New Facile Synthesis of Imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones via aza-Wittig Reaction

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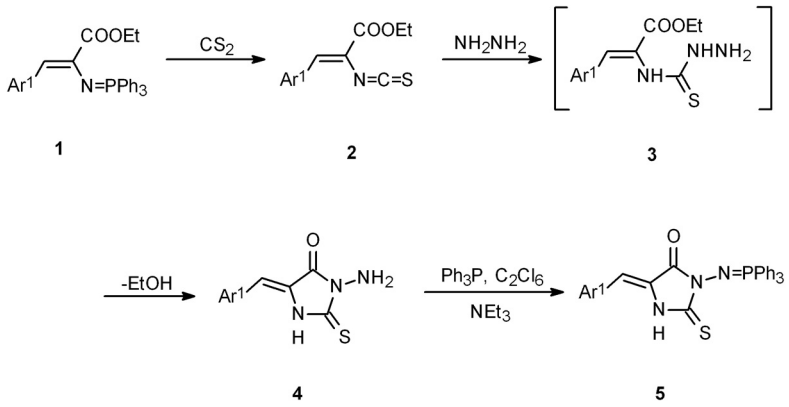
Abstract: The isothiocyanates **2**, obtained from aza-Wittig reactions of vinyliminophosphoranes **1** with CS_2, reacted with hydrazine to give 3-amino-2-thioxo-4-imidazolidinones **4**. Reactions of **4** with triphenyphosphine, hexachloroethane and Et_3N produced iminophosphoranes **5**. A tandem aza-Wittig reaction of iminophosphoranes **5** with isocyanates generated imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones **7** in moderate yield.

Key words: imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-one, iminophosphorane, carbodiimide, aza-Wittig reaction, synthesis

The derivatives of 4*H*-imidazol-4-ones have shown biological and pharmaceutical activities.[1–3] Some of them exhibited good antibacterial, antifungal and angiotensin antagonistical activities,[4–6] whereas others appear in a variety of biologically active molecules, particularly in some alkaloids in which a common structural unit is a derivatized 4*H*-imidazol-4-one moiety.[7,8] The introduction of a thiadiazole ring to the imidazolone system is expected to influence the biological activities significantly. However, there are few reports on synthesis of imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones and the method hitherto reported for the preparation of this ring system generally started from 2-mercapto-1,3,4-thiadiazoles.[9] Over past twenty years, the aza-Wittig reactions of iminophosphoranes have received increased attention in view of their utility in the synthesis of nitrogen heterocyclic compounds.[10] Recently we have been interested in the synthesis of imidazolones, quinazolinones and thieno[2,3-*d*]pyrimidin-4(3*H*)-ones via aza-Wittig reaction, with the aim of evaluating their fungicidal activities.[11–15] Here we wish to report a new facile synthesis of imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones.

Iminophosphorane **1**[15,16] reacted with CS_2 to give isothiocyanates **2**, which were allowed to react with hydrazine to give 3-amino-2-thioxo-4-imidazolidinones **4** in 77–94% yields (Scheme 1, Table 1). The formation of **4** can be rationalized in terms of an initial nucleophilic addition of hydrazine to give the thiourea intermediate **3** which cyclizes to give **4**. Compounds **4** were easily converted to iminophosphoranes **5** via reaction with triphenylphosphine, hexachloroethane and Et_3N in good yields (72–85%) (Scheme 1, Table 1).

When solutions of iminophosphoranes **5** in anhydrous DMF were treated with aromatic isocyanate at room temperature, the color of the reaction mixture quickly turned red, becoming yellow after few minutes, and 2-arylamino-imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones **7** were isolated as crystalline solids in moderate yields (48–64%) (Scheme 2, Table 1). Presumably, the conversion of **5** into **7** involves initial aza-Wittig reaction between the iminophosphorane **5** and an isocyanate to give a carbodiimide **6** as highly reactive intermediate, which undergoes ring closure across the mercapto group to give the otherwise not readily available 2-arylamino substituted imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones **7**.



