Synthesis of substituted isoindolo[2,1-*a*]quinoxalin-6-yl-amino and 6-imino-5-yl thiourea derivatives

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Abstract

A series of substituted 1-(5-bromopyridin-2-yl)-3-[2-(isoindolo[2,1-*a*]quinoxalin-6-ylamino)ethyl]thiourea and 1-(5-bromopyridin-2-yl)-3-[2-(6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thiourea derivatives were prepared in good yields (63-85%) by reaction between the corresponding amino compounds with 5-bromo-2-isothiocyanatopyridine. All thiourea derivatives, tested for inhibition of HIV-1 RT, showed no significant antiviral activity.

Keywords: AIDS, NNRTIs, isoindolo-quinoxalines, quinoxalinyylethylpyridylthioureas, antiviral activity

Introduction

Human immunodeficiency virus (HIV) is a retrovirus responsible for transmission and development of the acquired immune deficiency syndrome (AIDS). It is characterized by the presence of a viral reverse transcriptase (RT) that is able to synthesize DNA from the viral RNA genome. Due to its important role in the viral life cycle, this enzyme is considered an excellent target in the chemotherapy against AIDS. In the current treatment strategy, called highly active antiretroviral therapy (HAART), HIV-1 RT inhibitors are used in combination with HIV-1 protease inhibitors.¹⁻³

There are two classes of HIV-1 RT inhibitors: nucleoside analogues (NRTIs), for example AZT, ddI, ddC, d4T and non-nucleoside analogues (NNRTIs), for example nevirapine, efavirenz, delarvidine. NRTIs are competitive inhibitors that act at the catalytic site of the enzyme by interrupting DNA synthesis.⁴ NNRTIs are non-competitive inhibitors, structurally diverse, that bind to a hydrophobic pocket located approximately 10 Å away from the catalytic

site. Their binding leads to a distortion of the catalytic pocket preventing the enzyme to carry out its normal functions.^{5,6}

Most NNRTIs are highly specific against HIV-1 RT and have a low toxicity for the human cells but show a reduced efficacy against mutated variants of RT.^{7,8}

For this reason in the last years many efforts have been done to find new NNRTIs able to inhibit both wild-type and mutants HIV-1 RT that are resistant to the common antiretroviral drugs.^{9,10}

The quinoxaline ring and structurally related quinoxalinone constitute the skeleton of many compounds showing a variety of biological activities.¹¹ Some quinoxaline derivatives (for example S-2720,¹² HBY097¹³ and GW420867X¹⁴) have been reported as excellent NNRTIs and in particular HBY 097 and GW420867X were also selected for clinical trials. They were highly potent inhibitors of HIV-1 replication in different human cell lines showing IC₅₀ values in the low nanomolar range. The compounds were also active against various HIV-1 subtypes and mutant reverse transcriptases. Compounds with a heteroarylsulfonylquinoxaline structure were also reported for their properties to inhibit the RT with IC₅₀ at submicromolar range (Figure 1).¹⁵

S-2720

HBY097

GW420867X

N⁴-(hetero)arylsulfonylquinoxalinones

Figure 1. NNRTIs having a quinoxaline skeleton.

Quinoxalinyldiethylpyridylthioureas (QXPTs) of type **1** and **2** (Figure 2) represent another class of NNRTIs; many compounds showed a potent activity against both HIV-1 wild-type RT and various HIV-1 mutants HIV-1 RT.¹⁶ Considering the good experience reached in the course of our researches on polycyclic nitrogen systems, bearing pyrrole,¹⁷⁻²⁴ indole,²⁵⁻³⁵ isoindole³⁶⁻³⁸ and indazole³⁹ moieties, we have decided to synthesize the QXPT analogues of type **3** and **4** bearing an isoindole moiety instead of the five-membered heterocyclic ring. Moreover the replacement

of the oxygen atom with a nitrogen atom could have increased the pharmacokinetic profile (Figure 2).

Figure 2. Quinoxalinyethylpyridylthioureas **1-4**.

Results and Discussion

The key intermediates for the synthesis of 1-(5-bromopyridin-2-yl)-3-[2-(isoindolo[2,1-*a*]-quinoxalin-6-ylamino)ethyl]thiourea **3a-d** and 1-(5-bromopyridin-2-yl)-3-[2-(6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thiourea derivatives **4a-d** were the isoindolo[2,1-*a*]quinoxalin-6(5*H*)-imine acetates **5a-d** prepared by us as previously reported³⁸ (Scheme 1).

The reaction of the latter compounds with 2-azidoethyl-4-methylbenzenesulfonate **6**, properly prepared from 2-chloroethanol with sodium azide and subsequent tosylation of the

alcohol group,⁴⁰ in dimethylformamide and in the presence of potassium carbonate as base, furnished both *N*-(2-azidoethyl)isoindolo[2,1-*a*]quinoxalin-6-amines **8a-d** (40-45%) and 5-(2-azidoethyl)isoindolo[2,1-*a*]quinoxalin-6(5*H*)-imines **7a-d** (46-51%) separated by column chromatography (Scheme 1).

a) R = R₁ = R₂ = H; b) R = R₂ = H, R₁ = OMe; c) R = H, R₁ = R₂ = Cl; d) R = Me, R₁ = R₂ = H

Scheme 1. *Reagents and conditions:* (i) K₂CO₃, DMF, 2 h, rt, then 2-azidoethyl-4-methylbenzenesulfonate **6**, 12 h, 90 °C.

