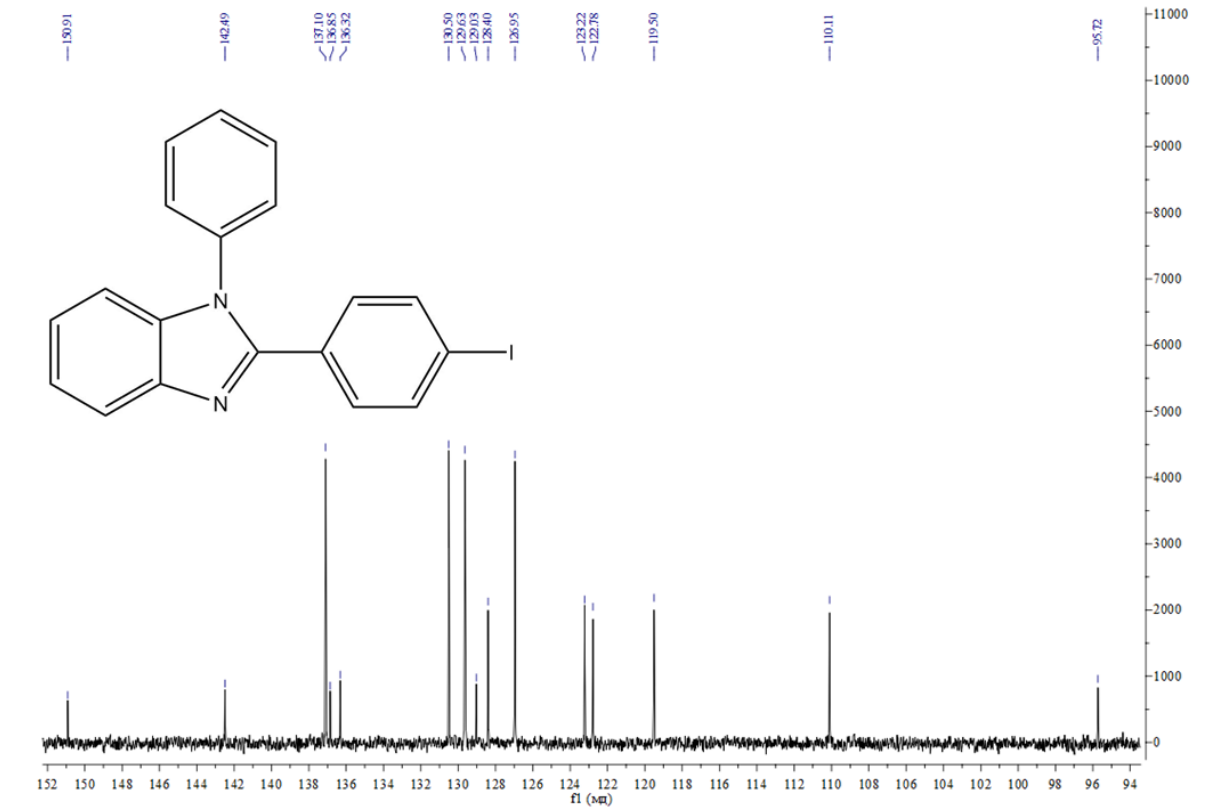

Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of the **3** ($CDCl_3$, 101 MHz, 25°C).

