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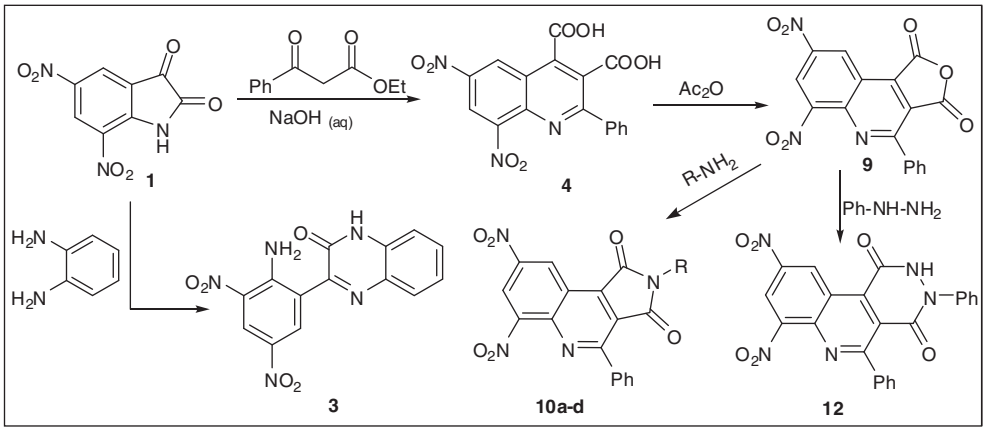
Received September 22, 2011
DOI 10.1002/jhet.1607
Published online 31 October 2013 in Wiley Online Library (wileyonlinelibrary.com).



2-(2-Amino-3,5-dinitrophenyl)-2-oxoacetic acid (**2**) was obtained from hydrolysis of 5,7-dinitroisatin (**1**) in alkaline media. A novel quinoxaline derivative (**3**) was synthesized from the reaction of the same compound (**1**) with *o*-phenylenediamine. Reacting **2** with ethyl 3-oxo-3-phenylpropanoate yields 6,8-dinitro-2-phenylquinoline-3,4-dicarboxylic acid (**4**). Then, **4** was converted into new quinoline-diacylchloride, quinoline-ester, quinoline-dicarboxamide, pyridazine, and pyrroledione derivatives (**5**, **6a–d**, **7a–d**, **8**, **9**, **10a–d**, **11a–b**, **12**) with $SOCl_2$, alcohols, amines, and hydrazines, respectively. The structures of synthesized compounds were clarified by ^{1}H NMR, ^{13}C NMR, IR, mass and elemental analysis methods.

J. Heterocyclic Chem., **51**, 224 (2014).

INTRODUCTION

Quinoxaline-2-one ring derivatives show various biological activities [1–4]. The heterocyclic quinoline ring building block of many natural compounds is widely used in medicinal chemistry. Substituted quinolines possess diverse biological activities including antibacterial [5,6], antifungal [7,8], antiamoebic [9,10], antileishmanial [11,12], antimalarial [13,14], and antitumor [15,16] activities.

The synthesis and some biological activities of various pyrroloquinoline (general structure **A**) and quinoline dicarboxylic acid (general structure **B**) derivatives have also been reported in the literature [17–19]. Among the quinoline derivatives, pyrrolo[3,4-*c*]quinolines constitute an interesting group of physiologically active molecules. For instance, pyrrolo[3,4-*c*]quinolines were described as potential antimalarial [20], cytotoxic agents [21], and caspase-3 inhibitors [22–24] (Fig. 1).

In the current report, we aimed to show synthesis, characterization of new quinoline, quinoxaline, pyrrole, and pyridazine derivatives as candidate drug molecules. Hence, we intended to contribute to the heterocyclic chemistry by showing synthetic routes to excellent yield percentages. To achieve that goal, first, hydrolysis reaction was performed on **1** in alkali medium. In this reaction, corresponding dicarboxylic acid derivative (**2**) was obtained via the cleavage of isatin ring (Scheme 1).

A new quinoxaline-2-one (**3**) derivative was synthesized from the reaction of **1** with *o*-phenylenediamine in THF at 25°C (Scheme 2). The interaction of **1** with ethyl 3-oxo-3-phenylpropanoate under the Pfitzinger reaction [25] conditions forms the corresponding quinoline dicarboxylic acid derivative (**4**) (Scheme 2). The carbonyl groups of **4** were activated by treating with $SOCl_2$ (**5**). In addition, the compound **4** was simply converted to the new ester derivatives (**6a–d**) by reacting with various alcohols in which the catalyst was H_2SO_4. Novel amide derivatives were synthesized (**7a–d**) by the reaction of **5** with various aryl and alkyl amines.

The interaction of **6a** and **6d** with hydrazine hydrate yielded the same product (**8**) (Scheme 2).

A new anhydride derivative (**9**) was synthesized from the reaction of **4** with acetic anhydride. Imide derivatives including the quinoline rings (**10a–d**) were obtained from the reaction of **9** with various alkyl and aryl amines. The reaction of the same compound (**9**) with aryl diamines yielded symmetric imide derivatives (**11a–b**) (Scheme 3).

N-Aminopyrrole derivative (**10e**) was obtained from the reaction of **9** with hydrazine hydrate in benzene, whereas the reaction of **9** with phenylhydrazine gave a pyridazine derivative (**12**) under the same conditions (Scheme 4).

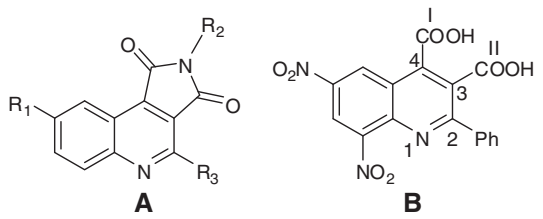
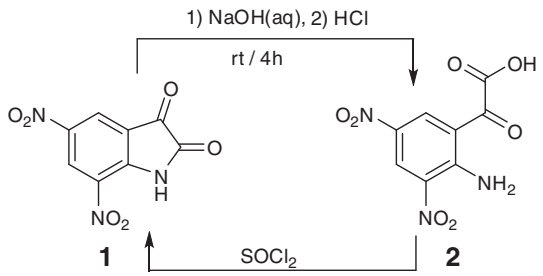


Figure 1. Structures of pyrrolo[3,4-*c*]quinoline and quinoline-3,4-dicarboxylic acid.

Scheme 1. The cleavage of isatin ring.



