Bromination of naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione*

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Investigations of bromination of naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione revealed that the reaction proceeded most efficiently with *N*-bromosuccinimide in sulfuric acid and depending on the reaction conditions, can give mono-, di-, tri- and tetrabromo derivatives of naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione. A series of the major isomers was isolated, and their structure was proven using heteronuclear multiple bond correlation NMR spectroscopy and high-resolution mass spectrometry.

Key words: naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione, bromination, non-fullerene acceptors.

1,2,5-Thiadiazoles fused with aromatic, carbocyclic, and heterocyclic moieties are among the most studied classes of compounds in both chemistry and materials science due to the combination of atmospheric stability, electrical conductivity, and electron-withdrawing properties comparable to fullerenes owing to their positive electron affinity.[1—3] Fused 1,2,5-thiadiazoles are applied as materials or components in design of devices used in various fields of technology, such as organic photovoltaic devices,[4,5] dye-sensitized solar cells (DSSCs),[6—8] organic field-effect transistors (OFETs),[9,10] and organic light-emitting diodes (OLEDs).[11—13] Benzo[*c*][1,2,5]thiadiazole derivatives are used as dyes for fluorescence imaging[14] and as non-fullerene acceptors in bulk heterojunction solar cells.[15—17] 4,7-Dibromobenzo-[*c*][1,2,5]thiadiazole containing the bromine atoms at *para*-positions relative to each other is used to introduce substituents into the benzene ring fused with 1,2,5-thiadiazole. Such compounds are of considerable interest for the preparation of both individual organic compounds and polymeric products, whereas the major reactions used for the synthesis of target compounds are the Suzuki or Stille cross-coupling reactions. 4,7-Dibromo[*c*][1,2,5]benzochalcogenadiazoles (chalcogen is O, S, or Se) are easily obtained *via* bromination of their unsubstituted precursors with bromine under various conditions.[3,18] However, the corresponding dibromo derivatives have not been reported for some polycyclic fused 1,2,5-thiadiazoles that are of interest for the design of new materials based on them. One of such polycyclic thiadiazoles is naphtho-[2,3-*c*][1,2,5]thiadiazole-4,9-dione (**1**) known for more than 60 years.[19] There are some methods for obtaining compound **1** from commercially available naphthalene-1,4-dione *via* the reaction with hardly accessible trithiazyl trichloride ($S_3N_3Cl_3$)[20] or from 2,3-dichloronaphthalene-1,4-dione *via* reaction with explosive tetrasulfur tetranitride (S_4N_4),[21] as well as from 2,3-diaminonaphthalene-1,4-dione[19] (Scheme 1). The simplest and most attractive method to synthesize compound **1** is the reaction of naphthalene-1,4-dione with Katz reagent gener-

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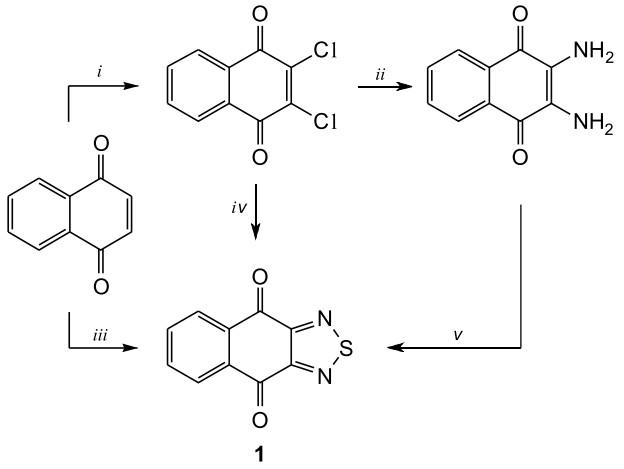
ated *in situ* from urethane, thionyl chloride, and pyridine.[20]

Scheme 1

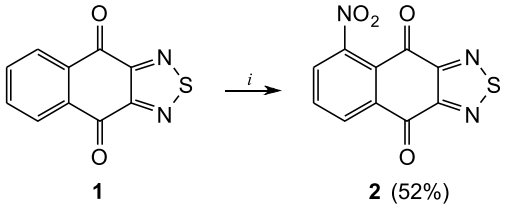


Reagents and conditions: *i*. $SOCl_2$, pyridine; *ii*. 1) potassium phthalimide, 2) N_2H_4; *iii*. Katz reagent or $S_3N_3Cl_3$; *iv*. S_4N_4; *v*. $SOCl_2$.