Scheme 1

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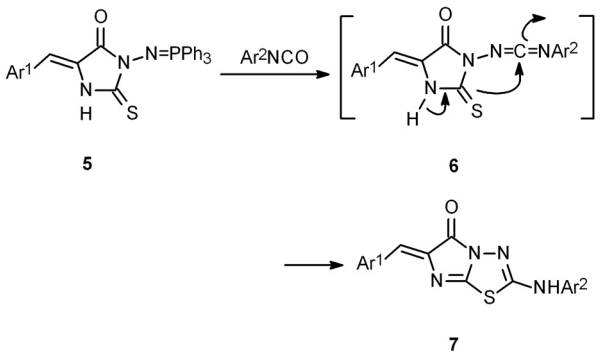

Scheme 2

The structure of **7** has been characterized spectroscopically. For example, the ^{1}H NMR spectrum data in **7a** showed the signals of NH at 10.46 ppm as a single absorption and ArH at 8.21–7.03 ppm as mutiple absorptions. The signals of OCH_3 and CH_3 appear at 3.83 ppm and 2.28 ppm, respectively, as a single absorption. The ^{13}C NMR spectrum data of **7a** showed the signals of C=O, C_8 and C_2 at 162.7, 159.8 and 152.8 ppm, respectively. In the IR spectral data of **7a**, the stretching resonance peak of NH and C=O appear at 3266 and 1693 cm^{-1}. The MS spectrum of **7a** shows molecule ion peak at *m*/*z* = 364 with 7% abundance.

Table 1 Preparation of 3-Amino-2-thioxo-4-imidazolidinones **4**, Iminophosphorane **5** and 2-Arylamino-imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones **7**

Entry	Ar^1	Ar^2	Reaction Condition	Yield (%)
4a	4-$MeOC_6H_4$		r.t./30 min	94
4b	Ph		r.t./20 min	91
4c	4-ClC_6H_4		r.t./10 min	77
5a	4-$MeOC_6H_4$		r.t./6 h	78
5b	Ph		r.t./4 h	85
5c	4-ClC_6H_4		r.t./6 h	72
7a	4-$MeOC_6H_4$	4-MeC_6H_4	r.t./2 h	56
7b	4-$MeOC_6H_4$	3-MeC_6H_4	r.t./2 h	51
7c	4-$MeOC_6H_4$	Ph	r.t./1 h	48
7d	4-$MeOC_6H_4$	4-ClC_6H_4	r.t./1 h	61
7e	Ph	4-MeC_6H_4	r.t./2 h	62
7f	Ph	3-MeC_6H_4	r.t./2 h	55
7g	Ph	Ph	r.t./2 h	54
7h	Ph	4-ClC_6H_4	r.t./1 h	49
7i	Ph	4-BrC_6H_4	r.t./1 h	50
7j	4-ClC_6H_4	4-MeC_6H_4	r.t./2 h	64
7k	4-ClC_6H_4	3-MeC_6H_4	r.t./2 h	55
7l	4-ClC_6H_4	Ph	r.t./2 h	51
7m	4-ClC_6H_4	4-ClC_6H_4	r.t./1 h	58

Melting points were uncorrected. MS were measured on a Finnigan Trace MS spectrometer. IR spectra were recorded on a PE-983 infrared spectrometer as KBr pellets with absorption in cm^{-1}. NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 on a Varian Mercury 400 spectrometer and resonances are given in ppm (δ) relative to TMS. Elemental analyses were performed on a Perkin-Elmer CHN 2400 elementary analysis instrument.

Preparation of 3-Amino-2-thioxo-4-imidazolidinones 4; General Procedure

To a solution of vinyliminophosphorane **1**[15,16] (2.25 g, 5 mmol) in anhyd CH_2Cl_2 (15 mL) was added excess CS_2 (5 mL). After the reaction mixture was refluxed for 28 h, the solvent was removed under reduced pressure and Et_2O–petroleum ether (1:2, 20 mL) was added to precipitate triphenylphosphine sulfide which was removed by filtration. The filtrate was evaporated to give isothiocyanate **2**, which was used directly without further purification. To a solution of the crude **2** in CH_3CN (15 ml) was added hydrazine hydrate (0.35 g, 6 mmol, 85%) and the mixture was stirred for 10–30 min at r.t. The precipitated solid was collected and washed with water and EtOH, crystallized from CH_2Cl_2–petroleum ether to give 3-amino-2-thioxo-4-imidazolidinone **4**.

