

Prediction of Suitable Catalyst by ^1H NMR: Asymmetric Synthesis of Multisubstituted Biaryls by Chiral Phosphoric Acid Catalyzed Asymmetric Bromination

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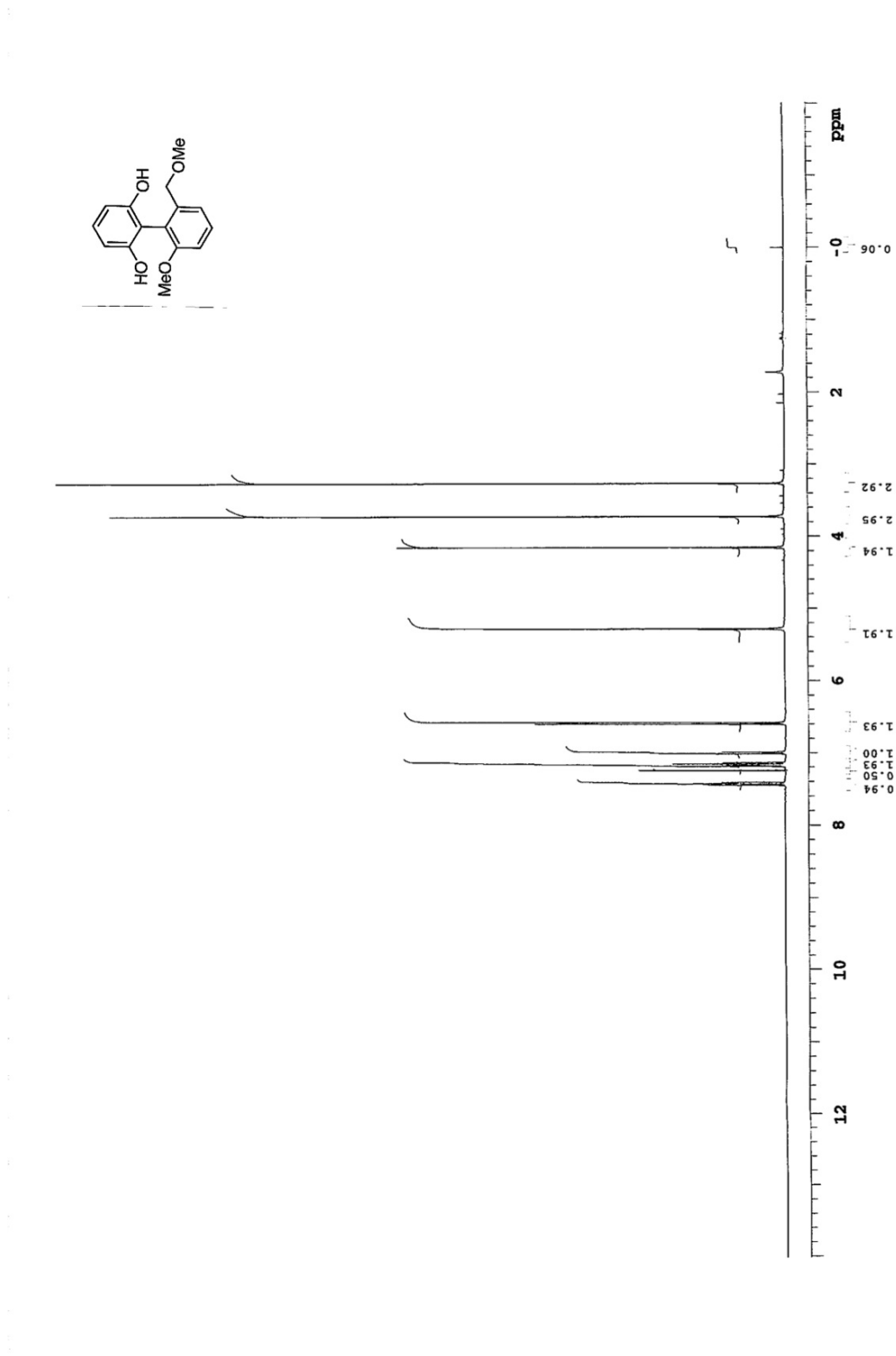
takahiko.akiyama@gakushuin.ac.jp

Supporting Information

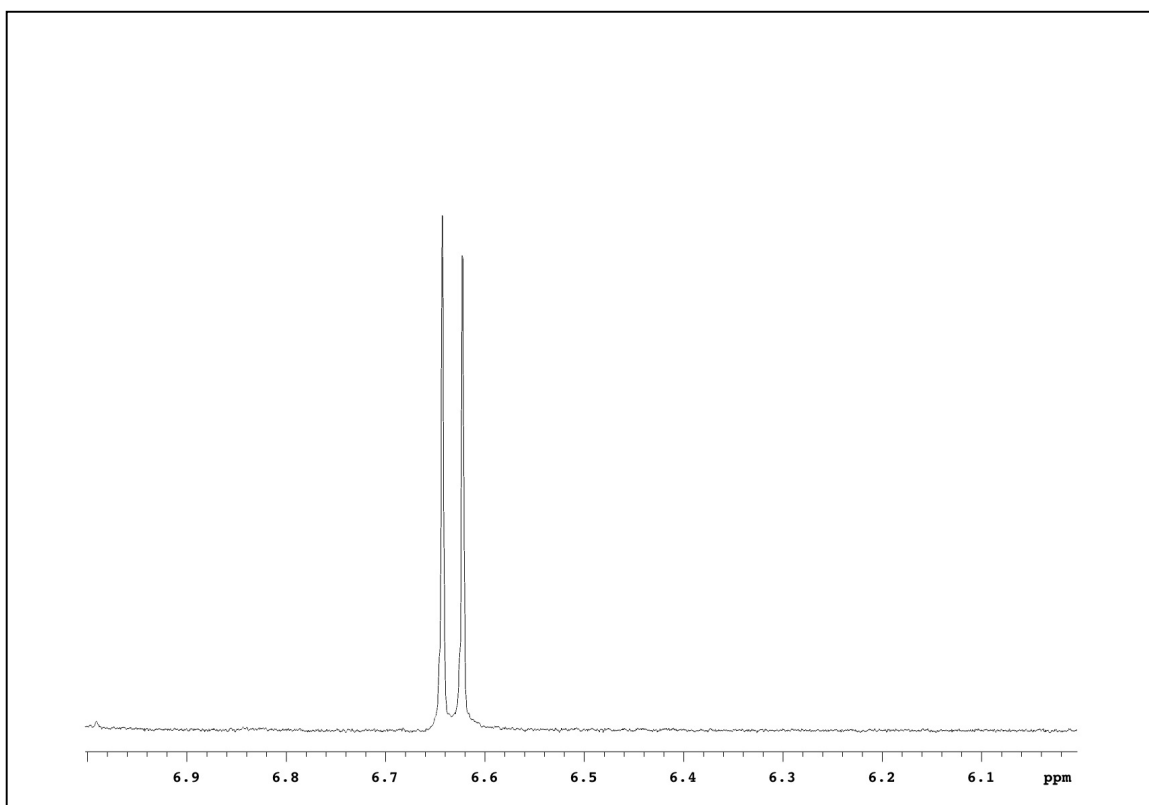
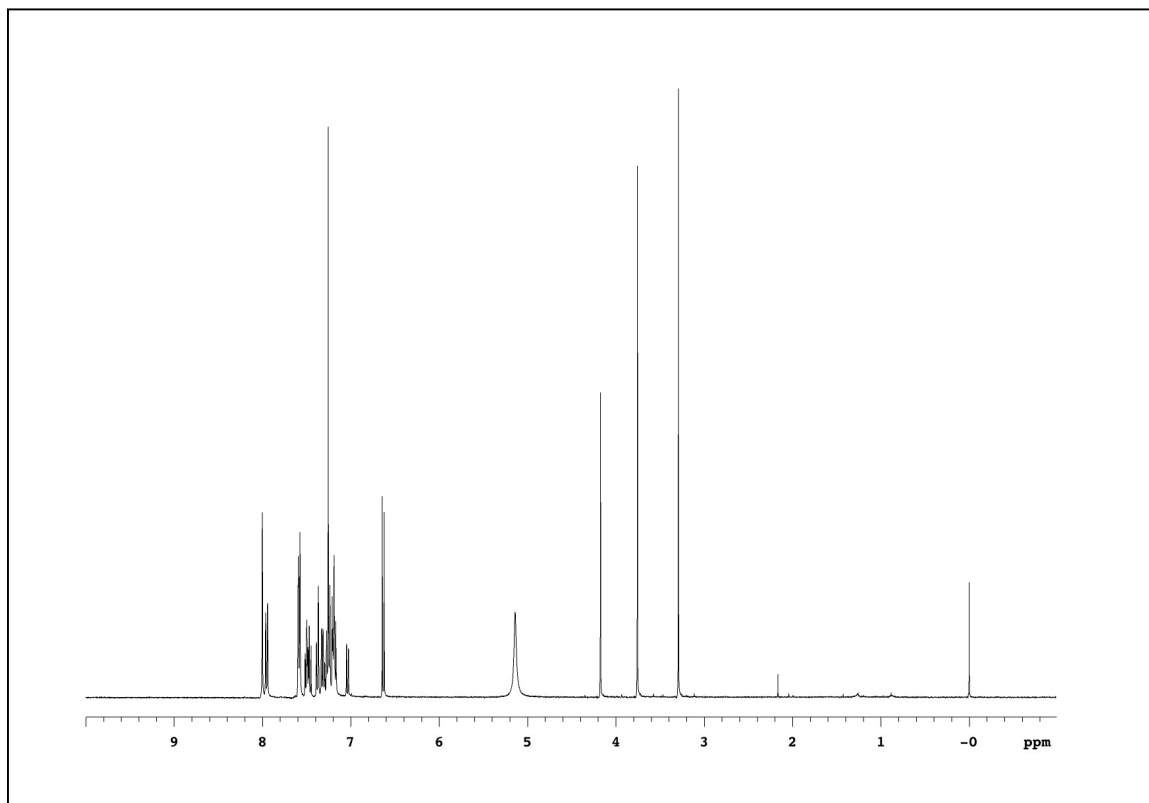
Scanned images of ^1H - and ^{13}C -NMR of new compounds

S1

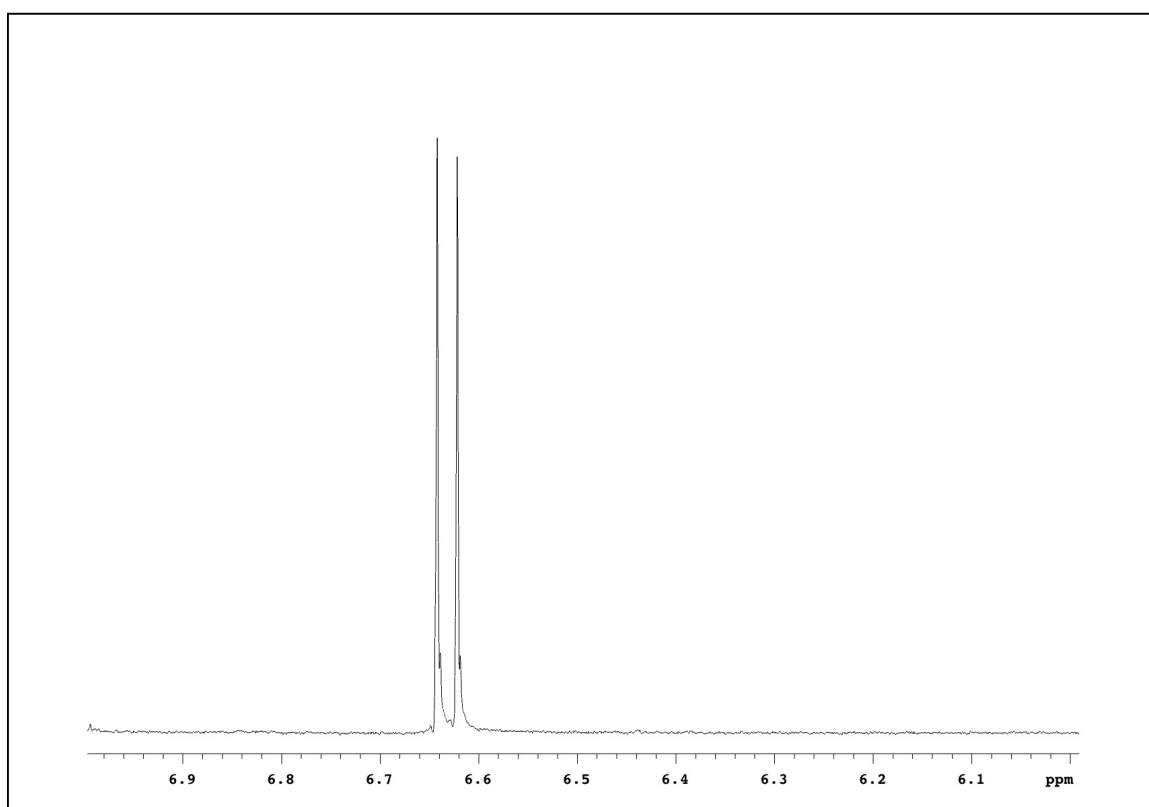
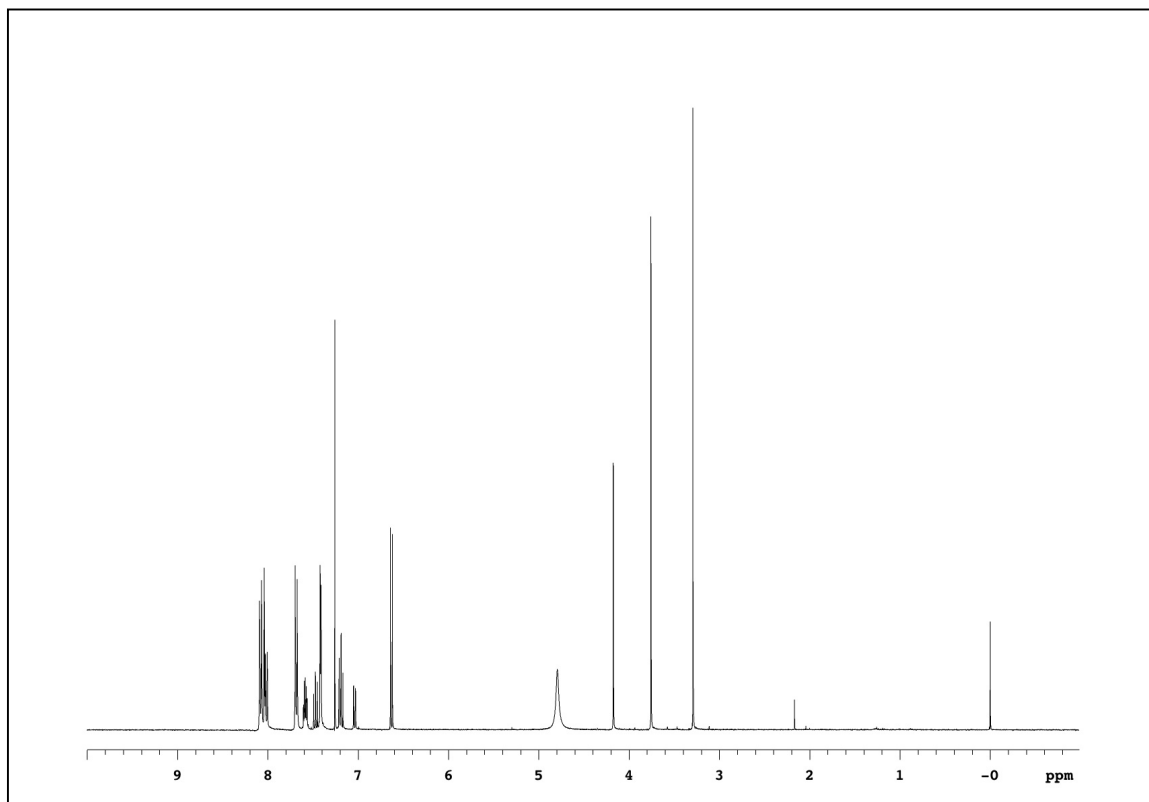
¹H NMR spectrum of **3a**.