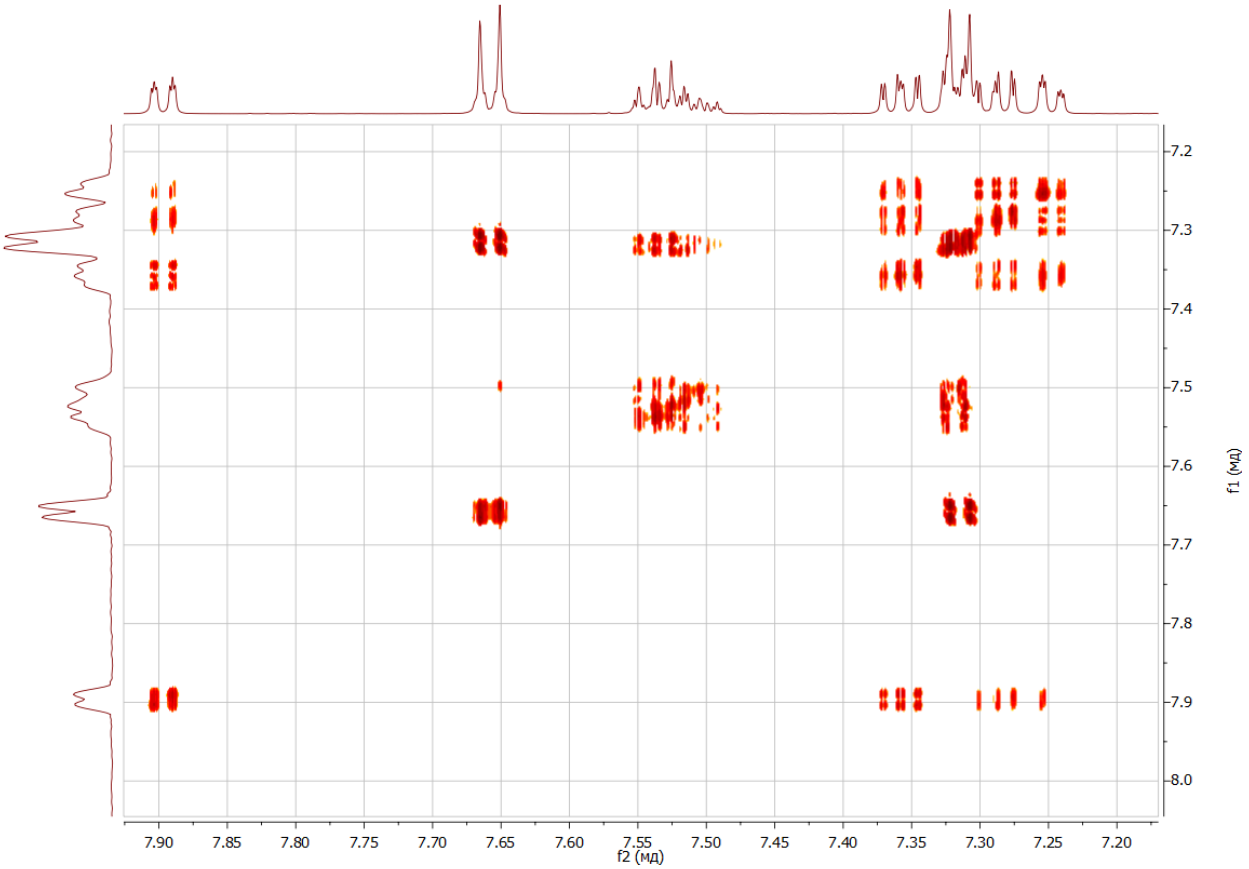

Figure S7. COSY NMR spectrum of the **3** ($CDCl_3$, 600 MHz, 25°C).

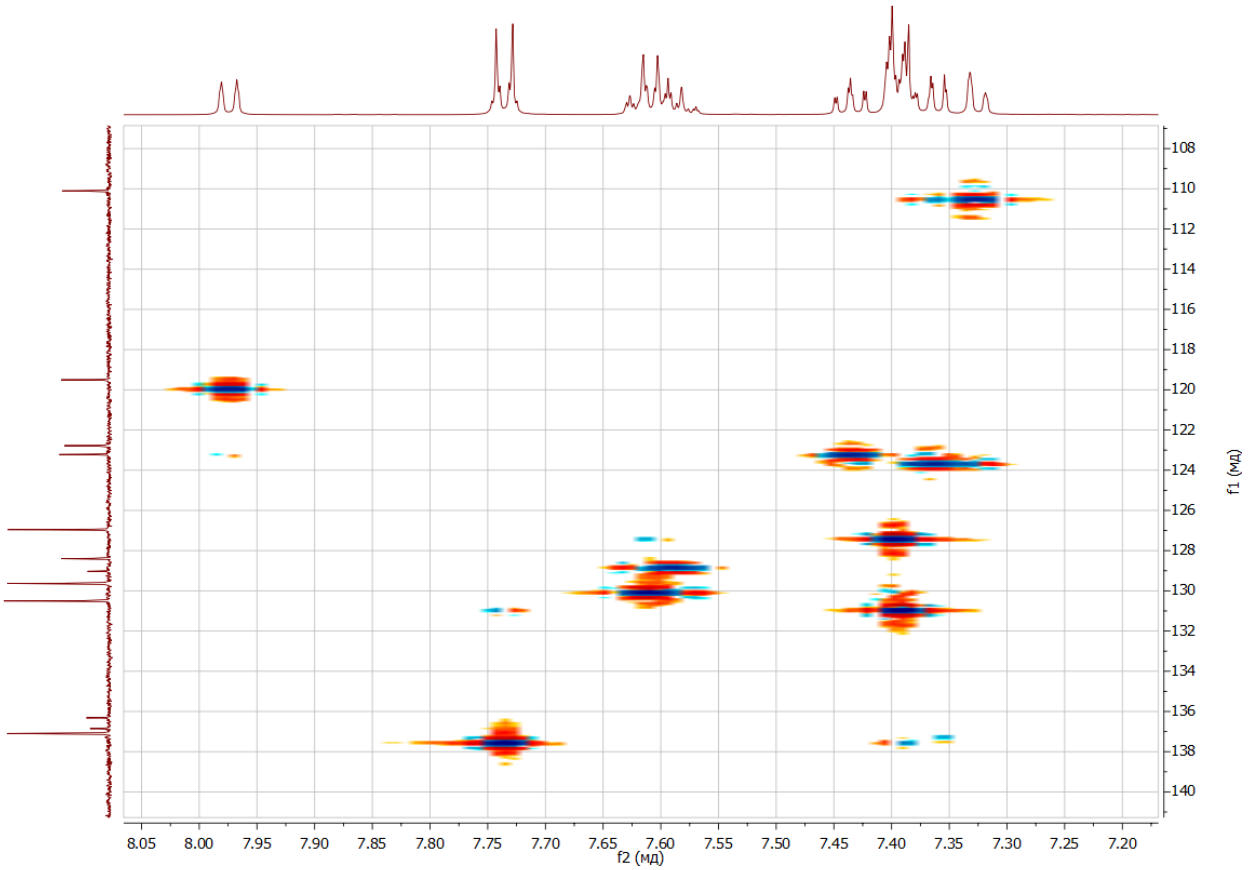

Figure S8. HSQC NMR spectrum of the **3** ($CDCl_3$, 600 MHz, 25°C).