RESULTS AND DISCUSSION

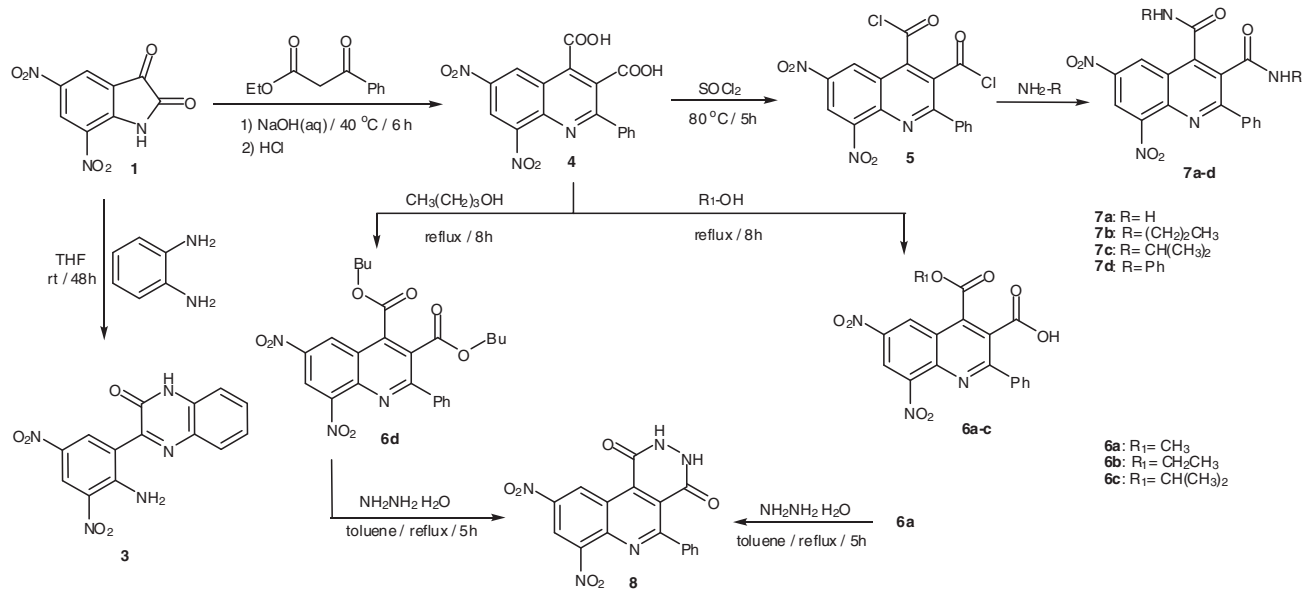
In the current study, further stage reaction of indole-2,3-dione (isatin) was performed. Thus, novel derivatives of quinoxaline, quinoline, pyridazinoquinoline, and pyrroloquinoline ring systems were systematically synthesized. The structures of the synthesized molecules were characterized by different techniques. ^{1}H NMR and ^{13}C NMR spectroscopy were employed to elucidate the chemical structures, whereas FTIR was applied for determining the frequencies of functional groups such as C═O and C═N. Molecular weight of some compounds was determined with LC/MS analysis. Elemental analysis was useful in determining variation of the fractions of elements that form the compounds.

Compound **2** was obtained from alkaline hydrolysis of 5,7-dinitroindole-2,3-dione (**1**). This compound (**2**) converted back to **1** after reacting with $SOCl_2$. In this reaction, first, acyl chloride of **2** was formed. Second, amino group of the same compound attacked the acyl carbonyl yielding back the starting compound (**1**) (Scheme 1).

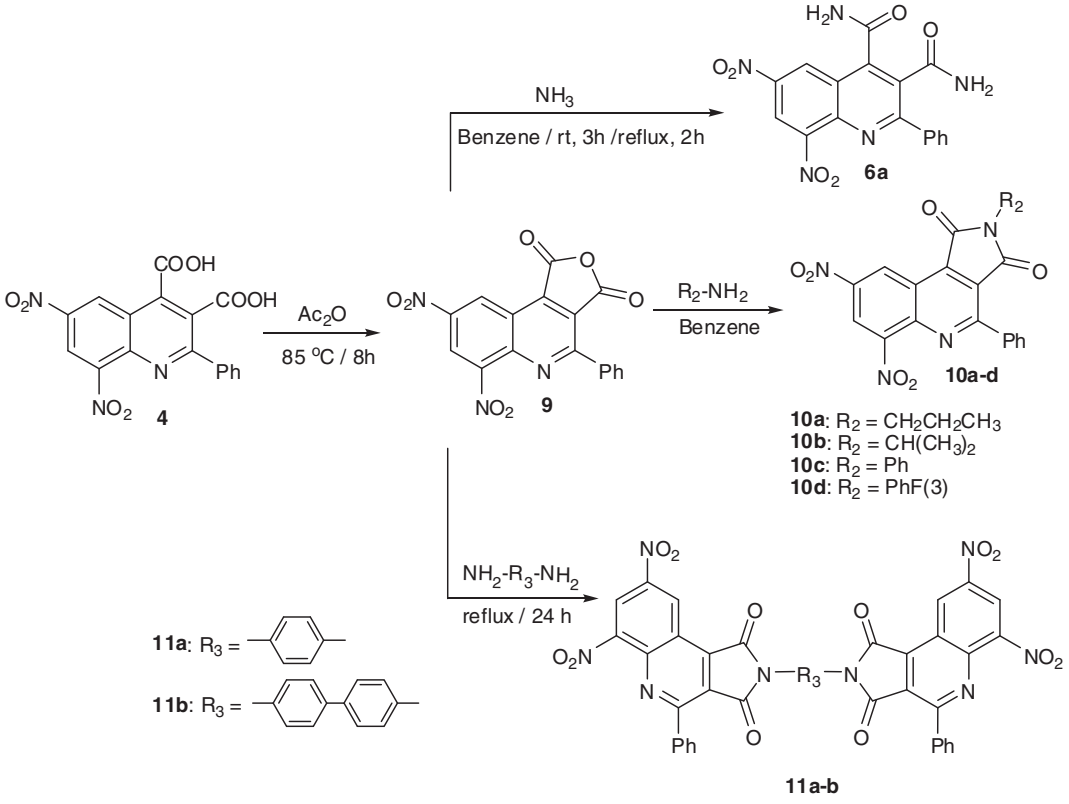
On the other hand, one of the amino groups of *o*-phenylenediamine attack the carbonyl group of **1** at the C-3 position. Elimination of one mol water formed an intermediate compound. Then, other amino group attack the carbonyl group at the C-2 position. Finally, rearrangement of the molecule led to novel indolo-[3,2-*b*]-quinoxaline derivative (**3**) (Figure 2).

The synthesis of β-dicarboxylic acid derivative (**4**) was performed under the Pfitzinger reaction conditions. In this reaction, first, **1** was hydrolyzed in alkaline media. Second, amino group of the hydrolysis product formed a Schiff

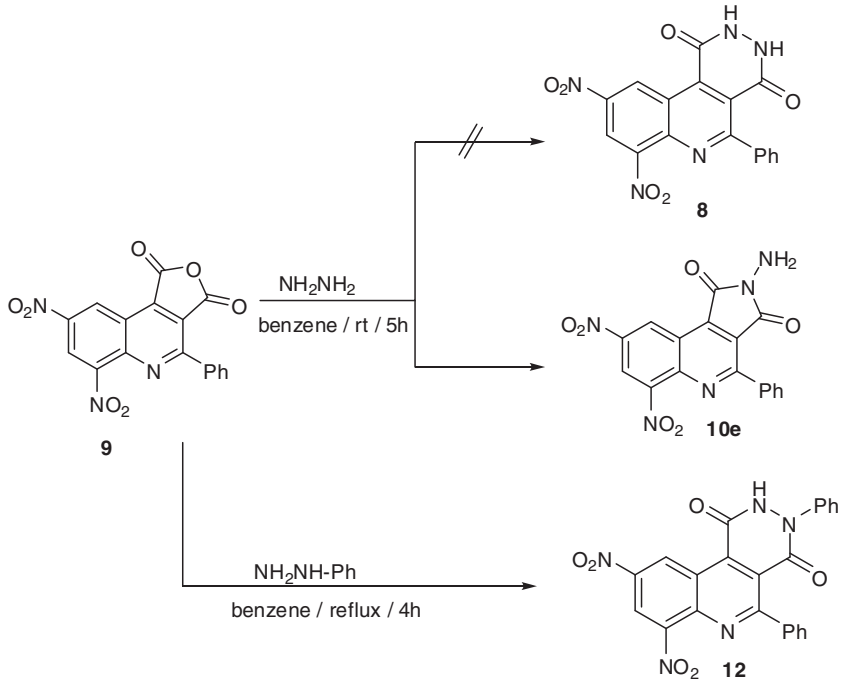
Scheme 2. Synthetic route of novel quinoline-3,4-dicarboxylic acid and quinoxaline derivatives.