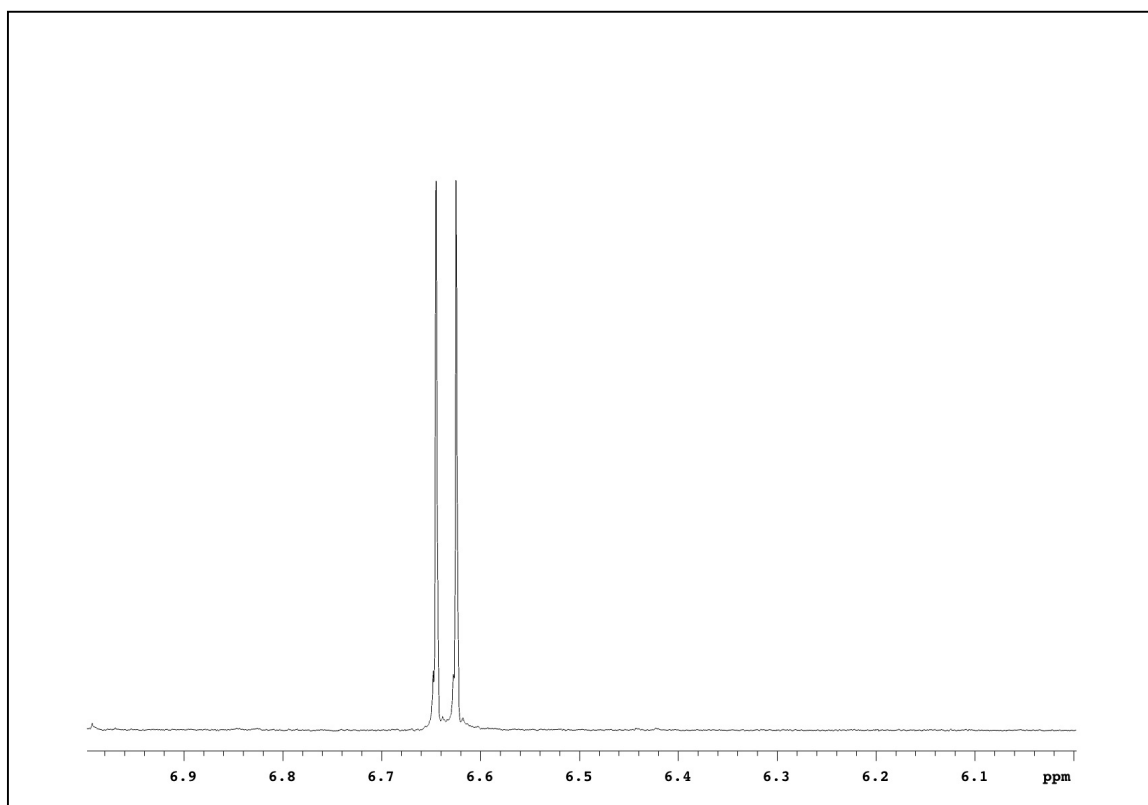
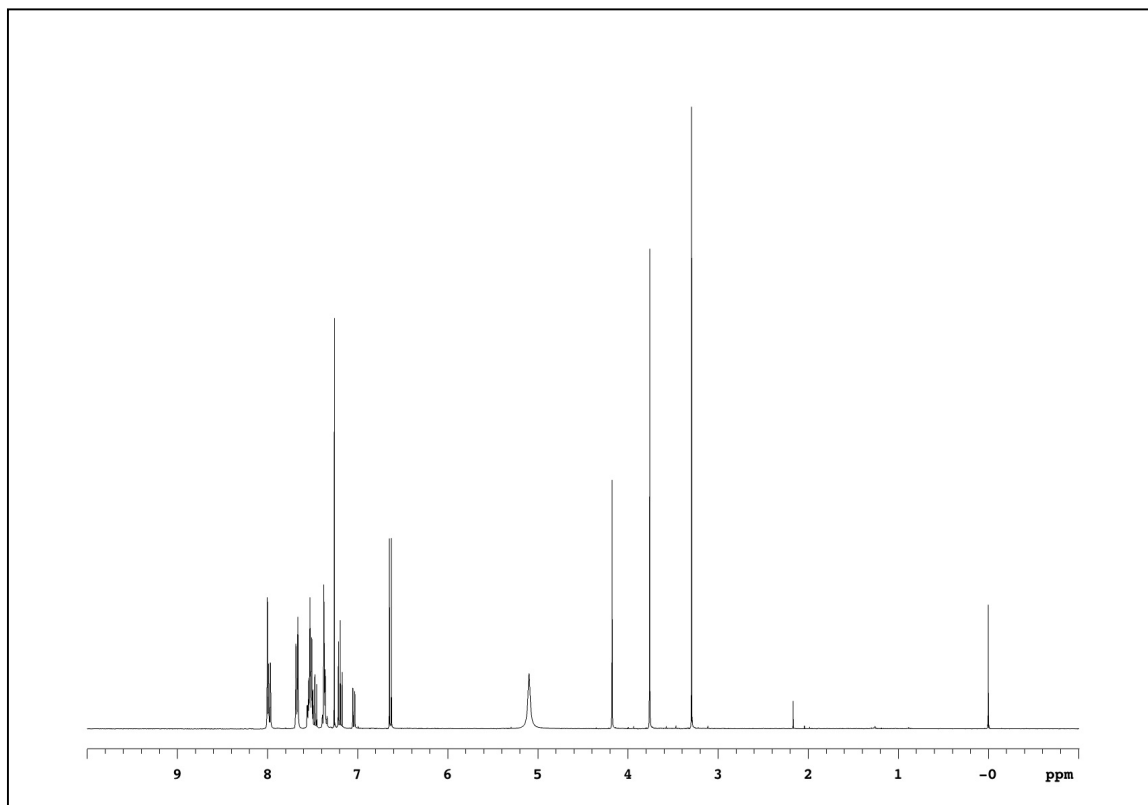
^1H NMR spectrum of the mixture of **3a** and **1a** (X = Ph).



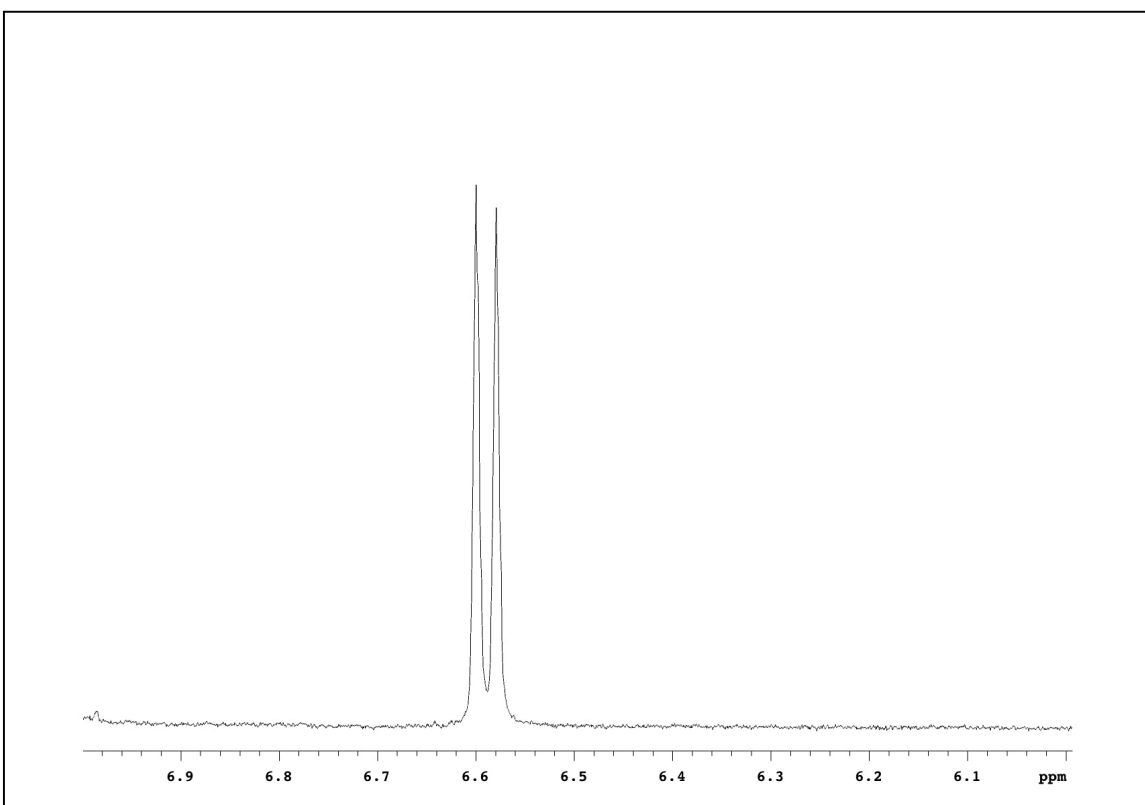
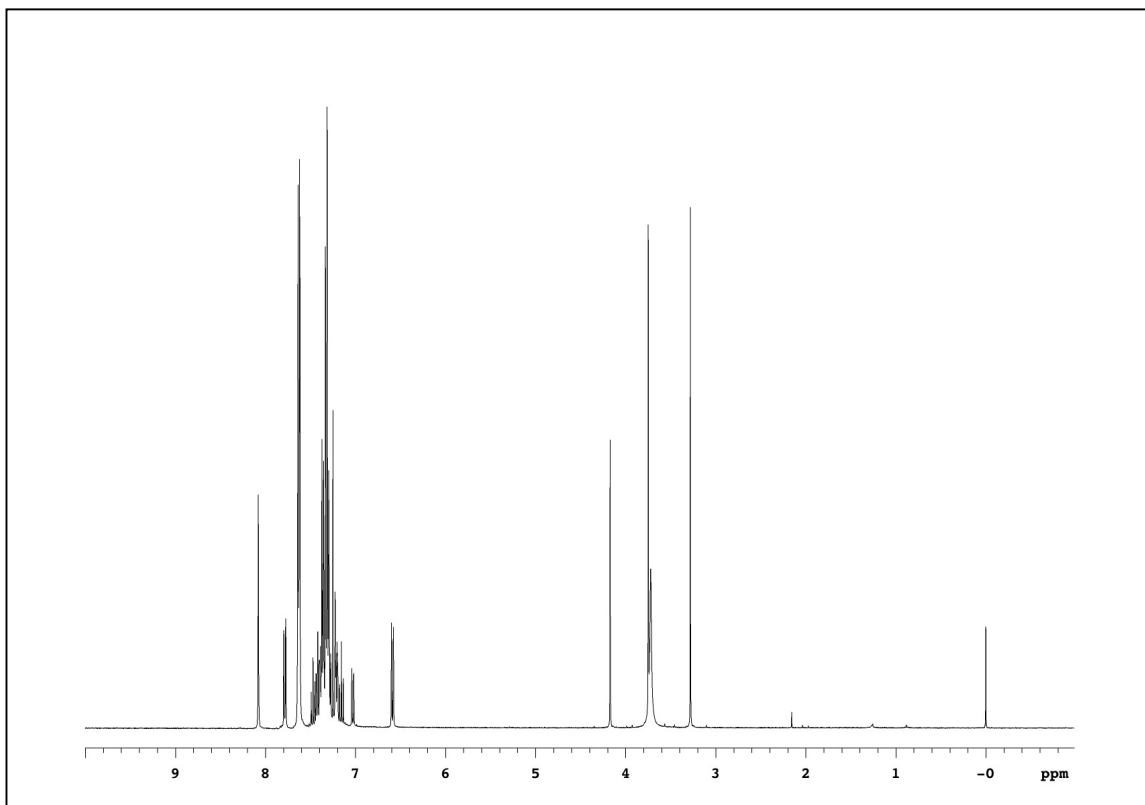
^1H NMR spectrum of the mixture of **3a** and **1b** ($\text{X} = p\text{-NO}_2\text{C}_6\text{H}_4$).



