Supplementary materials

Synthesis, crystal structure and cyclic voltammetric behavior of N-Aroyl-N′-(4′-cyanophenyl)thioureas

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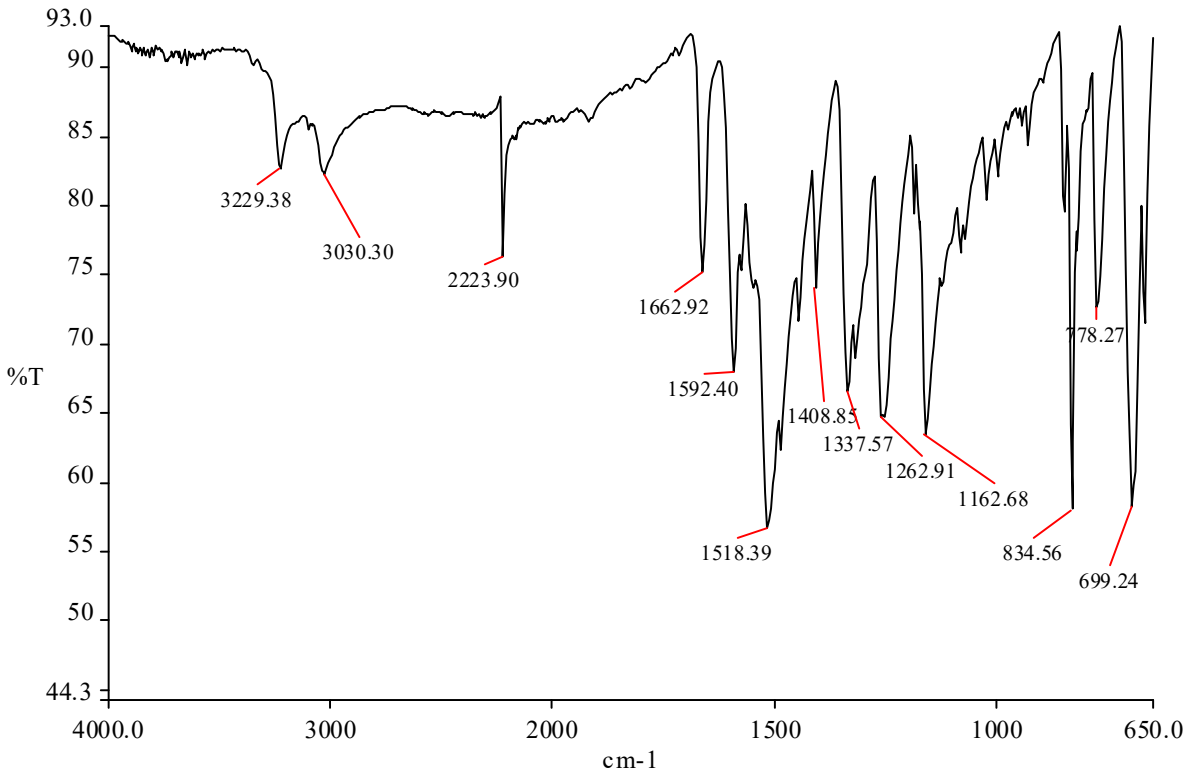

Figure S1. The FT-IR spectrum of N-benzoyl-N′-(4-cyanophenyl)-thiourea (**1**)

