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Iodine-catalyzed synthesis of pyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid derivatives in ionic liquids

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Abstract The iodine-catalyzed reaction of 2-aminobenzamide and 2-oxopentanedioic acid in ionic liquids is described in this paper. It gave 1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid derivatives in high yields. One of their structures was confirmed by X-ray diffraction analysis.

Keywords Pyrroloquinazoline · 2-aminobenzamide · Ionic liquid · Iodine · Synthesis

Introduction

Pyrroloquinazoline and its derivatives are important heterocycles found in a variety of biological molecules. It is reported that they possess a wide range of biologic activities, for example, antitumor [1–3] and anti-inflammatory activity [4]. In addition, some of them are used as thrombin receptor antagonists [5–7] and modulators of chemokine [8]. Therefore, much attention has been devoted to the synthesis of these active heterocyclic compounds both in organic synthesis and in pharmaceutical chemistry. In general, they could be achieved by a three-component reaction of isatoic anhydride, amine, and 2-formylbenzoic acid [9], or coupling cyclization of 2-aminobenzamide with 3-butynoic acid catalyzed by platinum salt [10, 11], or reduction reaction of 2-nitrobenzamide with γ-ketonic acid or

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halogenated ketone in the presence of $SnCl_2$ [12, 13], or condensation cyclization of 2-aminobenzamide with γ-ketone acid ester [14].

Although these reported reactions [9–14] have developed some useful synthetic procedures, several limitations still remain. For example, most of the procedures involve several steps, or low yields, or metal catalysts, or inorganic solvents. Thus, simple, efficient, and green methods to synthesize pyrroloquinazoline would be attractive.

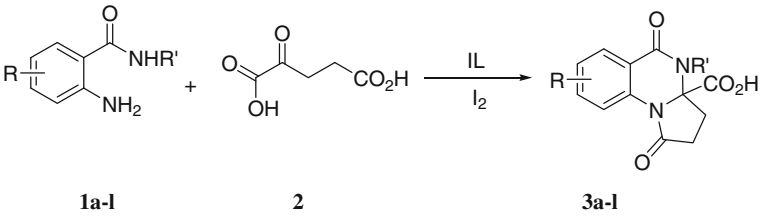
Ionic liquid containing catalytic iodine is a green system, because the ionic liquids have attracted increasing interest in the context of green chemistry in the past few years for a large number of organic transformations [15, 16]. In addition, iodine is also a novel and green Lewis metal-free catalyst for many organic reactions in recent years [17]. As a continuation of our research devoted to prepare heterocycles in ionic liquid and with iodine-catalyzed reaction [18, 19], we would like to report the synthesis of pyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid derivatives in ionic liquids. This method involves the reaction of 2-aminobenzamides with 2-oxopentanedioic acid catalyzed by iodine.

Results and discussion

The treatment of 2-aminobenzamides **1a–l** and 2-oxopentanedioic acid **2** in ionic liquid of [BMIm]Br in the presence of 5 mol% iodine at 80 °C resulted in the corresponding 1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid derivatives **3a–l** in high yields (Scheme 1).

Using the conversion of 2-aminobenzamide **1a** and 2-oxopentanedioic acid **2** as a model reaction, several parameters, such as Lewis acids, catalyst amount, reaction temperature, and ionic liquids, were explored as shown in Table 1. **3a** was obtained successfully in the presence of various quantities of the catalyst, reaching a maximum of 86 % yield, using 5 mol% iodine as a catalyst (Table 1, entry 4). Different imidazolium ionic liquids and Lewis acids were also tested, and the iodine-[BMIm]Br system appeared to be the best medium for this transformation.

First of all, these optimized conditions were applied for the conversion of various kinds of 2-aminobenzamides **1a–l** into the corresponding pyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid analogs (Table 2, entries 1–12). Entries 1–12 demonstrate that the reactions also tolerate significant functionalization of the 2-aminobenzamides **1**; both electron-donating (such as alkyl and alkoxyl group) and electron-withdrawing



