Supplementary Materials: Synthesis, Crystal Structure, Spectroscopic Properties, and DFT Studies of 7,9-Dibromobenzo[*h*]quinolin-10-ol

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Table S1. Bond lengths (Å) and angles (°) for **1**.

Br(1)-C(2)	1.892(6)
Br(2)-C(4)	1.901(6)
O-C(1)	1.337(8)
O-H(0A)	0.99(10)
N-C(11)	1.311(8)
N-C(12)	1.377(8)
C(1)-C(2)	1.378(9)
C(1)-C(13)	1.423(8)
C(2)-C(3)	1.386(9)
C(3)-C(4)	1.384(9)
C(3)-H(3A)	0.9300
C(4)-C(5)	1.393(9)
C(5)-C(13)	1.427(8)
C(5)-C(6)	1.448(9)
C(6)-C(7)	1.333(10)
C(6)-H(6A)	0.9300
C(7)-C(8)	1.412(10)
C(7)-H(7A)	0.9300
C(8)-C(12)	1.407(8)
C(8)-C(9)	1.416(9)
C(9)-C(10)	1.352(11)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.395(10)
C(10)-H(10A)	0.9300
C(11)-H(11A)	0.9300
C(12)-C(13)	1.440(8)
C(1)-O-H(0A)	108(6)
C(11)-N-C(12)	120.0(5)
O-C(1)-C(2)	120.3(5)
O-C(1)-C(13)	121.5(6)
C(2)-C(1)-C(13)	118.2(6)
C(1)-C(2)-C(3)	122.5(6)
C(1)-C(2)-Br(1)	118.6(5)
C(3)-C(2)-Br(1)	118.9(5)
C(2)-C(3)-C(4)	119.1(6)
C(2)-C(3)-H(3A)	120.5
C(4)-C(3)-H(3A)	120.5
C(3)-C(4)-C(5)	121.9(6)
C(3)-C(4)-Br(2)	115.9(5)
C(5)-C(4)-Br(2)	122.2(5)
C(4)-C(5)-C(13)	118.0(5)
C(4)-C(5)-C(6)	122.9(6)
C(13)-C(5)-C(6)	119.1(6)
C(7)-C(6)-C(5)	121.2(6)
C(7)-C(6)-H(6A)	119.4
C(5)-C(6)-H(6A)	119.4
C(6)-C(7)-C(8)	122.2(6)
C(6)-C(7)-H(7A)	118.9

C(8)-C(7)-H(7A)	118.9
C(12)-C(8)-C(7)	118.4(6)
C(12)-C(8)-C(9)	117.3(6)
C(7)-C(8)-C(9)	124.3(6)
C(10)-C(9)-C(8)	119.4(6)
C(10)-C(9)-H(9A)	120.3
C(8)-C(9)-H(9A)	120.3
C(9)-C(10)-C(11)	120.7(6)
C(9)-C(10)-H(10A)	119.6
C(11)-C(10)-H(10A)	119.6
N-C(11)-C(10)	121.4(7)
N-C(11)-H(11A)	119.3
C(10)-C(11)-H(11A)	119.3
N-C(12)-C(8)	121.1(5)
N-C(12)-C(13)	117.2(5)

Table S2. Total and relative energies of **1** and **2** in the ground state [a].

Species	**1**	**2**
Enol	−655.8191	−630.8095
keto	−655.8094	−630.7936

a: Total energies are in a.u.