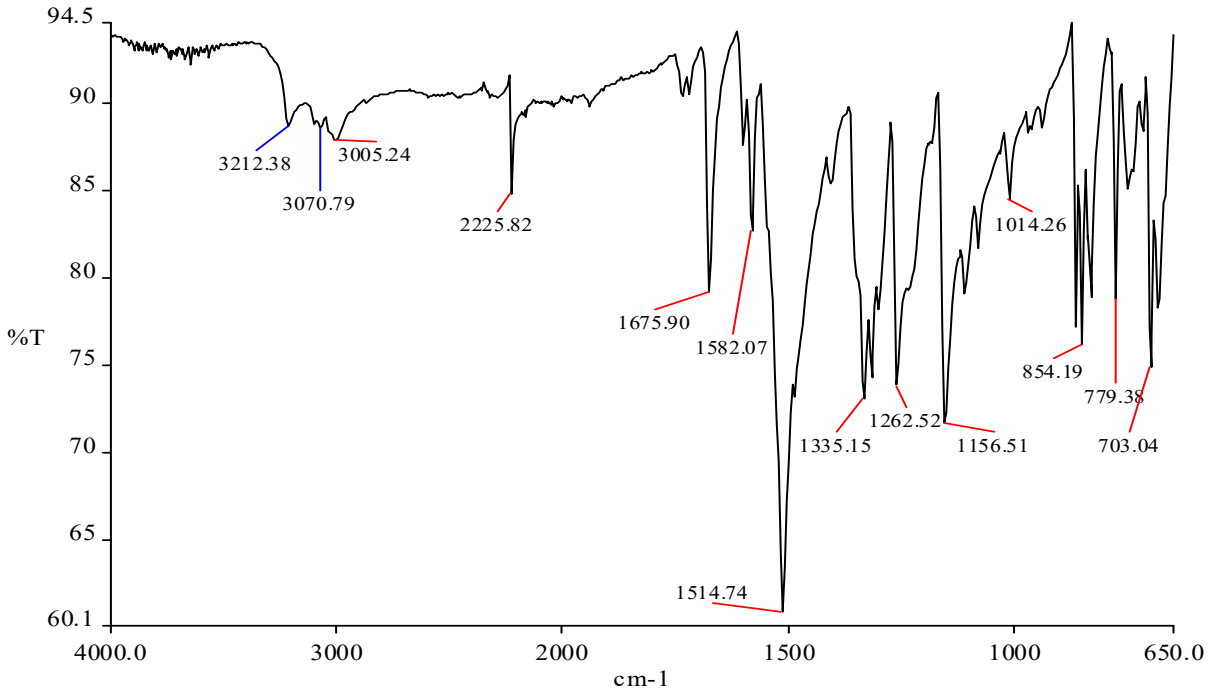

Figure S2. The FT-IR spectrum of N-(4-nitrobenzoyl)-N′-(4-cyanophenyl)-thiourea (**2**)

