Supplementary Material

Activation of 6-bromoquinoline by nitration. Synthesis of morpholinyl and piperazinyl quinolines

Osman Çakmak*[a], Salih Ökten[b], Dilek Alımlı[c], Aisha Saddiqa[d], Cem Cüneyt Ersanlı[e]

[a]*Department of Nutrition and Dietetics, School of Health Sciences, İstanbul Gelişim University, 34315, Avcılar, İstanbul, Turkey*

[b]*Department of Mathematic and Science Education, Division of Science Education, Faculty of Education, Kırıkkale University, 71450, Yahşihan, Kırıkkale, Turkey*

[c]*Department of Chemistry, Faculty of Science, Gebze Technical University, 41400, Gebze, Kocaeli, Turkey*

[d]*Department of Chemistry, Faculty of Natural Science, Government College Women University, Sialkot, Pakistan*

[e]*Department of Physics, Faculty of Arts and Science, Sinop University, 57010, Sinop, Turkey*

Email: cakmak.osman@gmail.com

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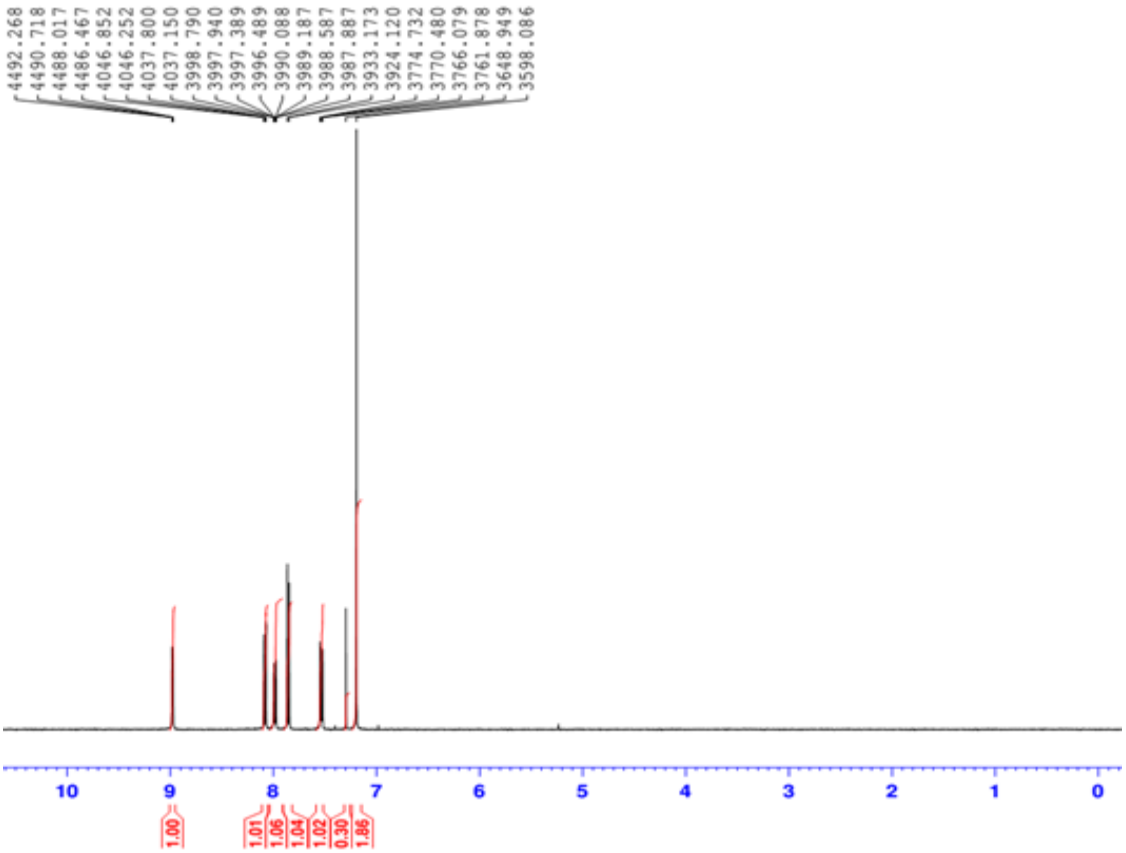

Figure 1. ^{1}H-NMR (400 MHz, $CDCl_3$) of 6-Bromo-5-nitroquinoline (**14**)