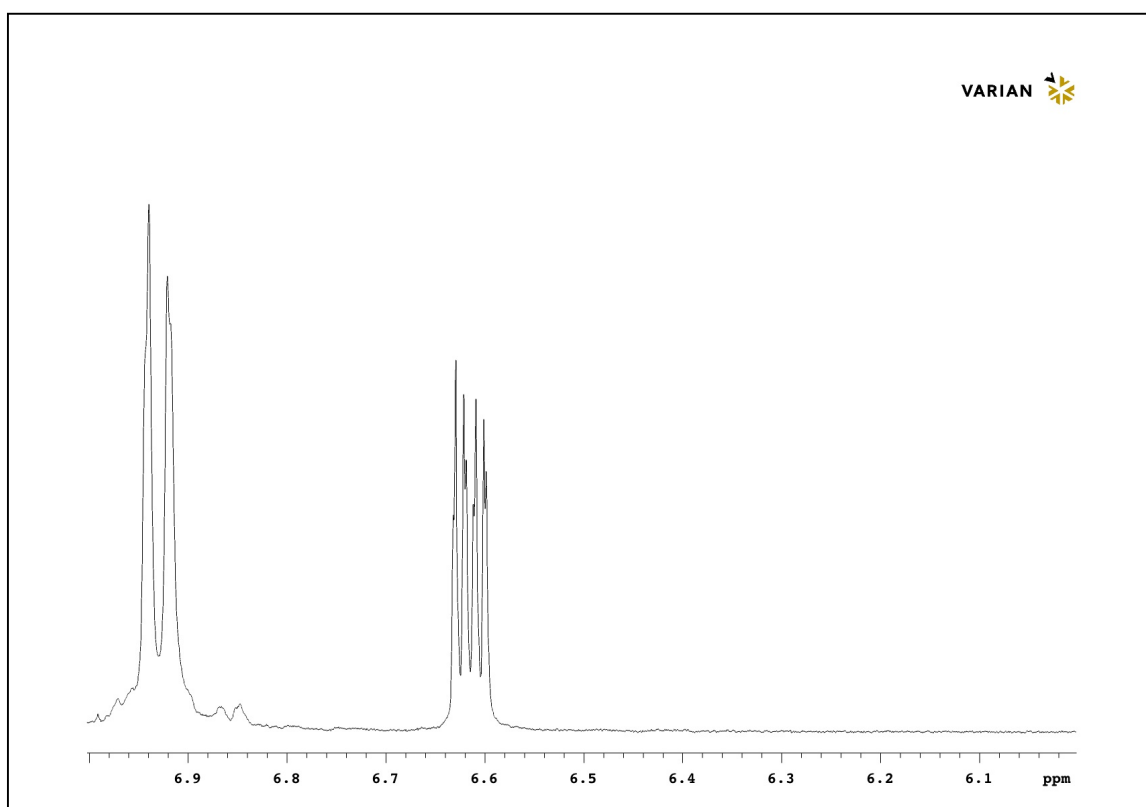
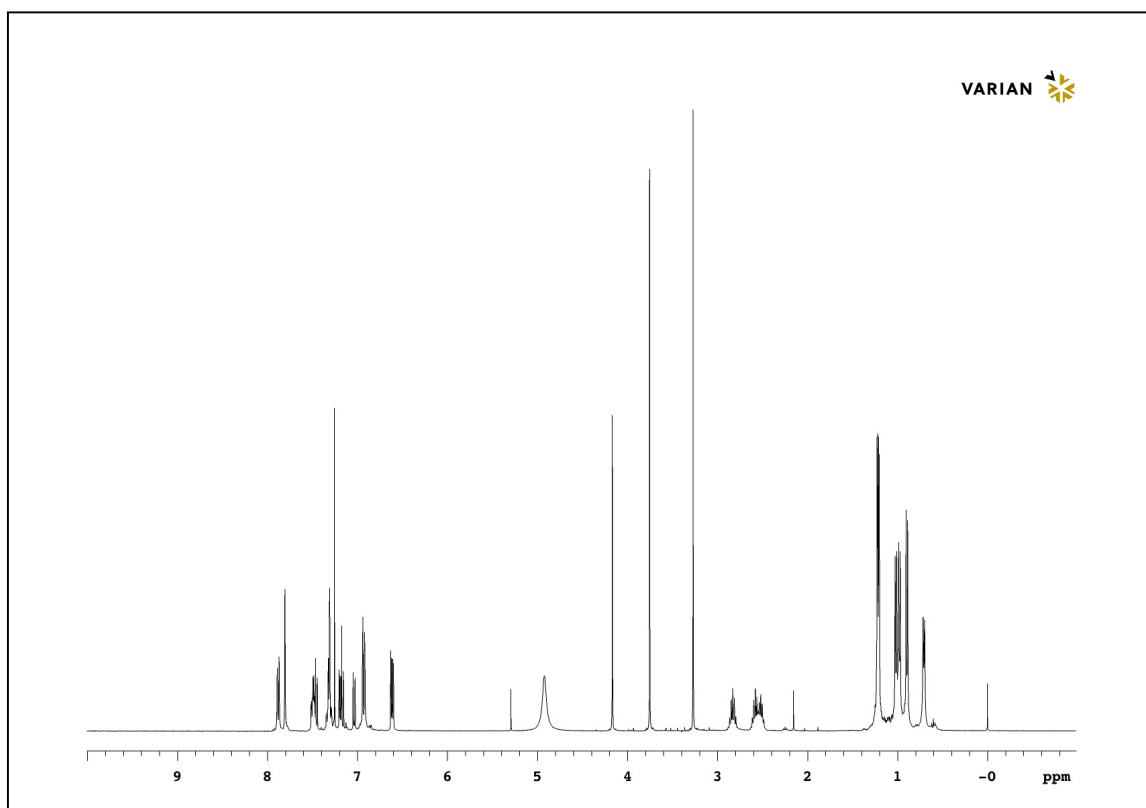
^1H NMR spectrum of the mixture of **3a** and **1c** ($\text{X} = p\text{-CF}_3\text{C}_6\text{H}_4$).



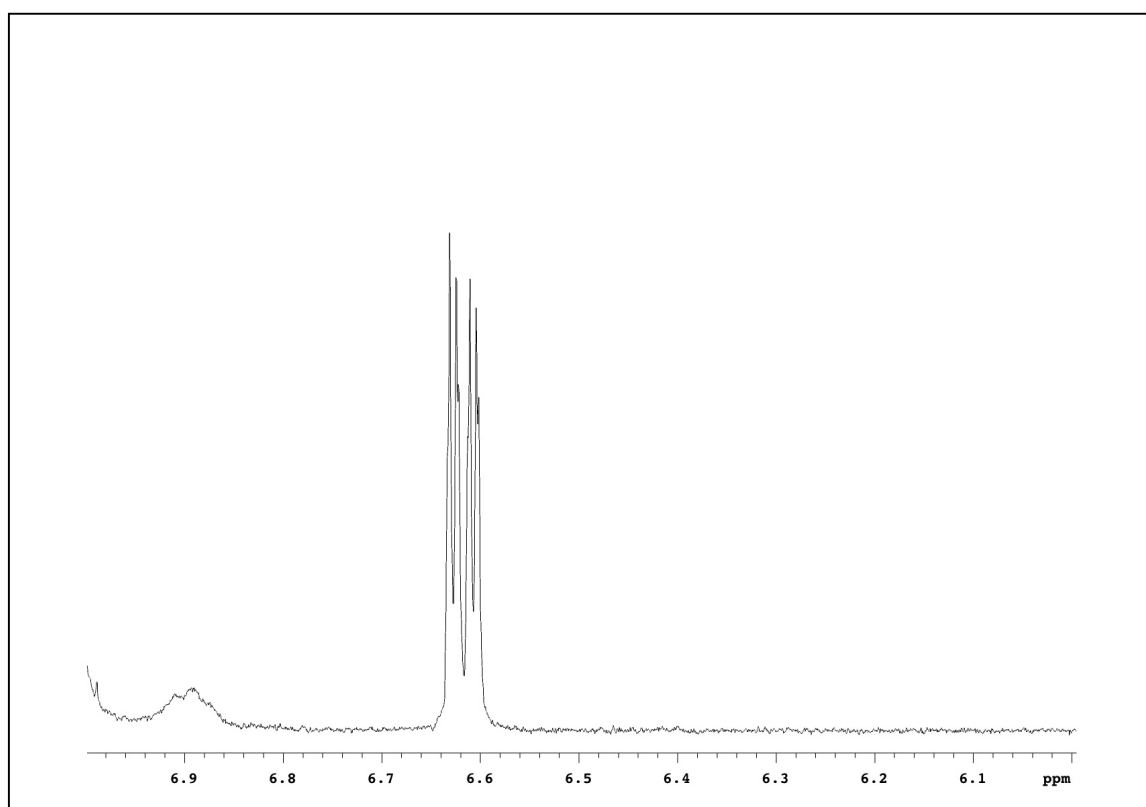
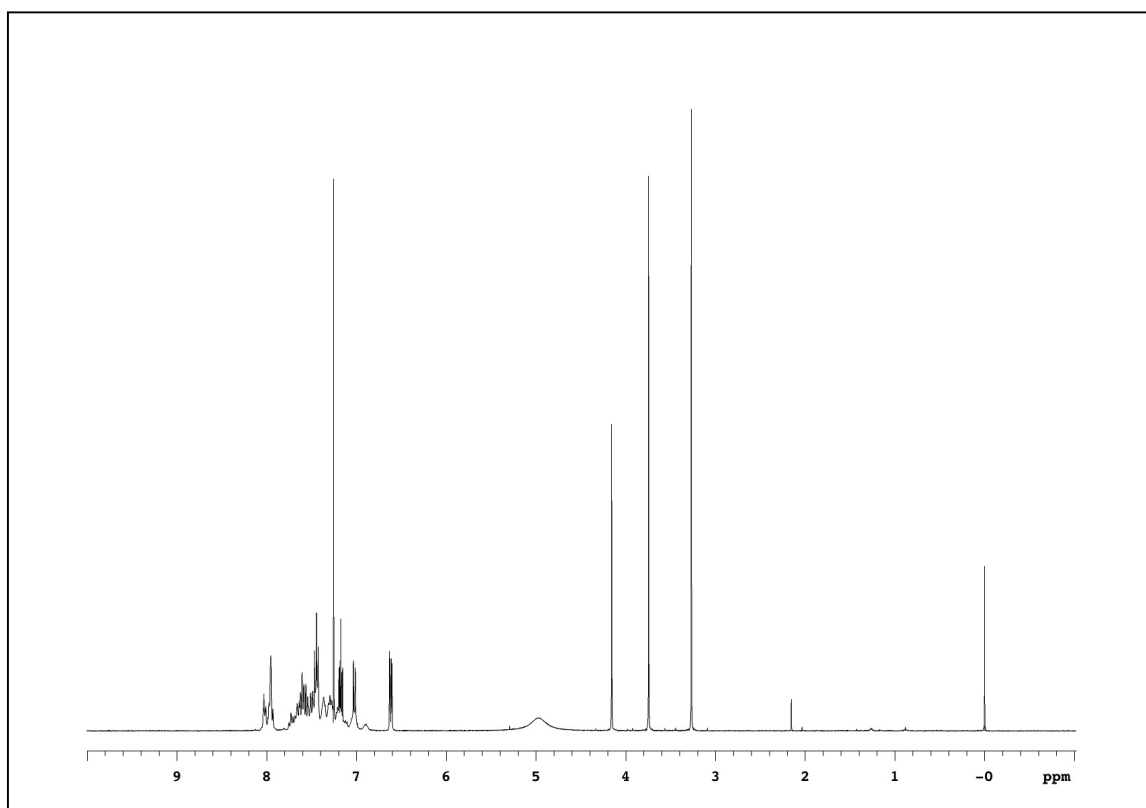
^1H NMR spectrum of the mixture of **3a** and **1d** ($\text{X} = \text{SiPh}_3$).



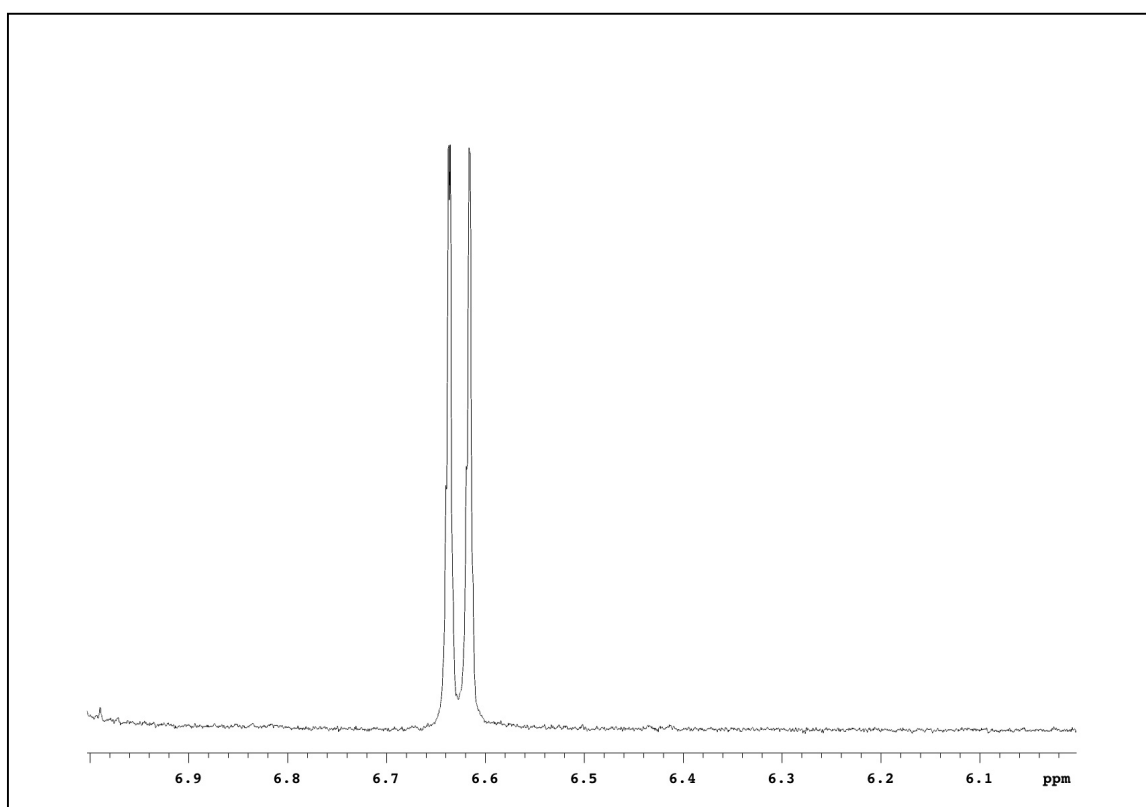
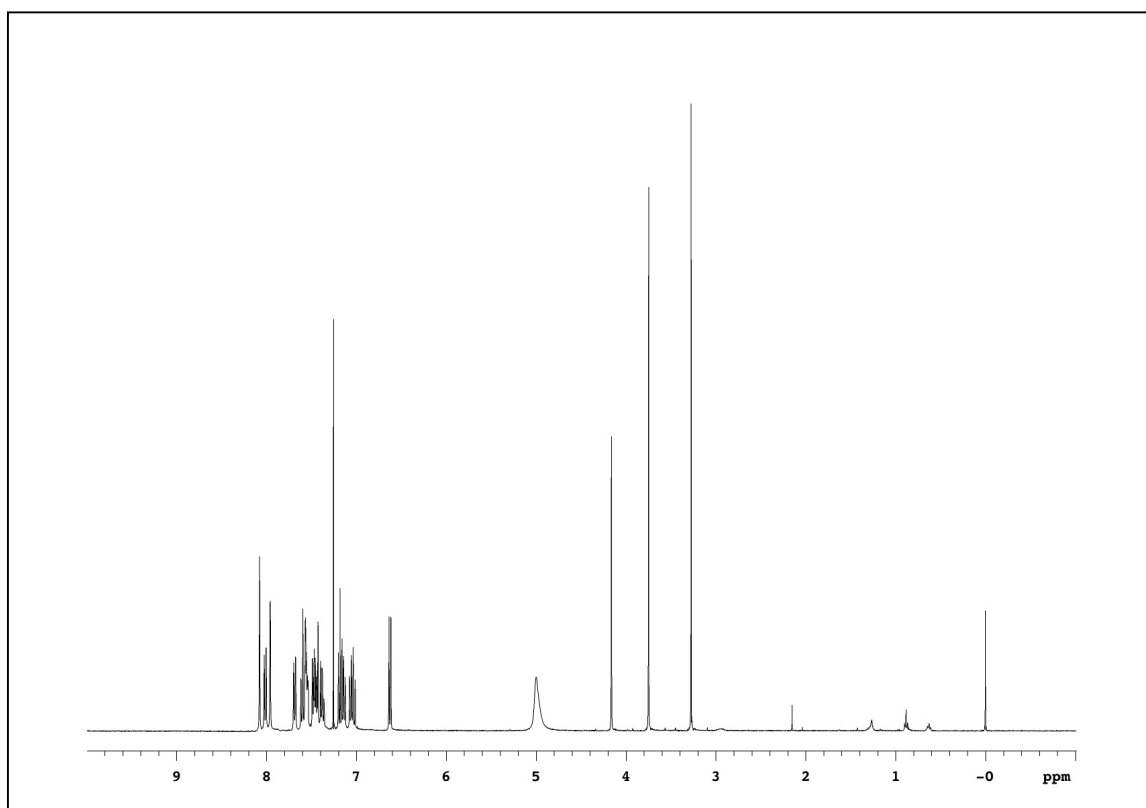
^1H NMR spectrum of the mixture of **3a** and **1e** ($\text{X} = 2,4,6\text{-}(i\text{-Pr})_3\text{C}_6\text{H}_2$).