The azidoethylquinoxalines **7a-d** and **8a-d** obtained were reduced to the corresponding amino compounds¹⁶ **9a-d** and **10a-d** in good yields (58-64% and 62-78% respectively) using propane-1,3-dithiol and triethylamine (TEA) (Scheme 2). The subsequent functionalization of the obtained amino derivatives gave the desired 1-(5-bromopyridin-2-yl)-3-[2-(isoindolo[2,1-*a*]quinoxalin-6-ylamino)ethyl]thiourea **3a-d** (63-85%) and 1-(5-bromopyridin-2-yl)-3-[2-(6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thiourea **4a-d** (67-81%) derivatives by a coupling reaction in dimethylformamide with 5-bromo-2-isothiocyanatopyridine obtained from a reaction between 2-amino-5-bromopyridine and thiocarbonyldiimidazole in chloroform⁴¹ (Scheme 2).

a) R = R₁ = R₂ = H; b) R = R₂ = H, R₁ = OMe; c) R = H, R₁ = R₂ = Cl; d) R = Me, R₁ = R₂ = H

Scheme 2. *Reagents and conditions:* (i) TEA, propane-1,3-dithiol, MeOH, 24 h, rt; (ii) 5-bromo-2-isothiocyanatopyridine, DMF, 16 h, 100 °C.

Furthermore, the antiviral activity of compounds **3** and **4** was assayed. In particular, their capacity to inhibit the activity of HIV-1 RT, was evaluated. Unfortunately, none of the derivatives **3** and **4** showed inhibition up to a concentration of 100 μM.

Experimental Section

General. All melting points were taken on a Büchi-Tottoly capillary apparatus and are uncorrected. IR spectra were determined in bromoform with a Shimadzu FT/IR 8400S spectrophotometer. ¹H and ¹³C NMR spectra were measured at 200 and 50.0 MHz, respectively, in DMSO-*d*₆ or CDCl₃ solution, using a Bruker Avance II series 200 MHz spectrometer. Column chromatography was performed with Merk silica gel 230–400 mesh ASTM or with Büchi Sepacor chromatography module (prepacked cartridge system). Elemental analyses (C, H, N) were within ±0.4% of theoretical values and were performed with a VARIO EL III elemental analyzer.

General procedure for the preparation of substituted *N*-(2-azidoethyl)isoindolo[2,1-*a*]quinoxalin-6-amines (8a-d) and 5-(2-azidoethyl)isoindolo[2,1-*a*]quinoxalin-6(5*H*)-imines (9a-d). To a solution of isoindolo[2,1-*a*]quinoxalin-6(5*H*)-imine acetates **5a-d**³⁸ (2.10 mmol) in DMF (7 mL), potassium carbonate (7.40 mmol, 1.05 g) was added and the reaction mixture was stirred for 2 hours at room temperature. Then 2-azidoethyl-4-methylbenzenesulfonate **6**⁴⁰ (6.40 mmol, 1.50 g) was added and the mixture was heated at 90 °C for 12 hours. Water was added and the resulted solution was extracted with ethyl acetate (3 x 60 mL), dried (Na₂SO₄) and evaporated under reduced pressure. The obtained residue was purified by column chromatography to give corresponding derivatives **7a-d** and **8a-d**.

***N*-(2-Azidoethyl)isoindolo[2,1-*a*]quinoxalin-6-amine (7a).** The residue was purified by chromatography eluting with DCM. White solid; yield: 45%; mp 156 °C; IR (CHBr₃) ν 3429 (NH), 2257 (N₃) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.74-3.80 (m, 2H, CH₂), 4.80 (t, *J* 5.9 Hz, 2H, CH₂), 7.45 (d, *J* 8.0 Hz, 1H, Ar-H), 7.63 (d, *J* 8.0 Hz, 1H, Ar-H), 7.79-8.08 (m, 4H, Ar-H), 8.22 (d, *J* 7.5 Hz, 1H, Ar-H), 8.41 (d, *J* 7.7 Hz, 1H, Ar-H), 8.89 (d, *J* 7.7 Hz, 1H, Ar-H), 11.20 (br, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 39.6 (CH₂), 48.1 (CH₂), 127.1 (C), 127.5 (CH), 127.6 (CH), 128.1 (CH), 128.6 (CH), 128.8 (CH), 129.8 (CH), 131.2 (CH), 131.7 (CH), 132.4 (C), 133.7 (CH), 138.5 (C), 140.2 (C), 143.4 (C), 161.2 (C). Anal. Calcd for C₁₇H₁₄N₆: C, 67.54; H, 4.67; N, 27.80. Found: C, 67.38; H, 4.89; N, 27.64.

Further elution with DCM/Ethyl acetate 8/2 gave **5-(2-azidoethyl)isoindolo[2,1-*a*]quinoxalin-6(5*H*)-imines (8a)**. White solid; yield: 50%; mp 165 °C; IR (CHBr₃) ν 3407 (NH), 2256 (N₃) 1711 (C=NH) cm⁻¹; ¹H NMR (200 MHz, CDCl₃) δ 3.83 (t, *J* 4.9 Hz, 2H, CH₂), 5.05 (t, *J* 4.9 Hz, 2H, CH₂), 7.80-7.93 (m, 4H, Ar-H), 8.01 (td, *J* 1.3, 7.2 Hz, 1H, Ar-H), 8.28-8.35 (m, 2H, Ar-H), 8.43 (dd, *J* 0.8, 7.9 Hz, 1H, Ar-H), 9.26 (dd, *J* 0.8, 7.9 Hz, 1H, Ar-H), 11.36 (br, 1H, NH); ¹³C NMR (50 MHz, CDCl₃) δ 50.2 (CH₂), 66.5 (CH₂), 121.01 (C), 122.7 (C), 124.8 (CH), 125.4 (CH), 129.2 (CH), 129.3 (CH), 129.4 (CH), 130.5 (CH), 130.8 (CH), 132.5 (CH), 134.9 (C), 137.6 (C), 140.8 (CH), 141.3 (C), 143.3 (C). Anal. Calcd for C₁₇H₁₄N₆: C, 67.54; H, 4.67; N, 27.80. Found: C, 67.76; H, 4.32; N, 27.92.