Note. Hereinbelow, compound **1** and its derivatives are shown in the quinoid form to avoid resonance superposition with the benzenoid form.

The most of works devoted to the reactivity of compound **1** explore reactions of the two keto groups,[21–23] and only the one work[24] was aimed at the reactivity of its benzene ring, revealing that the nitration with a mixture of 90% nitric acid and 20% oleum leads to the 5-mononitro derivative **2** (Scheme 2). Bromination of compound **1** has never been reported in the literature.

Scheme 2

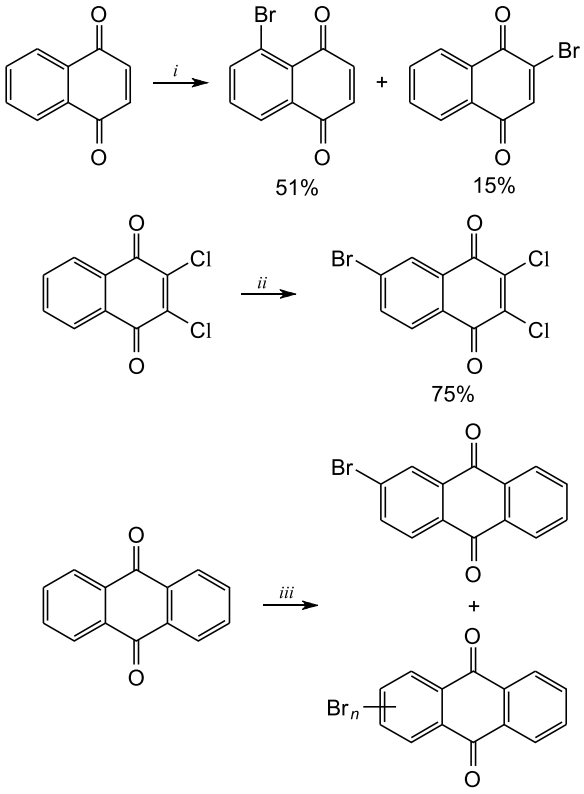


Reagents and conditions: *i*. $HNO_3/H_2SO_4/SO_3$.

The present work was aimed at the detailed investigations of bromination reaction of compound **1** in order to synthesize 5,8-dibromonaphtho[2,3-*c*]-[1,2,5]thiadiazole-4,9-dione that is a promising starting compound for obtaining various functional materials for organic electronics, including non-fullerene acceptors for solar cells with a bulk heterojunction.

An analysis of literature on the bromination of benzene ring in naphthoquinone derivatives demonstrated that the reaction results are very dependent on the structure of starting compound and often contradict each other (Scheme 3). The reaction can give α- and β-bromination products, as well as polybrominated derivatives. Thus, selective *ortho*-bromination occurs[25] in the reaction of naphthoquinone with 1,3-dibromo-5,5-dimethylhydantoin in the presence of a Rh catalyst, the reaction of 2,3-dichloronaphthoquinone with *N*-bromosuccinimide (NBS) in trifluoromethanesulfonic acid leads to a 6-bromo derivative in a high yield,[26] and bromination of anthraquinone with bromine in oleum gives a difficult-to-separate mixture of mono-, di-, and

Scheme 3



n = 2, 3

Reagents and conditions: *i*. 1,3-dibromo-5,5-dimethylhydantoin, $[RhCp^*Cl_2]_2$, $AgNTf_2$, $Cu(OAc)_2$, 65 °C, microwave irradiation, 5 h;[25] *ii*. NBS, CF_3SO_3H, 40 °C, 16 h;[26] *iii*. Br_2, oleum, 80 °C.[24]

tribromo derivatives in low yields.[27] Therefore, it seemed difficult to predict how the bromination of compound **1** would proceed.