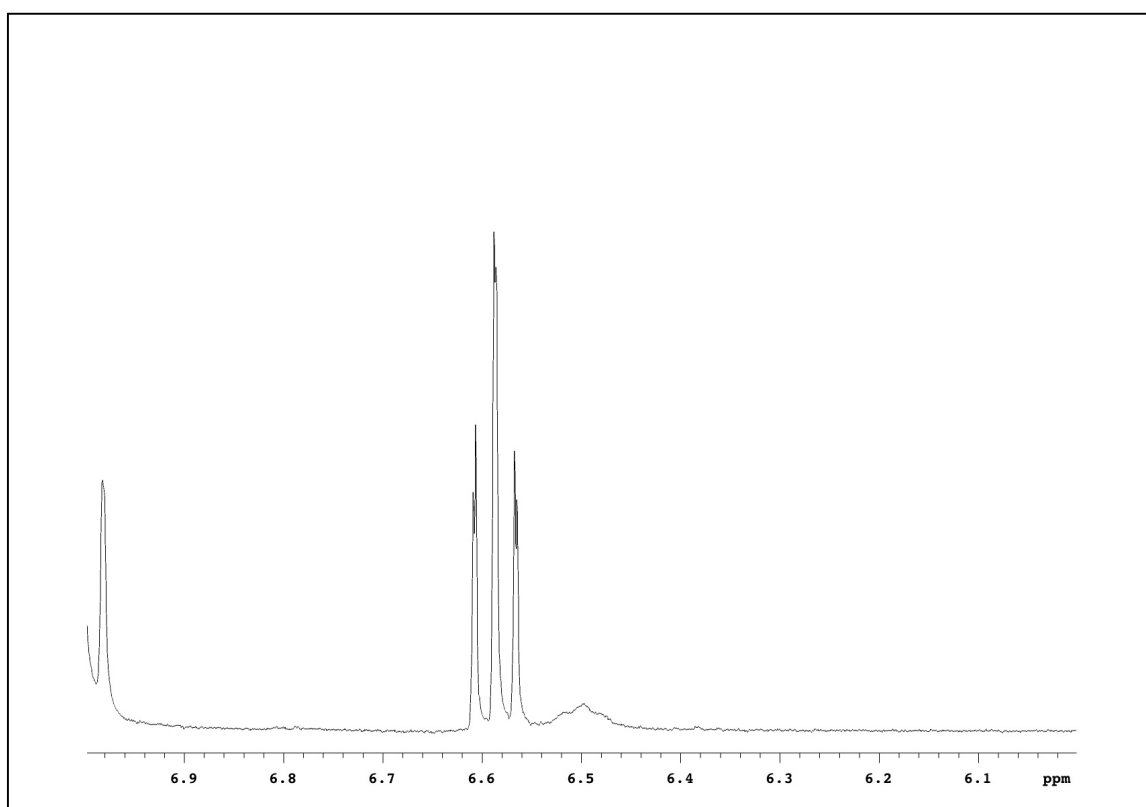
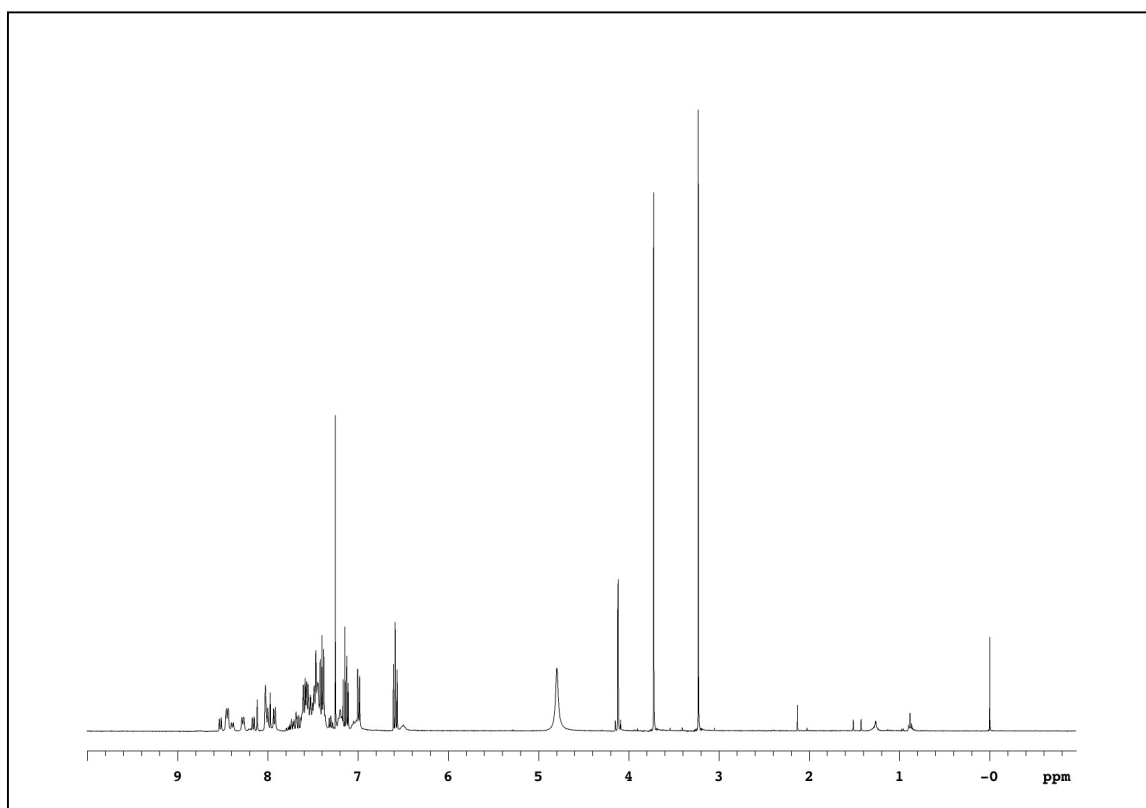
^1H NMR spectrum of the mixture of **3a** and **1f** (X = 1-naphthyl).



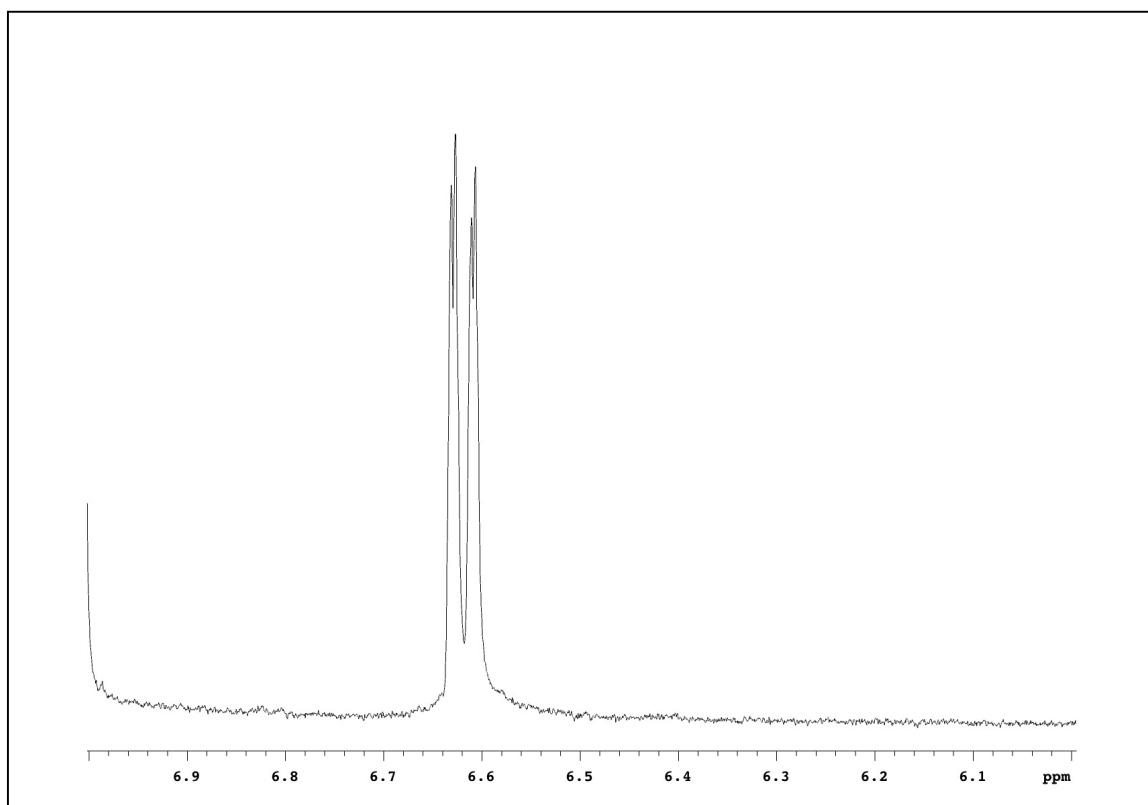
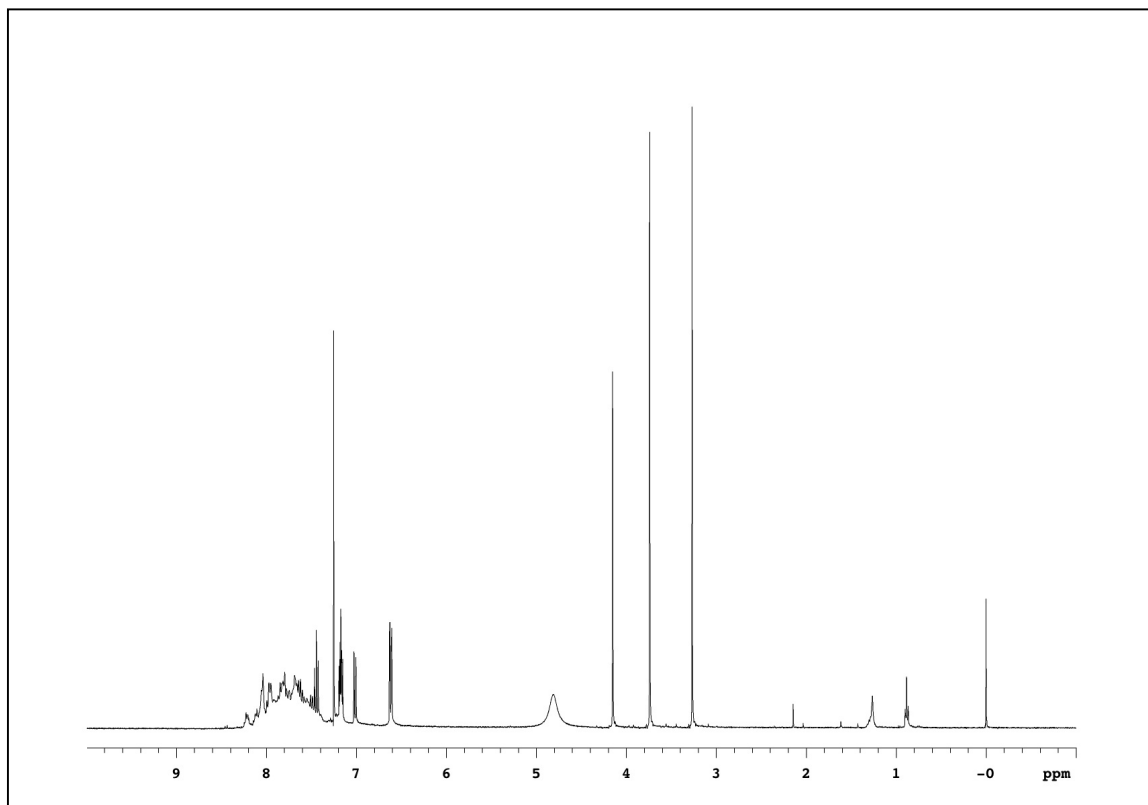
^1H NMR spectrum of the mixture of **3a** and **1g** (X = 2-naphthyl).