***N*-(2-Azidoethyl)-3-methoxyisoindolo[2,1-*a*]quinoxalin-6-amine (7b).** The residue was purified by chromatography eluting with DCM/Ethyl acetate 9/1. White solid; yield: 43%; mp 189 °C; IR (CHBr₃) ν 3480 (NH), 2256 (N₃) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.75-3.81 (m, 2H, CH₂), 3.99 (s, 3H, OCH₃), 4.79 (t, *J* 6.0 Hz, 2H, CH₂), 7.40-7.50 (m, 2H, Ar-H), 7.82-8.08 (m, 4H, Ar-H), 8.39 (dd, *J* 0.9, 7.1 Hz, 1H, Ar-H), 8.84 (dd, *J* 0.9, 7.1 Hz, 1H, Ar-H), 11.18 (br, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 39.5 (CH₂), 48.1 (CH₂), 56.0 (CH₃), 105.7 (CH), 121.7 (CH), 123.6 (CH), 126.5 (C), 128.0 (CH), 130.0 (CH), 130.9 (CH), 132.6 (C), 132.7 (C), 133.6 (CH), 134.6 (C), 139.9 (CH), 142.3 (C), 161.3 (C), 161.5 (C). Anal. Calcd for C₁₈H₁₆N₆O: C, 65.05; H, 4.85; N, 25.29. Found: C, 64.81; H, 4.69; N, 25.50.

Further elution with DCM/Ethyl acetate 8/2 gave **5-(2-azidoethyl)-3-methoxyisoindolo[2,1-*a*]quinoxalin-6(5*H*)-imine (8b)**. White solid; yield: 46%; mp 189 °C; IR (CHBr₃) ν 3021 (NH), 2104 (N₃), 1695 (C=NH) cm⁻¹; ¹H NMR (200 MHz, CDCl₃) δ 3.83 (t, *J* 6.0 Hz, 2H, CH₂), 4.02 (s, 3H, OCH₃), 5.08 (t, *J* 6.0 Hz, 2H, CH₂), 7.46-7.55 (m, 2H, 2 x Ar-H), 7.80-8.02 (m, 3H, 3 x

Ar-H), 8.18 (d, J 9.1 Hz, 1H, Ar-H), 8.41 (d, J 8.0 Hz, 1H, Ar-H), 9.19 (d, J 8.0 Hz, 1H, Ar-H), 11.34 (br, 1H, NH); ^{13}C NMR (50 MHz, CDCl_3) δ 29.7 (CH_2), 50.2 (CH_2), 55.8 (CH_3), 105.6 (CH), 122.1 (C), 123.8 (CH), 124.2 (CH), 124.5 (C), 125.3 (CH), 129.0 (CH), 130.1 (CH), 130.3 (CH), 132.4 (CH), 135.0 (C), 135.4 (C), 137.9 (C), 145.1 (C), 161.4 (C). Anal. Calcd for $\text{C}_{18}\text{H}_{16}\text{N}_6\text{O}$: C, 65.05; H, 4.85; N, 25.29. Found: C, 64.75; H, 5.12; N, 25.41.

***N*-(2-Azidoethyl)-2,3-dichloroisindolo[2,1-*a*]quinoxalin-6-amine (7c).** The residue was purified by chromatography eluting with DCM/Ethyl acetate 9/1. White solid; yield: 40%; mp 152 °C; IR (CHBr_3) ν 3429 (NH), 2256 (N_3) cm^{-1} ; ^1H NMR (200 MHz, CDCl_3) δ 3.73-3.80 (m, 2H, CH_2), 4.92 (t, J 6.3 Hz, 2H, CH_2), 7.83-7.93 (m, 3H, Ar-H), 8.21 (s, 1H, Ar-H), 8.33 (s, 1H, Ar-H), 8.52 (d, J 7.7 Hz, 1H, Ar-H), 8.95 (d, J 7.7 Hz, 1H, Ar-H), 11.19 (br, 1H, NH); ^{13}C NMR (50 MHz, CDCl_3) δ 39.9 (CH_2), 47.6 (CH_2), 124.8 (CH), 125.1 (C), 127.5 (C), 128.6 (CH), 128.8 (CH), 129.6 (CH), 131.8 (CH), 131.9 (CH), 132.4 (C), 133.7 (CH), 135.5 (C), 139.5 (C), 139.7 (C), 158.6 (C), 161.9 (C). Anal. Calcd for $\text{C}_{17}\text{H}_{12}\text{Cl}_2\text{N}_6$: C, 55.00; H, 3.26; N, 22.64. Found: C, 54.79; H, 3.42; N, 22.43.

Further elution with DCM/Ethyl acetate 8/2 gave **5-(2-azidoethyl)-2,3-dichloroisindolo[2,1-*a*]quinoxalin-6(5*H*)-imine (8c).** White solid; yield: 51%; mp 169 °C; IR (CHBr_3) ν 3409 (NH), 2105 (N_3), 1722 (C=NH) cm^{-1} ; ^1H NMR (200 MHz, CDCl_3) δ 3.83 (t, J 4.9 Hz, 2H, CH_2), 5.03 (t, J 4.9 Hz, 2H, CH_2), 7.83-8.06 (m, 3H, Ar-H), 8.36-8.43 (m, 3H, Ar-H), 9.18 (dd, J 1.2, 8.0 Hz, 1H, Ar-H), 11.35 (br, 1H, NH); ^{13}C NMR (50 MHz, CDCl_3) δ 50.1 (CH_2), 66.7 (CH_2), 122.8 (CH), 124.9 (CH), 125.5 (CH), 129.4 (CH), 129.6 (CH), 131.4 (CH), 132.8 (CH), 133.9 (C), 134.5 (C), 135.2 (C), 138.5 (C), 139.7 (C), 141.8 (C), 148.0 (C), 163.5 (C). Anal. Calcd for $\text{C}_{17}\text{H}_{12}\text{Cl}_2\text{N}_6$: C, 55.00; H, 3.26; N, 22.64. Found: C, 55.32; H, 3.48; N, 22.42.

