Supporting information for

N-Heterocyclization of Naphthylamines with 1,2- and 1,3-Diols Catalyzed by Iridium Chloride/BINAP System

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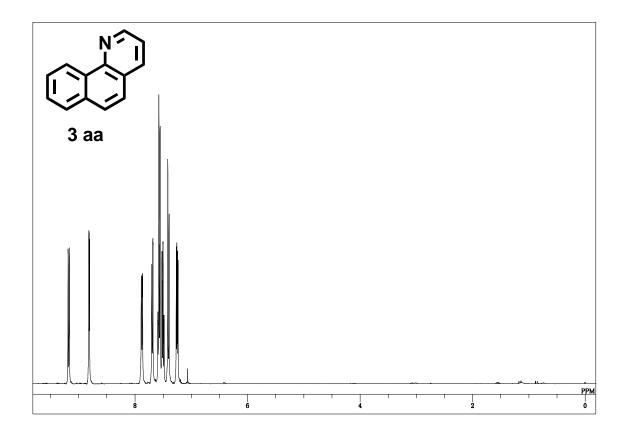
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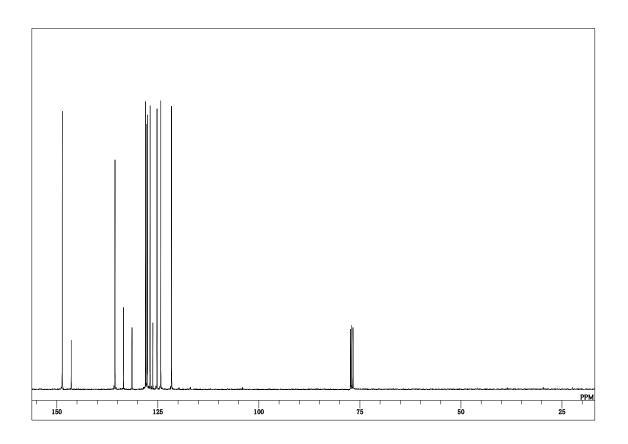
General Experimental Methods

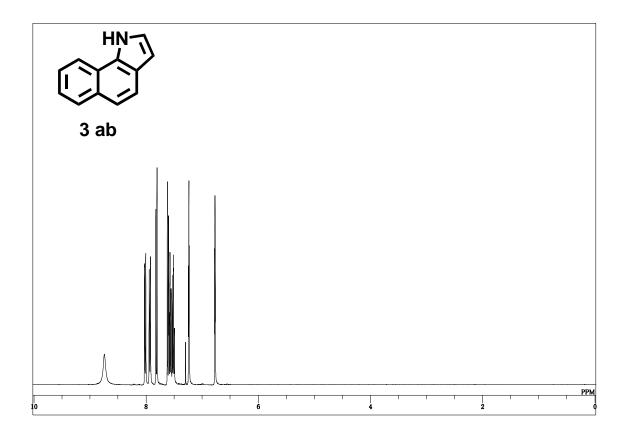
GLC analysis was performed with a flame ionization detector using a 0.22 mm \times 25 m capillary column (BP-5). 1 H and 13 C NMR were measured at 400 and 100 MHz, respectively, in CDCl₃ with Me₄Si as the internal standard. The products were characterized by 1 H NMR, 13 C NMR, NOESY, DEPT, HMQC, and GC-MS. The yields of products were estimated from the peak areas based on the internal standard technique using GLC.