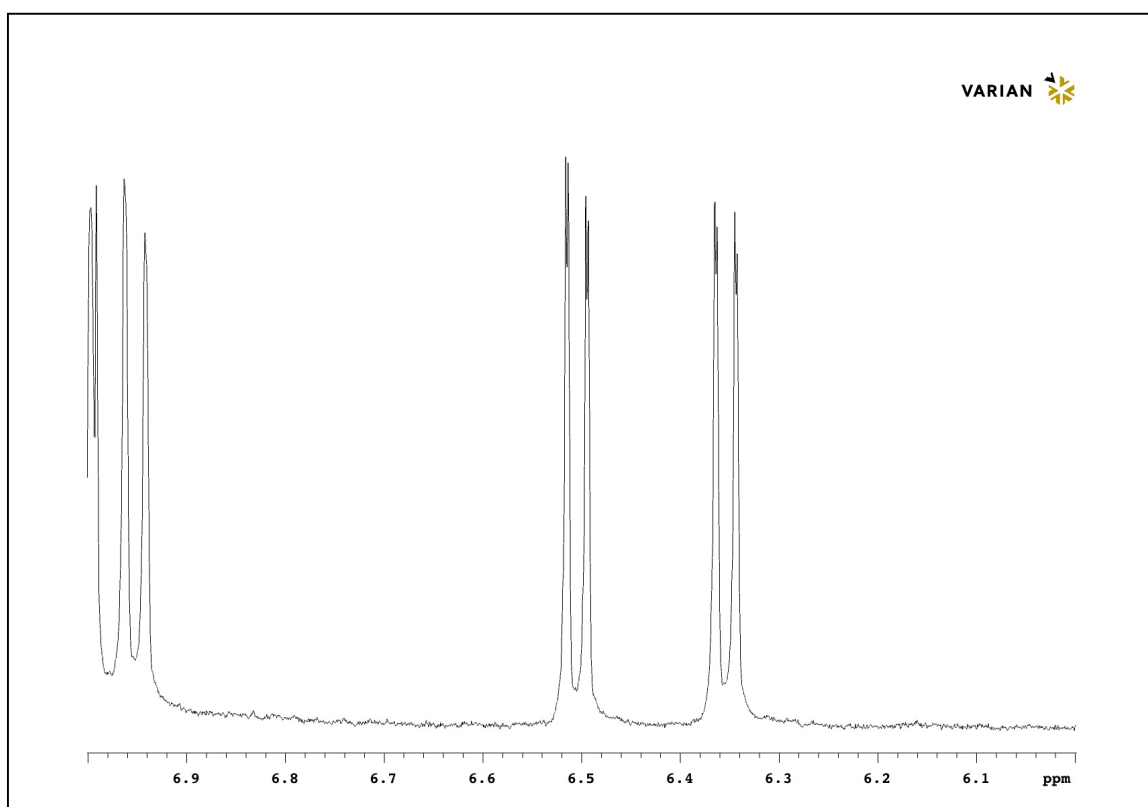
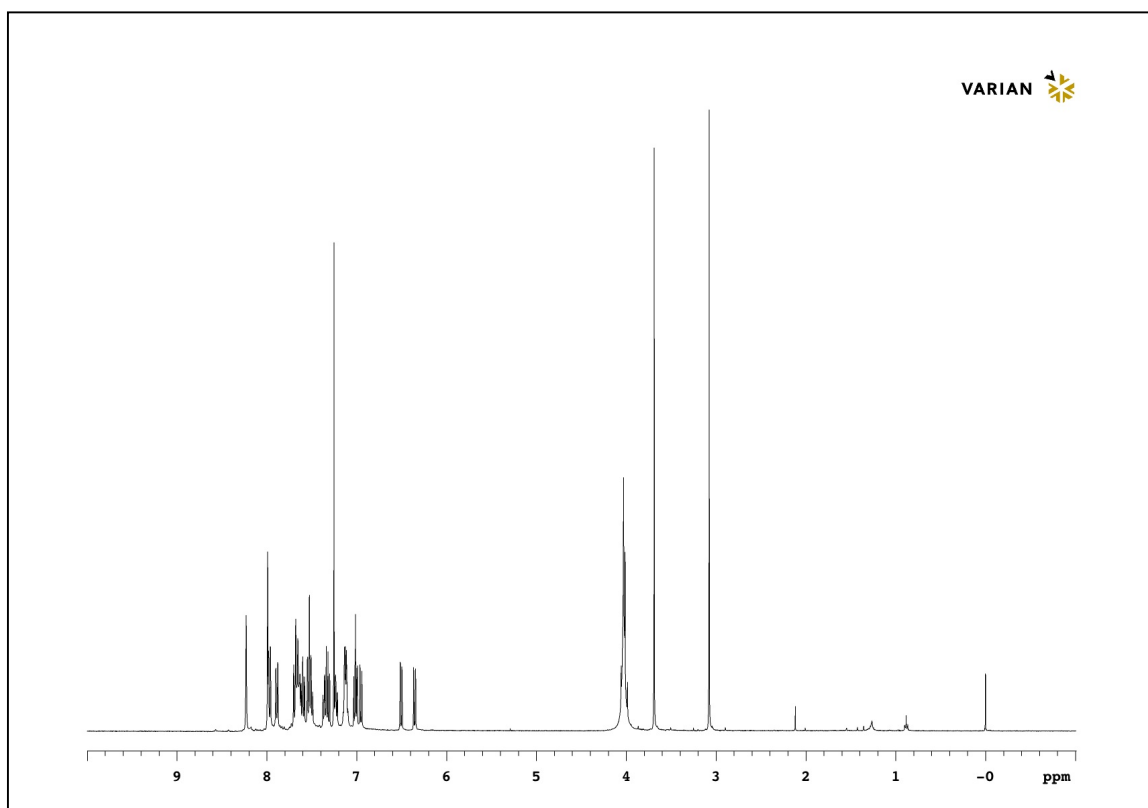
^1H NMR spectrum of the mixture of **3a** and **1h** (X = 9-phenanthryl).



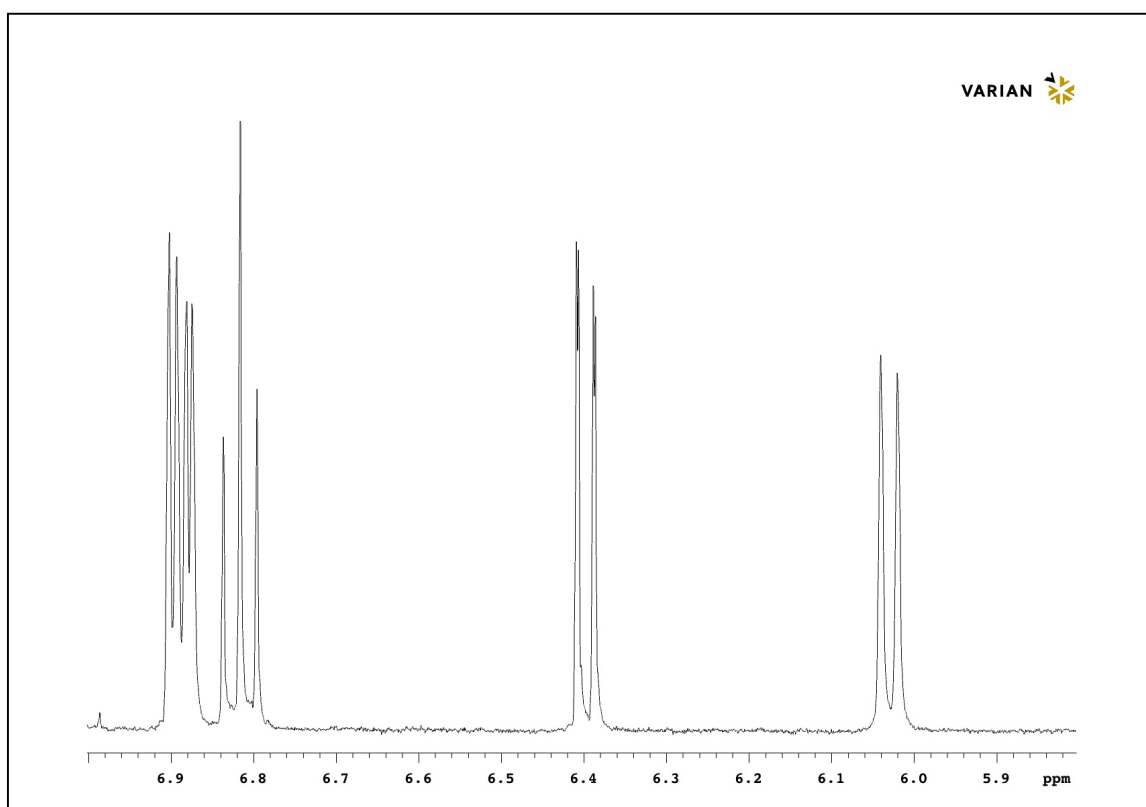
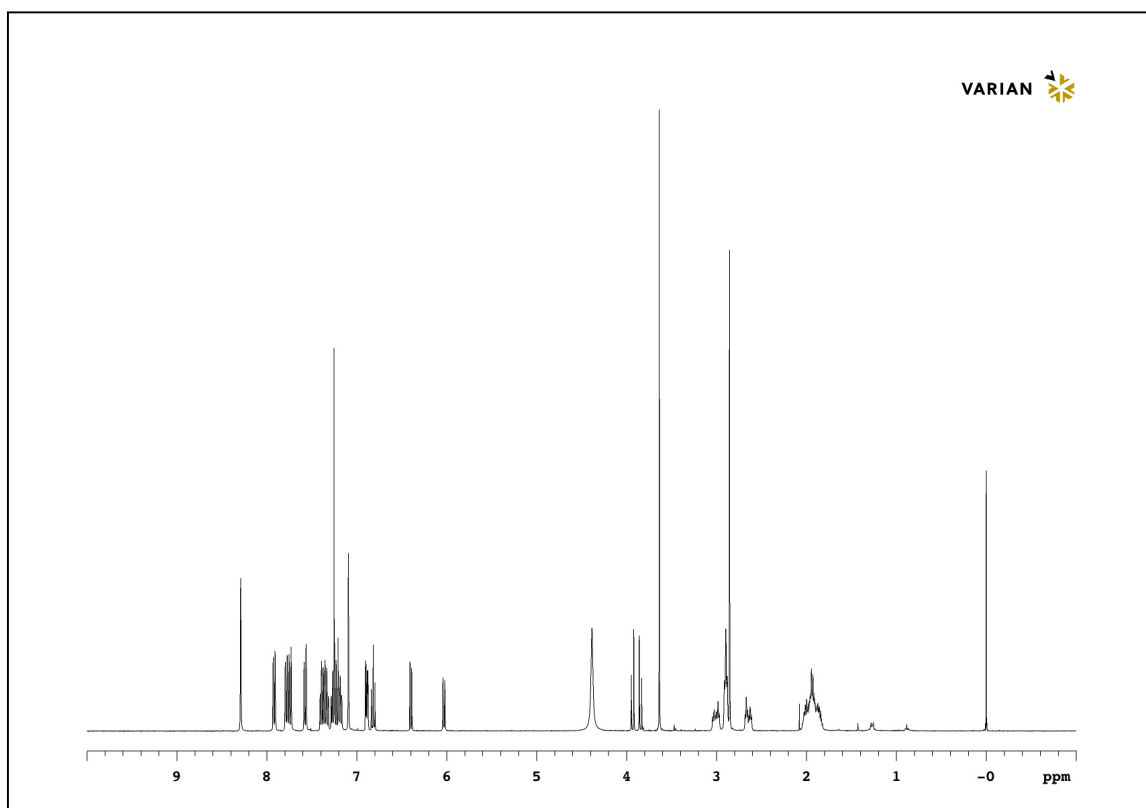
^1H NMR spectrum of the mixture of **3a** and **1i** (X = 1-pyrenyl).



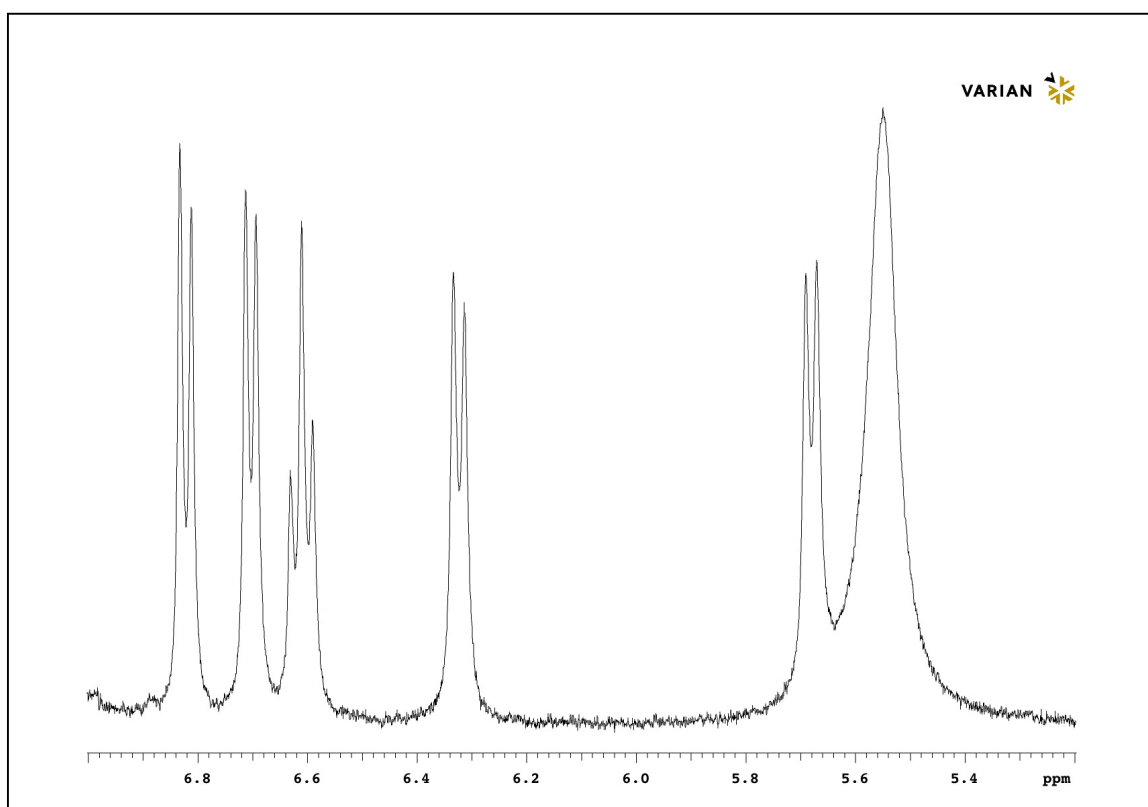
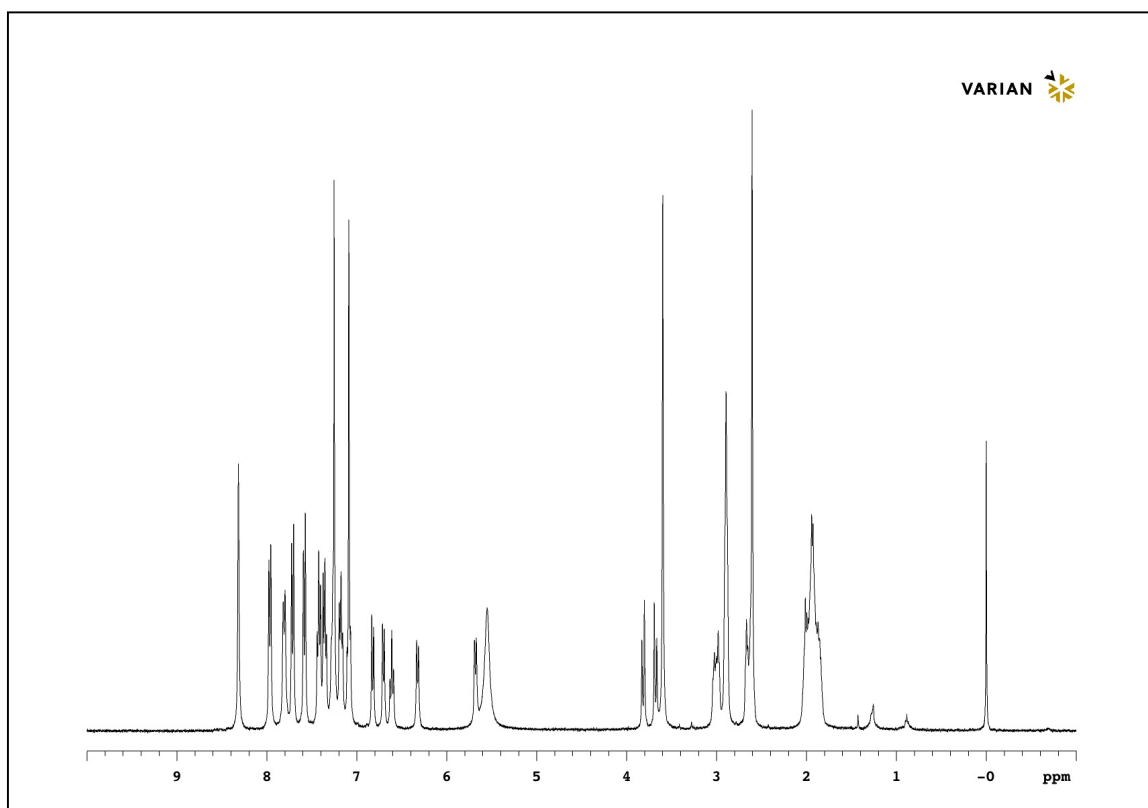
^1H NMR spectrum of the mixture of **3a** and **1j** (X = 9-anthryl).