Scheme 3. Synthesis of various pyrrolo[3,4-*c*]quinoline derivatives.



Scheme 4. Synthesis of pyrrolo[3,4-*c*]quinoline and pyridazino[4,5-*c*]quinoline derivatives.



base by the reaction with ketone carbonyl of ethyl benzoyl acetate. Then, the rearranged Schiff base turned into an enaminone derivative. And then, sodium salt of **4** formed after the elimination of water and cyclocondensation reaction. Finally, this salt turned into a dicarboxlic acid (**4**) after the addition of HCl (Fig. 3).

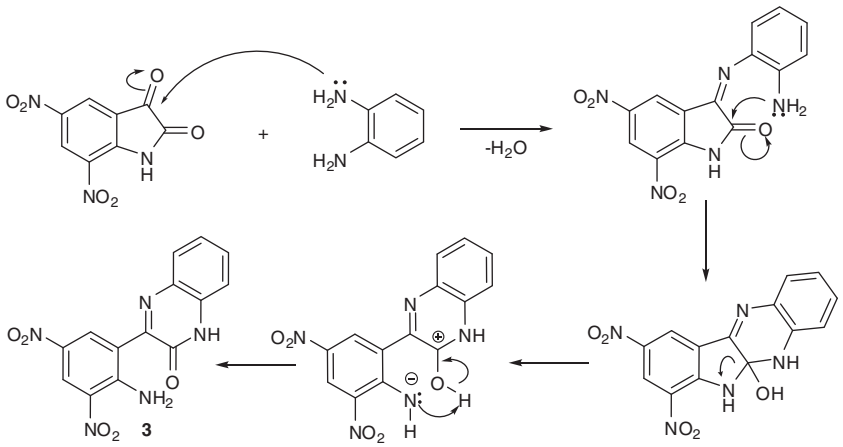


Figure 2. The reaction mechanism for quinoxaline-2-one derivative.

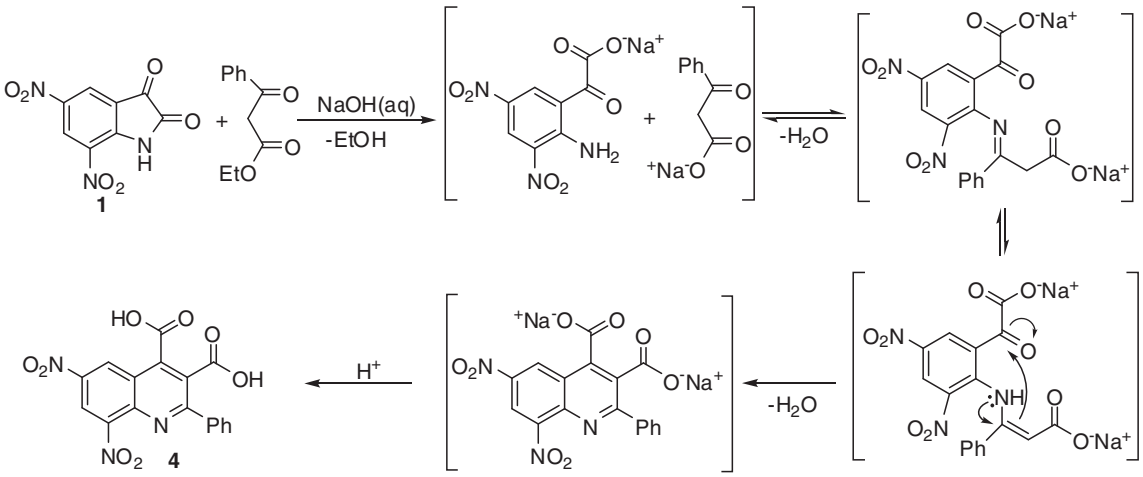


Figure 3. The reaction mechanism for quinoline-3,4-dicarboxylic acid synthesized via Pfitzinger reaction.

Interestingly, it was observed that in the reaction of **4** with alcohols having lower molecular weight and lower boiling point (such as methanol, ethanol, and 2-propanol) with H_2SO_4 catalyst, only one of the carboxyl group yielded an ester (**6a–c**) molecule. However, after the reaction of the same compound (**4**) with butanol having higher molecular weight and higher boiling point, both carboxyl groups have given esters (**6d**).

In mono esterification reactions of dicarboxylic acid (general structure **B**) (Fig. 1), it was considered that esterification occurred at the carboxyl group adjacent to the C-4 of quinoline ring. Because of the mesomeric effect of the phenyl group of **4** substituting to the C-2 position, the C-4 position in quinoline ring became less electronegative. Consequently, the carbonyl group next to the C-4 position (**I**) also turned out to be less electronegative. Thus, this carbonyl group (**I**) had higher activity for the possible nucleophilic attacks compared with the other carboxyl group (**II**) (Fig. 1). Because alcohol molecules are more nucleophilic, the alcohol molecules attack the **I** position of **4** first. Consequently, **6a–c** compounds were formed including an ester in **I** position and also a carboxylic acid in **II** position (Scheme 3).

The spectroscopic data depicted that same product (**6a**) was obtained by the reaction of both **5** and **9** with NH_3 (see Experimental).

An anhydride derivative (**9**) was formed in high yield (92%) and purity from intramolecular cyclocondensation of **4** in acetic anhydride at 85°C. The structure of the product was confirmed by spectral data. Characteristic absorption bands were observed at 3100 cm^{-1} (aromatic CH), 1788 and 1706 cm^{-1} (anhydride C═O), and 1618–1455 cm^{-1} (aromatic C═C and C═N). In ^1H NMR spectrum of **9**, the peak at 12.05 ppm arising from the COOH group was not observed. In ^{13}C NMR spectrum, the peaks at 169.64 and 165.96 ppm indicated the existence of two C═O groups having different chemical environments. The LC/MS results have confirmed the molecular weight. LC-MSD $m/z = 365.9$ $[M+H]^+$ *Anal.* Calcd for, $C_{17}H_7N_3O_7$: 365.25 g/mol.

An *N*-amino imide derivative (**10e**) was obtained from the reaction of **9** with hydrazine hydrate [26] rather than the expected pyridazine dione ring (**8**). The spectral data of the synthetic molecule were consistent with the assigned structure. In the ^{1}H NMR spectrum of compound **10e**, two exchangeable protons appeared as a broad singlet shifted to 4.59 ppm that was in agreement with N-NH_2. As expected, from the reaction of **9** with phenylhydrazine gave a pyridazine derivative (**12**) [27]. In the ^{1}H NMR spectrum of **12**, an exchangeable proton (CO-NH-N-) shifted to 11.78 ppm confirmed the conversion of the structure to a pyridazinedione ring.