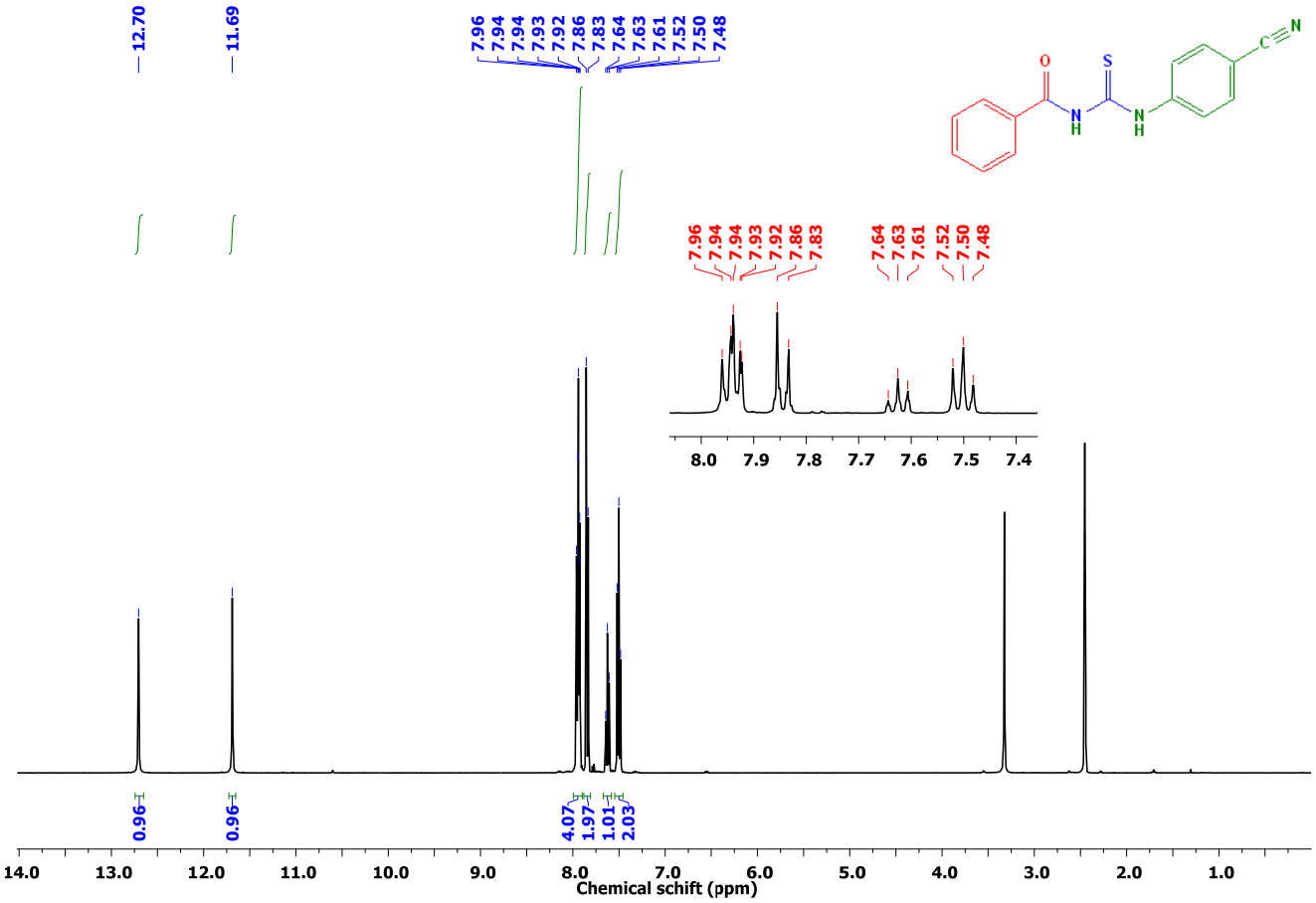

Figure S3. The ^{1}H-NMR spectrum of the N-benzoyl-N′-(4-cyanophenyl)-thiourea (**1**)