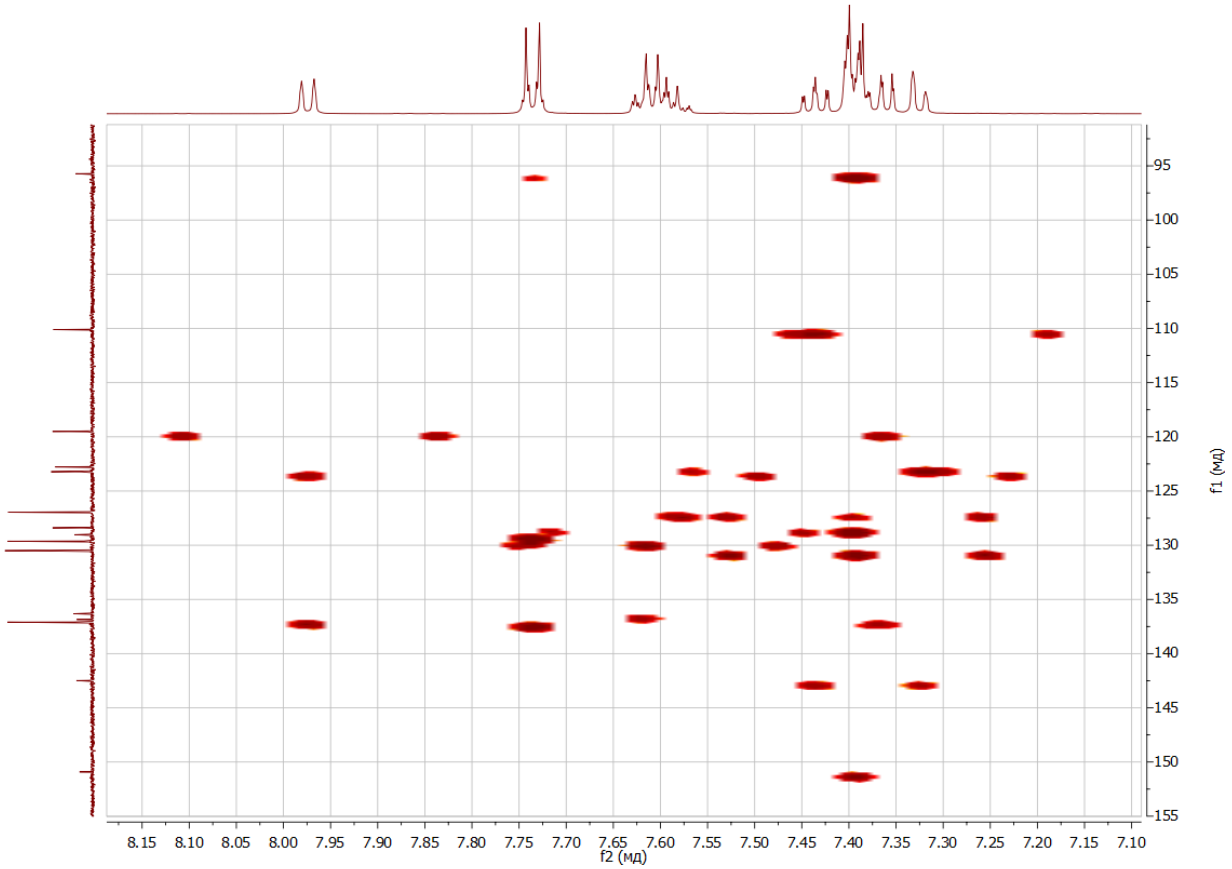

Figure S9. HMBC NMR spectrum of the **3** ($CDCl_3$, 600 MHz, 25°C).

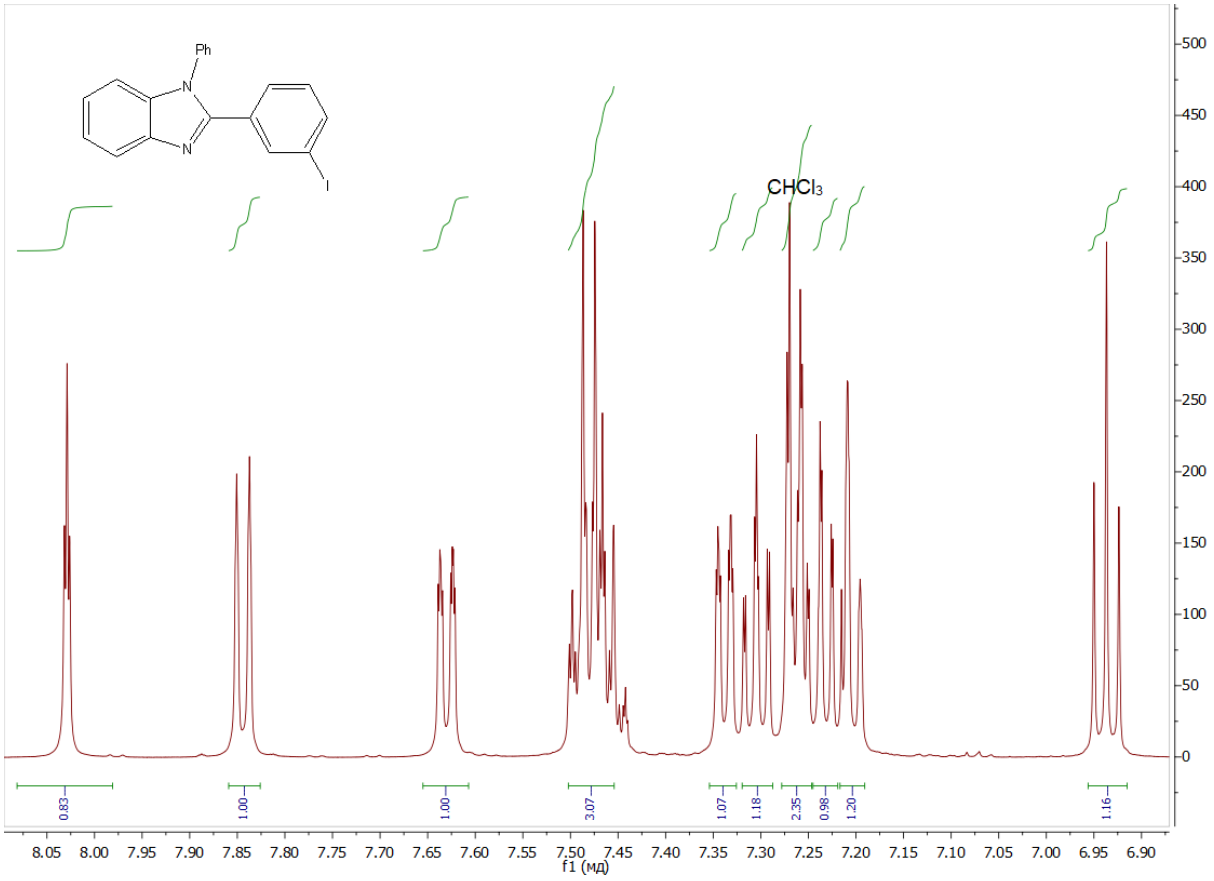

Figure S10. ^1H NMR spectrum of the **4** ($CDCl_3$, 600 MHz, 25°C).