4a

Yellow solid; mp 174–176 °C.

IR (KBr): 3321, 3211 (NH), 1681 (C=O), 1595, 1258, 1143 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 12.20 (s, 1 H, NH), 7.72–6.87 (m, 4 H, ArH), 6.68 (s, 1 H, =CH), 5.20 (s, 2 H, NH_2), 3.82 (s, 3 H, OCH_3).

MS: *m*/*z* (%) = 249 (93) [M$^+$], 218 (14), 190 (25), 147 (99), 132 (100).

Anal. Calcd for $C_{11}H_{11}N_3O_2S$: C, 53.00; H, 4.45; N, 16.86. Found: C, 53.18; H, 4.55; N, 16.84.

4b

Yellow solid; mp 228–230 °C.

IR (KBr): 3316, 3288 (NH), 1711 (C=O), 1613, 1460, 1262 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 12.24 (s, 1 H, NH), 7.78–7.40 (m, 5 H, ArH), 6.64 (s, 1 H, =CH), 5.22 (s, 2 H, NH_2).

MS: *m*/*z* (%) = 219 (69) [M$^+$], 188 (11), 190 (25), 147 (99), 132 (100).

Anal. Calcd for $C_{10}H_9N_3OS$: C, 54.78; H, 4.14; N, 19.16. Found: C, 54.71; H, 4.02; N, 19.25.

4c

Yellow solid; mp 254–255 °C.

IR (KBr): 3323, 3274 (NH), 1713 (C=O), 1607, 1470, 1268 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 12.28 (s, 1 H, NH), 7.80–7.48 (m, 4 H, ArH), 6.63 (s, 1 H, =CH), 5.22 (s, 2 H, NH_2).

MS: *m*/*z* (%) = 255 (24), 253 (62) [M$^+$], 222 (10), 194 (31), 151 (88), 89 (100).

Anal. Calcd for $C_{10}H_8ClN_3OS$: C, 47.34; H, 3.18; N, 16.56. Found: C, 47.27; H, 3.22; N, 19.61.

Preparation of Iminophosphorane 5; General Procedure

To a mixture of 3-amino-2-thioxo-4-imidazolidinone **4** (8 mmol), PPh_3 (3.14 g, 12 mmol) and C_2Cl_6 (2.84 g, 12 mmol) in anhyd CH_3CN (40 mL), was added dropwise Et_3N (2.42 g, 24 mmol) at r.t. The color of the reaction mixture quickly turned red, becoming yellow after 4–6 h. The precipitate was filtered and washed with CH_3CN to give iminophosphorane **5**.

5a

Yellow solid; mp >300 °C.

IR (KBr): 3420 (NH), 1740 (C=O), 1642 (C=C), 1477, 1170 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 12.31 (s, 1 H, NH), 8.03–6.82 (m, 19 H, ArH), 6.64 (s, 1 H, =CH), 3.83 (s, 3 H, OCH_3).

MS: *m*/*z* (%) = 509 (2) [M^+], 294 (9), 277 (45), 262 (15), 183 (63), 44 (100).

Anal. Calcd for $C_{29}H_{24}N_3O_2PS$: C, 68.36; H, 4.75; N, 8.25. Found: C, 68.21; H, 4.68; N, 8.31.

5b

Yellow solid; mp 267–269 °C.

IR (KBr): 3425 (NH), 1745 (C=O), 1643 (C=C), 1475, 1170 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 12.35 (s, 1 H, NH), 8.00–7.40 (m, 20 H, ArH), 6.60 (s, 1 H, =CH).

MS: *m*/*z* (%): 479 (11) [M^+], 294 (38), 277 (100), 262 (49), 183 (91).

Anal. Calcd for $C_{28}H_{22}N_3OPS$: C, 70.13; H, 4.62; N, 8.76. Found: C, 70.01; H, 4.77; N, 8.72.

5c

Yellow solid; mp >300 °C.

IR (KBr): 3417 (NH), 1738 (C=O), 1645 (C=C), 1474, 1162 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 12.30 (s, 1 H, NH), 8.06–7.42 (m, 19 H, Ar-H), 6.63 (s, 1 H, =CH).