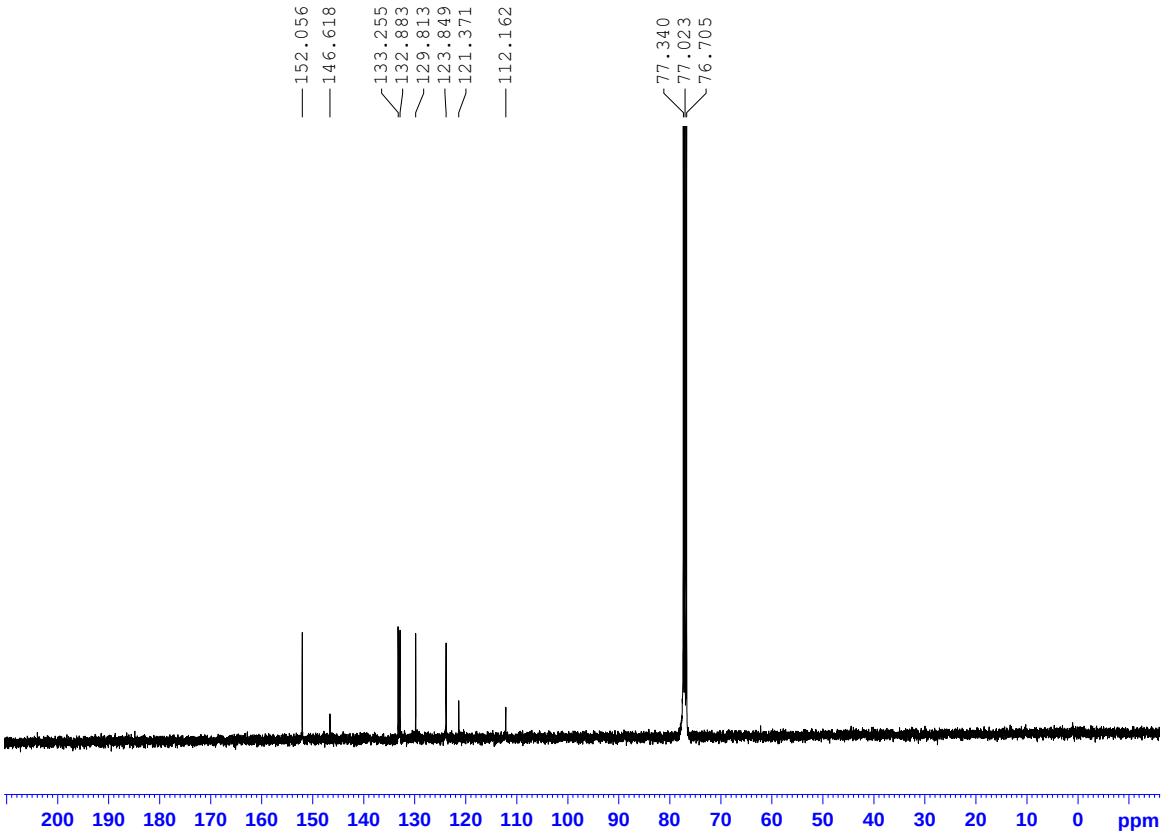

Figure 2. ^{13}C-NMR (100 MHz, $CDCl_3$) of 6-Bromo-5-nitroquinoline (**14**)

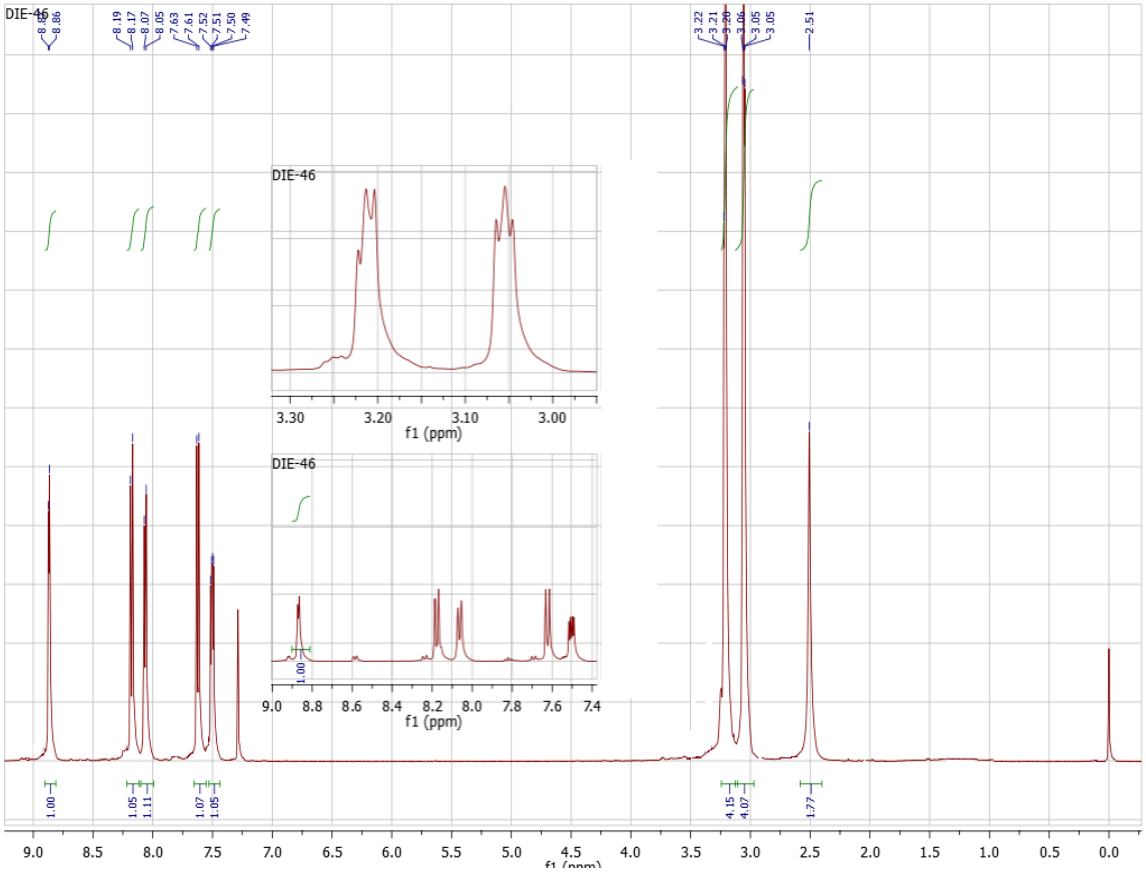

Figure 3. ^{1}H-NMR (500 MHz, $CDCl_3$) of 5-nitro-6-(piperazin-1-yl)quinoline (**18**)