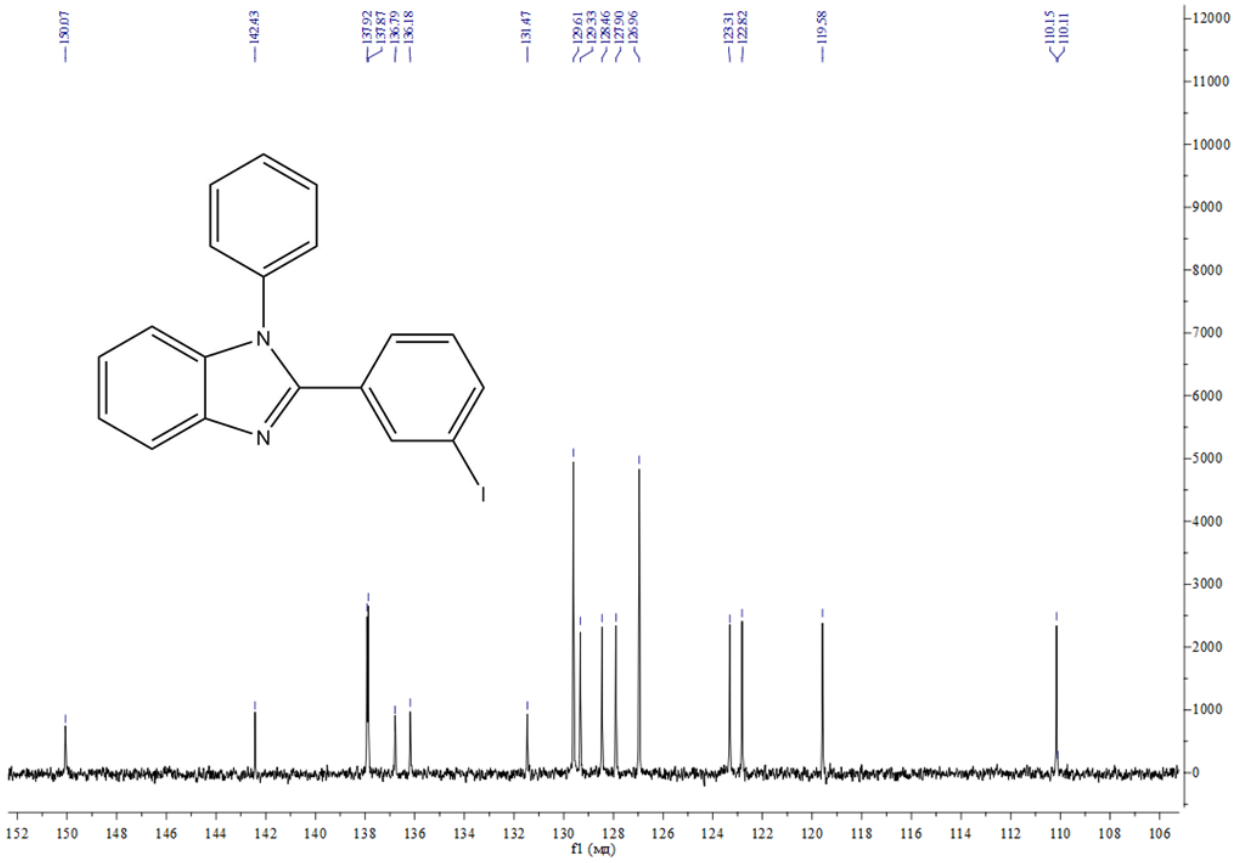

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of the **4** ($CDCl_3$, 101 MHz, 25°C).