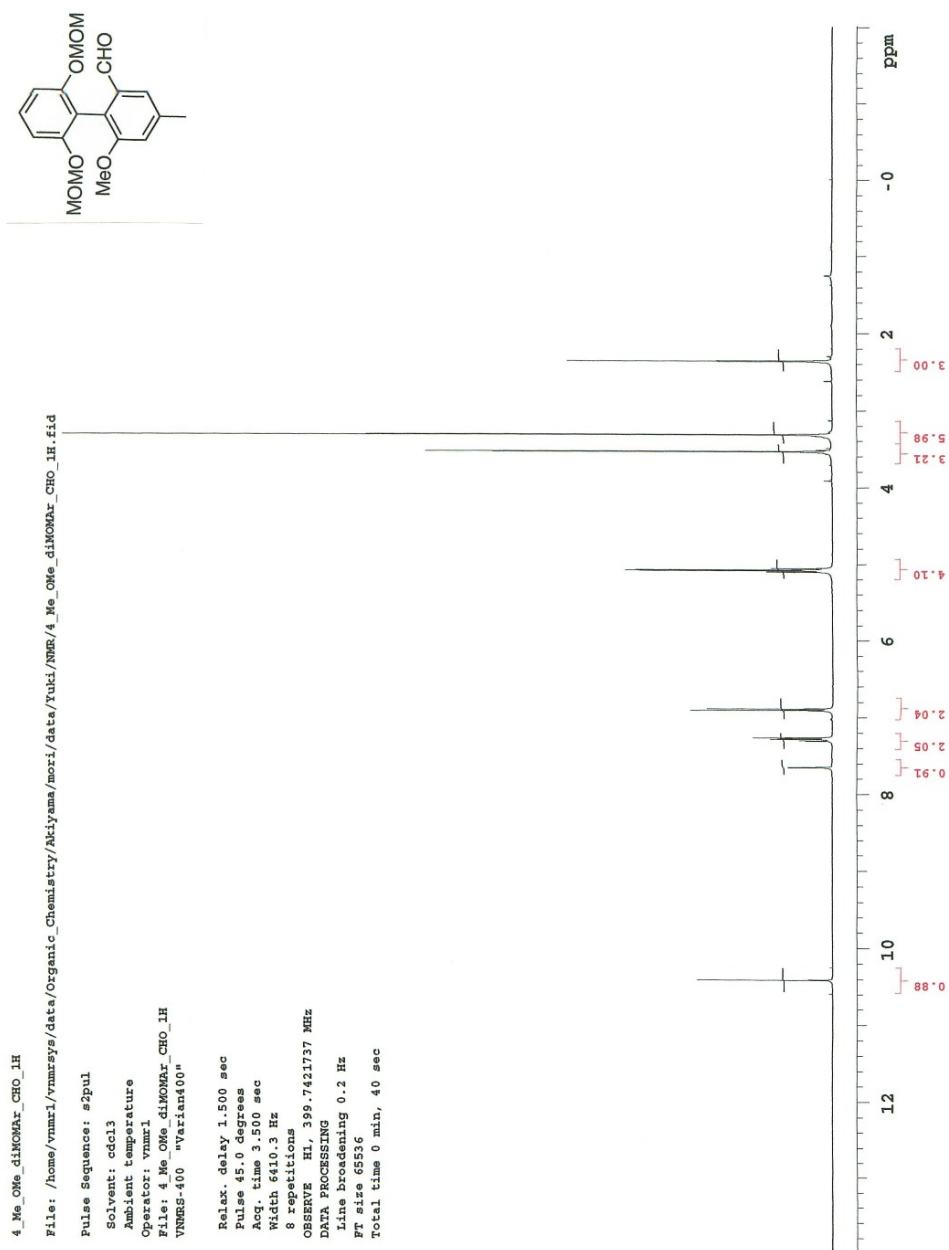
^1H NMR spectrum of the mixture of **3a** and **2j** (X = 9-anthryl).



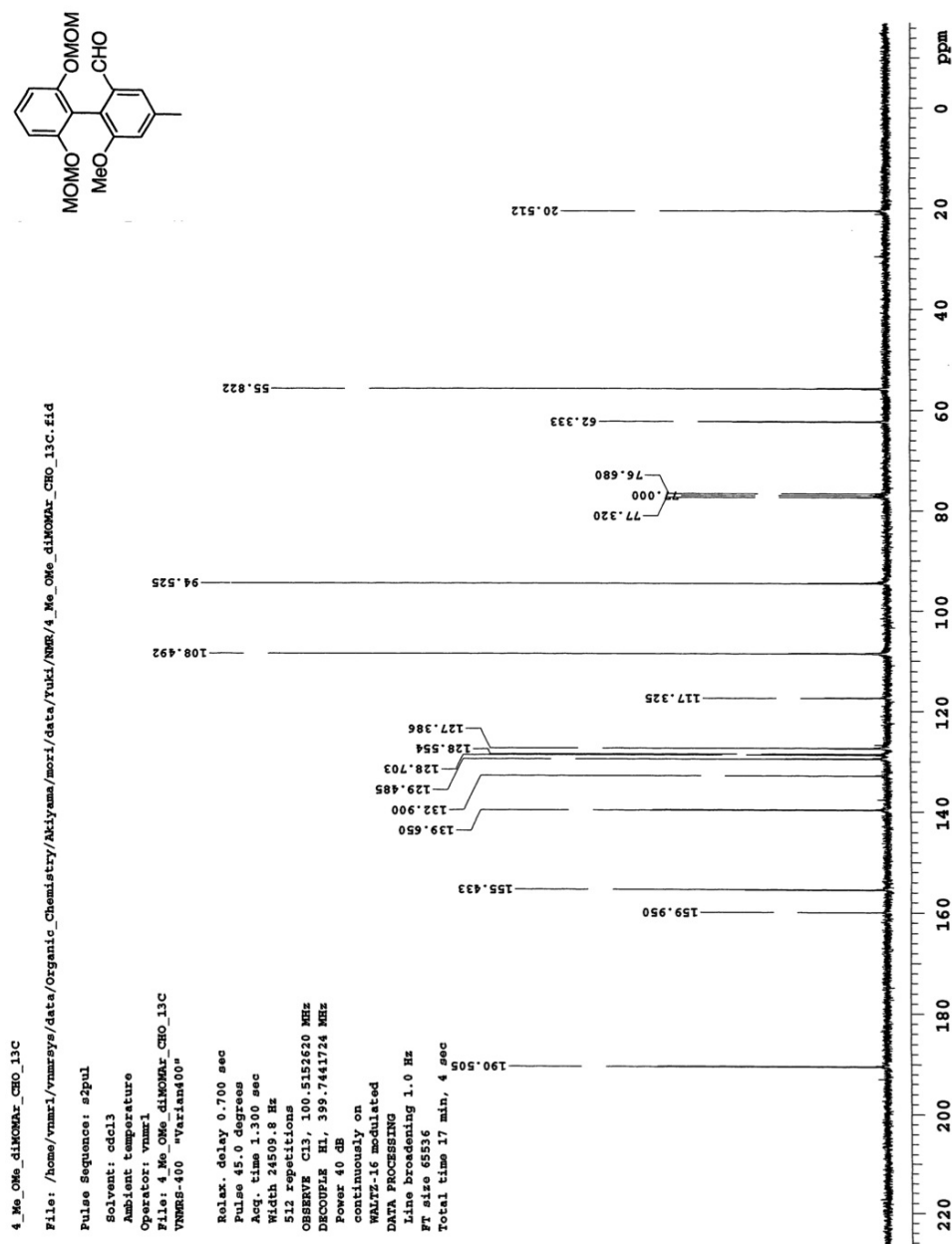
^1H NMR spectrum of the mixture of **3a** and **2j** (X = 9-anthryl) and MS13X.



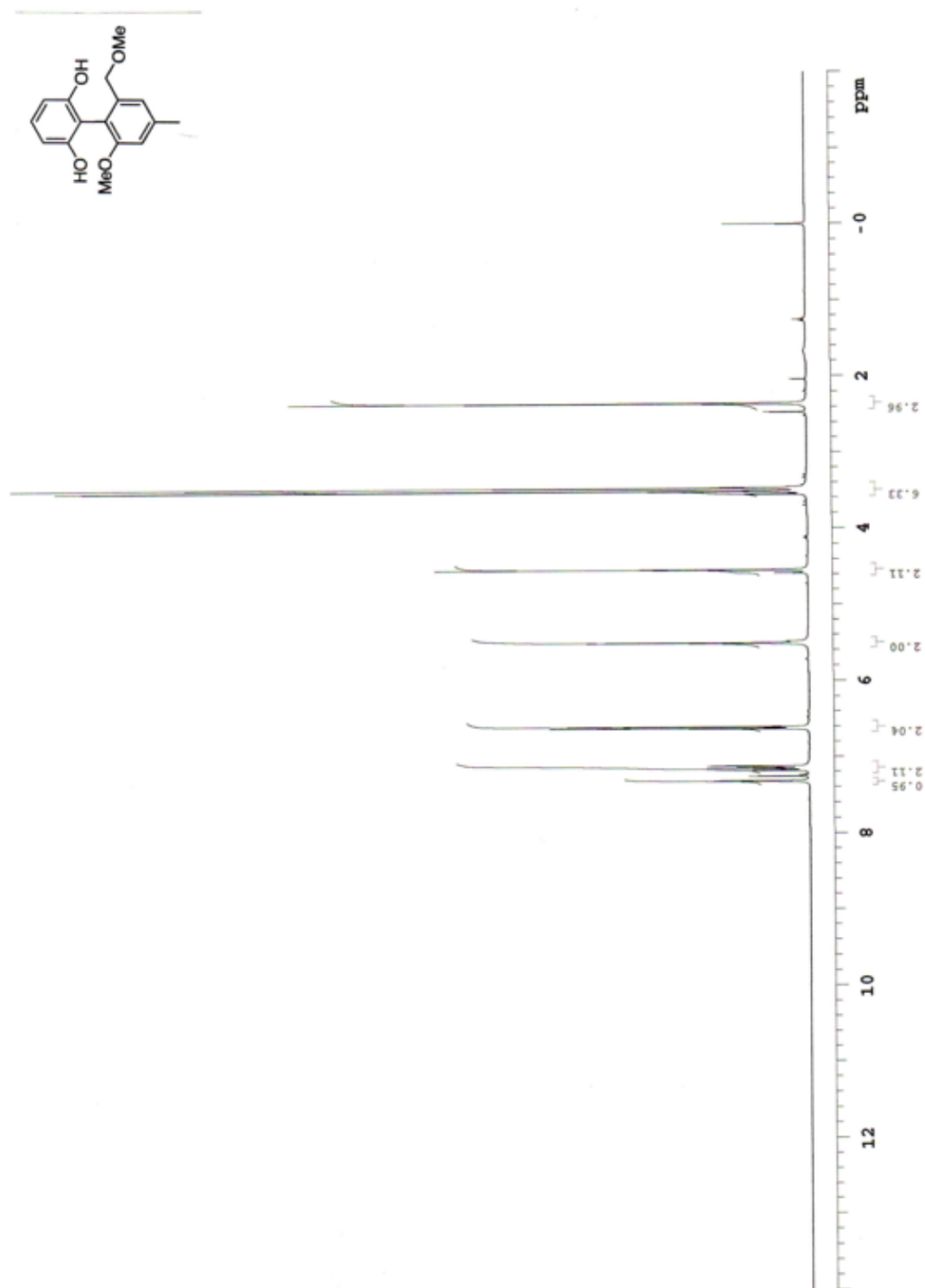
^1H NMR spectrum of **s15**.