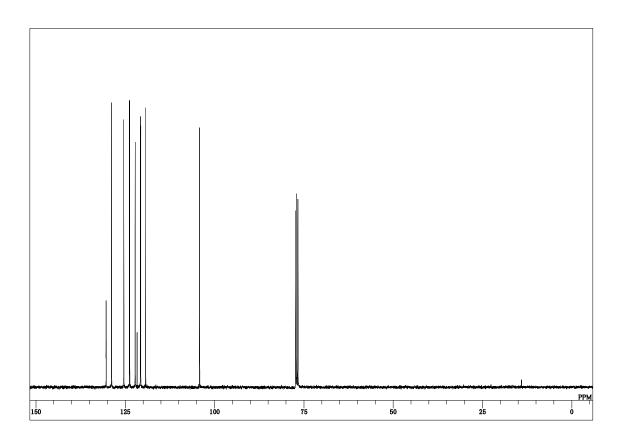
Reaction of 3-(1-Naphtylamino)-propanol (D) and 1a in the Presence of Ir catalyst (Eq. 2): To a mixture of $IrCl_3 \cdot H_2O$ (18 mg, 0.05 mmol), BINAP (47 mg, 0.075 mmol), and Na_2CO_3 (9 mg, 0.08 mmol) was added to the mixture of 3-(1-naphtylamino)-1-propanol (201 mg, 1 mmol) and 1a (143 mg, 1 mmol) in mesitylene (1.5 mL) under O_2 (1 atm). The reaction mixture was stirred at refluxing temperature of mesitylene (169 °C) for 15 h. GC analysis of the reaction mixture showed that 3aa and 1a was formed in 72% and 19% yields, respectively.

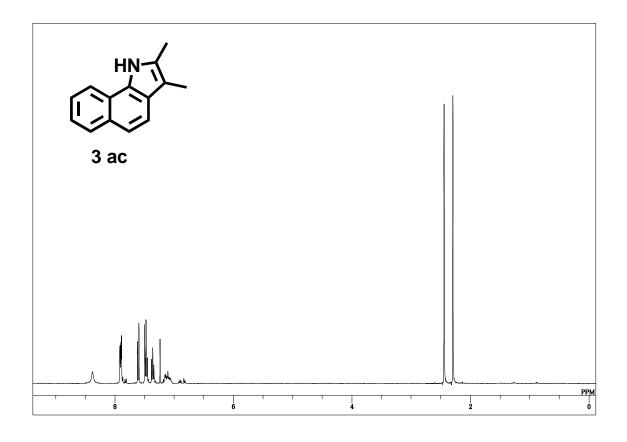
Reaction of N,N'-di(naphthalene-1-yl)propane-1,3-diamine (E) in the Presence of Ir catalyst (Eq. 4): To a mixture of IrCl₃·H₂O (35 mg, 0.10 mmol), BINAP (93 mg, 0.15 mmol), Na₂CO₃ 0.16 mmol) was added and (17 mg, N,N'-di(naphthalene-1-yl)propane-1,3-diamine (E) (326 mg, 1 mmol) in mesitylene (1.5 mL) under O₂ (1 atm). The reaction mixture was stirred at refluxing temperature of mesitylene (169 °C) for 15 h. GC analysis of the reaction mixture showed that 3aa and 1a was formed in 76% and 83% yield, respectively.