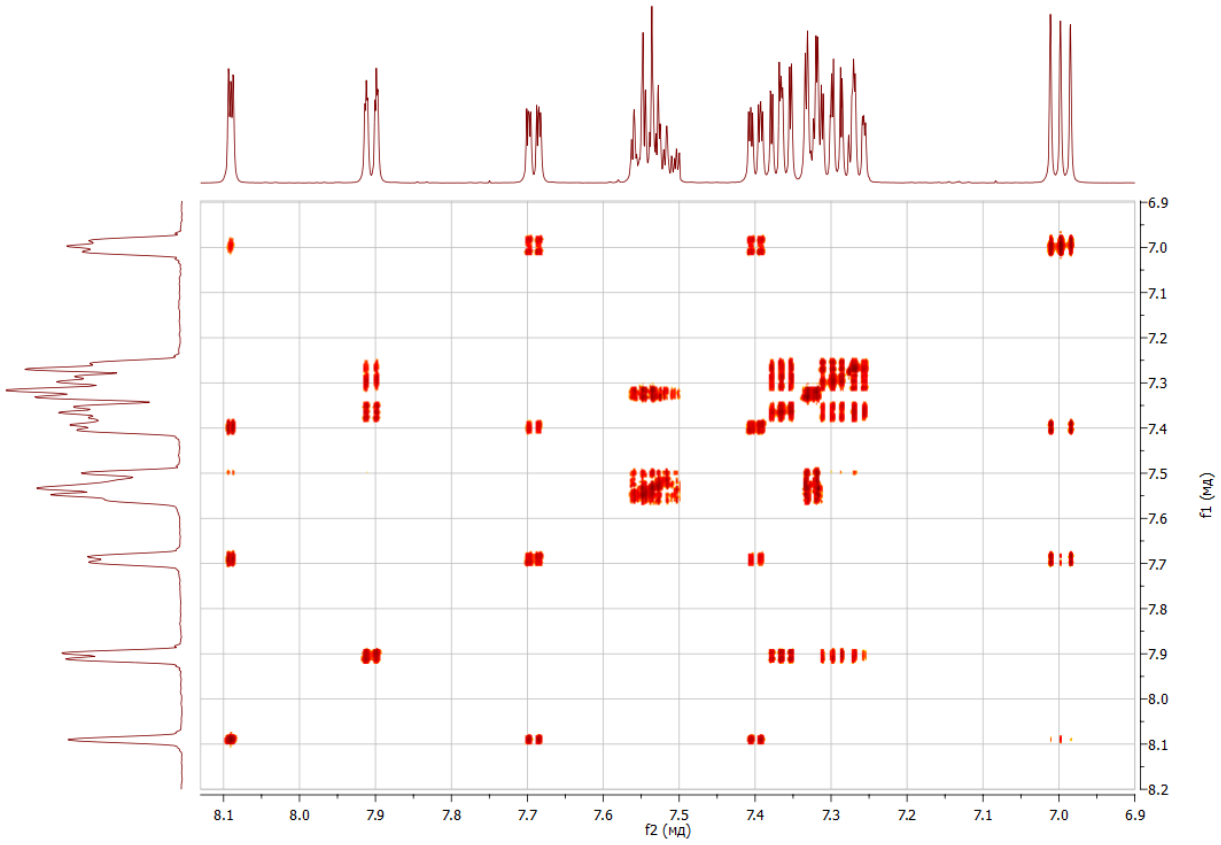

Figure S12. COSY NMR spectrum of the **4** ($CDCl_3$, 600 MHz, 25°C).

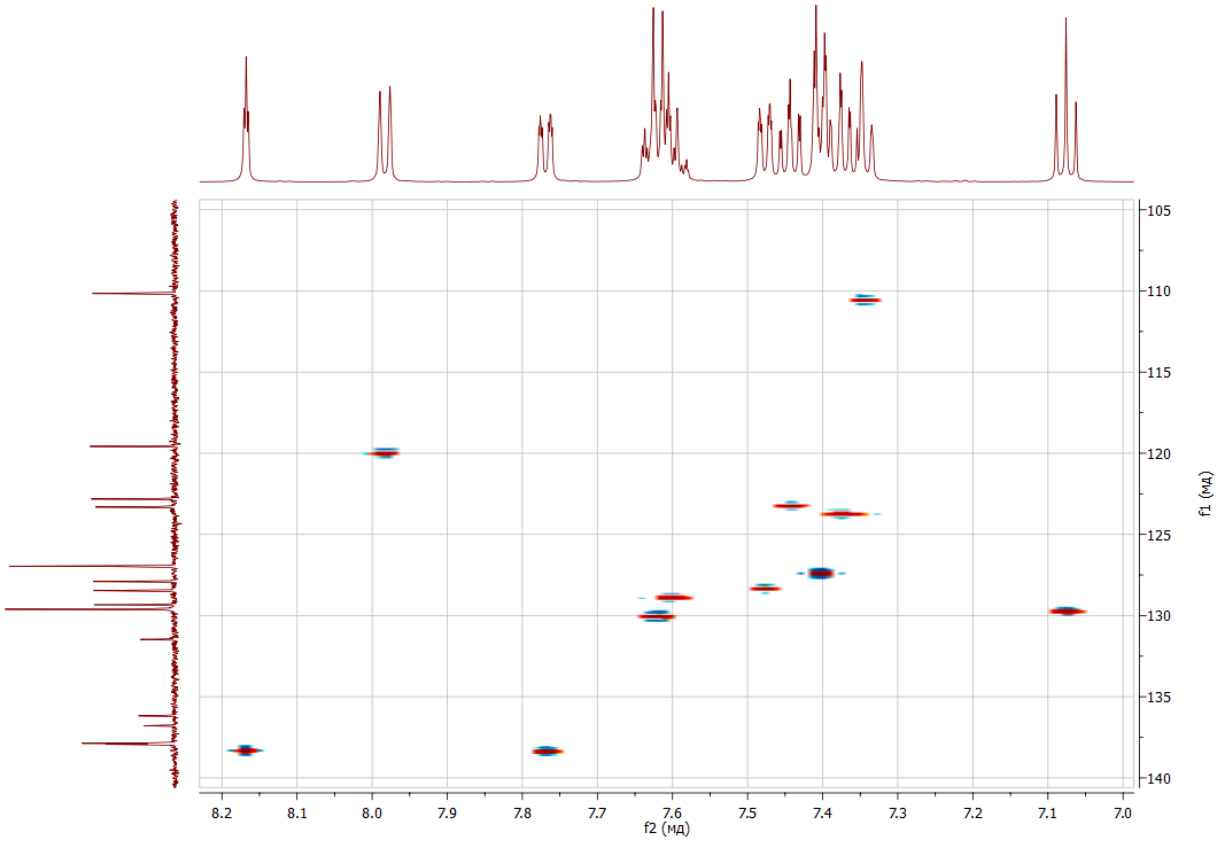

Figure S13. HSQC NMR spectrum of the **4** ($CDCl_3$, 600 MHz, 25°C).