EXPERIMENTAL

Chemical compounds used in this research were analytically pure, and the solvents were purified using appropriate purifying agents and distillation. All reactions were monitored by analytical thin-layer chromatography (TLC) (E. Merck Co., Darmstadt, Germany) on 0.25 mm precoated Kieselgel 60 F 254 plates (Merck); compounds were visualized by Camag TLC devices UV (254 and 366 nm) Barnstead Electrothermal 9200 (Camag, Upland, CA) capillary melting point apparatus (Electrothermal Co, Essex, UK) and remained uncorrected. The IR data (Agilent Technologies Inc., Santa Clara, CA) were recorded on a Bruker Vertex 70 Sample compartment spectrometer using potassium bromide pellets. ^{1}H NMR and ^{13}C NMR spectra were recorded on Varian spectrometers (400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) in DMSO-d_6 using TMS as an internal standard. LC/MS spectra were recorded on an Agilent 1100 LC-MSD mass spectrometer operating at 55–100 eV (Agilent Technologies Inc., Santa Clara, CA, USA). Elemental analyses were carried out on a Leco CHNS-932 instrument (LECO Corporation, Saint Joseph, MI). The starting compound (**1**) was synthesized from isatin as described in reference [28] and crystallized from xylene in bright yellow leaflets.

2-(2-Amino-3,5-dinitrophenyl)-2-oxoacetic acid (2). Compound **1** (1 g, 4.2 mmol) was added at 25°C to a stirred solution of NaOH (0.5 g, 12.5 mmol) in distilled water (80 mL). The mixture was stirred at 25°C for 4 h. The obtained solution was cooled to 0°C and acidified with 2N HCl till reaching pH 1. The resulting mixture was kept at 5°C overnight. Then, the precipitate was filtered off and washed with water (3 × 15 mL). The product was crystallized from xylene and dried in vacuo at 70°C. Yield: 0.75 g (70%); mp 158–159°C; IR (ν, cm^{-1}): 3421 (NH), 3600–2600 (COOH), 3089 (Ar CH), 1748 (C═O, ketone), 1667 (C═O, acid), 1595–1433 (aromatic C═C), 1523 and 1337 (NO_2 asym. and sym.); ^{1}H NMR (400 MHz, DMSO- d_6) δ (ppm): 9.25 (br, s, 3H, NH_2 and COOH), 9.01 (d, J = 2.56 Hz, 1H, H-4), 8.73 (d, J = 2.56 Hz, 1H, H-6); ^{13}C NMR (100 MHz, DMSO- d_6) δ (ppm): 189.60 (C═O, ketone), 164.95 (C═O, acid), 150.20 (C-NH_2), 136.34, 134.34, 133.29, 129.28, 116.28; LC-MSD (API-ES (−) 70 eV) *m/z*: 255.0 $[M+H]^+$; *Anal*. Calcd for $C_8H_5N_3O_7$: C, 37.66; H, 1.98; N, 16.47. Found: C, 36.51; H, 2.03; N, 16.23.

3-(2-Amino-3,5-dinitrophenyl)quinoxalin-2(1H)-one (3). A solution of **1** (0.7 g, 3 mmol) in THF (50 mL) was added at room temperature to a stirred solution of *o*-phenylenediamine (0.32 g, 3 mmol) in THF (20 mL). The mixture was stirred at 25°C for 48 h. The formed precipitate was filtered off, washed with ether (3 × 15 mL). The product was crystallized from DMF and dried in vacuo at 70°C. Yield: 0.88 g (91%); mp over 300°C; IR (ν, cm^{-1}): 3466–3390 (NH), 3103 (Ar CH), 1656 (C═O, amide), 1617–1581 (Ar C═C and C═N), 1526 (NO_2 asym.), 1302 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 8.93 (d, J = 2.92 Hz, 1H, H-4′) 8.92 (br, s, 1H, NH) 8.74 (br, s, 2H, NH_2), 7.82 (d, J = 7.68 Hz, 1H, H-6′) 7.57 (t, J = 7.31 Hz, 1H, H-8) 7.36 (m, 3H, H-5, H-6 and H-7); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 155.09 (C-3, bicyclic ring), 154.40 (C═O), 148.93 (C-NH_2), 134.59, 133.37, 132.19, 132.00, 131.78, 131.14, 129.39, 124.84, 124.57, 124.04, 115.98; *Anal*. Calcd for $C_{14}H_9N_5O_5$: C, 51.38; H, 2.77; N, 21.40. Found: C, 50.42; H, 2.85; N, 21.35.

6,8-Dinitro-2-phenylquinoline-3,4-dicarboxylic acid (4). Compound **1** (4 g, 16.9 mmol) was added at 25°C to a stirred solution of NaOH (2.1 g, 52.5 mmol) in water (250 mL). Ethyl benzoylacetate (3.5 mL, 20.3 mmol) was added. The resulting mixture was stirred and heated in an oil bath (40°C) for 6 h. The obtained solution was cooled to 0°C and acidified with 2N HCl till reaching pH 1. Then, the mixture was kept at 0°C overnight; the precipitate was filtered off and washed with ether (3 × 15 mL). The product was crystallized from methanol and dried in vacuo at 70°C. Yield: 1.29 g (20%); mp 289–291°C; IR (ν, cm^{-1}): 3416–2459 (COOH), 3084 (Ar CH), 1740 and 1676 (C═O, acid), 1630–1453 (Ar C═C and C═N), 1569 (NO_2 asym.), 1343 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 12.05 (br, s, 2H, 2COOH), 9.21 (d, J = 2.56 Hz, 1H, H-5,), 9.07 (d, J = 2.56 Hz, 1H, H-7), 7.86–7.49 (m, 5H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.71 (2C═O), 159.40 (quinoline, C-2), 141.22, 137.67, 136.28, 136.12, 135.96, 134.08, 134.02, 129.47, 129.23, 128.11, 123.48, 118.41; LC-MSD (API-ES (−) 70 eV) *m/z*: 383.0 $[M+H]^+$; *Anal*. Calcd for $C_{17}H_9N_3O_8$: C, 53.27; H, 2.37; N, 10.96. Found: C, 52.42; H, 2.39; N, 10.99.

6,8-Dinitro-2-phenylquinoline-3,4-dicarbonyl dichloride (5). A mixture of **4** (0.383 g, 1 mmol) and $SOCl_2$ (95%; 5 mL) was heated in an oil bath (80°C) for 5 h. The solvents were removed on a rotary evaporator at 50°C. The residue was washed with ether (3 × 15 mL). The product was crystallized from toluene and dried in vacuo at 70°C. Yield: 0.36 g (85%); mp 246–248°C; IR (ν, cm^{-1}): 3082 (Ar CH), 1783 and 1719 (C═O), 1615–1463 (aromatic C═C and C═N), 1550 (NO_2 asym.), 1357 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.39 (d, J = 2.56 Hz, 1H, H-5), 9.11 (d, J = 2.56 Hz, 1H, H-7), 7.79–7.48 (m, 5H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.29 (2C═O), 155.59 (quinoline, C-2), 145.00, 141.62, 138.15, 135.72, 134.87, 132.09, 131.38, 129.34, 127.36, 125.75, 124.33, 116.47; *Anal*. Calcd for $C_{17}H_7Cl_2N_3O_6$: C, 48.60; H, 1.68; N, 10.00. Found: C, 47.98; H, 1.85; N, 10.02.