MS: *m*/*z* (%): 513 (3) [M^+], 294 (4), 277 (6), 201 (12), 183 (25), 77 (100).

Anal. Calcd for $C_{28}H_{21}ClN_3OPS$: C, 65.43; H, 4.12; N, 8.18. Found: C, 65.58; H, 4.03; N, 8.12.

Preparation of 2-Arylamino-imidazo[2,1-*b*]-1,3,4-thiadiazol-5(6*H*)-ones 7; General Procedure

To a solution of iminophosphorane **5** (3 mmol) in anhyd DMF (20 mL) was added aromatic isocyanate (3 mmol) at r.t. The color of the reaction mixture turned red, becoming yellow after few minutes. The yellow solution was stirred at r.t. for 1–2 h. The solution was condensed and the residue was recrystallized from CH_3CN to give **7**.

7a

Yellow crystals, mp 267–268 °C.

IR (KBr): 3266 (NH), 1693 (C=O), 1635 (C=C), 1594, 1259, 1172 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 10.46 (s, 1 H, NH), 8.21–7.03 (m, 9 H, ArH, =CH), 3.83 (s, 3 H, OCH_3), 2.28 (s, 3 H, CH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 162.7 (C=O), 161.1 (MeOC), 159.8 (C_8), 152.8 (C_2), 139.1, 138.1, 134.3, 132.1, 131.4, 129.2, 128.4, 126.1, 125.2, 119.0, 114.2 (ArC), 55.3 (OCH_3), 21.0 (CH_3).

MS: *m*/*z* (%) = 364 (7) [M^+], 336 (11), 146 (36), 132 (100).

Anal. Calcd for $C_{19}H_{16}N_4O_2S$: C, 62.62; H, 4.43; N, 15.37. Found: C, 62.55; H, 4.56; N, 15.27.

7b

Yellow crystals; mp 283–285 °C.

IR (KBr): 3273 (NH), 1691 (C=O), 1634 (C=C), 1596, 1255, 1172 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 10.44 (s, 1 H, NH), 8.19–6.90 (m, 9 H, ArH, =CH), 3.83 (s, 3 H, OCH_3), 2.28 (s, 3 H, CH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 163.0 (C=O), 161.2 (MeOC), 159.9 (C_8), 152.8 (C_2), 139.3, 137.2, 134.3, 132.1, 131.5, 129.3, 128.6, 126.5, 125.3, 119.1, 114.0 (ArC), 55.2 (OCH_3), 20.7 (CH_3).

MS: *m*/*z* (%) = 364 (52) [M^+], 336 (54), 321 (22), 234 (220), 132 (100).

Anal. Calcd for $C_{19}H_{16}N_4O_2S$: C, 62.62; H, 4.43; N, 15.37. Found: C, 62.74; H, 4.48; N, 15.31.

7c

Yellow crystals; mp 211–212 °C.

IR (KBr): 3266 (NH), 1695 (C=O), 1636 (C=C), 1595, 1254, 1170 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 10.74 (s, 1 H, NH), 8.21–6.95 (m, 10 H, ArH, =CH), 3.83 (s, 3 H, OCH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 162.7 (C=O), 161.2 (MeOC), 159.8 (C_8), 152.7 (C_2), 139.3, 138.1, 134.1, 132.0, 131.4, 129.4, 128.3, 126.3, 124.7, 118.8, 114.6 (ArC), 55.3 (OCH_3).

MS: *m*/*z* (%) = 350 (16) [M^+], 322 (18), 147 (15), 119 (100).

Anal. Calcd for $C_{18}H_{14}N_4O_2S$: C, 61.70; H, 4.03; N, 15.99. Found: C, 61.59; H, 4.21; N, 15.86.

7d

Yellow crystals; mp 233–234 °C.

IR (KBr): 3295 (NH), 1691 (C=O), 1633 (C=C), 1595, 1239, 1172 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 10.73 (s, 1 H, NH), 8.21–7.03 (m, 9 H, ArH, =CH), 3.83 (s, 3 H, OCH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 162.9 (C=O), 161.2 (MeOC), 159.8 (C_8), 152.6 (C_2), 139.2, 138.1, 134.0, 132.0, 131.5, 129.1, 128.8, 126.4, 125.4, 119.5, 114.4 (ArC), 55.4 (OCH_3).