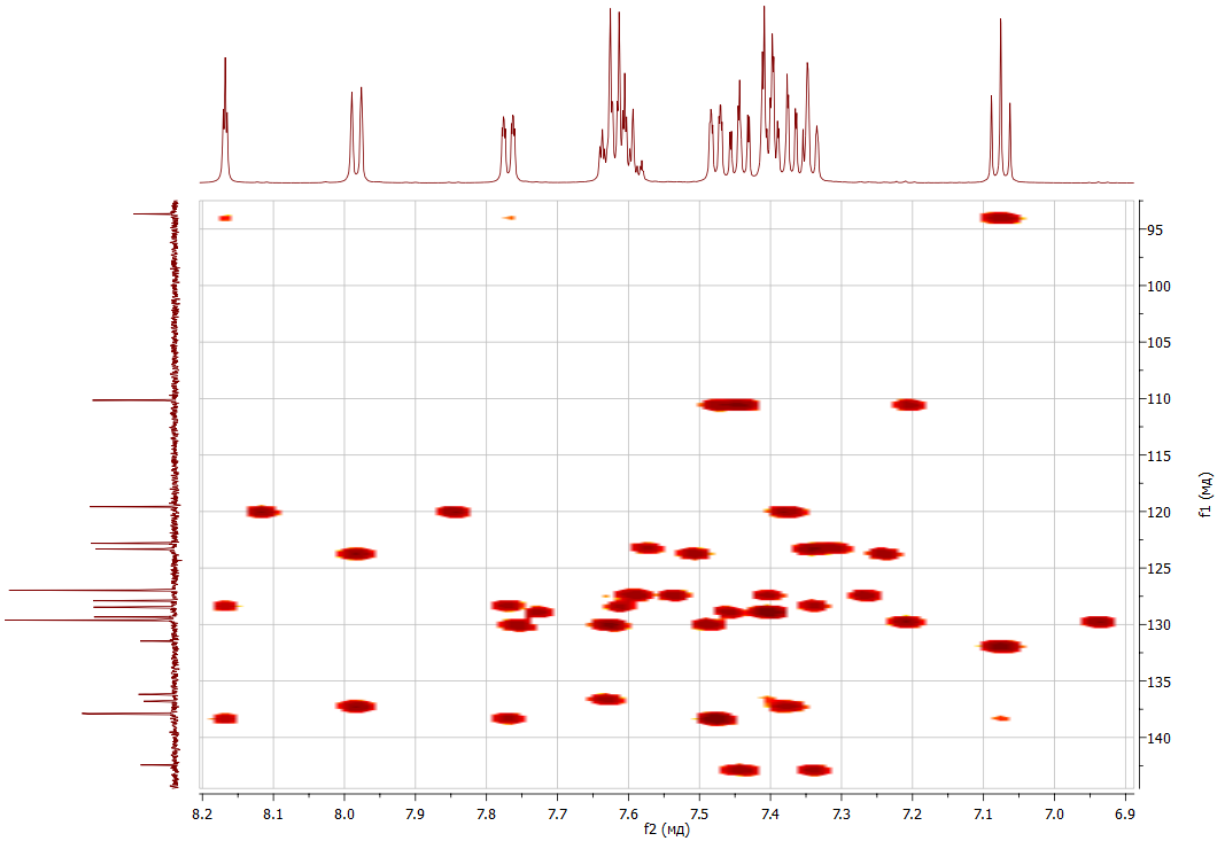

Figure S14. HMBC NMR spectrum of the **4** ($CDCl_3$, 600 MHz, 25°C).

2. X-ray crystallography

Table S1. Details of the X-ray crystal data collection and structure refinement for the title compounds.

Compound	**1**	**2**	**3**	**4**
Formula	$C_{19}H_{13}N_2Br$	$C_{19}H_{13}N_2Br$	$C_{19}H_{13}N_2I$	$C_{19}H_{13}N_2I$
M_w	349.22	349.22	396.21	396.21
Temperature (K)	150(2)	150(2)	150(2)	100(2)
Cryst. system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$	$P2_1/n$	$P2_1/c$
a (Å)	8.3061(15)	8.6166(7)	8.1539(2)	8.4708(5)
b (Å)	9.4657(14)	10.1262(8)	9.6185(2)	10.0913(6)
c (Å)	19.288(4)	17.6938(14)	19.6442(5)	18.2452(12)
α (°)	90	90	90	90
β (°)	90.276(7)	98.201(3)	91.9830(10)	98.622(2)
γ (°)	90	90	90	90
V (Å^3)	1516.5(5)	1528.1(2)	1539.74(6)	1542.00(16)
Z	4	4	4	4
ρ_{calc} (g·cm^{-3})	1.530	1.518	1.709	1.707
μ (mm^{-1})	2.708	2.687	2.077	2.074
F(000)	704.0	704.0	776.0	776.0
Size (mm)	0.25 × 0.22 × 0.15	0.32 × 0.30 × 0.16	0.18 × 0.15 × 0.10	0.12 × 0.10 × 0.09
2θ range (deg)	4.22 − 50.10	4.65 − 61.81	4.15 − 63.07	4.52 − 62.99
collected/unique rflns	15241 / 2681	71674 / 4740	19425 / 5125	17807 / 5060
Completeness to θ (%)	100.0	97.9	99.9	98.8
data/restraints/params	2681/0/199	4740/0/199	5125/0/199	5060/0/199
Goodness of fit on F^2	1.050	1.072	1.045	1.023
Final R indices ($I > 2\sigma(I)$)	R_1 = 0.0327, wR_2 = 0.0654	R_1 = 0.0271, wR_2 = 0.0700	R_1 = 0.0235, wR_2 = 0.0510	R_1 = 0.0210, wR_2 = 0.0444
Final R indices (all data)	R_1 = 0.0531, wR_2 = 0.0750	R_1 = 0.0309, wR_2 = 0.0724	R_1 = 0.0310, wR_2 = 0.0534	R_1 = 0.0266, wR_2 = 0.0461
Largest diff peak/hole (e/Å^3)	0.24 / −0.44	0.56 / −0.57	0.41 / −0.68	0.52 / −0.46