4-(Methoxycarbonyl)-6,8-dinitro-2-phenylquinoline-3-carboxylic acid (6a). H_2SO_4 (95–97%, 0.5 mL) was added to a solution of **4** (0.4 g, 1 mmol) in methanol (40 mL) at 25°C, and the mixture was stirred and heated to reflux for 8 h. The resulting mixture was kept at 25°C overnight. Then, the precipitate was filtered off, washed with ether (3 × 15 mL). The product was recrystallized from methanol and dried in vacuo at 70°C. Yield: 0.36 g (86%); mp 228–230°C; IR (ν, cm^{-1}): 3550–2521 (COOH), 3109 (Ar CH), 2965 (aliphatic CH), 1735 (C═O, ester), 1675 (C═O, acid), 1620–1451 (Ar C═N and C═C), 1544 (NO_2 asym.), 1340 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 12.21 (br, s, 1H, COOH), 9.07 (br, s, 2H, H-5 and H-7), 7.91–7.55 (m, 5H, other ArH), 3.63 (s, 3H, OCH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 192.31 (C═O, acid), 164.12 (C═O, ester), 159.74 (quinoline, C-2), 141.23, 138.88, 137.69, 136.06, 135.90, 135.08, 129.64, 128.53, 123.59, 118.50, 54.08 (OCH_3); *Anal*. Calcd for $C_{18}H_{11}N_3O_8$: C, 54.42; H, 2.79; N, 10.58. Found: C, 53.62; H, 2.86; N, 10.59.

4-(Ethoxycarbonyl)-6,8-dinitro-2-phenylquinoline-3-carboxylic acid (6b). H_2SO_4 (95–97%, 0.5 mL) was added to a solution of **4** (0.4 g, 1 mmol) in ethanol (60 mL) at 25°C, and the mixture was stirred and heated to reflux for 8 h. The resulting mixture was kept at 25°C overnight; the precipitate was filtered off and washed with ether (3 × 15 mL). The product was recrystallized from ethanol and dried in vacuo at 70°C. Yield: 0.36 g (84%); mp 214–216°C; IR (ν, cm^{-1}): 3417–2511 (COOH), 3123 (Ar CH), 2989 (aliphatic CH), 1728 (C═O, ester), 1690 (C═O, acid), 1621–1449 (Ar C═N and C═C), 1550 (NO_2 asym.), 1338 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 12.20 (br, s, 1H, COOH), 9.11 (d, J = 2.19 Hz, 1H, H-5), 9.07 (d, J = 2.56 Hz, 1H, H-7), 7.92–7.55 (m, 5H, other ArH), 4.17 (q, J = 7.10 Hz, 2H, OCH_2), 0.89 (t, J = 7.32 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 192.31 (C═O, acid), 163.53 (C═O, ester), 159.81 (quinoline, C-2), 141.17, 138.66, 137.65, 136.13, 135.12, 129.77, 129.61, 128.45, 123.51, 118.53, 63.63 (OCH_2), 13.42 (CH_3); *Anal*. Calcd for $C_{13}H_{13}N_3O_8$: C, 55.48; H, 3.19; N, 10.22. Found: C, 55.17; H, 3.21; N, 10.09.

4-(Isopropoxycarbonyl)-6,8-dinitro-2-phenylquinoline-3-carboxylic acid (6c). H_2SO_4 (95–97%, 0.5 mL) was added to a solution of **4** (0.4 g, 1 mmol) in isopropanol (80 mL) at 25°C, and the mixture was stirred and heated to reflux for 8 h. The resulting mixture was kept at 25°C overnight. Then, the precipitate was filtered off and washed with ether (3 × 15 mL). The product was recrystallized from isopropanol and dried in vacuo at 70°C. Yield: 0.27 g (62%); mp 232–234°C; IR (ν, cm^{-1}): 3415–2363 (COOH), 3123 (Ar CH), 2989 (aliphatic CH), 1721 (C═O, ester), 1692 (C═O, acid), 1621–1449 (Ar C═N and C═C), 1547 (NO_2 asym.), 1341 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 12.19 (br, s, 1H, COOH), 9.11 (d, J = 2.56 Hz, 1H, H-5), 9.07 (d, J = 2.56 Hz, 1H, H-7), 7.94–7.56 (m, 5H, other ArH), 5.07 (heptet, J = 6.22 Hz, 1H, OCH), 0.95 (d, J = 6.22 Hz, 6H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 192.29 (C═O, acid), 162.97 (C═O, ester), 159.87 (quinoline, C-2), 141.19, 138.73, 137.68, 136.22, 135.14, 129.89, 129.59, 128.32, 123.46, 118.55, 72.22 (OCH), 21.13 (CH_3); LC-MSD (API-ES (+) 55 eV) *m/z*: 426.0 $[M+H]^+$; *Anal*. Calcd for $C_{20}H_{15}N_3O_8$: C, 56.47; H, 3.55; N, 9.88. Found: C, 56.31; H, 3.62; N, 9.58.

Dibutyl 6,8-dinitro-2-phenylquinoline-3,4-dicarboxylate (6d). H_2SO_4 (95–97%, 0.5 mL) was added to a solution of **4** (0.4 g, 1 mmol) in *n*-butanol (90 mL) at 25°C, and the mixture was stirred and heated to reflux for 8 h. The resulting mixture was kept at 25°C overnight. Then, the precipitate was filtered off and washed with ether (3 × 15 mL). The product was recrystallized from *n*-butanol and dried in vacuo at 70°C. Yield: 0.35 g (67%); mp 159–161°C; IR (ν, cm^{-1}): 3112 (Ar CH), 2966 (aliphatic CH), 1725 (C═O, ester), 1621–1453 (Ar C═N and C═C), 1548 (NO_2 asym.), 1341 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.09 (d, J = 2.56 Hz, 1H, H-5), 9.07 (d, J = 2.56 Hz, 1H, H-7), 7.93–7.55 (m, 5H, other ArH), 4.10 (t, J = 6.22 Hz, 4H, OCH_2), 1.22 (pentet, J = 6.95 Hz, 4H, $2OCH_2\underline{CH_2}CH_2$), 0.95 (hextet, J = 7.32 Hz, 4H, $2CH_2\underline{CH_2}CH_3$), 0.63 (t, J = 7.32 Hz, 6H, $2CH_3$); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 163.73 (C═O, ester), 159.80 (quinoline, C-2), 141.17, 138.80, 137.66, 136.20, 136.10, 135.98, 135.12, 129.82, 129.57, 128.49, 123.54, 118.56, 67.40 ($O\underline{CH_2}$), 29.92 ($OCH_2\underline{CH_2}$), 19.04 ($\underline{CH_2}CH_3$), 14.01 (CH_3); LC-MSD (API-ES (+) 70 eV) *m/z*: 496.0 $[M+H]^+$; *Anal*. Calcd for $C_{25}H_{25}N_3O_8$: C, 60.60; H, 5.09; N, 8.48. Found: C, 59.69; H, 5.15; N, 8.51.

6,8-Dinitro-2-phenylquinoline-3,4-dicarboxamide (7a). Method A. A mixture of **5** (0.36 g, 0.86 mmol) and THF (20 mL) was cooled to 0°C. The obtained solution was slowly added to ammonium hydroxide solution (0.25 mL, 3.44 mmol) at 0°C, stirred, and kept at this temperature for 1 h. The solvents were removed on a rotary evaporator at 50°C. The residue was washed with water (3 × 20 mL) and ether (3 × 15 mL). The product was crystallized from methanol and dried in vacuo at 70°C. Yield: 0.3 g (94%).