MS: *m*/*z* (%) = 384 (7) [M^+], 356 (9), 234 (4), 185 (9), 153 (100).

Anal. Calcd for $C_{18}H_{13}ClN_4O_2S$: C, 56.18; H, 3.40; N, 14.56. Found: C, 56.05; H, 3.36; N, 14.58.

7e

Yellow crystals; mp 279–280 °C.

IR (KBr): 3281 (NH), 1696 (C=O), 1632 (C=C), 1594, 1113 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 10.54 (s, 1 H, NH), 8.22–6.91 (m, 9 H, ArH), 7.09 (s, 1 H, =CH), 2.33 (s, 3 H, CH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.0 (C=O), 159.8 (C_8), 152.7 (C_2), 141.4, 139.1, 138.6, 133.7, 132.0, 130.4, 129.2, 128.8, 125.7, 123.9, 118.5, 115.4 (Ar-C), 21.3 (CH_3).

MS: *m*/*z* (%): 334 (6) [M^+], 306 (9), 163 (11), 116 (100).

Anal. Calcd for $C_{18}H_{14}N_4OS$: C, 64.65; H, 4.22; N, 16.75. Found: C, 64.78; H, 4.17; N, 16.80.

7f

Yellow crystals; mp 270–271 °C.

IR (KBr): 3269 (NH), 1702 (C=O), 1635 (C=C), 1593, 1115 cm^{-1}.

^1H NMR (400 MHz, DMSO-d_6): δ = 10.65 (s, 1 H, NH), 8.22–7.20 (m, 9 H, ArH), 7.08 (s, 1 H, =CH), 2.29 (s, 3 H, CH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.4 (C = O), 159.9 (C_8), 152.7 (C_2), 141.6, 137.1, 133.7, 132.0, 130.5, 129.6, 128.9, 125.6, 123.9, 118.1, 114.8 (ArC), 20.5 (CH_3).

MS: *m*/*z* (%) = 334 (53) [M^+], 306 (61), 204 (22), 131 (100).

Anal. Calcd for $C_{18}H_{14}N_4OS$: C, 64.65; H, 4.22; N, 16.75. Found: C, 64.57; H, 4.12; N, 16.86.

7g
Yellow crystals; mp 277–278 °C.

IR (KBr): 3290 (NH), 1696 (C=O), 1636 (C=C), 1588, 1116 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.59 (s, 1 H, NH), 8.22–7.12 (m, 10 H, ArH), 7.09 (s, 1 H, =CH).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.1 (C=O), 159.8 (C_8), 152.4 (C_2), 141.8, 139.2, 138.7, 133.5, 132.2, 130.2, 129.1, 128.8, 124.8, 122.6, 118.0, 115.1 (ArC).

MS: *m*/*z* (%) = 320 (72) [M^+], 292 (77), 204 (6), 118 (100).

Anal. Calcd for $C_{17}H_{12}N_4OS$: C, 63.73; H, 3.78; N, 17.49. Found: C, 63.78; H, 3.71; N, 17.63.

7h
Yellow crystals, mp 254-256 °C.

IR (KBr): 3269 (NH), 1694 (C=O), 1659 (C=C), 1581, 1114 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.73 (s, 1 H, NH), 8.22–7.35 (m, 9 H, ArH), 7.10 (s, 1 H, =CH).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.4 (C=O), 159.9 (C_8), 152.6 (C_2), 141.2, 139.6, 138.5, 133.7, 132.3, 130.3, 129.8, 127.8, 125.3, 123.4, 118.0, 115.2 (ArC).

MS: *m*/*z* (%) = 354 (5) [M^+], 326 (8), 152 (52), 116 (100).

Anal. Calcd for $C_{17}H_{11}ClN_4OS$: C, 57.55; H, 3.12; N, 15.79. Found: C, 57.41; H, 3.06; N, 15.80.

7i
Yellow crystals; mp 251–252 °C.