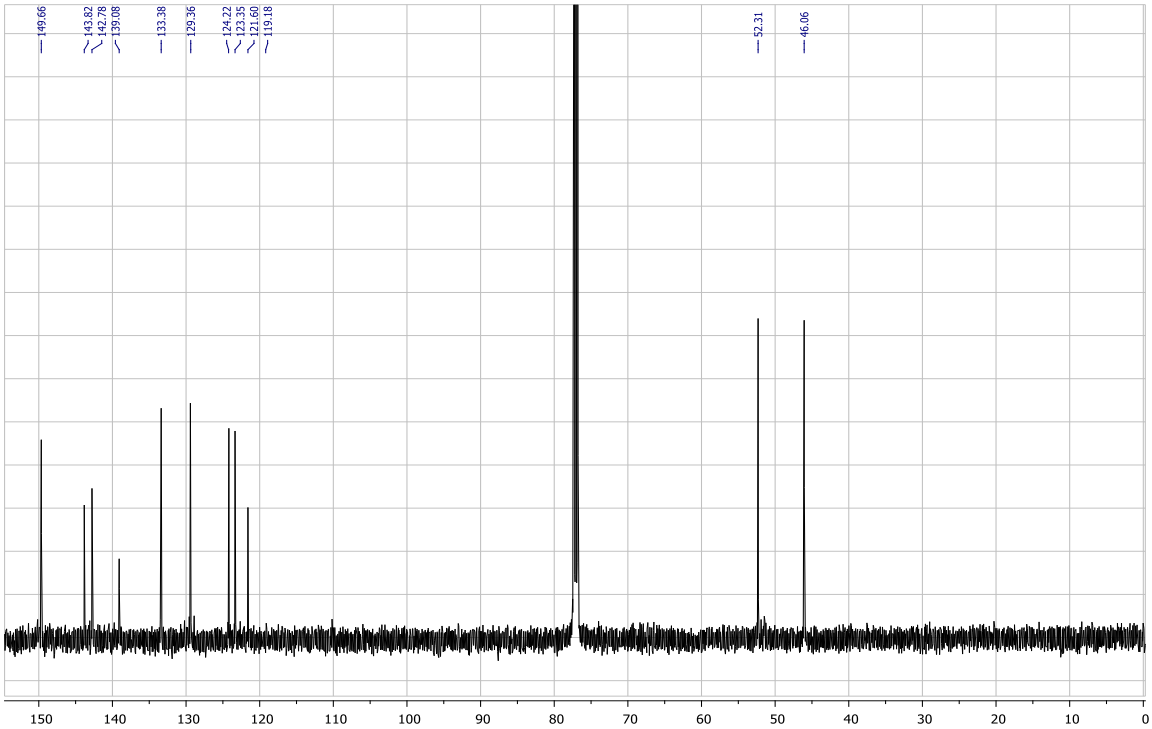

Figure 4. ^{13}C NMR (125 MHz, $CDCl_3$) of 5-nitro-6-(piperazin-1-yl)quinoline (**18**)

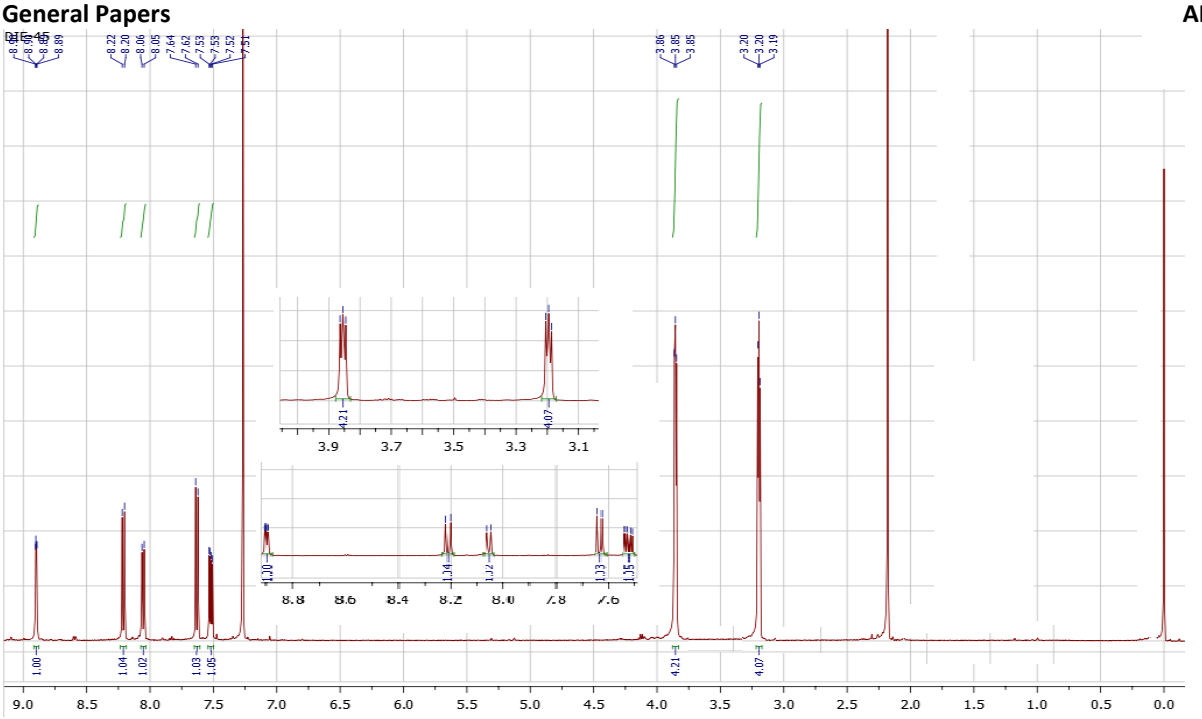

Figure 5. ^{1}H-NMR (500 MHz, $CDCl_3$) of 5-nitro-6-(morpholin-1-yl)quinoline (**17**)