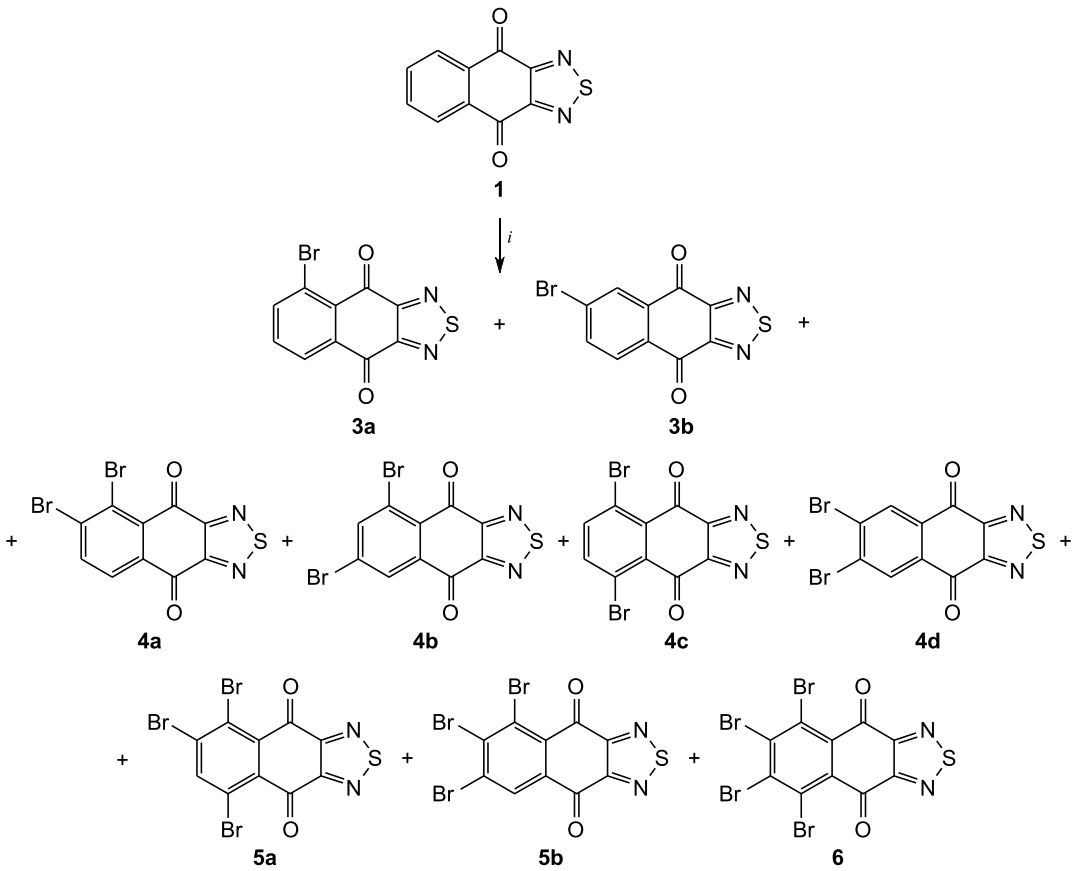
Taking into account these data and methods known for the preparation of 4,7-dibromo[*c*][1,2,5]-benzochalcogenadiazoles (chalcogen is O, S, or Se),[3,18] we explored the following methods for the bromination of naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (**1**): heating with a solution of bromine in hydrobromic acid and reactions with NBS in various acids.

It was found that compound **1** does not react with an excess of bromine in hydrobromic acid at 100 °C within 2 h and with NBS in acetic acid at 75 °C within 5 h. The starting compound **1** was recovered in a high yield in both cases. Heating compound **1** with NBS (4 equiv.) in sulfuric acid at 50 °C according to the procedure for obtaining 4,7-dibromobenzo-[*d*][1,2,3]thiadiazole[28] gave a mixture of tri- (**5a,b**) and tetrabromination products (**6**), wherein tribromo derivatives **5** were the major ones (Scheme 4, Table 1, entry *1*). Thus, the bromination of compound **1** with NBS in sulfuric acid does not stop at the step of formation of dibromo derivatives **4**, but proceeds further until obtaining tetrabromo derivative **6**.

It is obvious that it was necessary to decrease the reaction temperature and the amount of NBS used in order to obtain dibromo derivatives of compound **1**, including the target product **4c**. At this end, the reaction of compound **1** with NBS in sulfuric acid was investigated in order to obtain all the possible products of stepwise bromination. The acquired results are listed in Table 1.

It was shown that the reaction of compound **1** with NBS (**1** : NBS = 1 : 1.5) both at 0 °C and at room temperature proceeds very slowly: monobromo derivatives **3a** and **3b** were obtained only in trace amounts (see Table 1, entries *2* and *3*). Increasing the amount of NBS up to the ratio of **1** : NBS = = 1 : 2.5 in the reaction carried out at room temperature gave isomer **3b** in low yield (16%) and a mixture of isomers **4a—d** in moderate yield (57%),

Scheme 4



Reagents and conditions: *i*. NBS, H_2SO_4.