***N*-(2-Azidoethyl)-2-methylisindolo[2,1-*a*]quinoxalin-6-amine (7d).** The residue was purified by chromatography eluting with DCM/Ethyl acetate 9/1. White solid; yield: 44%; mp 147 °C; IR (CHBr_3) ν 3391 (NH), 2257 (N_3) cm^{-1} ; ^1H NMR (200 MHz, CDCl_3) δ 2.80 (s, 3H, CH_3), 3.77-3.83 (m, 2H, CH_2), 4.95 (t, J 6.6 Hz, 2H, CH_2), 7.58-7.68 (m, 3H, Ar-H), 7.78 (td, J 1.4, 7.3 Hz, 1H, Ar-H), 7.90 (td, J 1.4, 7.3 Hz, 1H, Ar-H), 8.00-8.06 (m, 1H, Ar-H), 8.53 (dd, J 0.8, 7.9 Hz, 1H, Ar-H), 8.98 (dd, J 0.8, 7.9 Hz, 1H, Ar-H), 11.20 (br, 1H, NH); ^{13}C NMR (50 MHz, CDCl_3) δ 17.3 (CH_3), 40.0 (CH_2), 48.5 (CH_2), 124.5 (CH), 127.0 (CH), 127.4 (C), 128.1 (CH), 128.2 (CH), 128.6 (CH), 129.6 (C), 130.8 (CH), 131.2 (CH), 133.0 (C), 133.4 (CH), 136.2 (C), 139.6 (C), 139.9 (C), 162.2 (C). Anal. Calcd for $\text{C}_{18}\text{H}_{16}\text{N}_6$: C, 68.34; H, 5.10; N, 26.56. Found: C, 68.62; H, 4.86; N, 26.82.

Further elution with DCM/Ethyl acetate 8/2 gave **5-(2-azidoethyl)-2-methylisindolo[2,1-*a*]quinoxalin-6(5*H*)-imine (8d).** Yellow solid; yield: 50%; mp 161 °C; IR (CHBr_3) ν 3442 (NH), 2256 (N_3), 1729 (C=NH) cm^{-1} ; ^1H NMR (200 MHz, CDCl_3) δ 2.98 (s, 3H, CH_3), 3.82 (t, J 4.9 Hz, 2H, CH_2), 5.08 (t, J 4.9 Hz, 2H, CH_2), 7.67-8.04 (m, 5H, Ar-H), 8.17 (dd, J 2.5, 7.5 Hz, 1H, Ar-H), 8.43 (dt, J 0.8, 8.0 Hz, 1H, Ar-H), 9.26 (dt, J 0.8, 8.0 Hz, 1H, Ar-H), 11.33 (br, 1H, NH); ^{13}C NMR (50 MHz, CDCl_3) δ 18.0 (CH_3), 50.3 (CH_2), 66.4 (CH_2), 122.6 (CH), 124.7 (CH), 125.3 (CH), 127.2 (CH), 129.1 (CH), 130.2 (CH), 130.6 (CH), 132.4 (CH), 135.1 (C), 137.1 (C),

137.4 (C) 141.4 (C), 142.6 (C), 146.7 (C), 162.7 (C). Anal. Calcd for $C_{18}H_{16}N_6$: C, 68.34; H, 5.10; N, 26.56. Found: C, 68.72; H, 5.02; N, 26.73.

General procedure for the preparation of substituted *N*-(isoindolo[2,1-*a*]quinoxalin-6-yl)ethane-1,2-diamines (9a-d) and 2-(6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethanamines (10a-d). To a mixture of propane-1,3-dithiol (0.90 mmol, 0.09 mL) and triethylamine (0.90 mmol, 0.13 mL) a solution of the proper *N*-(2-azidoethyl)isoindolo[2,1-*a*]quinoxalin-6-amine **7a-d** or 5-(2-azidoethyl)isoindolo[2,1-*a*]quinoxalin-6(5*H*)-imine **8a-d** (0.30 mmol) in anhydrous methanol (3 mL) was added under argon atmosphere. The reaction mixture was stirred at room temperature for 24 hours then the solvent was evaporated under reduced pressure and the obtained residue was purified by chromatography eluting with DCM/Ethyl acetate 8/2 to give derivatives **9a-d** and **10a-d**.

***N*-(Isoindolo[2,1-*a*]quinoxalin-6-yl)ethane-1,2-diamine (9a).** White solid; yield: 58%; mp 177 °C; IR (CHBr₃) ν 3688, 3557 (NH₂), 3370 (NH) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.73-3.79 (m, 2H, CH₂), 4.78 (t, *J* 6.2 Hz, 2H, CH₂), 7.77-8.07 (m, 6H, Ar-H), 8.20 (dd, *J* 1.3, 8.1 Hz, 1H, Ar-H), 8.39 (dd, *J* 1.3, 8.1 Hz, 1H, Ar-H), 8.86 (dd, *J* 1.0, 7.9 Hz, 1H, Ar-H), 11.23 (br, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 39.6 (CH₂), 48.1 (CH₂), 124.1 (CH), 127.1 (C), 127.5 (CH), 127.6 (C), 128.1 (CH), 128.6 (CH), 128.8 (CH), 129.8 (CH), 131.2 (CH), 131.7 (CH), 132.4 (C), 133.8 (CH), 138.6 (C), 140.3 (C), 161.2 (C). Anal. Calcd for $C_{17}H_{16}N_4$: C, 73.89; H, 5.84; N, 20.27. Found: C, 74.15; H, 6.02; N, 20.53.

***N*-(3-Methoxyisoindolo[2,1-*a*]quinoxalin-6-yl)ethane-1,2-diamine (9b).** White solid; yield: 60%; mp 192.4 °C; IR (CHBr₃) ν 3440, 3429 (NH₂), 3398 (NH) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.73-3.79 (m, 2H, CH₂), 3.97 (s, 3H, OCH₃), 4.75 (t, *J* 6.3 Hz, 2H, CH₂), 7.32 (d, *J* 2.8 Hz, 1H, Ar-H), 7.41 (dd, *J* 2.8, 9.1 Hz, 1H, Ar-H), 7.79-8.06 (m, 4H, Ar-H), 8.35 (dd, *J* 0.8, 7.5 Hz, 1H, Ar-H), 8.77 (dd, *J* 0.8, 7.5 Hz, 1H, Ar-H), 11.25 (br, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 56.0 (CH₃), 39.5 (CH₂), 48.1 (CH₂), 105.6 (CH), 121.7 (CH), 123.6 (CH), 126.5 (C), 128.0 (CH), 128.7 (CH), 130.0 (CH), 130.9 (CH), 132.6 (C), 132.7 (C), 133.6 (CH), 134.6 (C), 142.2 (C), 143.6 (C), 161.5 (C). Anal. Calcd for $C_{18}H_{18}N_4O$: C, 70.57; H, 5.92; N, 18.29. Found: C, 70.32; H, 5.62; N, 18.52.