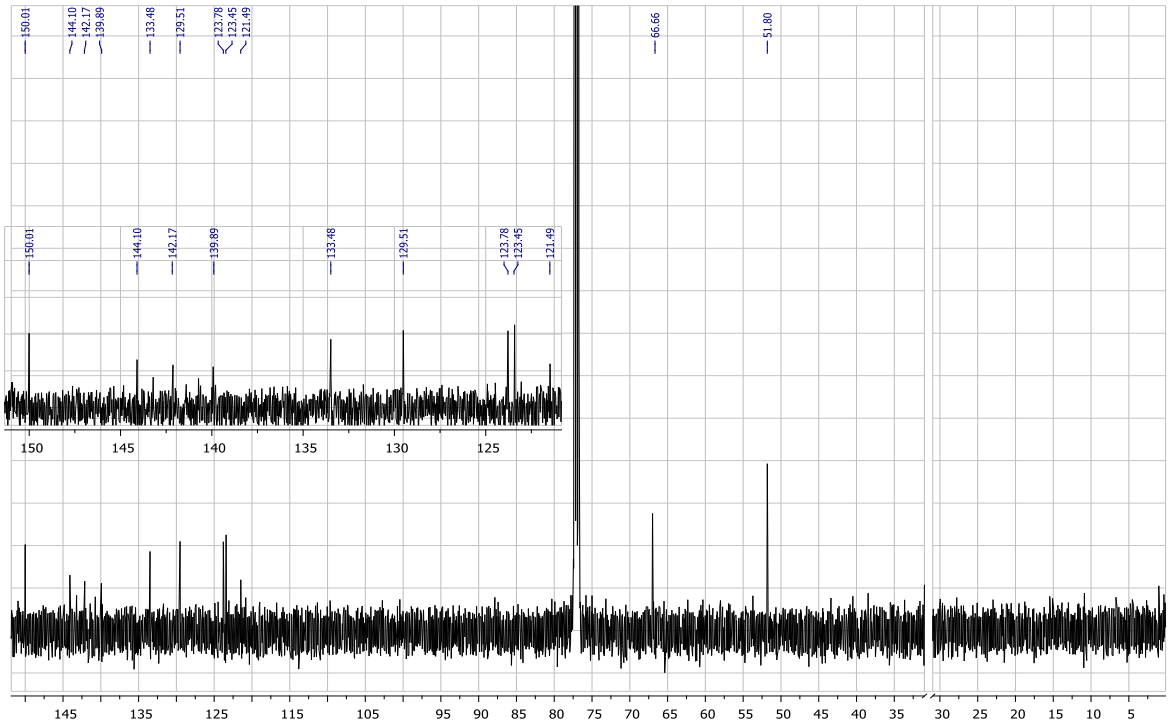

Figure 6. ^{13}C NMR (125 MHz, $CDCl_3$) of 5-nitro-6-(morpholin-1-yl)quinoline (**17**)

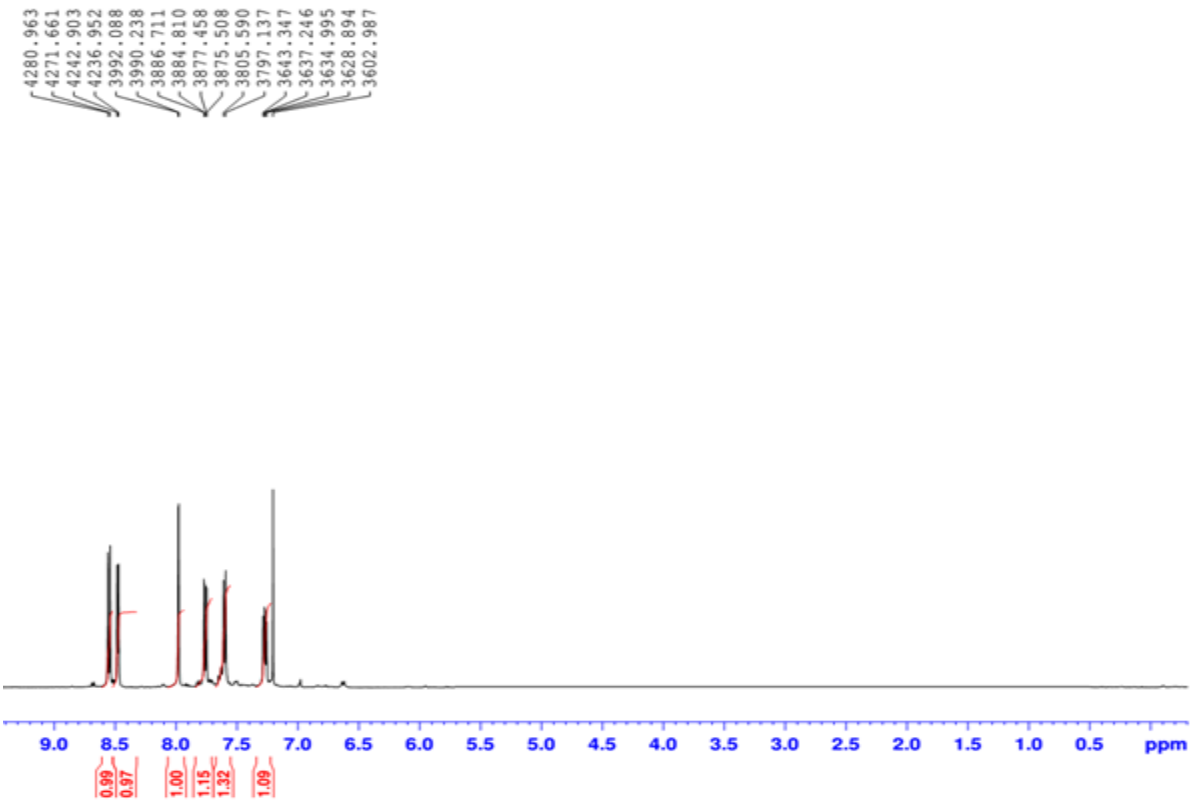

Figure 7. ^{1}H-NMR (400 MHz, $CDCl_3$) of 6-bromoquinoline-1-oxide (**20**)