Table 1. Reaction of compound **1** with NBS in sulfuric acid[a]

Entry	NBS/mmol	Reaction conditions	Products and yields (%)				
			3a	**3b**	**4a—d**	**5a,b**	**6**
1	4.0	50 °C, 5 h	0	0	—[b]	39[c]	21
2	1.5	0 °C, 3 days	—[b]	—[b]	0	0	0
3	1.5	20 °C, 24 h	—[b]	—[b]	0	0	0
4	2.5	20 °C, 16 h	0	16	57	—[b]	0
5	2.5	0 °C, 7 days	4	72	—[b]	0	0
6	2.0	0 °C, 10 days	16	51	0	0	0
7	3.0	20 °C, 3 h	8	0	61	0	0
8	4.0	20 °C, 24 h	0	0	0	61	3
9	4.0	0 °C, 3 days	7	51	13[c]	6[c]	0
10	4.0	0 °C, 5 days	0	0	60[c]	24[c]	0
11	4.0	0 °C, 10 days	0	0	5[c]	53[c]	0
12	6.0	0 °C, 7 days	0	0	0	76	0
13	6.0	55 °C, 12 h	0	0	0	0	53

[a] Reactions were carried out using compound **1** (1 mmol) in H_2SO_4 (25 mL).
[b] Trace amounts.
[c] Product yields were estimated by ^{1}H NMR spectroscopy.

which indicates a low selectivity of the reaction at room temperature (see Table 1, entry *4*). Therefore, we lowered the reaction temperature to 0 °C to increase the selectivity of reaction. It turned out that the reaction proceeds much more slowly under these conditions, *viz*. within 7 days (see Table 1, entry *5*), and is terminated upon the formation of a mixture of monobromo-substituted products **3**. Double chromatography on silica gel allowed us to isolate pure monobromo derivatives **3a** and **3b**. The major product was isomer **3b** (72%), and isomer **3a** was isolated in a low yield (4%). A twofold decrease in the amount of NBS under the same conditions resulted in a longer reaction time (up to 10 days) and in decreased reaction selectivity, while product **3b** was also the major one in this case (see Table 1, entry *6*). Increasing the amount of NBS up to 3 equiv. and carrying out the reaction at room temperature did not improve its selectivity (see Table 1, entry *7*). In this case, a mixture of dibromo derivatives **4a—d** was formed, whereas monobromo-substituted isomer **3b** was completely converted into a mixture of dibromides **4a—d**, while isomer **3a** was preserved apparently due to its lower reactivity. Increasing the amount of NBS up to 4 equiv. led to subsequent bromination giving a mixture of isomers of tribromo derivatives **5a,b** and tetrabromo-substituted compound **6** as a minor product (see Table 1, entry *8*). Taking into account the acquired results, we decided to evaluate carrying out this reaction at 0 °C.

It turned out that the composition of products changes significantly upon increasing the reaction time. Thus, a complex mixture of mono- (**3**), di- (**4**) and trisubstituted (**5**) isomers was formed after three days, the yields were determined after the isolation of pure products by column chromatography, as well as by ^{1}H NMR spectroscopy (see Table 1, entry *9*). After 5 days from the reaction onset, monoisomers **3** disappeared, and a mixture of di- (**4**) and tribrominated (**5**) isomers can be isolated (see Table 1, entry *10*). After 10 days of maintaining the reaction mixture at 0 °C, the major product was a mixture of tribromo-containing isomers **5**, but dibrominated isomers **4** did not disappear completely (see Table 1, entry *11*). The highest yield for the mixture of trisubstituted isomers **5** was achieved only upon using 6 equiv. of NBS and carrying out the reaction at 0 °C for 7 days (see Table 1, entry *12*). Tetrabromo derivative **6** was not formed at 0 °C, and it is most convenient for its preparation to heat the reaction mixture at 55 °C in the presence of 6 equiv. NBS for 12 h (see Table 1, entry *13*).

Therefore, the bromination of compound **1** proceeds non-selectively and affects all the possible positions. Some of the resulting brominated derivatives of naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (**1**) were isolated in pure form.