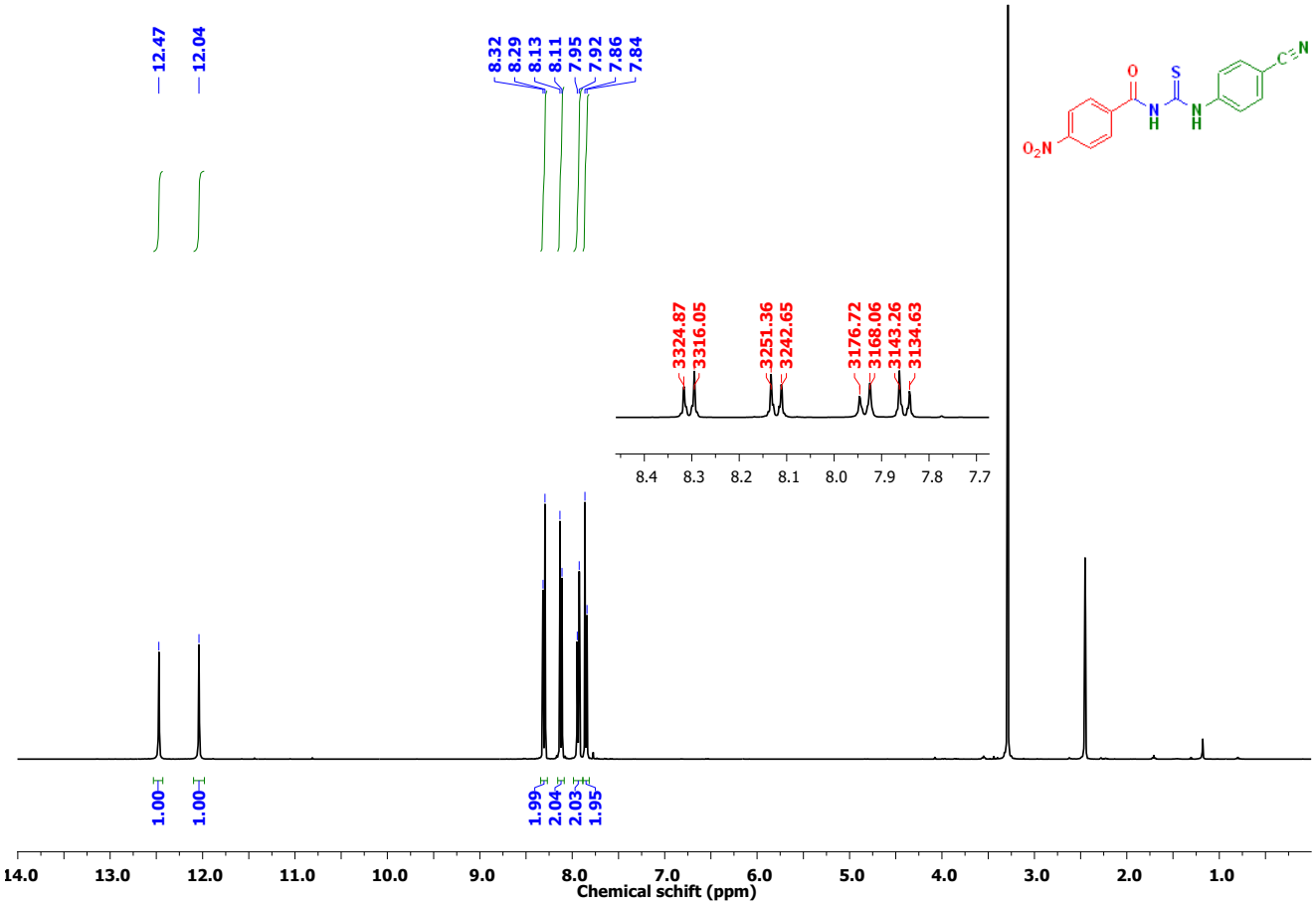

Figure S4. The ^{1}H-NMR spectrum of the N-(4-nitrobenzoyl)-N′-(4-cyanophenyl)-thiourea (**2**)