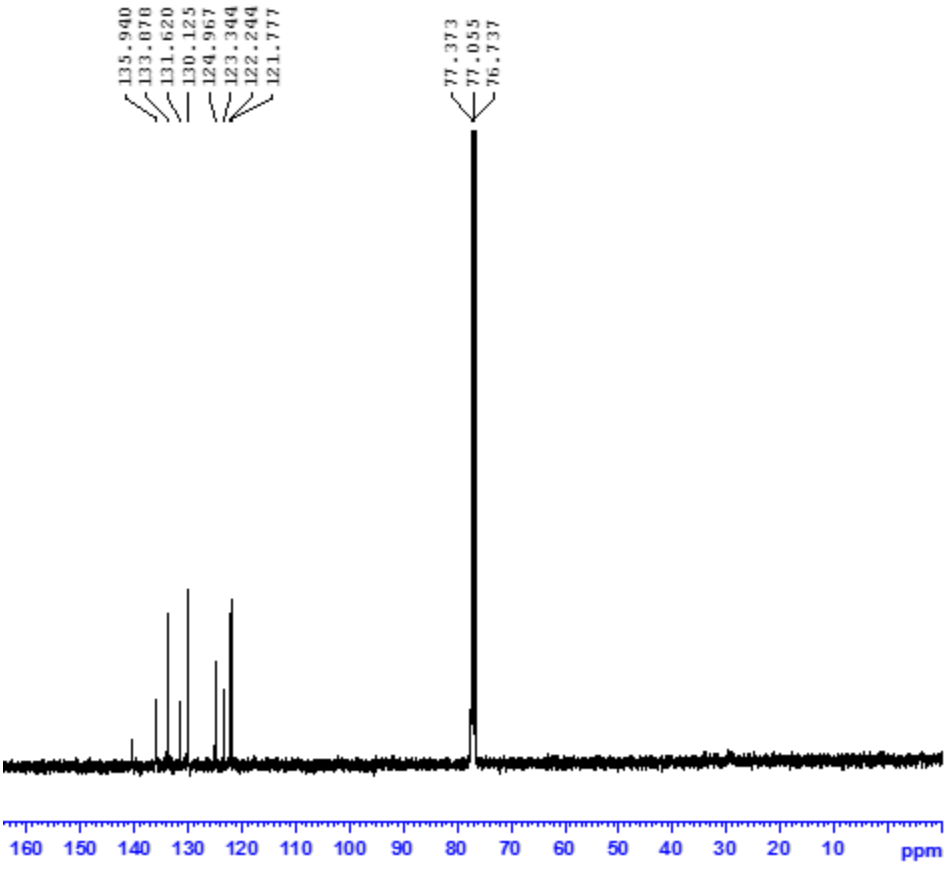

Figure 8. ^{13}C NMR (100 MHz, $CDCl_3$) of 6-bromoquinoline-1-oxide (**20**)

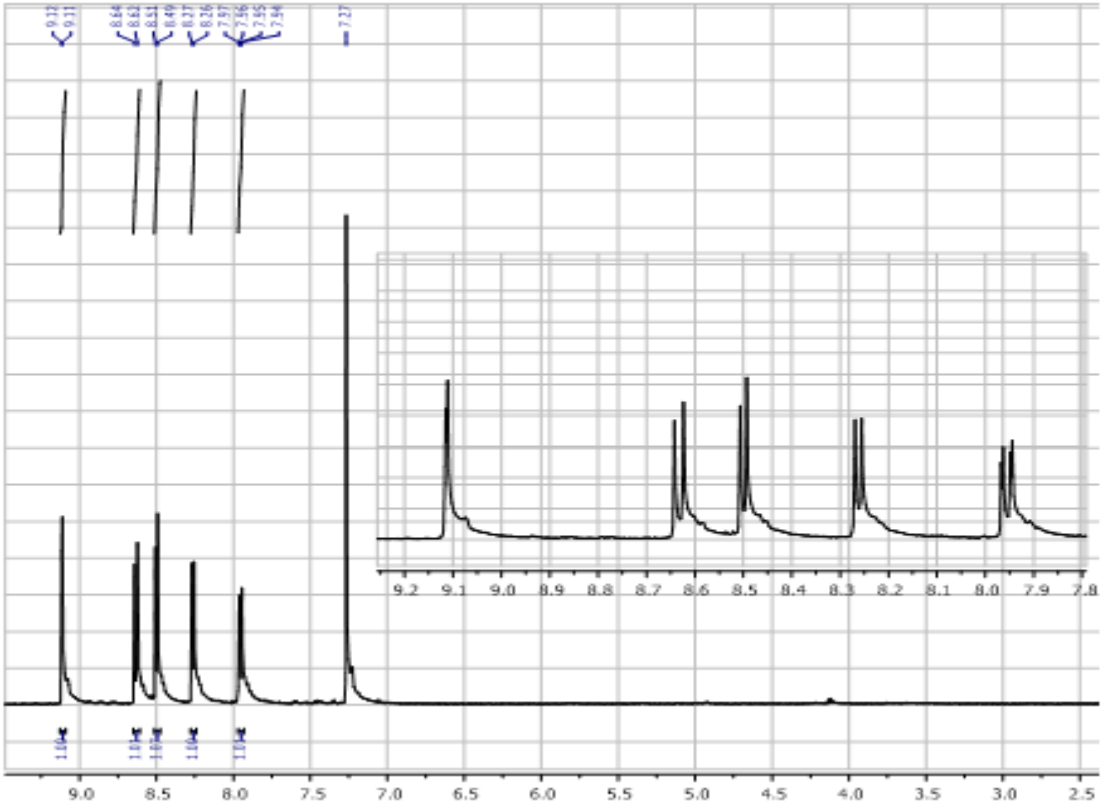

Figure 9. ^{1}H-NMR (500 MHz, $CDCl_3$) of 6-bromo-5-nitroquinoline-1-oxide (**25**)