Method B. Triethylamine (0.1 mL, 0.7 mmol) and ammonium hydroxide solution (0.25 mL, 3.44 mmol) were added to a solution of **9** (0.5 g, 1.4 mmol) in benzene (70 mL) at room temperature, and the resulting mixture was stirred for 3 h. The reaction mixture was continued and heated to reflux for an additional 2 h. The formed precipitate was filtered while it was still hot and washed with ether (3 × 15 mL). The product was crystallized from ethanol and dried in vacuo at 70°C. Yield: 0.31 g (60%); mp 280–282°C; IR (ν, cm^{-1}): 3279 (NH), 3078 (Ar CH), 1677 (C═O, amide), 1609–1454 (aromatic C═C and C═N), 1548 (NO_2 asym.), 1344 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 10.01 (s, 2H, $CONH_2$) 9.82 (d, J = 2.56 Hz, 1H, H-5), 9.04 (d, J = 2.56 Hz, 1H, H-7), 7.60–7.33 (m, 5H, other ArH), 7.15 (s, 2H, $CONH_2$); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 167.05 (2C═O, amide), 156.44 (quinoline, C-2), 143.94, 141.33, 138.68, 138.20, 135.91, 134.84, 128.99, 128.68, 126.92, 126.12, 123.17, 117.78; LC-MSD (API-ES (−) 70 eV) *m/z*: 381.0 $[M+H]^+$; *Anal*. Calcd for $C_{17}H_{11}N_5O_6$: C, 53.55; H, 2.91; N, 18.37. Found: C, 52.75; H, 2.98; N, 18.38.

6,8-Dinitro-2-phenyl-N^3,N^4-dipropylquinoline-3,4-dicarboxamide (7b). *n*-Propylamine (0.4 mL, 4.8 mmol) was added to a solution of **5** (0.5 g, 1.2 mmol) in toluene (60 mL) at 25°C. The mixture was stirred and heated to reflux for 5 h. The reaction mixture was filtered while it was still hot. The obtained solution was kept at 25°C overnight. The formed precipitate was filtered off, washed with water (3 × 20 mL) and ether (3 × 15mL). The product was recrystallized from toluene and dried in vacuo at 70°C. Yield: 0.4 g (72%); mp 254–256°C; IR (ν, cm^{-1}): 3291 (NH), 3094 (Ar CH), 2968 (aliphatic CH), 1672 (C═O, amide), 1612–1451 (Ar C═N and C═C), 1551 (NO_2 asym.), 1342 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.83 (d, J = 2.56 Hz, 1H, H-5), 9.04 (d, J = 2.56 Hz, 1H, H-7), 7.46 (br, s, 2H, 2CONH) 7.32 (m, 5H, other ArH), 3.29 (s, 4H, $2N\underline{CH_2}$), 1.39 (m, 4H, $2CH_2$), 0.74 (s, 6H, $2CH_3$); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.24 (2C═O), 156.12 (quinoline, C-2), 142.70, 141.35, 138.07, 136.88, 136.22, 129.27, 128.98, 126.89, 126.24, 123.23, 117.53, 41.39 (NCH_2), 21.89 (CH_2), 12.15 (CH_3); *Anal*. Calcd for $C_{23}H_{23}N_5O_6$: C, 59.35; H, 4.98; N, 15.05. Found: C, 58.85; H, 5.02; N, 15.09.

N^3,N^4-diisopropyl-6,8-dinitro-2-phenylquinoline-3,4-dicarboxamide (7c). A mixture of **5** (0.55 g, 1.3 mmol) and THF (60 mL) was cooled to 0°C. The obtained solution was slowly added into isopropylamine (0.45 mL, 5.2 mmol) at 0°C, and the resulting mixture was stirred for 30 min. The reaction mixture was continued and heated to reflux for an additional 4 h. The solvents were removed on a rotary evaporator at 50°C. The residue was washed with water (3 × 20 mL) and ether (3 × 15 mL). The product was crystallized from a chloroform–hexane mixture and dried in vacuo at 70°C. Yield: 0.37 g (61%); mp 154–156°C; IR (ν, cm^{-1}): 3392 (NH), 3062 (Ar CH), 2985 (aliphatic CH), 1678 (C═O, amide), 1633–1422 (Ar C═N and C═C), 1545 (NO_2 asym.), 1334 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.54 (d, J = 2.56 Hz, 1H, H-5), 8.57 (d, J = 2.56 Hz, 1H, H-7), 7.89 (br, s, 2H, 2CONH), 7.40–6.80 (m, 5H, other ArH), 3.41 (m, 2H, 2CH), 1.11 (d, J = 5.85 Hz, 6H, $2CH_3$), 1.06 (d, J = 6.58 Hz, 6H, $2CH_3$); ^{13}C NMR (100 MHz, DMSO-d_6)

δ (ppm): 166.87 and 165.88 (2C=O, amide), 147.40 (quinoline, C-2), 141.97, 141.47, 138.75, 136.13, 134.87, 128.41, 128.34, 126.99, 123.35, 118.17, 117.37, 44.20 and 43.60 (CH), 21.10 and 20.11 (CH_3); *Anal*. Calcd for $C_{23}H_{23}N_5O_6$: C, 59.35; H, 4.98; N, 15.05. Found: C, 58.73; H, 4.99; N, 15.07.

6,8-Dinitro-N³,N⁴,2-triphenylquinoline-3,4-dicarboxamide (7d). Aniline (0.6 mL, 6.4 mmol) was added to a solution of **5** (0.65 g, 1.6 mmol)) in toluene (70 mL) at 25°C. The mixture was stirred and heated to reflux for 5 h. The formed precipitate was filtered while it was still hot and washed with water (3 × 20 mL) and ether (3 × 15 mL). The product was crystallized from methanol and dried in vacuo at 70°C. Yield: 0.59 g (72%); mp 264–266°C; IR (ν, cm^{-1}): 3408 (NH), 3097 (Ar CH), 1704 and 1648 (C=O, amide), 1613–1453 (Ar C=N and C=C), 1548 (NO_2 asym.), 1343 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.89 (d, J = 2.56 Hz, 1H, H-5), 9.08 (d, J = 2.56 Hz, 1H, H-7), 7.90 (s, 1H, CONH), 7.51–7.17 (m, 16H, other ArH and CONH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.01 (2C=O), 156.09 (quinoline, C-2), 142.56, 141.46, 138.06, 136.59, 135.72, 135.47, 129.27, 129.13, 128.79, 127.46, 127.23, 126.40, 126.30, 123.37, 117.41; *Anal*. Calcd for $C_{29}H_{19}N_5O_6$: C, 65.29; H, 3.59; N, 13.13. Found: C, 64.79; H, 3.65; N, 13.18.

7,9-Dinitro-5-phenyl-2,3-dihydropyridazino[4,5-c]quinoline-1,4-dione (8). Method A. Hydrazine hydrate (80%, 0.051 mL, 0.85 mmol) was added to a solution of **6a** (0.34 g, 0.85 mmol) in toluene (80 mL) at 25°C. The mixture was stirred and heated to reflux for 5 h. The formed precipitate was filtered while it was still hot and washed with water (3 × 20 mL) and ether (3 × 15 mL). The product was crystallized from a methanol–THF mixture and dried in vacuo at 70°C. Yield: 0.3 g (91%).

Method B. Hydrazine hydrate (80%, 0.055 mL, 0.9 mmol) was added to a solution of **6d** (0.45 g, 0.9 mmol) in toluene (60 mL) at 25°C. Then, the mixture was stirred and heated to reflux for 5 h. The formed precipitate was filtered while it was still hot and washed with water (3 × 20 mL) and ether (3 × 15 mL). The product was crystallized from an *n*-butanol–THF mixture and dried in vacuo at 70°C. Yield: 0.23 g (68%); mp over 300°C; IR (ν, cm^{-1}): 3220 (NH), 3112 (Ar CH), 1701 (C=O, amide), 1616–1434 (Ar C=N and C=C), 1535 (NO_2 asym.), 1343 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 12.20 (br, s, 2H, CONH), 9.10 (d, J = 2.56 Hz, 1H, H-10), 9.08 (d, J = 2.19 Hz, 1H, H-8), 7.93–7.55 (m, 5H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 159.50 and 158.29 (C=O, amide), 146.00 (quinoline, C-2), 141.11, 138.00, 137.32, 134.86, 131.68, 129.84, 129.28, 128.72, 128.06, 126.04, 123.75, 119.04; LC-MSD (API-ES (−) 70 eV) m/z = 379.0 $[M+H]^+$; *Anal*. Calcd for $C_{17}H_9N_5O_6$: C, 53.83; H, 2.39; N, 18.46. Found: C, 53.28; H, 2.43; N, 18.51.