Scheme 1 The reaction of 2-aminobenzamides and 2-oxopentanedioic acid

Table 1 Synthetic results of **3a** under different reaction conditions

Entry	T/ °C	Ionic liquid	Cat. (mol%)	Yield (%)[a]
1	80	[BMIm]Br	I_2(0)	0
2	r.t.	[BMIm]Br	I_2(5)	Trace
3	50	[BMIm]Br	I_2(5)	80
4	**80**	**[BMIm]Br**	**I_2(5)**	**86**
5	100	[BMIm]Br	I_2(5)	86
6	80	[BMIm]Br	I_2(1)	78
7	80	[BMIm]Br	I_2(10)	86
8	80	[EMIm]Br	I_2(5)	82
9	80	[PMIm]Br	I_2(5)	82
10	80	[EMIm][BF_4]	I_2(5)	85
11	80	[PMIm][BF_4]	I_2(5)	84
12	80	[BMIm][BF_4]	I_2(5)	82
13	80	[BMIm]Br	CuI(5)	Trace
14	80	[BMIm]Br	$ZnCl_2$(5)	Trace
15	80	[BMIm]Br	$Yb(OTf)_3$(5)	79

Reaction conditions: ionic liquids (2.0 mL), 2-aminobenzamide (0.272 g, 2.0 mmol), **2** (0.292 g, 2.0 mmol)

BMIm 1-butyl-3-methylimidazolium, *EMIm* 1-ethyl-3-methylimidazolium, *PMIm* 1-propyl-3-methylimidazolium

[a] Isolated yields

Bold value indicates the best reaction condition

(such as halide) groups can be accommodated, and aliphatic groups can all be generated. They all reacted well to provide a library of pyrrolo[1,2-*a*]quinazoline derivatives **3a–l** (Table 2). All the structures of the products were characterized by ^{1}H NMR, IR, and HRMS, and their data were in good agreement with the preconceived structures. Of which, the structure of **3a** was further confirmed by X-ray diffraction analysis, indicating that there are two independent molecules in a unit and one of them is shown in Fig. 1.

The X-ray diffraction analysis indicates that the center pyrimidine ring is slightly distorted, and adopts a skew-boat confirmation: the atoms of C1, C6, C7, and N2 are coplanar, with the atoms of N1 and C8 deviating from the defined plane by 0.235(2) and 0.691(2) Å, respectively. The adjacent pyrrole ring adopts a typical envelope confirmation, the atom of C9 deviates from the defined plane (including atoms of C8, C10, C11, and N2) by 0.278(3) Å. It makes a dihedral angle of 30.8(1)° to the pyrimidine ring. The latter is nearly parallel to the benzene ring, forming a dihedral angle of 1.5(3)°.

The typical N–H···O and O–H···O hydrogen bonds (Table 3) are presented in the crystal structure. They link the adjacent molecules forming polymers along the *a*-axis (Fig. 2).

According to the structure of product **3**, we hypothesize that the subsequent condensation, cyclization, and intra-molecular dehydration reactions may take place. The possible reaction mechanism is outlined in Scheme 2.

Experimental

Melting points were determined in open capillaries and are uncorrected. IR spectra were recorded on a Tensor 27 spectrometer in KBr pellet. ^{1}H NMR spectra were

Table 2 The reaction time and yields of the products **3a–l**

Entry	R	R′	Product	Time (h)	Yields (%)
1	H	H	**3a**	6	86
2	H	4-MeC_6H_4	**3b**	8	82
3	H	4-$MeOC_6H_4$	**3c**	8	89
4	H	4-FC_6H_4	**3d**	5	79
5	H	4-*i*-PrC_6H_4	**3e**	9	85
6	H	3-Cl-4-FC_6H_3	**3f**	10	80
7		C_6H_5	**3g**	8	88
8	H	4-*n*-BuC_6H_4	**3h**	8	92
9	H	$C_6H_5CH_2$	**3i**	6	90
10	5-Br	H	**3j**	6	86
11	5-Me	H	**3k**	8	90
12	5-Cl	$C_6H_5CH_2CH_2$	**3l**	6	87

Reaction conditions: 2-aminobenzamides **1** (2.0 mmol), **2** (0.307 g, 2.1 mmol), iodine (0.025 g, 0.1 mmol), [BMIm]Br (2.0 mL), 80 °C

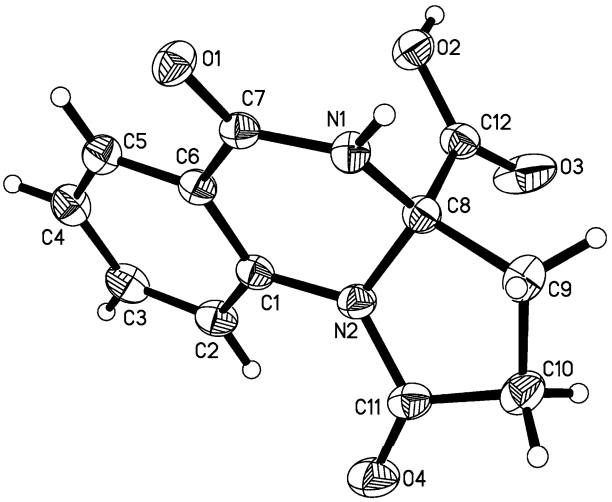


Fig. 1 The crystal structure of product **3a**

obtained from a solution in DMSO-d_6 or $CDCl_3$ with Me_4Si as the internal standard using a Bruker 400 spectrometer. HRMS analyses were carried out using a Bruker micrOTOF-Q MS analyzer.