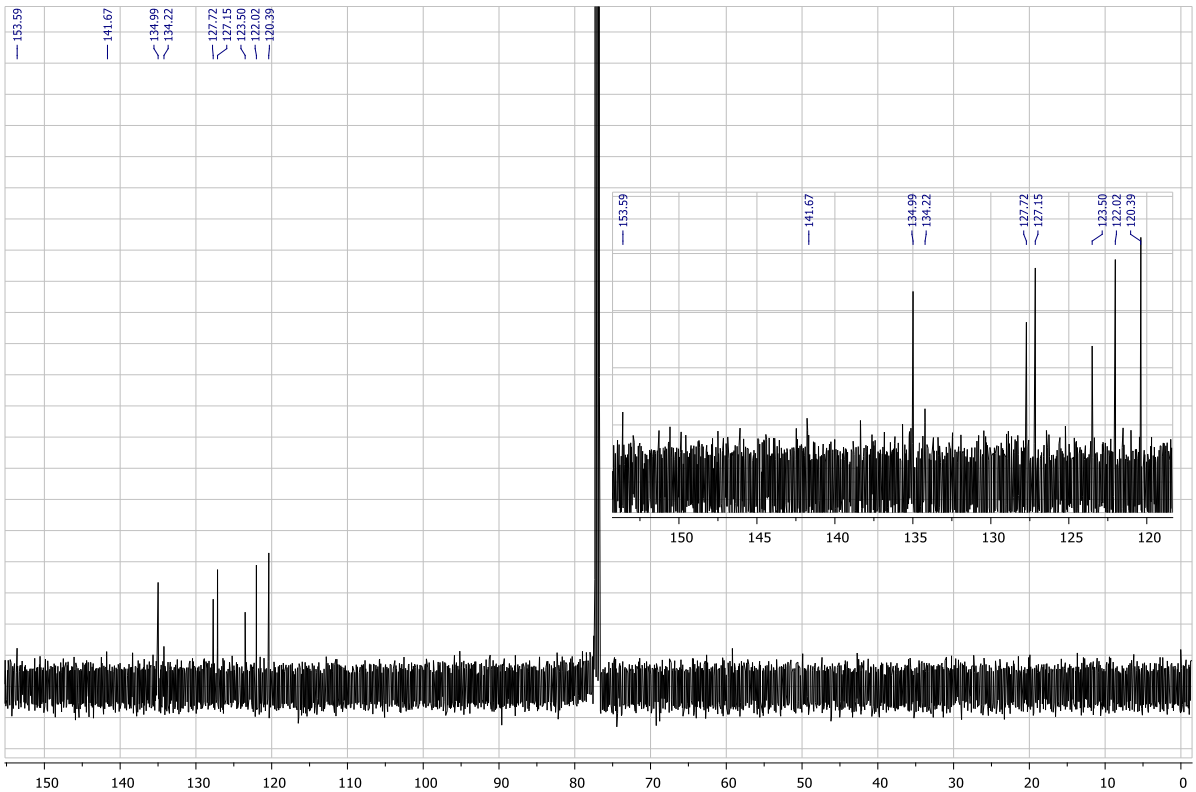

Figure 10. ^{13}C-NMR (125 MHz, $CDCl_3$) of 6-bromo-5-nitroquinoline-1-oxide (**23**)

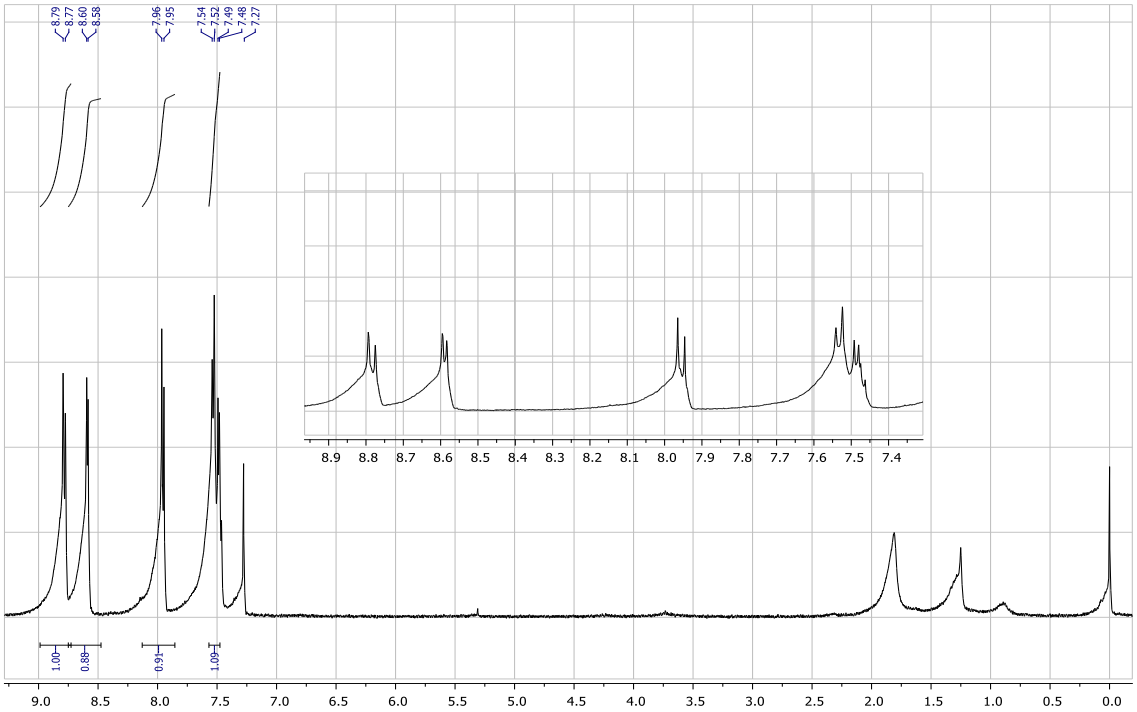

Figure 11. ^{1}H-NMR (500 MHz, $CDCl_3$) of 6-bromo-4-nitroquinoline-1-oxide (**24**)