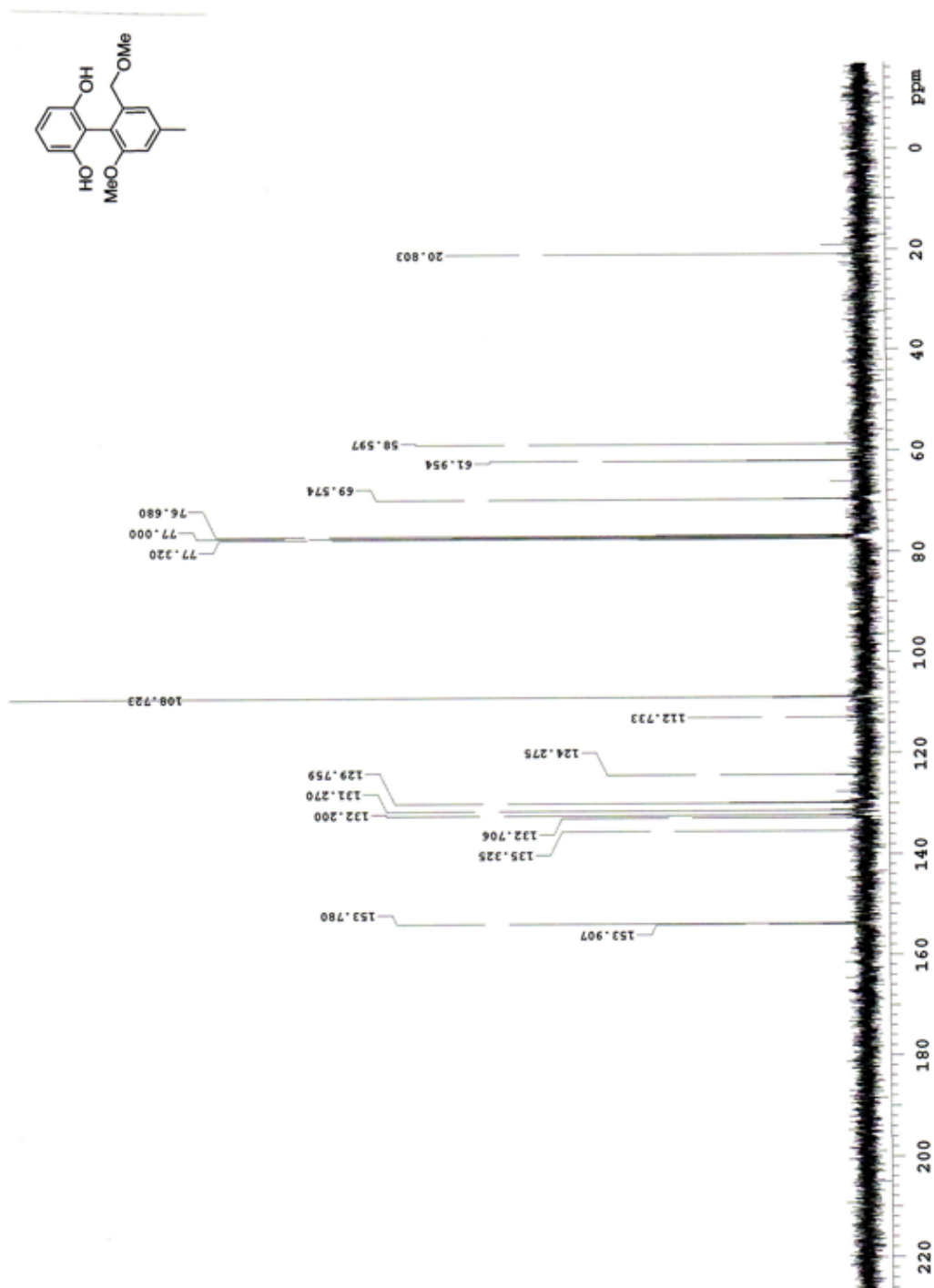
^{13}C NMR spectrum of **s15**.



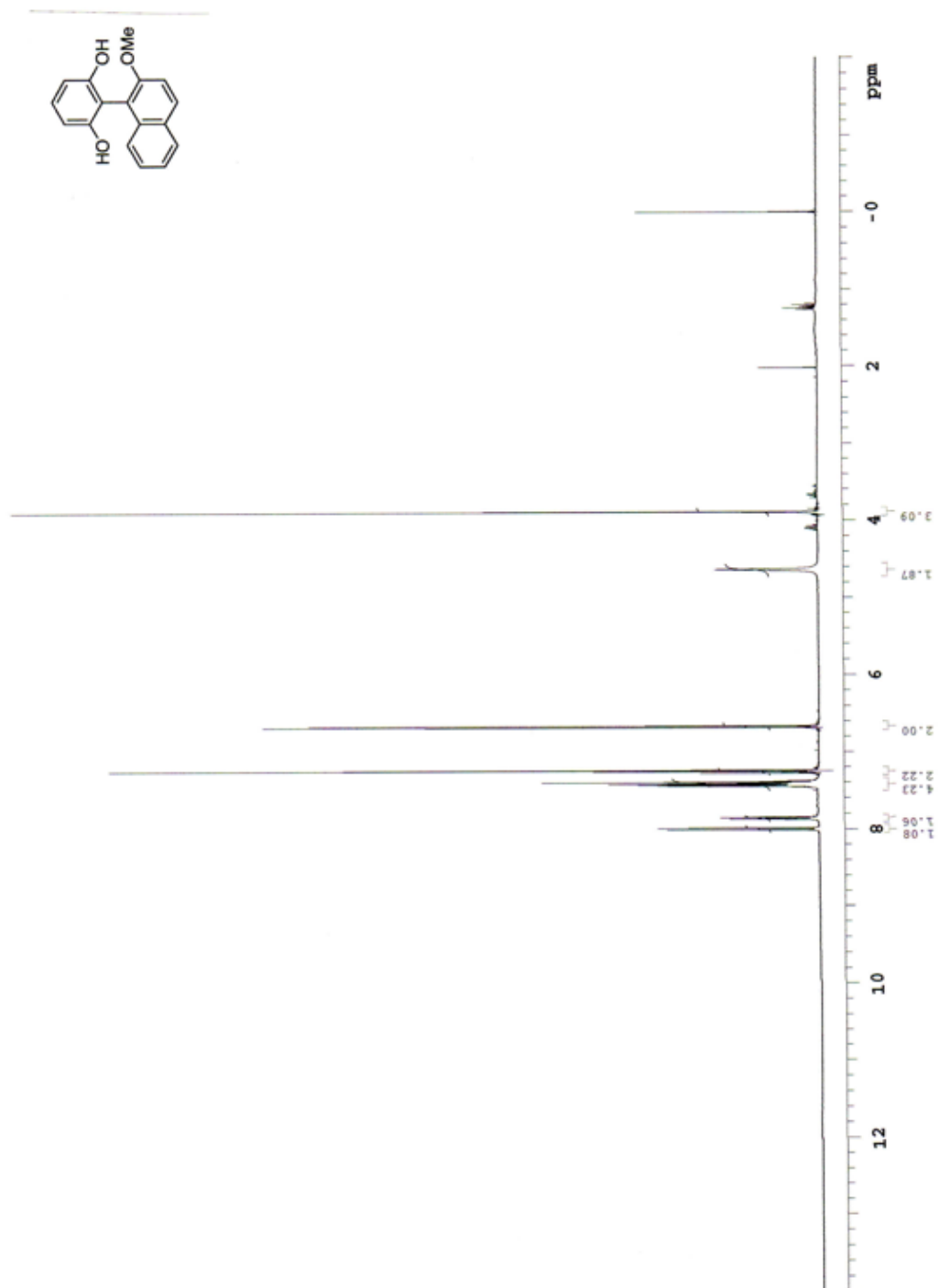
^1H NMR spectrum of **3n**.



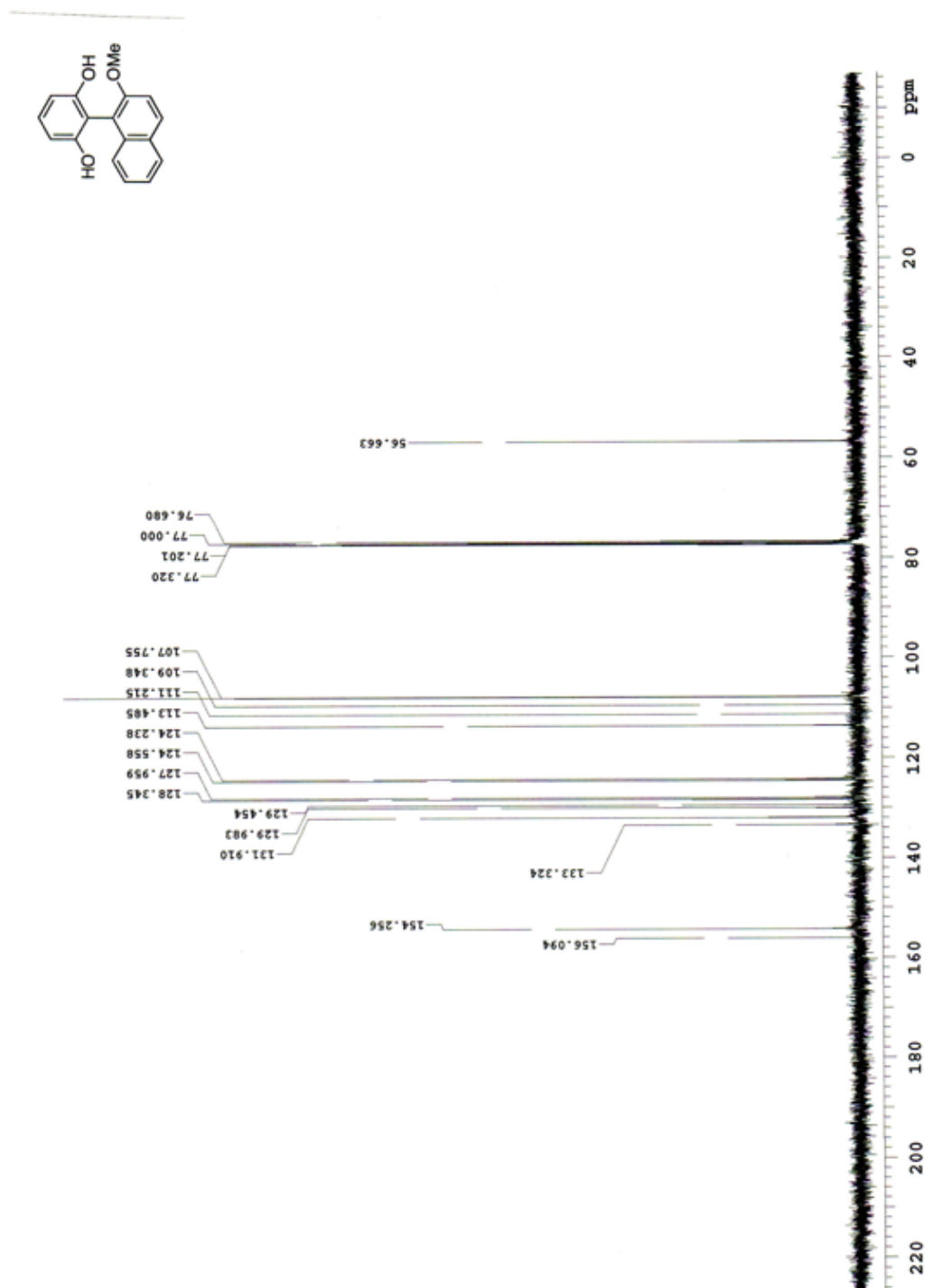
^{13}C NMR spectrum of **3n**.



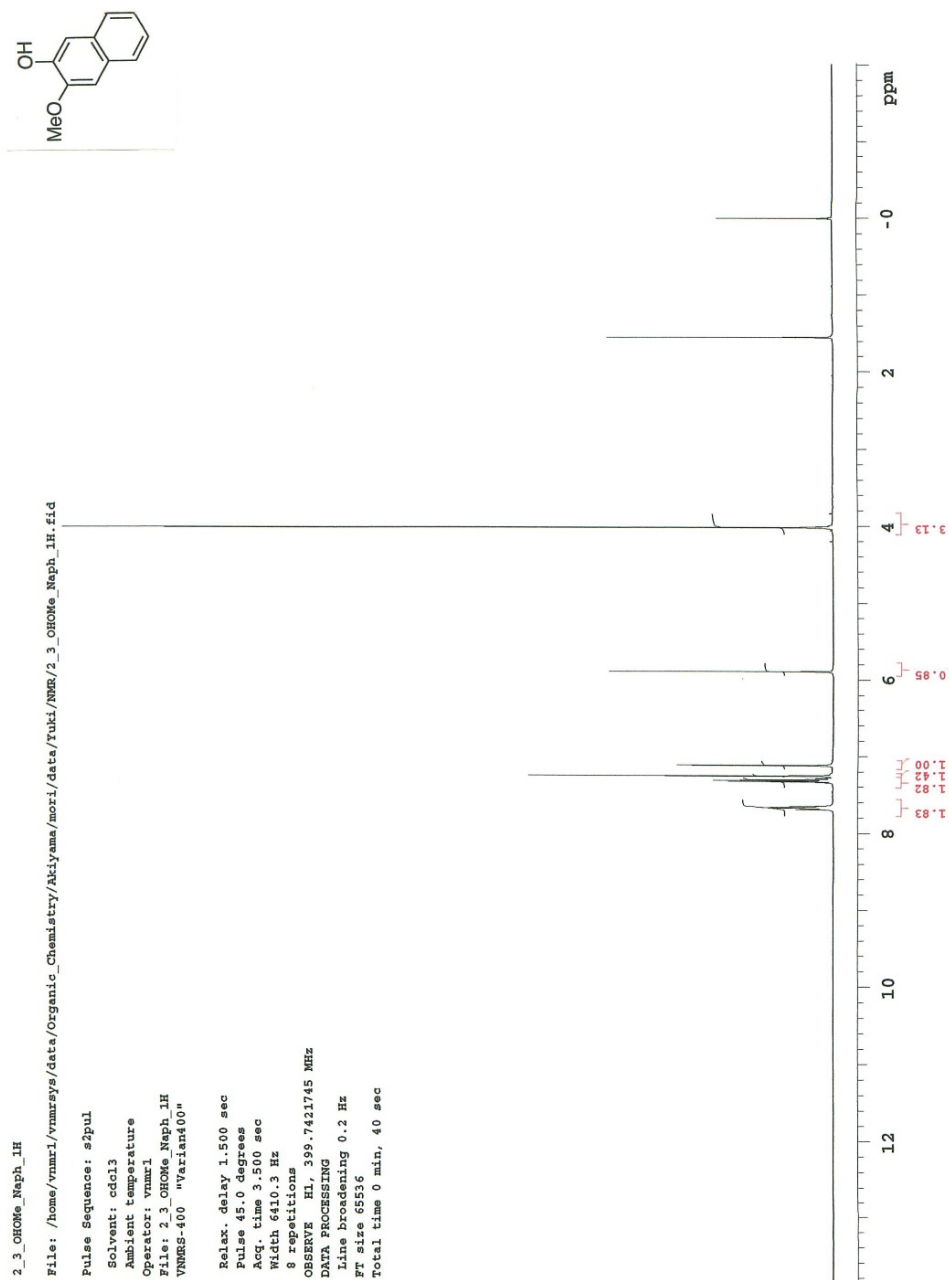
^1H NMR spectrum of **3o**.