6,8-Dinitro-4-phenylfuro[3,4-c]quinoline-1,3-dione (9). A mixture of **4** (0.383 g, 1 mmol) and acetic anhydride (95%; 60 mL) was heated in an oil bath (85°C) for 8 h. The solvents were removed on a rotary evaporator at 75°C. The residue was washed with ether (3 × 15 mL). The product was crystallized from a methanol–THF mixture and dried in vacuo at 70°C. Yield: 0.34 g (92%); mp 271–273°C; IR (ν, cm^{-1}): 3100 (Ar CH), 1788 and 1706 (C=O, anhydride asym. and sym.), 1618–1455 (Ar C=N and C=C), 1550 (NO_2 asym.), 1344 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.40 (d, J = 2.56 Hz, 1H, H-9), 9.10 (d, J = 2.56 Hz, 1H, H-7), 7.73–7.46 (m, 5H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 169.64 and 165.96 (2C=O, anhydride), 155.87 (quinoline, C-2), 143.70, 141.80, 138.14, 135.85, 133.62, 133.16, 131.07, 129.34, 126.80, 125.71, 124.13, 116.24; LC-MSD (API-ES (+) 100 eV) m/z: 365.9 $[M+H]^+$; *Anal*. Calcd for $C_{17}H_7N_3O_7$: C, 55.90; H, 1.93; N, 11.50. Found: C, 55.30; H, 1.98; N, 11.51.

6,8-Dinitro-4-phenyl-2-propyl-2H-pyrrolo[3,4-c]quinoline-1,3-dione (10a). Triethylamine (0.1 mL, 0.7 mmol) and *n*-propylamine (0.12 mL, 1.4 mmol) were added to a solution of **9** (0.5 g, 1.4 mmol) in benzene (70 mL) at 25°C, and the resulting mixture was stirred for 3 h. The reaction mixture was heated to reflux for an additional 2 h. The formed precipitate was filtered while it was still hot and washed with hexane (3 × 15 mL). The product was crystallized from a hexane–chloroform mixture and dried in vacuo at 70°C. Yield: 0.37 g (66%); mp 260–262°C; IR (ν, cm^{-1}): 3094 (Ar CH), 2968 (aliphatic CH), 1673 and 1641 (C=O, imide), 1612–1452 (aromatic C=N and C=C), 1551 (NO_2 asym.), 1342 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.84 (d, J = 2.92 Hz, 1H, H-9), 9.05 (d, J = 2.56 Hz, 1H, H-7), 7.48–7.32 (m, 5H, other ArH), 3.29 (t, J = 5.85 Hz, 2H, NCH_2), 1.41 (m, 2H, CH_2CH_3), 0.74 (t, J = 7.68 Hz, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.24 (2C=O), 156.15 (quinoline, C-2), 142.71, 141.35, 138.05, 136.89, 136.23, 129.29, 128.99, 126.90, 126.23, 123.24, 117.51, 41.39 (N-CH_2), 21.90 (CH_2-CH_3), 12.16 (CH_3); LC-MSD (API-ES (+) 55 eV) m/z: 407.0 $[M+H]^+$; *Anal*. Calcd for $C_{20}H_{14}N_4O_6$: C, 59.12; H, 3.47; N, 13.79. Found: C, 58.62; H, 3.47; N, 13.76.

2-Isopropyl-6,8-dinitro-4-phenyl-2H-pyrrolo[3,4-c]quinoline-1,3-dione (10b). Triethylamine (0.1 mL, 0.7 mmol) and isopropylamine (0.12 mL, 1.4 mmol) were added to a solution of **9** (0.5 g, 1.4 mmol) in benzene (70 mL) at 25°C. The mixture was stirred and heated to reflux for 5 h. The reaction mixture was filtered while it was still hot. The obtained solution was kept at room temperature overnight. The formed precipitate was filtered off and washed with ether (3 × 15 mL). The product was recrystallized from benzene and dried in vacuo at 70°C. Yield: 0.46 g (82%); mp 190–192°C; IR (ν, cm^{-1}): 3095 (Ar CH), 2982 (aliphatic CH), 1690 and 1645 (C=O, imide), 1613–1454 (aromatic C=N and C=C), 1550 (NO_2 asym.), 1343 (NO_2 sym.); ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 10.14 (d, J = 2.56 Hz, 1H, H-9), 9.39 (d, J = 2.56 Hz, 1H, H-7), 7.48–7.40 (m, 5H, other ArH), 3.70 (heptet, J = 6.96 Hz, 1H, CH), 1.25 (d, J = 6.59 Hz, 6H, $2CH_3$); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm): 164.28 (2C=O, imide), 156.01 (quinoline, C-2), 142.05, 141.89, 138.20, 137.13, 134.88, 132.82, 129.80, 129.12, 128.27, 126.05, 123.81, 118.07, 46.00 (N-CH), 20.94 (CH_3); *Anal*. Calcd for $C_{20}H_{14}N_4O_6$: C, 59.12; H, 3.47; N, 13.79. Found: C, 58.76; H, 3.50; N, 13.80.

6,8-Dinitro-2,4-diphenyl-2H-pyrrolo[3,4-c]quinoline-1,3-dione (10c). Triethylamine (0.1 mL, 0.7 mmol) and aniline (0.13 mL, 1.4 mmol) were added to a solution of **9** (0.5 g, 1.4 mmol) in benzene (70 mL) at 25°C. The mixture was stirred and heated to reflux for 5 h. The formed precipitate was filtered while it was still hot and washed with ether (3 × 15 mL). The product was crystallized from ethanol and dried in vacuo at 70°C. Yield: 0.45 g (75%); mp 248–250°C; IR (ν, cm^{-1}): 3096 (aromatic CH), 1703 and 1648 (C=O, imide), 1613–1453 (aromatic C=N and C=C), 1548 (NO_2 asym.), 1343 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.90 (d, J = 2.56 Hz, 1H, H-9), 9.08 (d, J = 2.56 Hz, 1H, H-7), 7.91–7.19 (m, 10H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.02 (C=O, imide), 156.13 (quinoline, C-2), 142.55, 141.42, 138.08, 136.58, 135.72, 135.45, 129.28, 129.13, 128.79, 127.46, 127.23, 126.39, 126.29, 123.36, 117.39; *Anal*. Calcd for $C_{23}H_{12}N_4O_6$: C, 62.73; H, 2.75; N, 12.72. Found: C, 62.27; H, 2.78; N, 12.75.