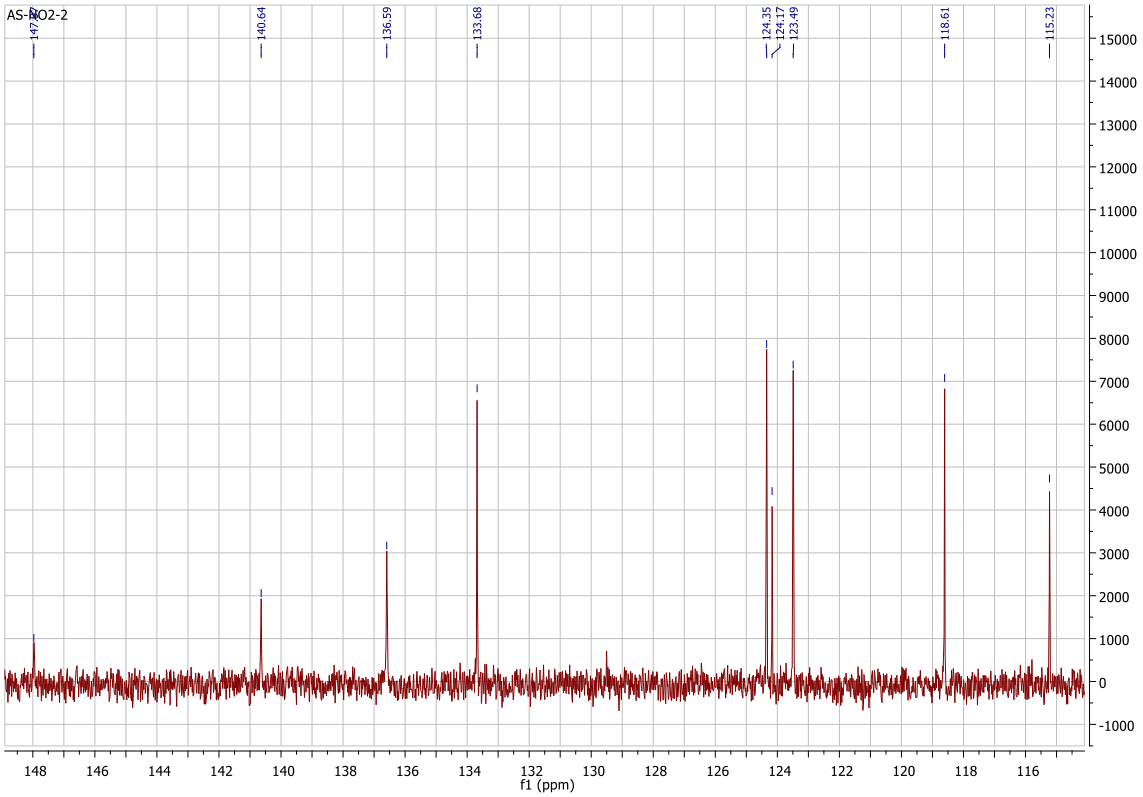

Figure 12. ^{13}C-NMR (125 MHz, $CDCl_3$) of 6-bromo-4-nitroquinoline-1-oxide (**24**)

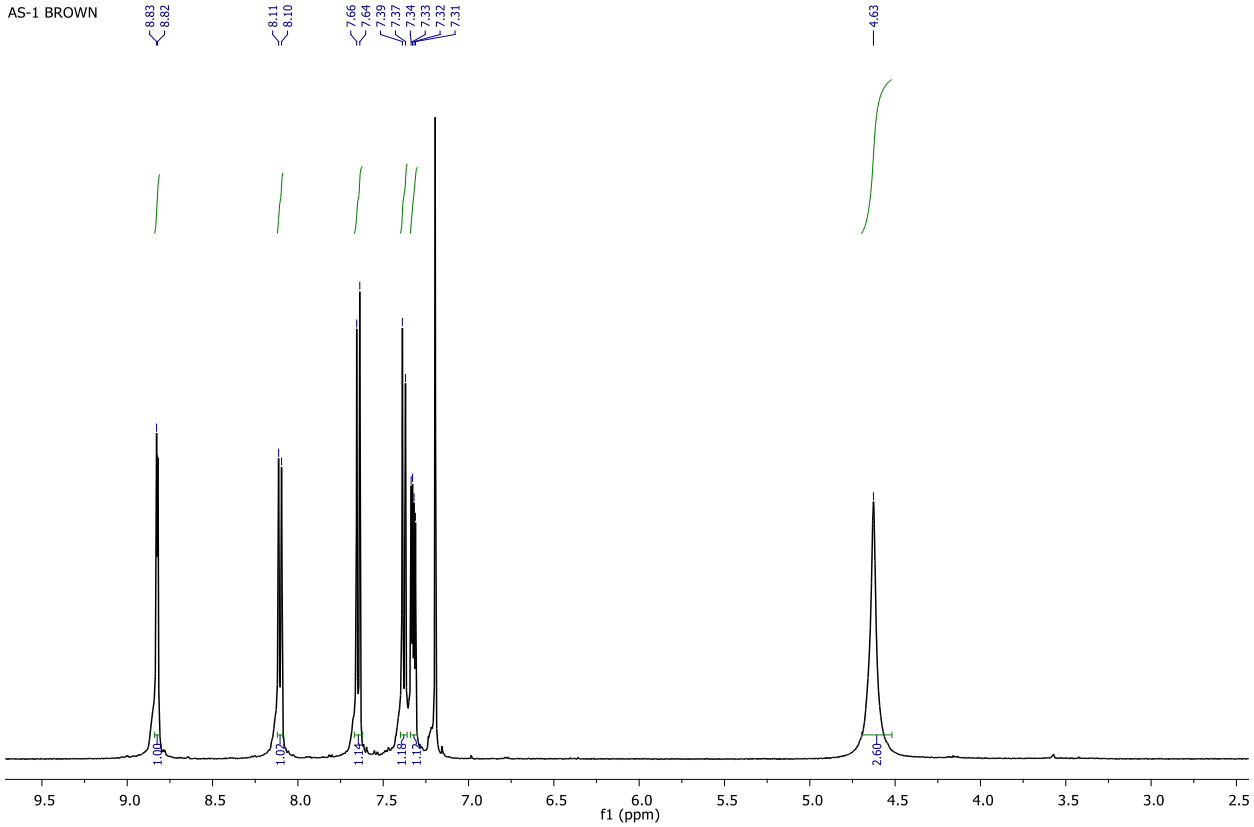

Figure 13. ^{1}H-NMR (500 MHz, $CDCl_3$) of 5-nitro-6-bromoquinoline-1-oxide (**25**)