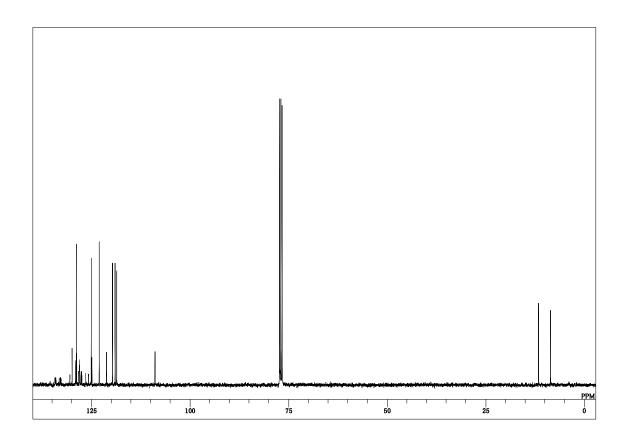


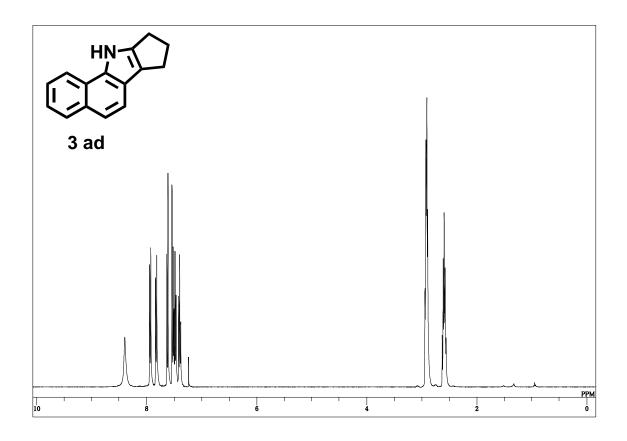


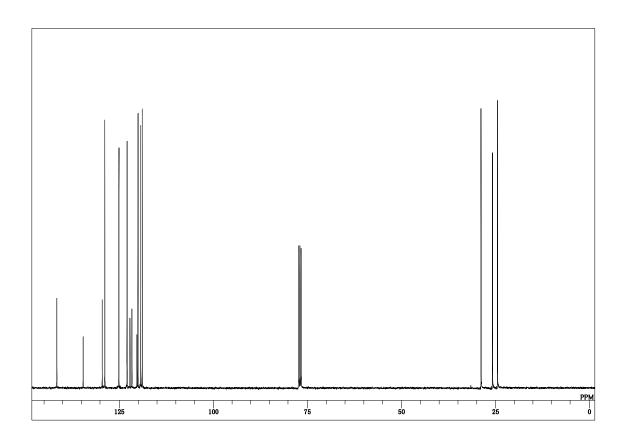


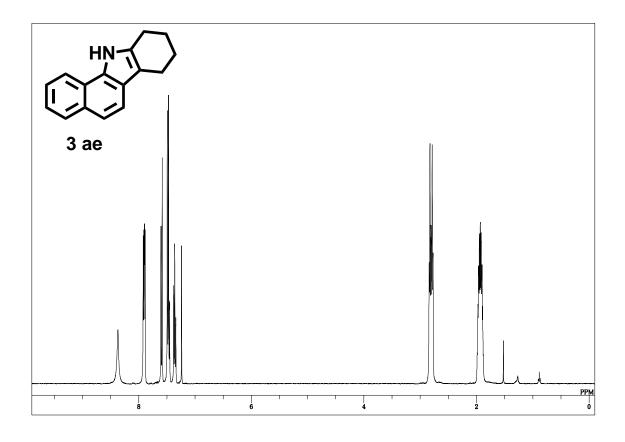


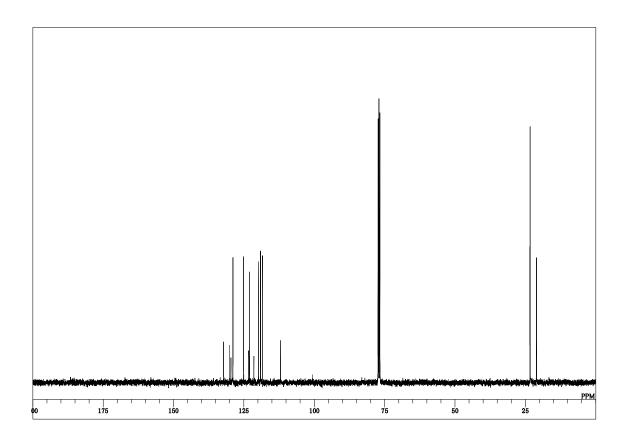