***N*-(2,3-Dichloroisoindolo[2,1-*a*]quinoxalin-6-yl)ethane-1,2-diamine (9c).** Brown solid; yield: 60%; mp 164 °C; IR (CHBr₃) ν 3671, 3584 (NH₂), 3419 (NH) cm⁻¹; ¹H NMR (200 MHz, CDCl₃) δ 3.76-3.80 (m, 2H, CH₂), 4.92 (t, *J* 6.4 Hz, 2H, CH₂), 7.78-7.97 (m, 3H, Ar-H), 8.20 (s, 1H, Ar-H), 8.32 (s, 1H, Ar-H), 8.54 (dd, *J* 1.2, 7.4 Hz, 1H, Ar-H), 8.92 (d, *J* 1.2 Hz, 1H, Ar-H), 11.25 (br, 1H, NH); ¹³C NMR (50 MHz, CDCl₃) δ 40.0 (CH₂), 48.7 (CH₂), 119.1 (C), 124.8 (CH), 127.5 (C), 128.6 (CH), 128.8 (CH), 129.5 (CH), 129.6 (CH), 131.9 (CH), 132.4 (C), 132.9 (C), 133.7 (CH), 135.5 (C), 138.1 (C), 139.7 (C), 161.9 (C). Anal. Calcd for $C_{17}H_{14}Cl_2N_4$: C, 59.14; H, 4.09; N, 16.23. Found: C, 58.86; H, 4.15; N, 16.47.

***N*-(2-Methylisoindolo[2,1-*a*]quinoxalin-6-yl)ethane-1,2-diamine (9d).** Yellow solid; yield: 64%; mp 168 °C; IR (CHBr₃) ν 3689, 3567 (NH₂), 3372 (NH) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 2.73 (s, 3H, CH₃), 3.78-3.83 (m, 2H, CH₂), 4.78 (t, *J* 6.4 Hz, 2H, CH₂), 7.62-8.05 (m, 6H, Ar-H), 8.40 (dd, *J* 0.9, 7.8 Hz, 1H, Ar-H), 8.85 (dd, *J* 0.9, 7.8 Hz, 1H, Ar-H), 11.24 (br,

1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 16.7 (CH₃), 39.6 (CH₂), 47.8 (CH₂), 124.0 (CH), 126.6 (CH), 127.1 (C), 127.5 (CH), 128.2 (CH), 129.8 (CH), 130.8 (CH), 131.5 (CH), 132.3 (C), 133.6 (CH), 135.5 (C), 138.5 (C), 139.1 (C), 142.2 (C), 161.1 (C). Anal. Calcd for C₁₈H₁₈N₄: C, 74.46; H, 6.25; N, 19.30. Found: C, 74.72; H, 6.01; N, 19.07.

2-(6-Iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethanamine (9a). White solid; yield: 72%; mp 194 °C; IR (CHBr₃) ν 3679, 3556 (NH₂), 3393 (NH), 1719 (C=NH) cm⁻¹; ¹H NMR (200 MHz, CDCl₃) δ 3.83 (t, *J* 4.9 Hz, 2H, CH₂), 5.05 (t, *J* 4.9 Hz, 2H, CH₂), 7.80-7.92 (m, 4H, Ar-H), 8.01 (td, *J* 1.4, 7.3 Hz, 1H, Ar-H), 8.27-8.35 (m, 2H, Ar-H), 8.43 (dd, *J* 0.8, 7.9 Hz, 1H, Ar-H), 9.25 (dd, *J* 0.8, 7.9 Hz, 1H, Ar-H), 11.32 (br, 1H, NH); ¹³C NMR (50 MHz, CDCl₃) δ 50.2 (CH₂), 66.5 (CH₂), 124.6 (CH), 125.2 (CH), 125.3 (CH), 129.1 (C), 129.2 (C), 129.2 (CH), 129.3 (CH), 129.4 (CH), 129.5 (C), 129.7 (C), 130.4 (CH), 130.9 (CH), 132.2 (C), 132.8 (CH), 136.8 (C). Anal. Calcd for C₁₇H₁₆N₄: C, 73.89; H, 5.84; N, 20.27. Found: C, 73.96; H, 6.01; N, 19.93.

2-(6-Imino-3-methoxyisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethanamine (9b). White solid; yield: 62%; mp 198.8 °C; IR (CHBr₃) ν 3584, 3437 (NH₂), 3319 (NH), 1666 (C=NH) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.77 (t, *J* 6.2 Hz, 2H, CH₂), 3.98 (s, 3H, OCH₃), 4.77 (t, *J* 6.2 Hz, 2H, CH₂), 7.35-7.46 (m, 2H, Ar-H), 7.70-8.09 (m, 4H, 4 x Ar-H), 8.37 (d, *J* 7.5 Hz, 1H, Ar-H), 8.80 (d, *J* 7.5 Hz, 1H, Ar-H), 11.30 (br, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 39.5 (CH₂), 48.1 (CH₂), 56.0 (CH₃), 105.6 (CH), 121.6 (CH), 123.6 (CH), 126.4 (C), 128.0 (CH), 129.9 (CH), 130.9 (CH), 131.7 (CH), 132.5 (C), 132.6 (C), 133.6 (CH), 134.5 (C), 142.2 (C), 143.6 (C), 161.2 (C). Anal. Calcd for C₁₈H₁₈N₄O: C, 70.57; H, 5.92; N, 18.29. Found: C, 70.83; H, 5.68; N, 18.01.