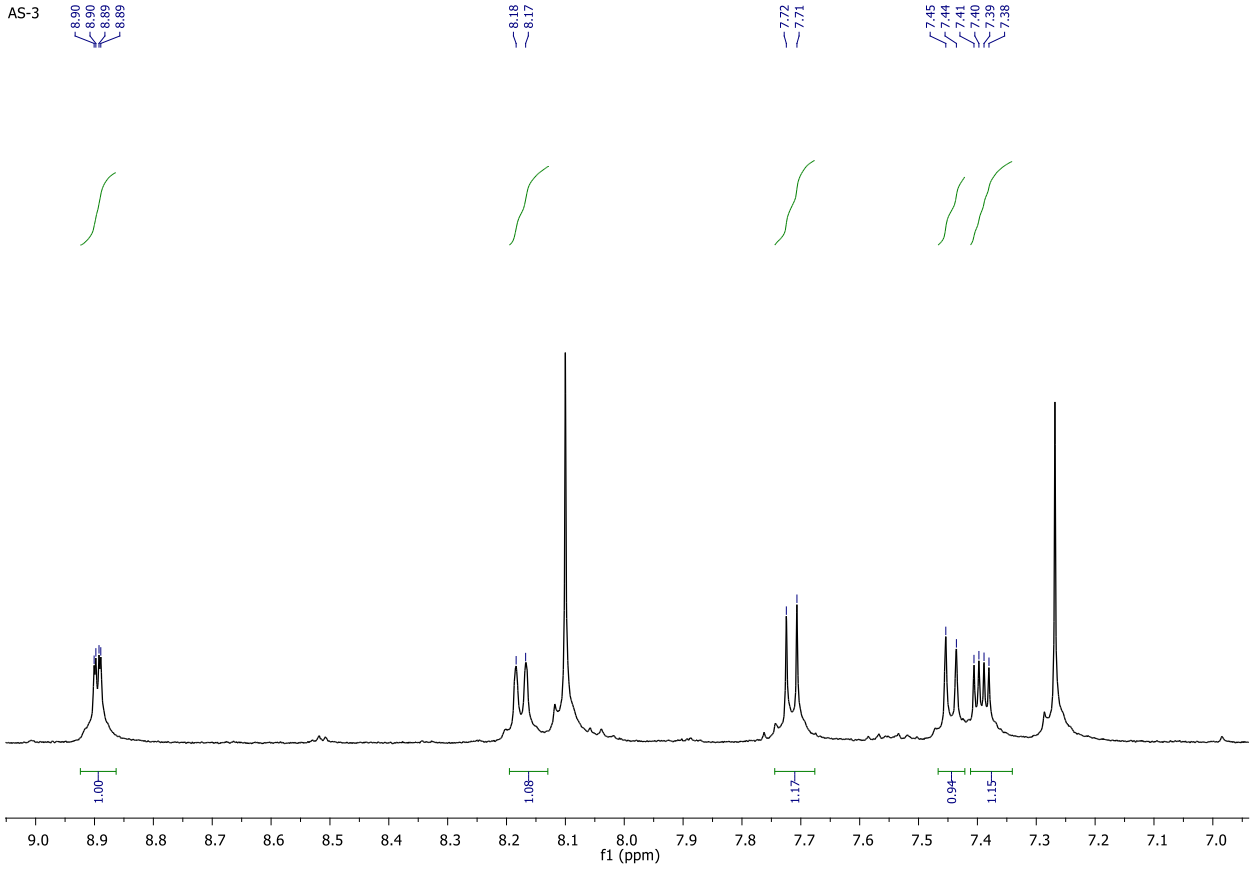

Figure 14. ^{1}H-NMR (500 MHz, $CDCl_3$) of 4-nitro-6-bromoquinoline-1-oxide (**26**)

Table 1. Experimental geometries of (**23**) in the ground state. Bond lengths (Å) and angles (º) with estimated standard deviations in parentheses.

Bond lengths (Å)		*Bond lengths* (Å)	
C1-N1	1.315(13)	C18-N3	1.404(8)
C5-N2	1.488(11)	N3-O3	1.310(8)
C6-Br1	1.861(9)	N4-O4	1.213(8)
C9-N1	1.425(13)	N4-O5	1.206(8)
N1-O1	1.277(10)	C19-N5	1.325(12)
N2-O2	1.197(6)	C27-N5	1.404(11)
N2-O2	1.197(6)	C24-Br3	1.898(8)
C10-N3	1.330(10)	C23-N6	1.482(11)
C14-N4	1.480(8)	N5-O6	1.299(10)
C15-Br2	1.889(7)	N6-O7	1.167(7)
Bond angle (º)		*Bond angle* (º)	
N1-C1-C2	122.9(10)	O4-N4-O4	117.6(7)
O1-N1-C1	122.7(8)	C15-C14-N4	119.3(7)
O1-N1-C9	119.5(8)	C13-C14-N4	117.6(7)
C1-N1-C9	117.8(8)	C14-C15-Br2	121.7(5)
C6-C5-N2	118.8(9)	C16-C15-Br2	118.3(5)
C4-C5-N2	115.8(9)	C17-C18-N3	119.5(6)
C5-C6-Br1	123.5(7)	N5-C19-C20	121.4(8)
C7-C6-Br1	119.5(7)	O6-N5-C19	121.3(7)
C8-C9-N1	117.9(9)	O6-N5-C27	118.8(8)
C4-C9-N1	120.1(8)	C24-C23-N6	119.6(8)
N3-C10-C11	121.9(7)	C23-C24-N6	118.4(8)
O2-N2-C5	118.2(4)	C23-C24-Br3	120.1(8)
O3-N3-C10	121.7(6)	C25-C24-Br3	119.3(7)
O3-N3-C18	118.0(6)	C22-C27-N5	119.3(8)
O5-N4-O4	124.7(7)	C26-C27-N5	118.5(8)
Torsion angles (º)		*Torsion angles* (º)	
C2-C1-N1-O1	180.0(2)	C14-C13-C18-N3	-179.8(6)
N2-O2-C5-C6	-90.2(8)°		
N4-C14-C15-C16	-178.4(7)	C17-C18-N3-O3	-0.3(10)

Table 2. C-H…Br and C-H…O interactions parameters (Å, º) for **23**.

D–H···A	**D–H**	**H···A**	**D···A**	**D–H···A**
C8-H8…Br1^{i}	0.93	2.74	3.665(9)	171.2
C17-H17…Br2^{ii}	0.93	2.80	3.708(7)	166.3
C25-H25…O7^{i}	0.93	2.52	3.376(11)	153.9
C25-H25…O7^{iii}	0.93	2.52	3.376(11)	153.9

Symmetry codes: (*i*) -*x*+1, -*y*+2, *z*+1/2, (*ii*) *x*, -*y*+2, *z*-1/2, (*iii*) *x*+2, -*y*+1, *z*+1/2