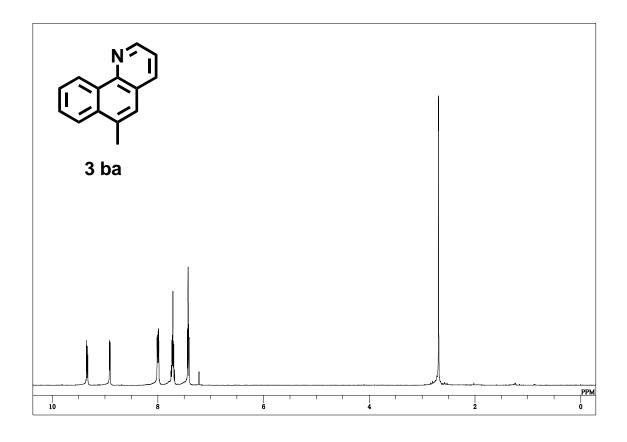


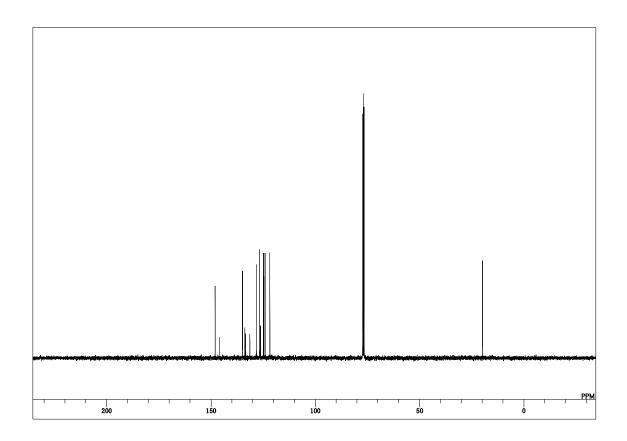


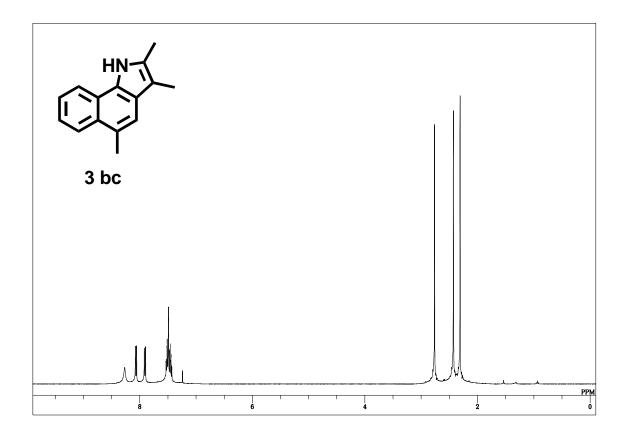


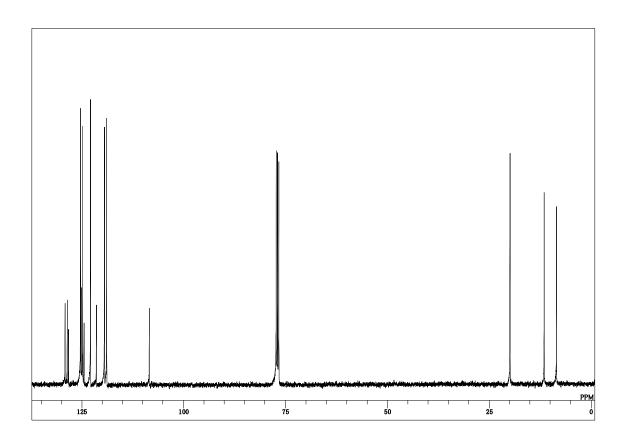


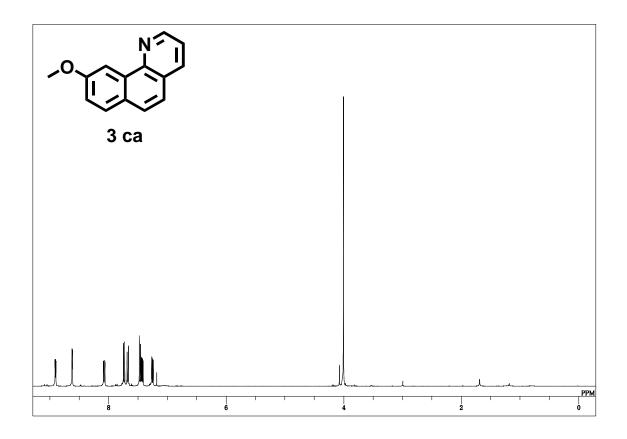