2-(2,3-Dichloro-6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethanamine (9c). Brown solid; yield: 78%; mp 182 °C; IR (CHBr₃) ν 3679, 3558 (NH₂), 3393 (NH), 1719 (C=NH) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.92 (t, *J* 5.0 Hz, 2H, CH₂), 4.90 (t, *J* 5.0 Hz, 2H, CH₂), 7.94-8.14 (m, 3H, Ar-H), 8.35 (d, *J* 8.1 Hz, 1H, Ar-H), 8.47 (s, 1H, Ar-H), 8.57 (s, 1H, Ar-H), 9.05 (d, *J* 8.1 Hz, 1H, Ar-H), 11.31 (br, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 50.1 (CH₂), 66.8 (CH₂), 122.9 (C), 124.9 (CH), 125.6 (CH), 129.4 (CH), 129.7 (CH), 131.4 (CH), 132.9 (CH), 133.9 (C), 134.5 (C), 135.2 (C), 139.8 (C), 141.8 (C), 143.1 (CH), 163.6 (C), 164.5 (C). Anal. Calcd for C₁₇H₁₄Cl₂N₄: C, 59.14; H, 4.09; N, 16.23. Found: C, 59.41; H, 4.36; N, 16.02.

2-(6-Imino-2-methylisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethanamine (9d). Yellow solid; yield: 64%; mp 189.6 °C; IR (CHBr₃) ν 3604, 3501 (NH₂), 3407 (NH), 1713 (C=NH) cm⁻¹; ¹H NMR (200 MHz, CDCl₃) δ 2.98 (s, 3H, CH₃), 3.82 (t, *J* 4.9 Hz, 2H, CH₂), 5.08 (t, *J* 4.9 Hz, 2H, CH₂), 7.60-7.80 (m, 3H, Ar-H), 7.87 (td, *J* 2.4, 7.4 Hz, 1H, Ar-H), 8.00 (td, *J* 1.4, 7.9 Hz, 1H, Ar-H), 8.17 (dd, *J* 2.4, 7.4 Hz, 1H, Ar-H), 8.43 (dd, *J* 1.3, 8.1 Hz, 1H, Ar-H), 9.25 (d, *J* 7.8 Hz, 1H, Ar-H), 11.39 (br, 1H, NH); ¹³C NMR (50 MHz, CDCl₃) δ 18.0 (CH₃), 29.7 (CH₂), 50.3 (CH₂), 122.6 (CH), 124.7 (CH), 125.3 (CH), 127.2 (CH), 129.1 (CH), 130.2 (CH), 130.6 (CH), 132.4 (CH), 135.0 (C), 137.1 (C), 137.4 (C), 141.4 (C), 142.6 (C), 146.7 (C), 162.8 (C). Anal. Calcd for C₁₈H₁₈N₄: C, 74.46; H, 6.25; N, 19.30. Found: C, 74.82; H, 6.17; N, 19.01.

General procedure for the preparation of substituted 1-(5-bromopyridin-2-yl)-3-[2-(isoindolo[2,1-*a*]quinoxalin-6-ylamino)ethyl]thioureas (3a-d) and 1-(5-bromopyridin-2-yl)-

3-[2-(6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thioureas (4a-d). To a suspension of 5-bromo-2-isothiocyanatopyridine⁴¹ (4.0 mmol) in DMF (15 mL) the suitable *N*-(isoindolo[2,1-*a*]quinoxalin-6-yl)ethane-1,2-diamine **9a-d** or 2-(6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethanamine **10a-d** (1.0 mmol) was added and the reaction was stirred at 100 °C for 16 hours. Then the reaction mixture was cooled to room temperature, poured into iced water and the resulting precipitate collected by filtration. The crude obtained was purified by column chromatography to give derivatives **3a-d** and **4a-d**.

1-(5-Bromopyridin-2-yl)-3-[2-(isoindolo[2,1-*a*]quinoxalin-6-ylamino)ethyl]thiourea (3a).

The residue eluted with DCM/Ethyl acetate 9/1. White solid; yield: 65%; mp 198 °C; IR (CHBr₃) ν 3678 (NH), 3563 (NH), 3403 (NH), 1328 (C=S) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.19-4.22 (m, 2H, CH₂), 4.89-4.91 (m, 2H, CH₂), 6.76 (d, *J* 9.1 Hz, 1H, Ar-H), 7.67-7.69 (m, 2H, Ar-H), 7.71-7.87 (m, 3H, Ar-H), 7.84-7.92 (m, 2H, Ar-H), 7.99-8.03 (m, 1H, Ar-H), 8.06-8.13 (m, 1H, Ar-H), 8.35 (d, *J* 7.5 Hz, 1H, Ar-H), 8.89 (d, *J* 7.5 Hz, 1H, Ar-H), 10.42 (br, 1H, NH), 10.62 (br, 1H, NH), 11.21 (t, *J* 4.9 Hz, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 40.3 (CH₂), 42.8 (CH₂), 111.5 (C), 113.8 (CH), 113.9 (CH), 124.0 (CH), 127.4 (CH), 127.9 (CH), 128.2 (CH), 128.5 (CH), 130.7 (CH), 131.4 (CH), 132.4 (C), 133.4 (CH), 135.4 (C), 138.2 (C), 140.0 (C), 140.7 (CH), 144.0 (C), 145.2 (CH), 151.7 (C), 161.4 (C), 180.0 (C). Anal. Calcd for C₂₃H₁₉BrN₆S: C, 56.22; H, 3.90; N, 17.10. Found: C, 56.39; H, 3.76; N, 17.43.

1-(5-Bromopyridin-2-yl)-3-{2-[(3-methoxyisoindolo[2,1-*a*]quinoxalin-6-yl)amino]ethyl}thiourea (3b).