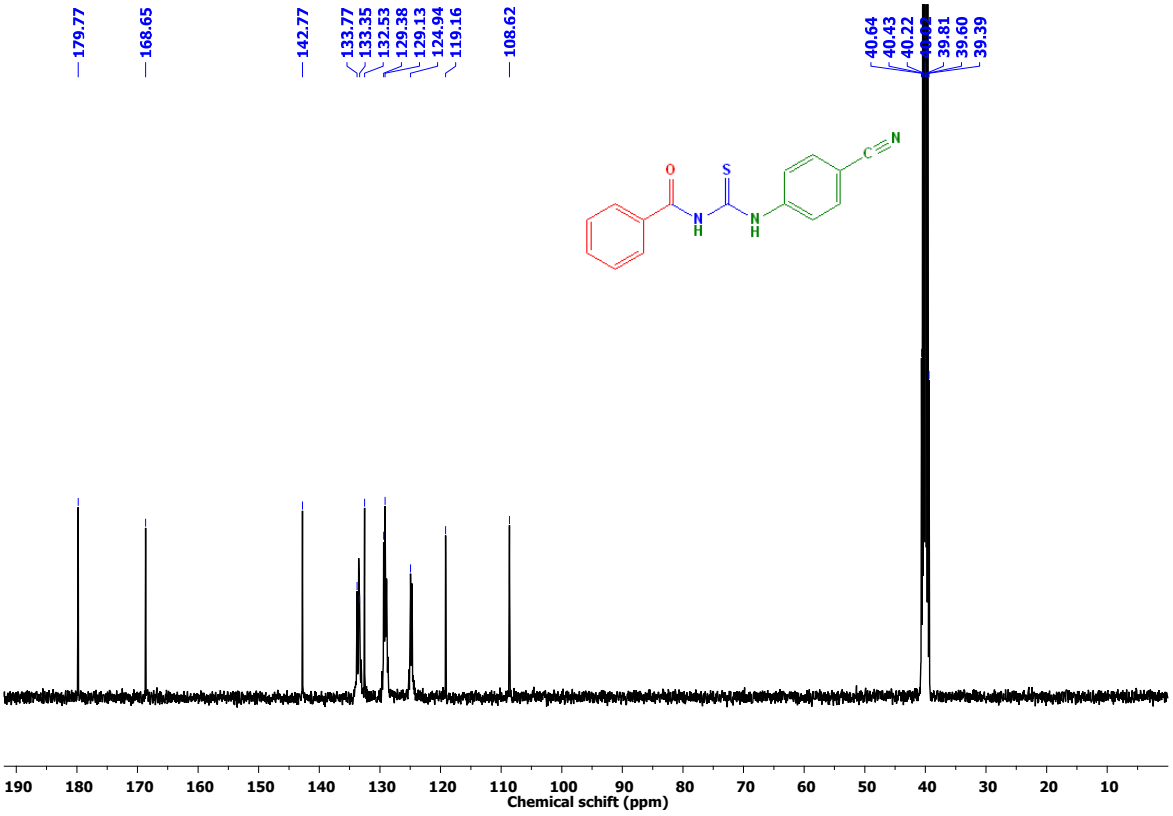

Figure S5. The ^{13}C-NMR spectrum of the N-benzoyl-N´-(4-cyanophenyl)-thiourea (**1**)