The elemental composition of bromination products was determined using high-resolution mass spectrometry (see Experimental). Signals in the ^{1}H NMR spectra were assigned using two-dimensional NMR spectra for all the isolated isomers and mixtures of isomers. The multiplicity of signals in the ^{1}H NMR spectra of monobrominated derivatives **3b** and **3a**, as well as the key interatomic couplings in the hetero-

nuclear multiple bond correlation (HMBC) spectra between protons at the positions 5 or 8 of benzene ring and the carbon atom of C=O group, allowed us to unambiguously determine the structure of each isomer (Fig. 1). ^{1}H NMR spectra of the mixture of dibrominated derivatives **4** contained two singlets corresponding to isomers **4c** and **4d**. The signals for these isomers can be unambiguously assigned by the presence/absence of couplings between protons at the benzene ring and the carbon atom of C=O group in the HMBC spectra. ^{1}H NMR spectra of dibromo isomers **4a** and **4b** contained two doublets with different *J* values. The *J* value for neighboring protons in isomer **4a** was greater than that for isomer **4b**. In both cases, one of the two protons in each isomer manifested a cross-peak with the carbon atom of C=O group in the HMBC spectra. The spectrum of mixture of tribromo derivatives **5a** and **5b** contained two singlets, one of which corresponds to isomer **5b** that exhibits a cross-peak with the carbon atom of C=O group, and the other does not.

The acquired data allowed us to propose a synthetic approach to the stepwise bromination of compound **1** with NBS in sulfuric acid. At the first step, a mixture of 5- and 6-bromo derivatives is formed, wherein the major one is isomer **3b** (Scheme 4). The subsequent bromination leads to an inseparable mixture of dibromo-substituted compounds **4a—d**. It should be noted that among the four possible isomers of dibromo derivatives **4a—d**, compounds **4a** and **4c** were initially formed in practically equal proportions, but an increased duration of the reaction and excess NBS resulted in the accumulation of isomer **4d**, while isomer **4b** was formed in trace amounts. Tribromo derivatives **5a,b** were isolated in a mixture with isomer **4d**, and the simplicity of analysis of their ^{1}H NMR spectra allowed us to estimate the approximate yields for the each isomer (see Table 1).

In summary, the present work reports on the optimal conditions for obtaining mono-, di-, tri-, and tetrabromo derivatives of naphtho[2,3-*c*][1,2,5]-thiadiazole-4,9-dione (**1**). A series of bromine-containing isomers were isolated in pure form, the structure of the obtained products was proven, and the main routes for the bromination of compound **1** were established. The acquired data can be useful for introducing bromine atoms into the benzene cycle of naphthoquinones fused with various heterocycles.