The residue eluted with DCM/Ethyl acetate 9/1. White solid; yield: 63%; mp 239 °C; IR (CHBr₃) ν 3688 (NH), 3584 (NH), 3405 (NH), 1360 (C=S) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.37 (s, 3H, OCH₃), 4.62-4.64 (m, 2H, CH₂), 5.30-5.36 (m, 2H, CH₂), 7.20 (d, *J* 8.6 Hz, 1H, Ar-H), 7.58 (d, *J* 2.7 Hz, 1H, Ar-H), 7.78 (dd, *J* 2.7, 8.6 Hz, 1H, Ar-H), 8.09-8.31 (m, 4H, Ar-H), 8.38-8.46 (m, 2H, Ar-H), 8.77 (d, *J* 7.9 Hz, 1H, Ar-H), 9.25 (d, *J* 7.9 Hz, 1H, Ar-H), 10.72 (br, 1H, NH), 10.86 (br, 1H, NH), 11.64 (t, *J* 4.7 Hz, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 40.7 (CH₂), 43.9 (CH₂), 56.7 (CH₃), 106.2 (CH), 112.4 (CH), 114.8 (CH), 122.3 (CH), 124.5 (CH), 127.7 (C), 128.8 (CH), 130.6 (CH), 131.6 (CH), 133.4 (C), 133.7 (C), 134.3 (CH), 135.1 (C), 141.6 (CH), 142.9 (C), 145.1 (C), 146.1 (CH), 152.6 (C), 162.1 (C), 162.4 (C), 180.9 (C). Anal. Calcd for C₂₄H₂₁BrN₆OS: C, 55.28; H, 4.06; N, 16.12. Found: C, 55.52; H, 3.86; N, 16.42.

1-(5-Bromopyridin-2-yl)-3-{2-[(2,3-dichloroisoindolo[2,1-*a*]quinoxalin-6-yl)amino]ethyl}thiourea (3c).

The residue eluted with DCM. Pale yellow solid; yield: 85%; mp 235 °C; IR (CHBr₃) ν 3671 (NH), 3558 (NH), 3414 (NH), 1311 (C=S) cm⁻¹; ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.19-4.23 (m, 2H, CH₂), 4.86-4.88 (m, 2H, CH₂), 6.77 (d, *J* 8.8 Hz, 1H, Ar-H), 7.68-7.75 (m, 2H, Ar-H), 7.84 (s, 1H, Ar-H), 7.89-8.08 (m, 3H, Ar-H), 8.35-8.39 (m, 2H, Ar-H), 8.83 (d, *J* 7.7 Hz, 1H, Ar-H), 10.01 (br, 1H, NH), 10.43 (br, 1H, NH), 11.18 (t, *J* 4.9 Hz, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 40.1 (CH₂), 42.9 (CH₂), 111.7 (CH), 113.8 (CH), 121.9 (C), 124.2 (CH), 127.7 (CH), 127.9 (CH), 128.0 (C), 129.1 (CH), 129.4 (C), 130.5 (C), 131.9 (C), 132.1 (CH), 133.2 (C), 133.6 (CH), 137.0 (C), 138.8 (C), 140.7 (CH), 145.1 (C), 145.2 (CH), 147.7

(C), 181.7 (C). Anal. Calcd for $C_{23}H_{17}BrCl_2N_6S$: C, 49.30; H, 3.06; N, 15.00. Found: C, 49.02; H, 3.33; N, 14.72.

1-(5-Bromopyridin-2-yl)-3-[2-[(2-methylisoindolo[2,1-*a*]quinoxalin-6-yl)amino]ethyl]thiourea (3d). The residue eluted with DCM/Ethyl acetate 98/2. Pale yellow solid; yield: 75%; mp 230 °C; IR (CHBr₃) ν 3757 (NH), 3570 (NH), 3406 (NH), 1297 (C=S) cm^{-1} ; ¹H NMR (200 MHz, DMSO-*d*₆) δ 2.71 (s, 3H, CH₃), 4.23-4.25 (m, 2H, CH₂), 4.90-4.95 (m, 2H, CH₂), 6.77 (d, *J* 8.9 Hz, 1H, Ar-H), 7.44 (d, *J* 2.4 Hz, 1H, Ar-H), 7.60-7.67 (m, 3H, Ar-H), 7.85-8.13 (m, 4H, Ar-H), 8.38 (d, *J* 7.8 Hz, 1H, Ar-H), 8.89 (d, *J* 7.9 Hz, 1H, Ar-H), 10.47 (br, 1H, NH), 10.62 (br, 1H, NH), 11.12 (t, *J* 5.8 Hz, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 16.7 (CH₃), 42.7 (CH₂), 59.7 (CH₂), 111.5 (CH), 113.8 (CH), 123.9 (CH), 126.2 (CH), 127.4 (CH), 127.9 (CH), 131.3 (CH), 132.4 (CH), 133.4 (CH), 134.9 (C), 135.5 (C), 138.2 (C), 139.0 (C), 140.7 (CH), 141.4 (C), 142.9 (C), 144.9 (CH), 151.6 (C), 161.4 (C), 170.3 (C), 179.9 (C). Anal. Calcd for $C_{24}H_{21}BrN_6S$: C, 57.03; H, 4.19; N, 16.63. Found: C, 56.82; H, 4.49; N, 16.32.

1-(5-Bromopyridin-2-yl)-3-[2-(6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thiourea (4a). The residue eluted with DCM/Ethyl acetate 9/1. Pale yellow solid; yield: 68%; mp 205 °C; IR (CHBr₃) ν 3670 (NH), 3557 (NH), 1704 (C=NH), 1323 (C=S) cm^{-1} ; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.74-3.80 (m, 2H, CH₂), 4.80 (t, *J* 6.1 Hz, 2H, CH₂), 7.38 (d, *J* 8.0 Hz, 1H, Ar-H), 7.83-7.95 (m, 3H, Ar-H), 8.01-8.10 (m, 2H, Ar-H), 8.16-8.25 (m, 3H, Ar-H), 8.42 (d, *J* 8.0 Hz, 1H, Ar-H), 8.61 (d, *J* 2.5 Hz, 1H, Ar-H), 8.90 (d, *J* 8.0 Hz, 1H, Ar-H), 10.25 (br, 1H, NH), 11.30 (br, 1H, NH), 11.38 (t, *J* 5.3 Hz, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 39.7 (CH₂), 48.1 (CH₂), 118.9 (C), 121.7 (CH), 124.1 (CH), 127.1 (C), 127.5 (C), 127.6 (CH), 127.9 (CH), 128.1 (CH), 128.6 (CH), 128.8 (CH), 131.2 (CH), 131.7 (CH), 132.4 (C), 133.7 (CH), 135.6 (C), 138.5 (C), 140.2 (C), 142.1 (CH), 143.5 (C), 150.7 (CH), 161.2 (C). Anal. Calcd for $C_{23}H_{19}BrN_6S$: C, 56.22; H, 3.90; N, 17.10. Found: C, 56.38; H, 4.07; N, 16.88.