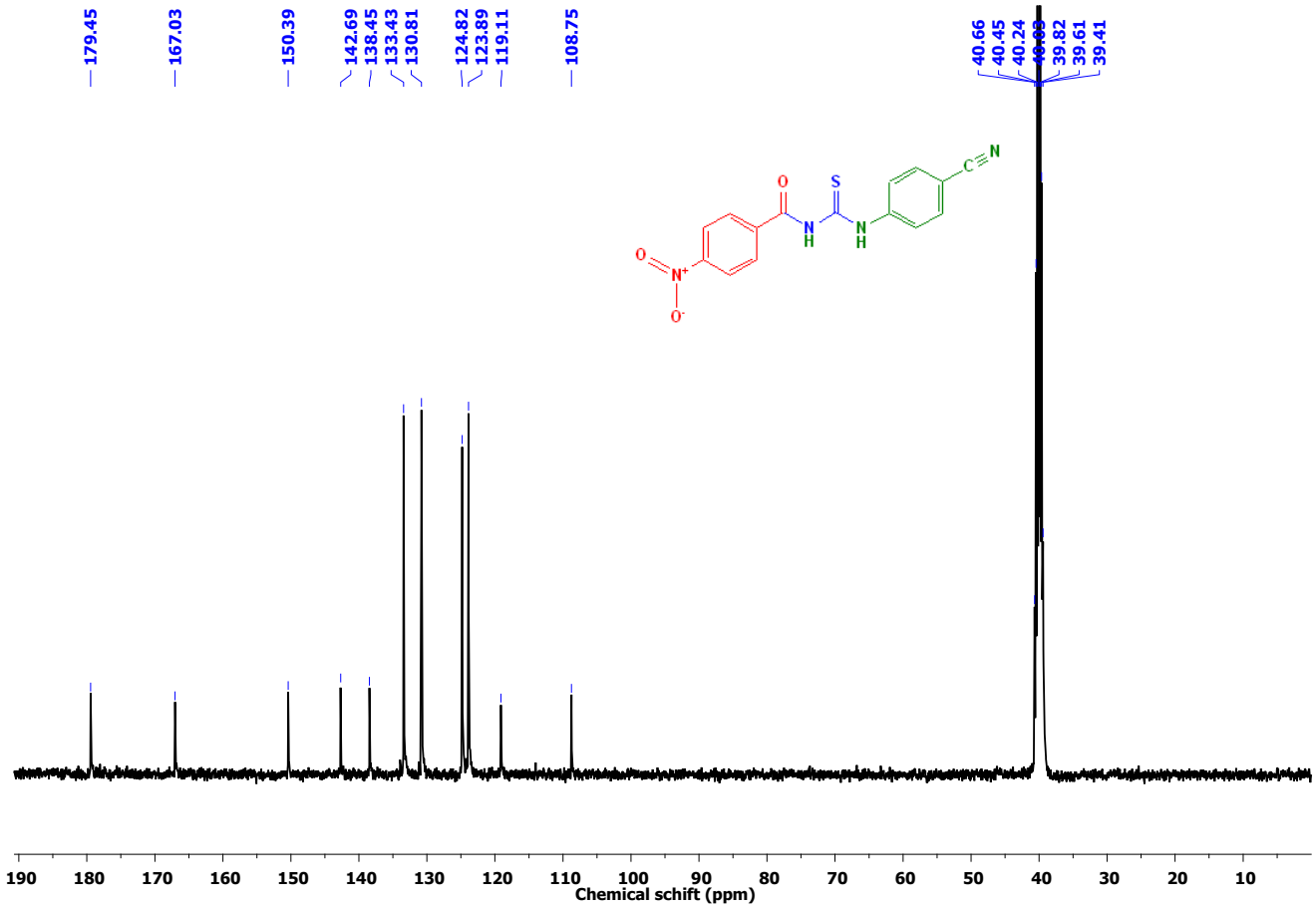

Figure S6. The ^{13}C-NMR spectrum of the N-(4-nitrobenzoyl)-N′-(4-cyanophenyl)-thiourea (**2**)

Table S1. Crystal data and structure refinement parameters for the N-Benzoyl-N′-(4-cyanophenyl)-thiourea (**1**).

Crystal data	
Chemical formula	$C_{15}H_{11}N_3OS$
Mr	281.33
Crystal system, space group	Triclinic, *P-1*
Temperature (K)	296
a, b, c (Å)	4.0684 (3), 12.3410 (11), 14.7486 (13)
α, β, γ (°)	69.009 (3) 89.918 (3), 83.018 (3)
V (Å^3)	685.52 (10)
Z	2
D_x mg/mm	1.363
Radiationtype, λ, Å	MoK_α, , 0.71073
No. of reflections for cell measurement	7562
θ range (°) for cell measurement	2.7 - 21.4
μ (mm^{-1})	0.23
F(000)	292
Crystalshape	Block, colourless
Crystal size (mm)	0.30 × 0.145 × 0.12
Index ranges	$-5 \le h \le 5$, $-19 \le k \le 19$, $-1\ 6 \le l \le 16$
Data collection	
Diffractometer	BrukerAPEX-II CCD
Absorption correction	Multi-scan
No. of measured, independent and observed [I> 2σ(I)] reflections	34359, 3430, 2170
R_{int}	0.069
Θ_{max}, θ_{min} (°)	28.3, 1.5
Refinement	
$R[F^2 > 2\sigma(F^2)]$, w$R(F^2)$, S	064, 0.213, 1.10
No. of reflections	3430
No. of parameters	181
H-atom treatment	H-atom parameters constrained
	w = $1/[\sigma 2(F_o^2) + (0.1242P)^2 + 0.0055P]$ where$P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	< 0.001
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.61, −0.38

Computer programs: Bruker*APEX2*, Bruker*SAINT*, SHELXT 2014/4 (Sheldrick, 2014), *SHELXL2016*/6 (Sheldrick, 2016).