IR (KBr): 3270 (NH), 1692 (C=O), 1632 (C=C), 1593, 1117 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.73 (s, 1 H, NH), 8.22–7.43 (m, 9 H, ArH), 7.10 (s, 1 H, =CH).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 164.7 (C=O), 159.8 (C_8), 152.6 (C_2), 141.2, 138.9, 138.5, 133.6, 132.0, 130.4, 129.0, 128.7, 125.9, 123.7, 120.2, 114.6 (ArC).

MS: *m*/*z* (%) = 400 (25) [M^+], 398 (24), 372 (23), 370 (23), 196 (47), 116 (100).

Anal. Calcd for $C_{17}H_{11}BrN_4OS$: C, 51.14; H, 2.78; N, 14.03. Found: C, 51.23; H, 2.64; N, 14.07.

7j
Yellow crystals; mp 246–247 °C.

IR (KBr): 3291 (NH), 1697 (C=O), 1638 (C=C), 1595, 1243 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.50 (s, 1 H, NH), 8.25–7.20 (m, 8 H, ArH), 7.10 (s, 1 H, =CH), 2.28 (s, 3 H, CH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.3 (C=O), 159.8 (C_8), 152.7 (C_2), 141.9, 139.9, 138.1, 133.4, 132.7, 130.3, 129.2, 128.7, 125.7, 123.8, 119.5, 114.3 (ArC), 21.4 (CH_3).

MS: *m*/*z* (%) = 370 (9), 368 (24) [M^+], 340 (31), 253 (14), 132 (100).

Anal. Calcd for $C_{18}H_{13}ClN_4OS$: C, 58.62; H, 3.55; N, 15.19. Found: C, 58.48; H, 3.65; N, 15.13.

7k
Yellow crystals; mp 232–234 °C.

IR (KBr): 3274 (NH), 1700 (C=O), 1636 (C=C), 1585, 1260 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.53 (s, 1 H, NH), 8.26–6.91 (m, 8 H, ArH), 7.10 (s, 1 H, =CH), 2.33 (s, 3 H, CH_3).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.7 (C=O), 159.9 (C_8), 152.5 (C_2), 141.7, 139.6, 138.0, 133.4, 132.7, 130.1, 129.4, 128.9, 125.7, 123.3, 119.8, 114.0 (ArC), 21.9 (CH_3).

MS: *m*/*z* (%) = 368 (6) [M^+], 340 (11), 253 (6), 150 (100).

Anal. Calcd for $C_{18}H_{13}ClN_4OS$: C, 58.62; H, 3.55; N, 15.19. Found: C, 58.52; H, 3.39; N, 15.29.

7l
Yellow crystals; mp 242–244 °C.

IR (KBr): 3265 (NH), 1694 (C=O), 1638 (C=C), 1596, 1242 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.99 (s, 1 H, NH), 8.26–7.38 (m, 9 H, ArH), 7.09 (s, 1 H, =CH).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.8 (C=O), 159.8 (C_8), 152.8 (C_2), 142.0, 139.9, 135.0, 133.6, 132.7, 130.3, 129.3, 128.7, 125.8, 123.6, 118.3, 114.0 (ArC).

MS: *m*/*z* (%): 356 (22), 354 (63) [M^+], 326 (68), 150 (46), 118 (100).

Anal. Calcd for $C_{17}H_{11}ClN_4OS$: C, 57.55; H, 3.12; N, 15.79. Found: C, 57.48; H, 3.25; N, 15.98.

7m
Yellow crystals; mp 235–236 °C.

IR (KBr): 3270 (NH), 1693 (C=O), 1631 (C=C), 1595, 1239 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 10.77 (s, 1 H, NH), 8.25–7.29 (m, 8 H, ArH), 7.11 (s, 1 H, =CH).

^{13}C NMR (400 MHz, DMSO-d_6): δ = 165.9 (C=O), 159.8 (C_8), 152.9 (C_2), 142.4, 139.6, 135.4, 133.5, 132.7, 130.7, 129.5, 128.5, 125.8, 123.8, 118.4, 114.5 (ArC).

MS: *m*/*z* (%) = 388 (6) [M^+], 360 (10), 185 (12), 153 (100).

Anal. Calcd for $C_{17}H_{10}Cl_2N_4OS$: C, 52.46; H, 2.59; N, 14.39. Found: C, 52.31; H, 2.44; N, 14.57.

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