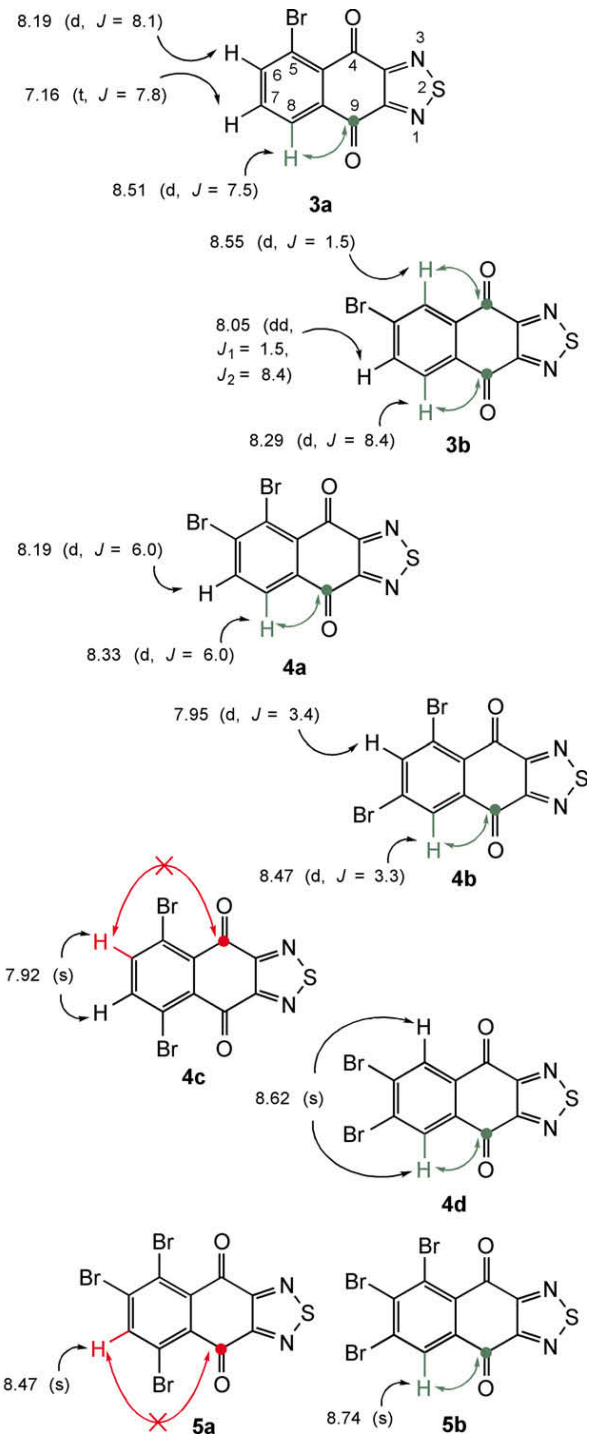


Fig. 1. Chemical shifts and multiplicity of the characteristic signals in ^{1}H NMR spectra and main correlations in the HMBC spectra of brominated derivatives of compound **1**.

Experimental

The solvents were purified by distillation over appropriate drying agents. Commercially available reagents were

used without further purification. All synthetic operations were carried out under dry argon. The progress of reactions and the purity of synthesized compounds were monitored by TLC on Merck TLC Silicagel 60 F254 plates, using petroleum ether, methylene chloride, ethyl acetate, diethyl ether, chloroform, carbon tetrachloride, and their various mixtures as eluents. The synthesized compounds were isolated by column chromatography on Merck silica gel 60.

Naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (**1**) was obtained according to the known procedure.[20]

^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker AM-300 (300 and 75 MHz, respectively) and QOne Quantum-I-plus AS600 (600 and 150 MHz, respectively) instruments. Chemical shifts are given relative to Me_4Si. IR spectra were recorded on a Bruker Alpha-T spectrometer in KBr pellets or in a thin neat layer placed between KBr disks. Melting points were determined on a Kofler apparatus at the heating rate near the melting point of 4 deg min^{-1} and also on a Stuart SMP10 apparatus. Mass spectra were recorded on a Finnigan MAT INCOS 50 instrument with direct sample introduction and electron impact ionization (EI) at the energy of 70 eV. High-resolution mass spectra (HRMS) were recorded on a Bruker micrOTOF instrument using electrospray ionization (ESI). Elemental analysis was performed on a Perkin-Elmer 2400 CHNS/O analyzer.

Reactions of naphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (1) with NBS in sulfuric acid (general procedure). *N*-Bromosuccinimide was added to a solution of compound **1** (216 mg, 1 mmol) in concentrated H_2SO_4 (25 mL), and the reaction mixture was kept under the conditions listed in Table 1. The mixture was poured into ice water (300 mL) and extracted with CH_2Cl_2 (2×150 mL). The combined organic layer was washed with aqueous solution (1%, 100 mL) of sodium carbonate, water (3×100 mL), and dried over $MgSO_4$. The solvent was evaporated under reduced pressure. The residue was separated by column chromatography (the eluent was CH_2Cl_2—hexane (10 : 1, by volume)).

5-Bromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (3a). Yellow crystalline product, m.p. 206—208 °C. R_f 0.46 (CH_2Cl_2). ^{1}H NMR (600 MHz), δ: 8.51 (d, 1 H, C(8)H, J = 7.5 Hz); 8.19 (d, 1 H, C(6)H, J = 8.1 Hz); 7.16 (t, 1 H, C(7)H, J = 7.8 Hz). ^{13}C NMR (75 MHz), δ: 176.1, 175.7, 157.1, 155.6, 143.6, 137.5, 135.5, 131.6, 129.6, 125.3. HRMS (ESI): found m/z 318.8966 $[M + Na]^+$; calculated for $C_{10}H_3BrN_2NaO_2S$ 318.8970. MS (EI, 70 eV), m/z (I_{rel} (%)): 296 (100), 294 (98), 215 (95), 182 (35), 154 (16), 75 (63). IR (KBr), ν/cm^{-1}: 1690, 1568, 1414, 1358, 1206, 1181, 997, 801.