General procedure for the synthesis of pyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid derivatives **3**

A dry 50-mL flask was charged with 2-aminobenzamides **1** (2.0 mmol), 2-oxopentanedioic acid **2** (0.307 g, 2.1 mmol), iodine (0.025 g, 0.1 mmol), and ionic liquid of [BMIm]Br (2.0 mL). The reaction mixture was stirred at 80 °C for 5–10 h. Then, a small amount of water (5 mL) was added to the mixture, and the

Table 3 The data of hydrogen bonds in **3a** (Å and °)

Entry	D–H···A	d(D–H, Å)	d(H···A, Å)	d(D···A, Å)	<(DHA, °)	Symmetry code
1	O2–H2···O1	0.879(10)	1.654(10)	2.5298(15)	174(3)	$x, -y + 3/2, z + 1/2$
2	O7–H7···O8	0.862(10)	1.793(10)	2.6533(15)	175(3)	$x, -y + 1/2, z-1/2$
3	N1–H1···O3	0.889(9)	1.955(10)	2.8345(17)	170.1(16)	$x, -y + 3/2, z-1/2$
4	N3–H3···O5	0.875(9)	1.967(10)	2.8349(16)	171.3(16)	$-x + 1, -y + 1, -z$

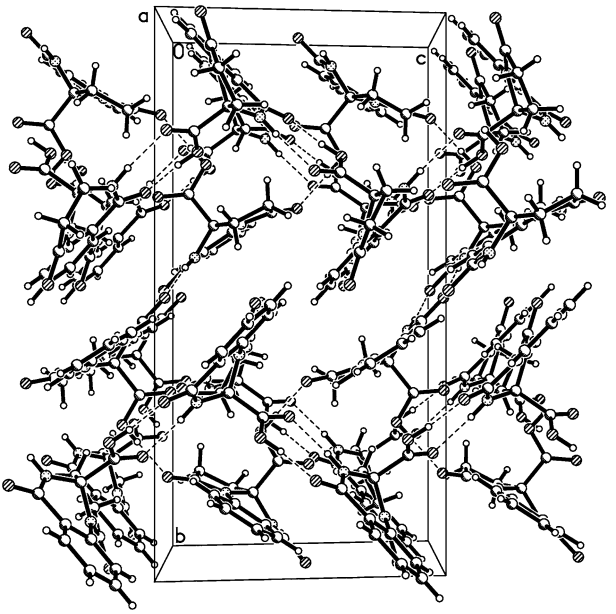
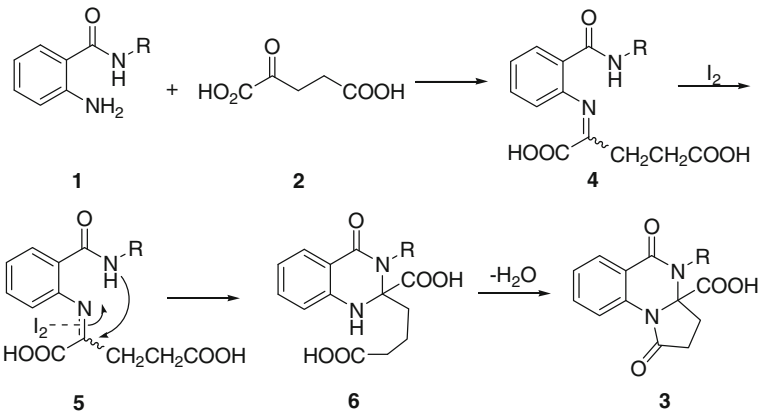


Fig. 2 The molecular packing diagram for **3a**



Scheme 2 The possible reaction mechanism for the formation of **3**

generated yellow solid was filtered off. The water in the filtrate was removed by distillation under reduced pressure, and the ionic liquid in the residue could be reusable by being evaporated at 80 °C for 4 h in a vacuum. The crude yellow products were washed with water and purified by recrystallization from 95 % EtOH, then dried at 80 °C for 2 h under vacuum to give **3**.