Table S2. The optimized geometry (bond lengths (Å), bond angles (°) and torsion angles (°) of the the *N*-Benzoyl-*N*′-(4′-cyanophenyl)thiourea (**1**)

Geometric parameters (Å, °)			
C1—C2	***1.387 (4)***	***C8—S1***	***1.650 (3)***
C1—C6	***1.392 (4)***	***C9—C10***	***1.387 (4)***
C1—H1	***0.9300***	***C9—C14***	***1.392 (4)***
C2—C3	***1.371 (5)***	***C9—N2***	***1.414 (3)***
C2—H2	***0.9300***	***C10—C11***	***1.383 (4)***
C3—C4	***1.370 (4)***	***C10—H10***	***0.9300***
C3—H3	***0.9300***	***C11—C12***	***1.380 (4)***
C4—C5	***1.384 (4)***	***C11—H11***	***0.9300***
C4—H4	***0.9300***	***C12—C13***	***1.385 (4)***
C5—C6	***1.382 (4)***	***C12—C15***	***1.443 (4)***
C5—H5	***0.9300***	***C13—C14***	***1.373 (4)***
C6—C7	***1.489 (4)***	***C13—H13***	***0.9300***
C7—O1	***1.220 (3)***	***C14—H14***	***0.9300***
C7—N1	***1.380 (3)***	***C15—N3***	***1.140 (4)***
C8—N2	***1.342 (3)***	***N1—H1A***	***0.8600***
C8—N1	***1.400 (3)***	***N2—H2A***	***0.8600***
C2—C1—C6	***119.3 (3)***	***C10—C9—N2***	***125.2 (2)***
C2—C1—H1	***120.3***	***C14—C9—N2***	***115.3 (2)***
C6—C1—H1	***120.3***	***C11—C10—C9***	***119.4 (3)***
C3—C2—C1	***120.4 (3)***	***C11—C10—H10***	***120.3***
C3—C2—H2	***119.8***	***C9—C10—H10***	***120.3***
C1—C2—H2	***119.8***	***C12—C11—C10***	***121.0 (3)***
C4—C3—C2	***120.5 (3)***	***C12—C11—H11***	***119.5***
C4—C3—H3	***119.8***	***C10—C11—H11***	***119.5***
C2—C3—H3	***119.8***	***C11—C12—C13***	***119.6 (3)***
C3—C4—C5	***119.9 (3)***	***C11—C12—C15***	***120.3 (3)***
C3—C4—H4	***120.1***	***C13—C12—C15***	***120.1 (3)***
C5—C4—H4	***120.1***	***C14—C13—C12***	***120.0 (3)***
C6—C5—C4	***120.3 (3)***	***C14—C13—H13***	***120.0***
C6—C5—H5	***119.9***	***C12—C13—H13***	***120.0***
C4—C5—H5	***119.9***	***C13—C14—C9***	***120.6 (3)***
C5—C6—C1	***119.6 (3)***	***C13—C14—H14***	***119.7***
C5—C6—C7	***122.6 (2)***	***C9—C14—H14***	***119.7***
C1—C6—C7	***117.7 (3)***	***N3—C15—C12***	***179.7 (5)***
O1—C7—N1	***122.4 (2)***	***C7—N1—C8***	***129.1 (2)***