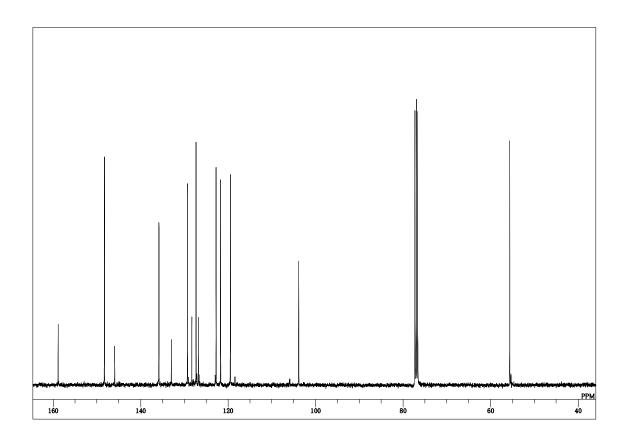


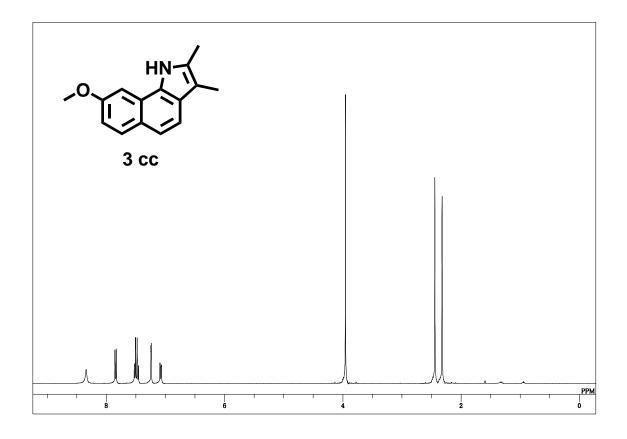


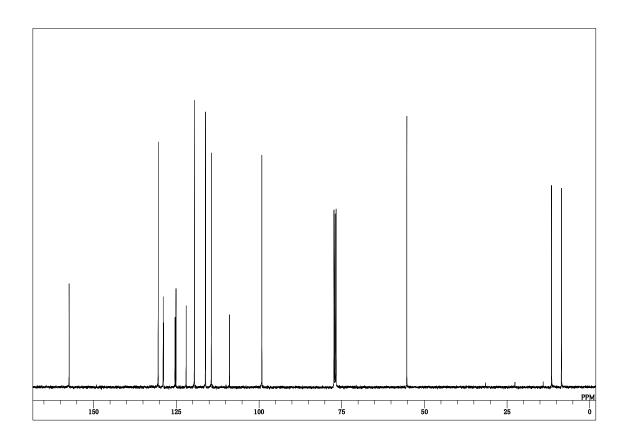




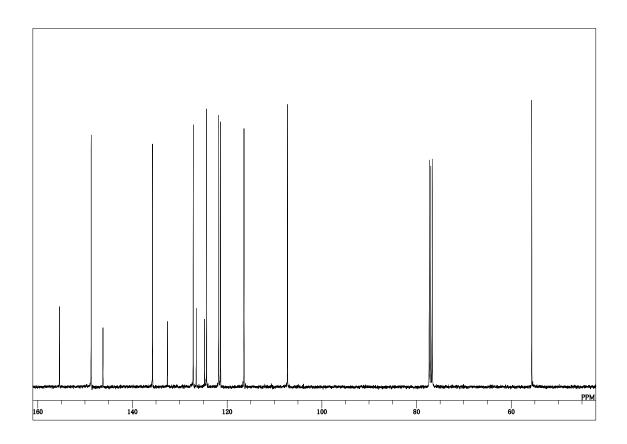












DEPT