1,5-Dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3a**): M.p. 266 ~ 268 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ_H 2.32 ~ 2.38 (m, 1H, CH), 2.46 ~ 2.51 (m, 1H, CH), 2.65 ~ 2.70 (m, 2H, CH_2), 7.27 ~ 7.31 (m, 1H, ArH), 7.60 ~ 7.64 (m, 1H, ArH), 7.88 (d, J = 7.6 Hz, 1H, ArH), 8.15 (d, J = 8.0 Hz, 1H, ArH), 9.35 (s, 1H, NH). ^{13}C NMR (DMSO-d_6, 100 MHz): δ_C 29.0, 29.7, 75.5, 118.7, 119.4, 124.7, 127.8, 133.4, 136.1, 161.8, 172.3, 172.5. IR (KBr): v 3349, 3160, 3,054, 2,918, 1,706, 1,671, 1,605, 1,579, 1,486, 1,468, 1,393, 1,366, 1,328, 1,290, 1277, 1227, 1208, 1169, 1157, 1075, 1035, 814, 793, 764 cm^{-1}. HRMS (ESI, m/z): calcd. for $C_{12}H_9N_2O_4$ $[M - H]^-$ 245.0563, found 245.0562.

1,5-Dioxo-4-(*p*-tolyl)-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3b**): M.p. 166 ~ 168 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ_H 2.16 ~ 2.21 (m, 2H, CH_2), 2.35 (s, 3H, CH_3), 2.53 ~ 2.70 (m, 2H, CH_2), 7.26 ~ 7.32 (m, 4H, ArH), 7.34 (d, J = 7.6 Hz, 1H, ArH), 7.65 ~ 7.69 (m, 1H, ArH), 7.93 ~ 7.95 (m, 1H, ArH), 8.26 (d, J = 8.4 Hz, 1H, ArH). IR (KBr): v 3008, 2927, 1731, 1711, 1654, 1604, 1582, 1512, 1487, 1470, 1397, 1352, 1299, 1286, 1265, 1238, 1218, 1198, 1173, 1148, 1106, 1073, 808, 756, 703 cm^{-1}. HRMS (ESI, m/z): calcd. for $C_{19}H_{16}N_2O_4Na$ $[M + Na]^+$ 359.1008, found 359.1034.

4-(4-Methoxyphenyl)-1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3c**): M.p. 255 ~ 257 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ_H 2.12 ~ 2.22 (m, 2H, CH_2), 2.60 ~ 2.70 (m, 2H, CH_2), 3.80 (s, 3H, OCH_3), 7.02 (d, J = 8.8 Hz, 2H, ArH), 7.31 ~ 7.37 (m, 3H, ArH), 7.65 ~ 7.69 (m, 1H, ArH), 7.93 ~ 7.95 (m, 1H, ArH), 8.26 (d, J = 8.4 Hz, 1H, ArH). ^{13}C NMR (DMSO-d_6, 100 MHz): δ_C 27.8, 30.3, 55.9, 80.4, 114.2, 118.2, 119.8, 124.9, 128.4, 129.5, 130.5, 133.6, 135.8, 158.7, 161.8, 171.8, 172.5. IR (KBr): v 3000, 2980, 2939, 1723, 1656, 1603, 1585, 1509, 1486, 1469, 1443, 1399, 1351, 1298, 1272, 1248, 1237, 1214, 1204, 1181, 1169, 1148, 1073, 1049, 1029, 879, 836, 820, 793, 767, 720 cm^{-1}. HRMS (ESI, m/z): calcd. for $C_{19}H_{16}N_2O_5Na$ $[M + Na]^+$ 375.0957, found 375.0977.

4-(4-Fluorophenyl)-1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3d**): M.p. 243 ~ 245 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ_H 2.18 ~ 2.23 (m, 2H, CH_2), 2.58 ~ 2.70 (m, 2H, CH_2), 7.31 ~ 7.36 (m, 3H, ArH), 7.48 ~ 7.52 (m, 2H, ArH), 7.66 ~ 7.71 (m, 1H, ArH), 7.93 ~ 7.96 (m, 1H, ArH), 8.27 (d, J = 8.4 Hz, 1H, ArH). IR (KBr): v 2974, 2938, 2900, 1648, 1610, 1572, 1511, 1497, 1481, 1471, 1439, 1387, 1358, 1337, 1241, 1216, 1196, 1177, 1146, 1133, 1120, 1109, 1045, 1027, 808, 754 cm^{-1}. HRMS (ESI, m/z): calcd. for $C_{18}H_{13}FN_2O_4Na$ $[M + Na]^+$ 363.0757, found 363.0770.