6-Bromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (3b). Yellow crystalline product, m.p. 218—220 °C. R_f 0.51 (CH_2Cl_2). ^{1}H NMR (600 MHz), δ: 8.55 (d, 1 H, C(5)H, J = 1.5 Hz); 8.29 (d, 1 H, C(8)H, J = 8.4 Hz); 8.05 (dd, 1 H, C(7)H, J_1 = 1.5 Hz, J_2 = 8.4 Hz). ^{13}C NMR (150 MHz), δ: 175.6, 141.9, 139.1, 138.5, 131.6, 131.4, 130.2, 128.9. HRMS (ESI): found m/z 318.8966 $[M + Na]^+$; calculated for $C_{10}H_3BrN_2NaO_2S$ 318.8970. MS (EI, 70 eV), m/z (I_{rel} (%)): 296 (100), 294 (98), 215 (95), 182 (35), 154 (16), 75 (63). IR (KBr), ν/cm^{-1}: 1690, 1568, 1414, 1358, 1206, 1181, 997, 801.

Dibromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-diones 4a—d (mixture of isomers). Yellow crystalline product. R_f 0.53 (CH_2Cl_2). HRMS (ESI): found m/z 396.8061 $[M + Na]^+$; calculated for $C_{10}H_2Br_2N_2NaO_2S$ 396.8075. MS (EI, 70 eV), m/z (I_{rel} (%)): 376 (12), 374 (16), 372 (10), 296 (100), 294 (98), 216 (38), 214 (36), 184 (41), 172 (45), 152 (13), 154 (15), 75 (40). IR (KBr), ν/cm^{-1}: 2956, 2924, 2853, 1694, 1542, 1465, 1359, 1191, 1106, 831.

5,6-Dibromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (4a). ^{1}H NMR (600 MHz), δ: 8.33 (d, 1 H, C(8)H, J = 6.0 Hz); 8.19 (d, 1 H, C(7)H, J = 6.0 Hz).

5,7-Dibromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (4b). ^{1}H NMR (600 MHz), δ: 8.47 (d, 1 H, C(8)H, J = 3.3 Hz); 7.95 (d, 1 H, C(6)H, J = 3.4 Hz).

5,9-Dibromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (4c). ^{1}H NMR (600 MHz), δ: 7.92 (s, 2 H, C(6)H, C(7)H).

6,7-Dibromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (4d). ^{1}H NMR (600 MHz), δ: 8.62 (s, 2 H, C(5)H, C(8)H). ^{13}C NMR (75 MHz), δ: 174.7, 155.9, 133.9, 133.5, 132.6.

Tribromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-diones 5a,b (mixture of isomers). Yellow crystalline product. R_f 0.55 (CH_2Cl_2). HRMS (ESI): found m/z 476.7167 $[M + Na]^+$; calculated for $C_{10}HBr_3N_2NaO_2S$ 476.7160. MS (EI, 70 eV), m/z (I_{rel} (%)): 456 (14), 454 (45), 452 (45), 450 (14), 373 (51), 342 (42), 340 (42), 314 (12), 312 (12), 233 (20), 152 (22), 150 (21), 32 (100). IR (KBr), ν/cm^{-1}: 1695, 1565. 1538, 1225, 1152, 1106, 1005, 838.

5,6,8-Tribromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (5a). ^{1}H NMR (600 MHz), δ: 8.47 (s, 1 H, C(7)H).

5,6,7-Tribromonaphtho[2,3-c][1,2,5]thiadiazole-4,9-dione (5b). ^{1}H NMR (600 MHz), δ: 8.74 (s, 1 H, C(8)H).

5,6,7,8-Tetrabromonaphtho[2,3-*c*][1,2,5]thiadiazole-4,9-dione (6). Yellow crystalline product, m.p. 272—274 °C. R_f 0.60 (CH_2Cl_2). ^{13}C NMR (75 MHz), δ: 175.1, 155.4, 138.8, 135.4, 125.9. Found (%): C, 22.52, N, 5.28. $C_{10}Br_4N_2O_2S$. Calculated (%): C, 22.58, N, 5.27. MS (EI, 70 eV), m/z (I_{rel} (%)): 534 (63), 532 (100), 530 (65), 453 (75), 451 (73), 420 (30), 392 (31), 339 (22), 313 (20), 232 (45), 179 (20), 153 (25). IR (KBr), ν/cm^{-1}: 1692, 1488, 1458, 1359, 1167, 1030, 838.

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Animal Testing and Ethics

No human or animal subjects were used in this research.

Conflict of Interest

The authors declare no competing interests.

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