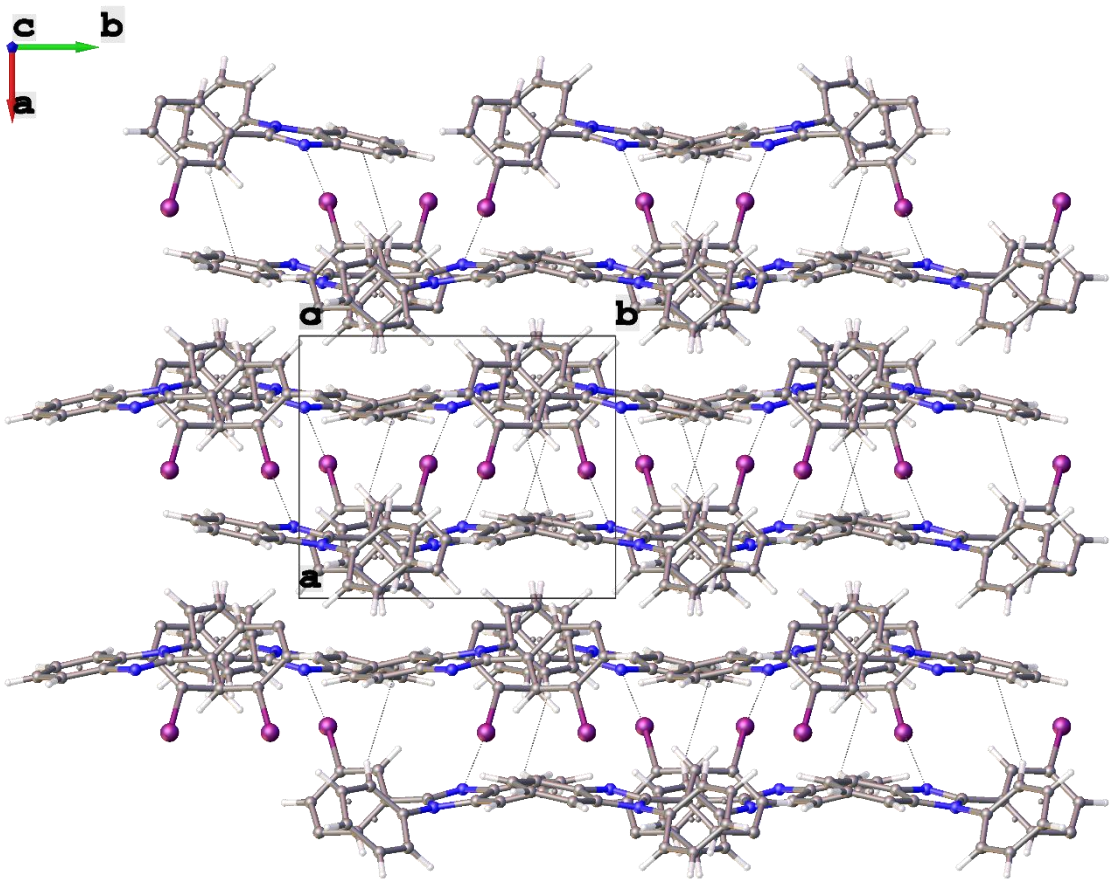

Figure S15. The fragment of the crystal packing of the 1-phenyl-2-(3-iodophenyl)benzimidazole.

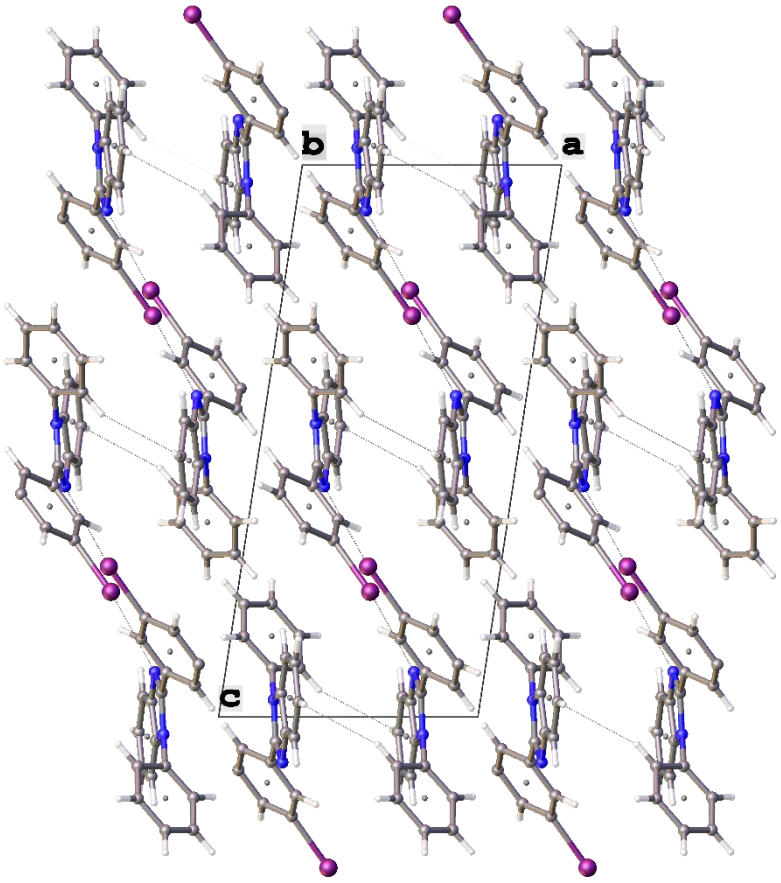

Figure S16. The fragment of the crystal packing of the 1-phenyl-2-(3-iodophenyl)benzimidazole