O1—C7—C6	***122.4 (2)***	***C7—N1—H1A***	***115.4***
N1—C7—C6	***115.2 (2)***	***C8—N1—H1A***	***115.4***
N2—C8—N1	***114.3 (2)***	***C8—N2—C9***	***131.8 (2)***
N2—C8—S1	***127.8 (2)***	***C8—N2—H2A***	***114.1***
N1—C8—S1	***117.88 (19)***	***C9—N2—H2A***	***114.1***
C10—C9—C14	***119.5 (2)***		

C6—C1—C2—C3	***−0.6 (5)***	***C10—C11—C12—C13***	***0.2 (5)***
C1—C2—C3—C4	***−0.6 (5)***	***C10—C11—C12—C15***	***179.6 (3)***
C2—C3—C4—C5	***0.9 (5)***	***C11—C12—C13—C14***	***0.2 (4)***
C3—C4—C5—C6	***0.0 (4)***	***C15—C12—C13—C14***	***−179.3 (3)***
C4—C5—C6—C1	***−1.2 (4)***	***C12—C13—C14—C9***	***0.0 (4)***
C4—C5—C6—C7	***−179.3 (3)***	***C10—C9—C14—C13***	***−0.5 (4)***
C2—C1—C6—C5	***1.5 (4)***	***N2—C9—C14—C13***	***178.6 (3)***
C2—C1—C6—C7	***179.6 (3)***	***O1—C7—N1—C8***	***−2.9 (4)***
C5—C6—C7—O1	***148.7 (3)***	***C6—C7—N1—C8***	***177.7 (2)***
C1—C6—C7—O1	***−29.4 (4)***	***N2—C8—N1—C7***	***−7.0 (4)***
C5—C6—C7—N1	***−31.9 (4)***	***S1—C8—N1—C7***	***173.7 (2)***
C1—C6—C7—N1	***150.0 (2)***	***N1—C8—N2—C9***	***179.9 (3)***
C14—C9—C10—C11	***0.9 (5)***	***S1—C8—N2—C9***	***−0.9 (4)***
N2—C9—C10—C11	***−178.1 (3)***	***C10—C9—N2—C8***	***−4.4 (5)***
C9—C10—C11—C12	***−0.7 (5)***	***C14—C9—N2—C8***	***176.6 (3)***

Table S3. Hydrogen bonds, intermolecular interactions and symmetry operations the *N*-Benzoyl-*N*′-(4′-cyanophenyl)thiourea (**1**) (A˚, °)

D—H···A	**D—H**	**H···A**	**D···A**	**D—H···A**
N1—H1A···S1^{i}	0.86	2.69	3.518 (2)	163
N2—H2A···O1	0.86	1.92	2.646 (3)	141
C5—H5···S1^{i}	0.93	2.87	3.239 (3)	105
C5—H5···S1^{ii}	0.93	2.87	3.773 (3)	164
C10—H10···S1	0.93	2.52	3.186 (3)	129

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

Table S4. Mulliken charges of title compounds

	Compound (**1**)	Compound (**2**)
Atoms	Charges	Charges
C1	-0.071	-0.087
C2	-0.184	-0.145
C3	-0.107	0.289
C4	-0.163	-0.116
C5	-0.082	-0.102
C6	-0.163	-0.125
C7	0.541	0.545
C8	0.203	0.200
C9	0.390	0.406
C10	-0.101	-0.089
C11	-0.089	-0.100
C12	0.070	0.072
C13	-0.066	-0.066
C14	-0.266	-0.265
C15	-0.241	-0.240
N1	-0.206	-0.699
N2	-0.823	-0.820
N3	-0.096	-0.090
N4	-	0.013
S	-0.082	-0.064
O1	-0.457	-0.445
O2	-	-0.253
O3	-	-0.255
H1	0.176	0.189
H2	0.156	0.219
H3	0.157	-
H4	0.195	0.219
H5	0.250	0.208
H1A	0.393	0.394
H2A	0.406	0.406
H10	0.183	0.186
H11	0.185	0.256
H12	0.187	0.187
H13		0.187