2-(3-Fluorophenyl)-6,8-dinitro-4-phenyl-2H-pyrrolo[3,4-c]quinoline-1,3-dione (10d). Triethylamine (0.1 mL, 0.7 mmol)

and 3-fluoroaniline (0.14 mL, 1.4 mmol) were added to a solution of **9** (0.5 g, 1.4 mmol) in benzene (70 mL) at 25°C. The mixture was stirred and heated to reflux for 8 h. The solvents were removed on a rotary evaporator at 50°C. The residue was washed with ether (3 × 15 mL). The product was crystallized from a benzene–hexane mixture and dried in vacuo at 70°C. Yield: 0.41 g (65%); mp 275–277°C; IR (ν, cm^{-1}): 3093 (aromatic CH), 1708 and 1678 (C═O, imide), 1615–1452 (aromatic C═N and C═C), 1549 (NO_2 asym.), 1342 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.89 (d, J = 2.56 Hz, 1H, H-9), 9.08 (d, J = 2.56 Hz, 1H, H-7), 8.03–7.02 (m, 9H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.24 (2C═O), 156.15 (quinoline, C-2), 142.71, 141.35, 138.05, 136.89, 136.23, 129.29, 128.99, 126.90, 126.23, 123.24, 117.51; LC-MSD (API-ES (+) 100 eV) *m/z*: 459.0 $[M+H]^+$; *Anal*. Calcd for $C_{23}H_{11}FN_4O_6$: C, 60.27; H, 2.42; N, 12.22. Found: C, 59.80; H, 2.40; N, 12.27.

2-Amino-6,8-dinitro-4-phenyl-2H-pyrrolo[3,4-c]quinoline-1,3-dione (10e). Hydrazine hydrate (80%, 0.06 mL, 1.4 mmol) was added to a solution of **9** (0.5 g, 1.4 mmol) in benzene (70 mL) at 25°C. Then, the resulting mixture was stirred for 5 h. The formed precipitate was filtered off and washed with ether (3 × 15 mL). The product was crystallized from an ethanol–methanol mixture and dried in vacuo at 70°C. Yield: 0.44 g (85%); mp over 300°C; IR (ν, cm^{-1}): 3093 (Ar CH), 1685 and 1640 (C═O, imide), 1613–1452 (aromatic C═N and C═C), 1551 (NO_2 asym.), 1341 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.83 (d, J = 2.56 Hz, 1H, H-9), 9.04 (d, J = 2.56 Hz, 1H, H-7), 7.47–7.27 (m, 5H, other ArH), 4.55 (br, s, 2H, NH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 163.57 (2C═O, imide), 155.99 (quinoline, C-2), 141.35, 141.16, 138.02, 136.47, 135.76, 129.07, 128.75, 127.46, 126.25, 123.25, 117.45; LC-MSD (API-ES (+) 100 eV) *m/z*: 380.0 $[M+H]^+$; *Anal*. Calcd for $C_{17}H_9N_5O_6$: C, 53.83; H, 2.39; N, 18.46. Found: C, 53.20; H, 2.38; N, 18.49.

2,2′-(1,4-Phenylene)bis(6,8-dinitro-4-phenyl-2H-pyrrolo[3,4-cquinoline-1,3-dione) (11a). *p*-Phenylenediamine (0.15 g, 1.4 mmol) was added to a solution of **9** (1.02 g, 2.8 mmol) in xylene (100 mL) at 25°C. The mixture was stirred and heated to reflux for 24 h. The formed precipitate was filtered while it was still hot, treated with warm ethanol, and washed with ether (3 × 15 mL). The product was crystallized from an ethyl acetate–hexane mixture and dried in vacuo at 70°C. Yield: 0.65 g (58%); mp over 300°C; IR (ν, cm^{-1}): 3091 (aromatic CH), 1694 and 1644 (C═O, imide), 1614–1454 (aromatic C═N and C═C), 1549 (NO_2 asym.), 1342 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.84 (d, J = 2.19 Hz, 2H, H-9 and H-9′), 9.03 (d, J = 1.83 Hz, 2H, H-7 and H-7′), 7.88–7.25 (m, 14H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.12 (4C═O), 156.69 (quinoline, C-4 and C-4′), 142.42, 141.06, 138.76, 136.61, 135.04, 133.89, 129.16, 128.83, 127.18, 127.05, 126.05, 125.72, 123.02, 117.28; *Anal*. Calcd for $C_{40}H_{18}N_8O_{12}$: C, 59.86; H, 2.26; N, 13.96. Found: C, 59.45; H, 2.28; N, 13.96.

2,2′-(Biphenyl-4,4′-diyl)bis(6,8-dinitro-4-phenyl-2H-pyrrolo[3,4-c]quinoline-1,3-dione) (11b). Triethylamine (0.1 mL, 0.7 mmol) and benzidine (0.17 g, 0.9 mmol) were added to a solution of **9** (0.65 g, 1.8 mmol) in benzene (90 mL) at 25°C. The mixture was stirred and heated to reflux for 24 h. The formed precipitate was filtered while it was still hot, treated with warm xylene, and washed with ether (3 × 15 mL). The product was crystallized from a THF–hexane mixture and dried in vacuo at 70°C. Yield: 0.52 g (66%); mp over 300°C; IR (ν, cm^{-1}): 3093 (aromatic CH), 1695 and 1649 (C═O, imide), 1613–1455 (aromatic C═N and C═C), 1550 (NO_2 asym.), 1341 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.86 (d, J = 2.93 Hz, 2H, H-9 and H-9′), 9.02 (d, J = 2.56 Hz, 2H, H-7 and H-7′), 7.94–7.20 (m, 18H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 165.30 (4C═O), 157.12 (quinoline, C-4 and C-4′), 142.47, 137.69, 136.81, 135.40, 134.99, 129.10, 128.82, 127.30, 127.25, 126.11, 126.09, 125.98, 125.85, 122.79, 117.31, 114.87; *Anal*. Calcd for $C_{46}H_{22}N_8O_{12}$: C, 62.88; H, 2.52; N, 12.75. Found: C, 62.88; H, 2.52; N, 12.75.

7,9-Dinitro-2,5-diphenyl-2,3-dihydropyridazino[4,5-c]quinoline-1,4-dione (12). Phenylhydrazine (98%, 0.14 mL, 1.4 mmol) was added to a solution of **9** (0.5 g, 1.4 mmol) in benzene (70 mL) at 25°C. Then, the resulting mixture was stirred for 1 h. The reaction mixture was heated to reflux for an additional 4 h. The formed precipitate was filtered while it was still hot and washed with ether (3 × 15 mL). The product was crystallized from isopropanol and dried in vacuo at 70°C. Yield: 0.42 g (68%); mp 203–205°C; IR (ν, cm^{-1}): 3300 (NH), 3092 (Ar CH), 1689 (C═O, amide), 1609–1452 (Ar C═C and C═N), 1550 (NO_2 asym.), 1343 (NO_2 sym.); ^{1}H NMR (400 MHz, DMSO-d_6) δ (ppm): 9.74 (d, J = 2.56 Hz, 1H, H-10), 9.07 (d, J = 2.56 Hz, 1H, H-8), 8.14 (s, 1H, NH), 7.62–6.68 (m, 10H, other ArH); ^{13}C NMR (100 MHz, DMSO-d_6) δ (ppm): 164.31 and 156.12 (C═O, amide), 148.40 (quinoline, C-2), 141.58, 141.42, 138.00, 136.51, 135.12, 129.16, 129.07, 128.71, 127.48, 126.23, 123.37, 119.82, 117.32, 113.51; LC-MSD (API-ES (+) 70 eV) *m/z*: 456.0 $[M+H]^+$; *Anal*. Calcd for $C_{23}H_{13}N_5O_6$: C, 60.66; H, 2.88; N, 15.38. Found: C, 60.23; H, 2.91; N, 15.39.

Acknowledgments. The authors would like to thank Dr. Salim Ok for useful comments and suggestions. Also, we gratefully acknowledge the Dumlupinar University Technology Research Fund for the financial support of this study through project number of 2007/6.

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