4-(4-*i*-Propylphenyl)-1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3e**): M.p. 147 ~ 148 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ_H 1.24 (d, J = 6.8 Hz, 6H, $2CH_3$), 2.17 ~ 2.21 (m, 2H, CH_2), 2.58 ~ 2.72 (m, 2H, CH_2), 2.91 ~ 3.00 (m, 1H, CH), 7.32 ~ 7.37 (m, 5H, ArH), 7.66 ~ 7.69 (m, 1H, ArH), 7.94 (d, J = 8.0 Hz, 1H, ArH), 8.27 (d, J = 8.4 Hz, 1H, ArH). IR (KBr):

v 2962, 2873, 1710, 1646, 1604, 1508, 1488, 1470, 1398, 1348, 1290, 1270, 1237, 1220, 1205, 1147, 1121, 1096, 1076, 1057, 1040, 1025, 884, 826, 757 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{21}H_{20}N_2O_4Na$ $[M + Na]^+$ 387.1321, found 387.1352.

4-(3-Chloro-4-fluorophenyl)-1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3f**): M.p. 181 ~ 183 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ_H 2.19 ~ 2.30 (m, 2H, CH_2), 2.59 ~ 2.71 (m, 2H, CH_2), 7.35 (t, $J = 7.6$ Hz, 1H, ArH), 7.50 ~ 7.59 (m, 2H, ArH), 7.68 ~ 7.74 (m, 2H, ArH), 7.94 (d, $J = 7.6$ Hz, 1H, ArH), 8.27 (d, $J = 8.4$ Hz, 1H, ArH). IR (KBr): *v* 3051, 1708, 1670, 1603, 1503, 1469, 1388, 1348, 1300, 1265, 1218, 1197, 1177, 1147, 1136, 1060, 1040, 828, 812, 760 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{18}H_{11}ClFN_2O_4$ $[M - H]^-$ 373.0392, found 373.0410.

1,5-Dioxo-4-phenyl-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3g**): M.p. 234 ~ 235 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ_H 2.13 ~ 2.24 (m, 2H, CH_2), 2.63 ~ 2.71 (m, 2H, CH_2), 7.33 ~ 7.36 (m, 1H, ArH), 7.37 ~ 7.39 (m, 3H, ArH), 7.42 ~ 7.47 (m, 2H, ArH), 7.66 ~ 7.71 (m, 1H, ArH), 7.95 (d, $J = 6.8$ Hz, 1H, ArH), 8.27 (d, $J = 8.0$ Hz, 1H, ArH). ^{13}C NMR (DMSO-d_6, 100 MHz): δ_C 27.8, 30.3, 80.3, 112.7, 112.8, 118.2, 119.7, 124.9, 128.0, 129.1, 133.8, 135.7, 137.0, 161.6, 171.8, 172.5. IR (KBr): *v* 3076, 2963, 2938, 1723, 1655, 1601, 1575, 1491, 1469, 1453, 1400, 1349, 1303, 1274, 1238, 1214, 1203, 1184, 1160, 1122, 1100, 1073, 1032, 884, 766, 755 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{18}H_{13}N_2O_4$ $[M - H]^-$ 321.0876, found 321.0916.

4-(4-*n*-Butylphenyl)-1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3h**): M.p. 212 ~ 213 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ_H 0.92 (t, $J = 7.2$ Hz, 3H, CH_3), 1.29 ~ 1.37 (m, 2H, CH_2), 1.55 ~ 1.63 (m, 2H, CH_2), 2.17 ~ 2.22 (m, 2H, CH_2), 2.61 ~ 2.64 (m, 3H, CH + CH_2), 2.67 ~ 2.72 (m, 1H, CH), 7.28 ~ 7.32 (m, 4H, ArH), 7.35 (d, $J = 7.6$ Hz, 1H, ArH), 7.66 ~ 7.69 (m, 1H, ArH), 7.94 (d, $J = 8.0$ Hz, 1H, ArH), 8.26 (d, $J = 8.0$ Hz, 1H, ArH). IR (KBr): *v* 3089, 3052, 2962, 2933, 2857, 1736, 1724, 1635, 1623, 1579, 1511, 1488, 1470, 1402, 1352, 1309, 1241, 1216, 1201, 1178, 1151, 1067, 1024, 882, 825, 792, 767, 709 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{22}H_{21}N_2O_4$ $[M - H]^-$ 377.1502, found 377.1515.