1-(5-Bromopyridin-2-yl)-3-[2-(6-imino-3-methoxyisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thiourea (4b). The residue eluted with DCM/Ethyl acetate 9/1. White solid; yield: 67%; mp 243 °C; IR (CHBr₃) ν 3680 (NH), 3558 (NH), 1696 (C=NH), 1297 (C=S) cm^{-1} ; ¹H NMR (200 MHz, DMSO-*d*₆) δ 3.95 (s, 3H, OCH₃), 4.16-4.24 (m, 2H, CH₂), 4.90 (t, *J* 5.1 Hz, 2H, CH₂), 6.77 (d, *J* 8.6 Hz, 1H, Ar-H), 7.15 (d, *J* 2.7 Hz, 1H, Ar-H), 7.35 (dd, *J* 2.7, 8.6 Hz, 1H, Ar-H), 7.67-7.74 (m, 2H, Ar-H), 7.84 (t, *J* 7.4 Hz, 1H, Ar-H), 7.95-8.10 (m, 3H, Ar-H), 8.35 (d, *J* 7.4 Hz, 1H, Ar-H), 8.83 (d, *J* 7.4 Hz, 1H, Ar-H), 10.44 (br, 1H, NH), 11.22 (t, *J* 5.4 Hz, 1H, NH), 11.28 (br, 1H, NH); ¹³C NMR (50 MHz, DMSO-*d*₆) δ 39.7 (CH₂), 43.0 (CH₂), 55.8 (CH₃), 105.2 (CH), 111.5 (C), 113.8 (CH), 121.3 (CH), 123.5 (CH), 126.8 (C), 127.8 (CH), 127.9 (CH), 129.6 (CH), 130.7 (CH), 132.5 (C), 132.7 (C), 133.3 (CH), 134.2 (C), 140.7 (CH), 141.9 (C), 144.1 (C), 145.2 (CH), 151.7 (C), 161.1 (C), 161.4 (C). Anal. Calcd for $C_{24}H_{21}BrN_6OS$: C, 55.28; H, 4.06; N, 16.12. Found: C, 55.53; H, 3.85; N, 16.42.

1-(5-Bromopyridin-2-yl)-3-[2-(2,3-dichloro-6-iminoisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thiourea (4c). The residue eluted with DCM. Pale yellow solid; yield: 78%; mp 228 °C; IR (CHBr₃) ν 3576 (NH), 3394 (NH), 1669 (C=NH), 1297 (C=S) cm^{-1} ; ¹H NMR (200 MHz, DMSO-*d*₆) δ 4.15-4.20 (m, 2H, CH₂), 4.87 (t, *J* 5.6 Hz, 2H, CH₂), 6.77 (d, *J* 8.4 Hz, 1H, Ar-H),

7.67-7.75 (m, 2H, 2 x Ar-H), 7.84 (s, 1H, Ar-H), 7.85-8.08 (m, 3H, Ar-H), 8.35-8.39 (m, 2H, Ar-H), 8.83 (d, J 7.0 Hz, 1H, Ar-H), 10.27 (br, 1H, NH), 10.43 (br, 1H, NH), 11.18 (t, J 5.6 Hz, 1H, NH); ^{13}C NMR (50 MHz, DMSO- d_6) δ 40.1 (CH_2), 42.9 (CH_2), 111.7 (C), 113.8 (CH), 116.4 (CH), 117.1 (C), 118.3 (C), 124.2 (CH), 127.7 (CH), 127.8 (CH), 128.0 (C), 129.1 (CH), 130.6 (C), 132.0 (CH), 133.2 (C), 133.6 (CH), 136.9 (C), 138.8 (C), 140.7 (CH), 145.1 (CH), 147.6 (C), 151.1 (C), 161.5 (C). Anal. Calcd for $\text{C}_{23}\text{H}_{17}\text{BrCl}_2\text{N}_6\text{S}$: C, 49.30; H, 3.06; N, 15.00. Found: C, 49.17; H, 3.34; N, 15.32.

1-(5-Bromopyridin-2-yl)-3-[2-(6-imino-2-methylisoindolo[2,1-*a*]quinoxalin-5(6*H*)-yl)ethyl]thiourea (4d). The residue eluted with DCM. Pale yellow solid; yield: 81%; mp 241 °C; IR (CHBr_3) ν 3570 (NH), 3384 (NH), 1674 ($\text{C}=\text{NH}$), 1343 ($\text{C}=\text{S}$) cm^{-1} ; ^1H NMR (200 MHz, CDCl_3) δ 2.78-2.80 (m, 5H, CH_2CH_3), 3.43-3.47 (m, 2H, CH_2), 7.61-7.64 (m, 2H, Ar-H), 7.77-8.05 (m, 6H, Ar-H), 8.42-8.54 (m, 3H, Ar-H), 9.01 (t, J 5.0 Hz, 1H, NH), 9.22 (br, 1H, NH), 9.27 (br, 1H, NH); ^{13}C NMR (50 MHz, CDCl_3) δ 17.3 (CH_3), 24.8 (CH_2), 29.7 (CH_2), 77.2 (CH), 108.3 (C), 115.4 (C), 120.1 (CH), 124.8 (CH), 127.3 (CH), 128.0 (CH), 128.3 (CH), 130.9 (CH), 131.2 (CH), 133.6 (CH), 133.9 (C), 134.7 (CH), 135.9 (C), 140.5 (C), 140.9 (CH), 141.9 (C), 149.4 (C), 154.8 (C), 162.1 (C), 165.1 (C). Anal. Calcd for $\text{C}_{24}\text{H}_{21}\text{BrN}_6\text{S}$: C, 57.03; H, 4.19; N, 16.63. Found: C, 56.83; H, 4.43; N, 16.91.

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