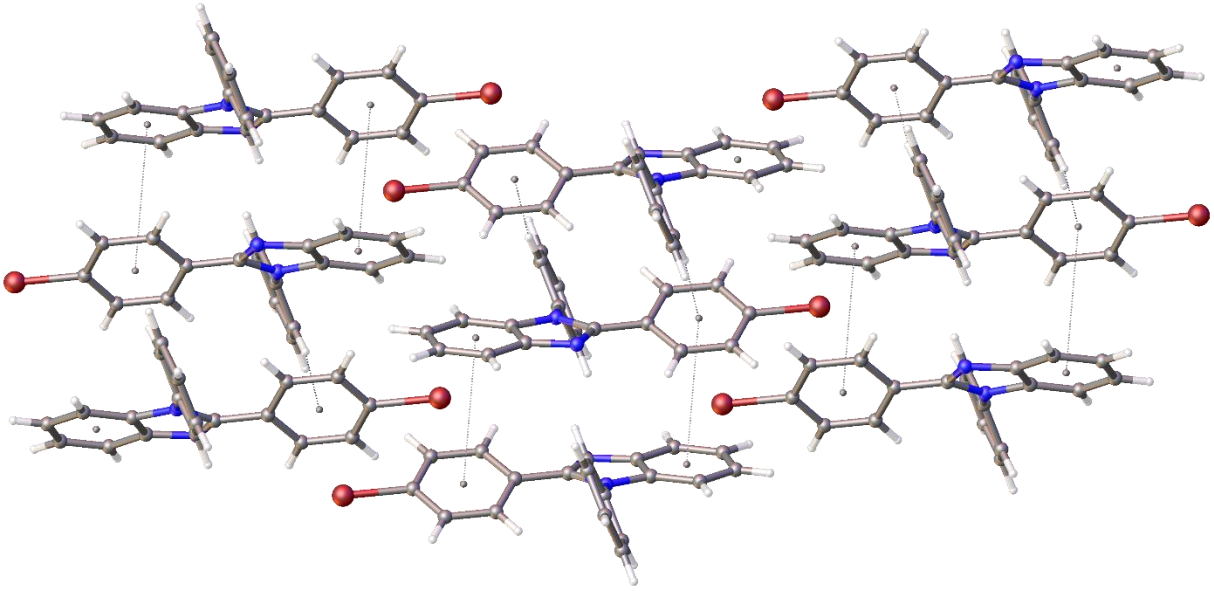

Figure S17. The fragment of the crystal packing of the 1-phenyl-2-(4-bromophenyl)benzimidazole.

3. Optical data

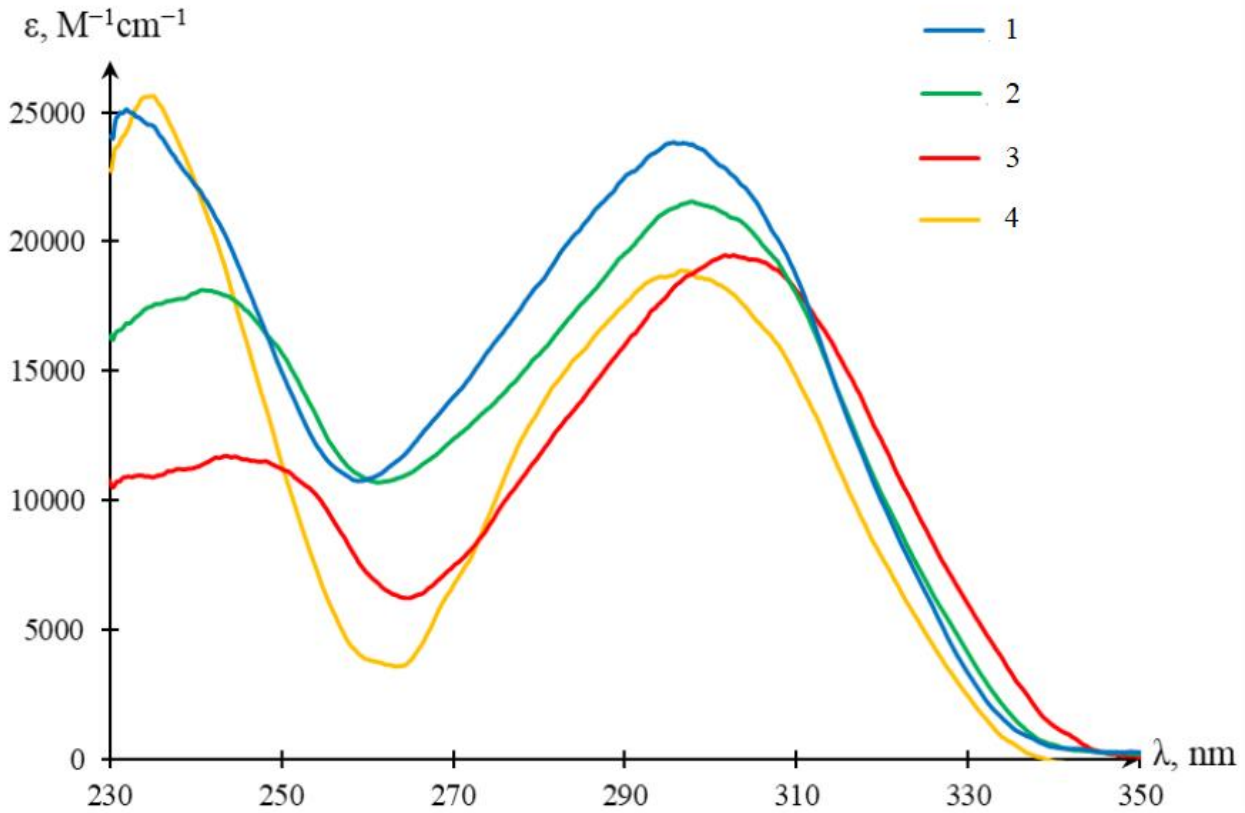

Figure S18. The UV-Vis spectrum of the study halogen-substituted 2-aryl-*N*-phenylbenzimidazoles.