4-Benzyl-1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3i**): M.p. 156 ~ 158 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ_H 2.26 ~ 2.35 (m, 2H, CH_2), 2.59 ~ 2.65 (m, 1H, CH), 2.69 ~ 2.70 (m, 1H, CH), 4.36 (d, $J = 16.4$ Hz, 1H, CH), 5.23 (d, $J = 16.4$ Hz, 1H, CH), 7.13 ~ 7.19 (m, 1H, ArH), 7.23 ~ 7.27 (m, 1H, ArH), 7.32 ~ 7.35 (m, 4H, ArH), 7.66 (t, $J = 7.6$ Hz, 1H, ArH), 7.96 (d, $J = 7.6$ Hz, 1H, ArH), 8.30 (d, $J = 8.4$ Hz, 1H, ArH). IR (KBr): *v* 3062, 3029, 2978, 2929, 1739, 1660, 1601, 1488, 1468, 1454, 1441, 1371, 1336, 1316, 1304, 1265, 1231, 1193, 1148, 1078, 1027, 977, 789, 740, 717, 701 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{19}H_{15}N_2O_4$ $[M - H]^-$ 355.1032, found 355.1064.

7-Bromo-1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3j**): m.p. 281 ~ 283 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ_H 2.30 ~ 2.38 (m, 1H, CH), 2.65 ~ 2.73 (m, 3H, CH + CH_2), 7.81 ~ 7.83 (m, 1H, ArH), 7.94 ~ 7.95 (m, 1H, ArH), 8.13 (d, $J = 8.8$ Hz, 1H, ArH), 9.53 (s, 1H, NH). IR (KBr): *v* 3247, 3177, 3068, 2913, 1720, 1685, 1597, 1483, 1433, 1365,

1337, 1274, 1235, 1196, 1162, 1106, 1072, 1029, 824, 782, 752, 722 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{12}H_8BrN_2O_4$ $[M - H]^-$ 322.9668, found 322.9666.

7-Methyl-1,5-dioxo-1,2,3,3a,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3k**): M.p. 288 ~ 289 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ_H 2.33 (s, 3H, CH_3), 2.36 ~ 2.37 (m, 1H, CH), 2.64 ~ 2.69 (m, 3H, CH + CH_2), 7.43 (d, $J = 7.2$ Hz, 1H, ArH), 7.68 (s, 1H, ArH), 8.03 (d, $J = 8.0$ Hz, 1H, ArH), 9.28 (s, 1H, NH). IR (KBr): *v* 3277, 3093, 2956, 2922, 1733, 1642, 1613, 1574, 1495, 1460, 1424, 1337, 1290, 1275, 1240, 1212, 1198, 1163, 1149, 1129, 1094, 1071, 1041, 1008, 851, 788, 742 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{13}H_{11}N_2O_4$ $[M - H]^-$ 259.0719, found 259.0736.

7-Chloro-1,2,3,3*a*,4,5-hexahydro-1,5-dioxopyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid (**3l**): M.p. 272 ~ 273 °C; ^1H NMR (DMSO-d_6, 400 MHz): δ_H 2.33 ~ 2.39 (m, 1H, CH), 2.66 ~ 2.69 (m, 3H, CH + CH_2), 7.68 ~ 7.71 (m, 1H, ArH), 7.82 ~ 7.83 (m, 1H, ArH), 8.19 (d, $J = 8.8$ Hz, 1H, ArH), 9.53 (s, 1H, NH). IR (KBr): *v* 3330, 3244, 3070, 2989, 2921, 1743, 1731, 1623, 1601, 1493, 1476, 1437, 1417, 1385, 1363, 1338, 1307, 1287, 1273, 1235, 1197, 1165, 1107, 1076, 1030, 842, 827, 783, 755, 723 cm^{-1}. HRMS (ESI, *m/z*): calcd. for $C_{12}H_8ClN_2O_4$ $[M - H]^-$ 279.0173, found 279.0176.

Conclusion

In conclusion, we found a mild and green method for the synthesis of 1,5-dioxo-1,2,3,3*a*,4,5-hexahydropyrrolo[1,2-*a*]quinazoline-3*a*-carboxylic acid derivatives catalyzed by iodine in ionic liquid. The novelty of this procedure is in using simple reactants to construct two fused heterocycles at the same time. In addition, the features of this procedure also include mild reaction conditions, high yields, operational simplicity, and the use of a metal-free catalyst.

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