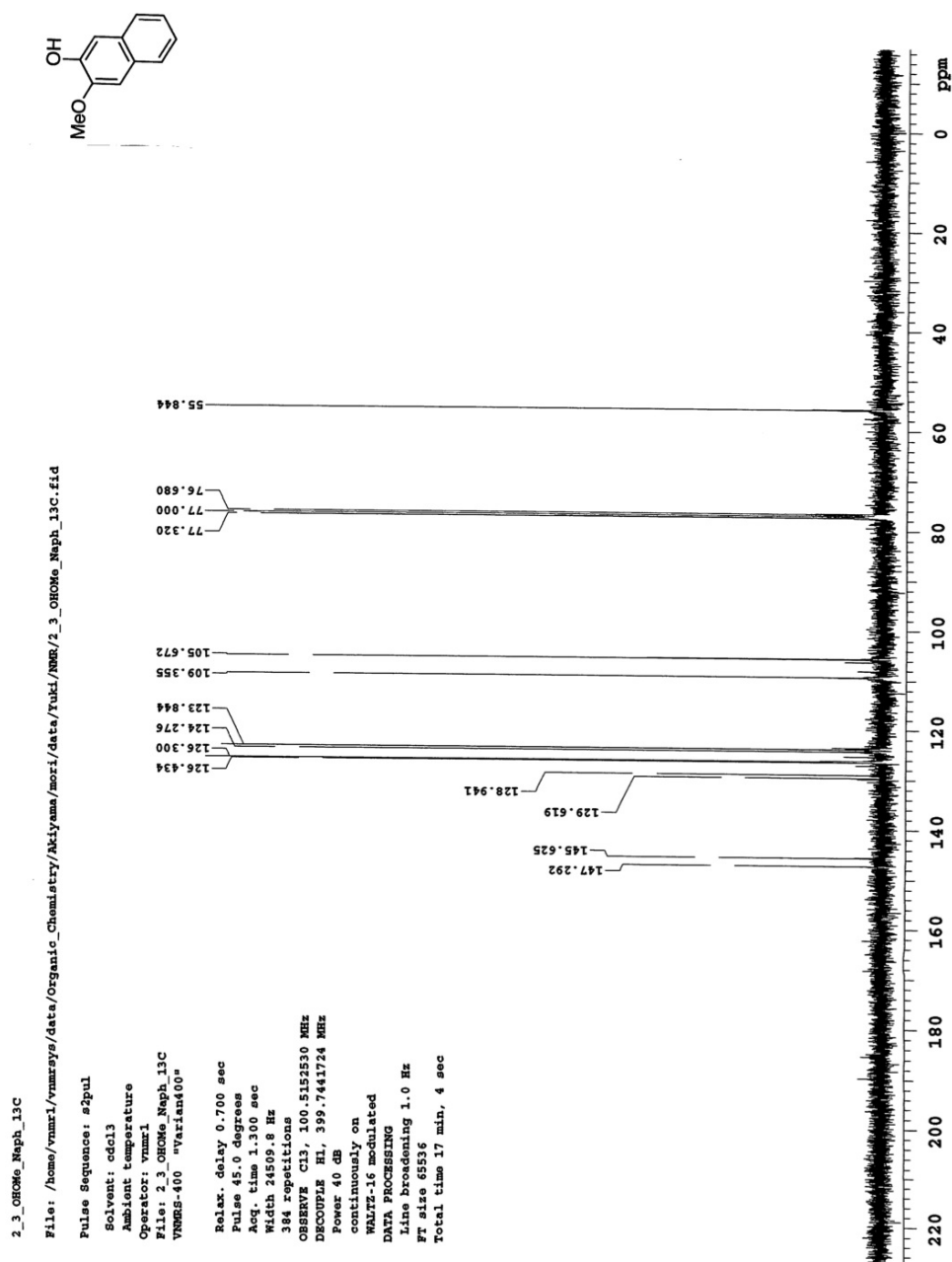
^{13}C NMR spectrum of **30**.



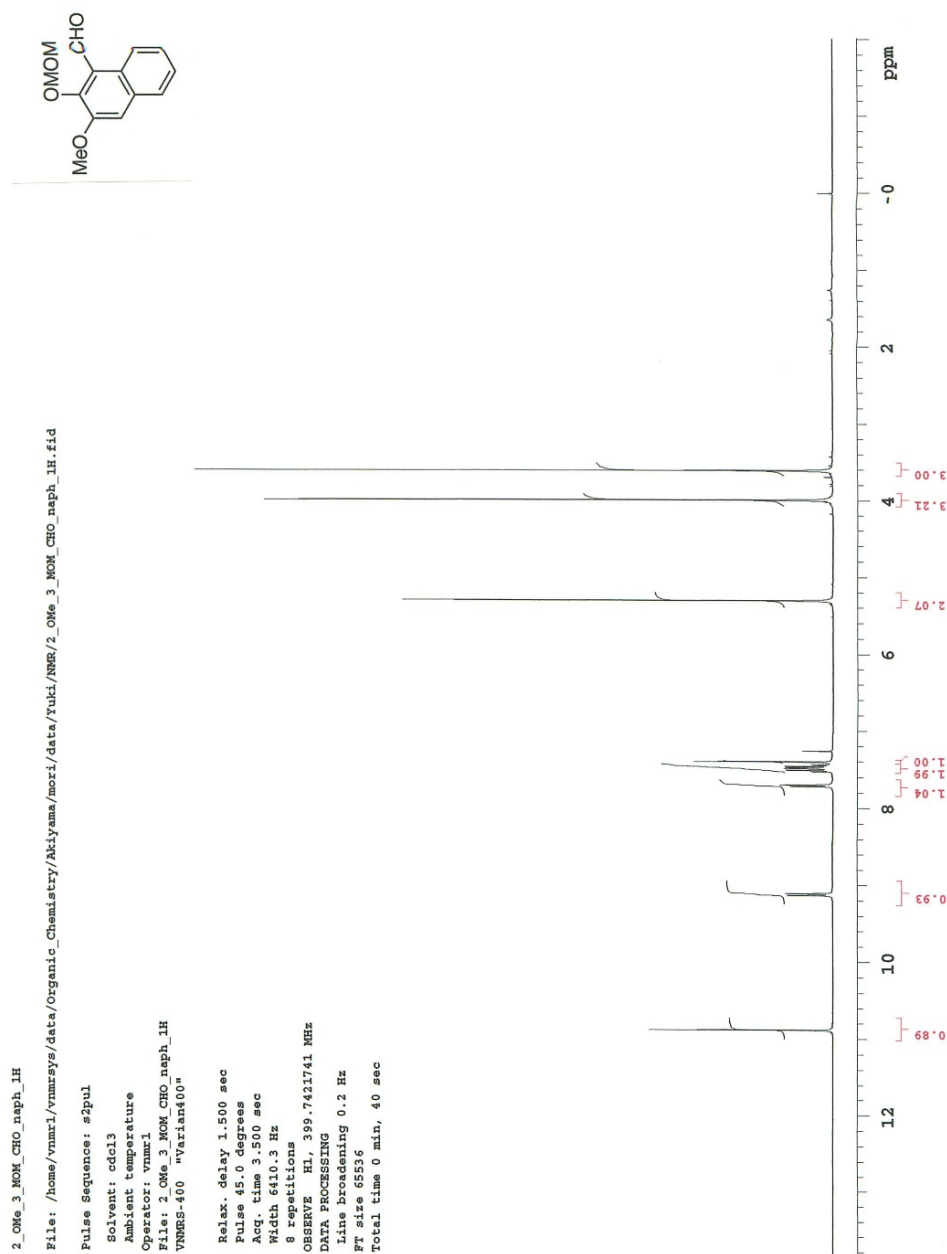
^1H NMR spectrum of **s23**.



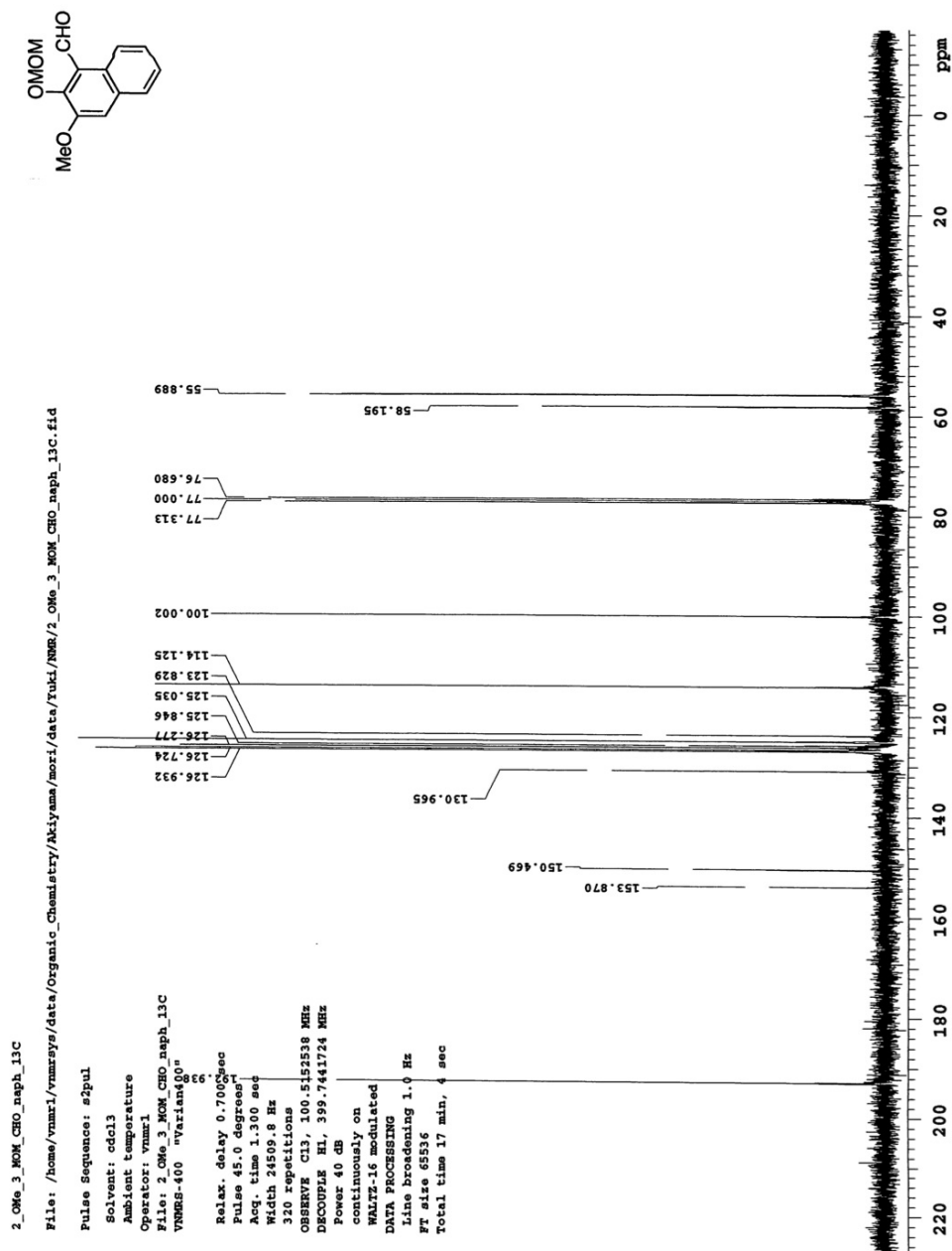
¹³C NMR spectrum of **s23**.



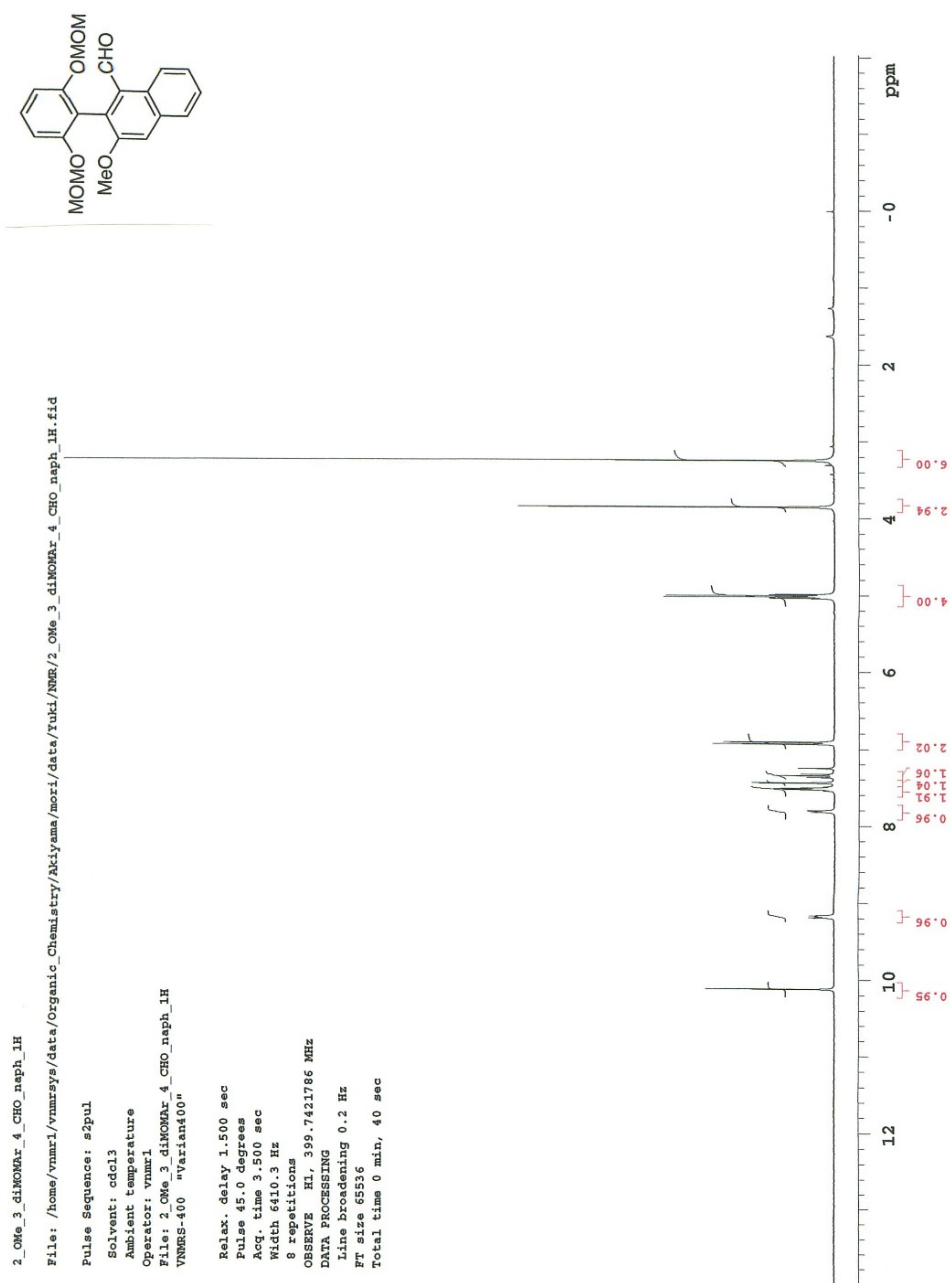
^1H NMR spectrum of **s25**.



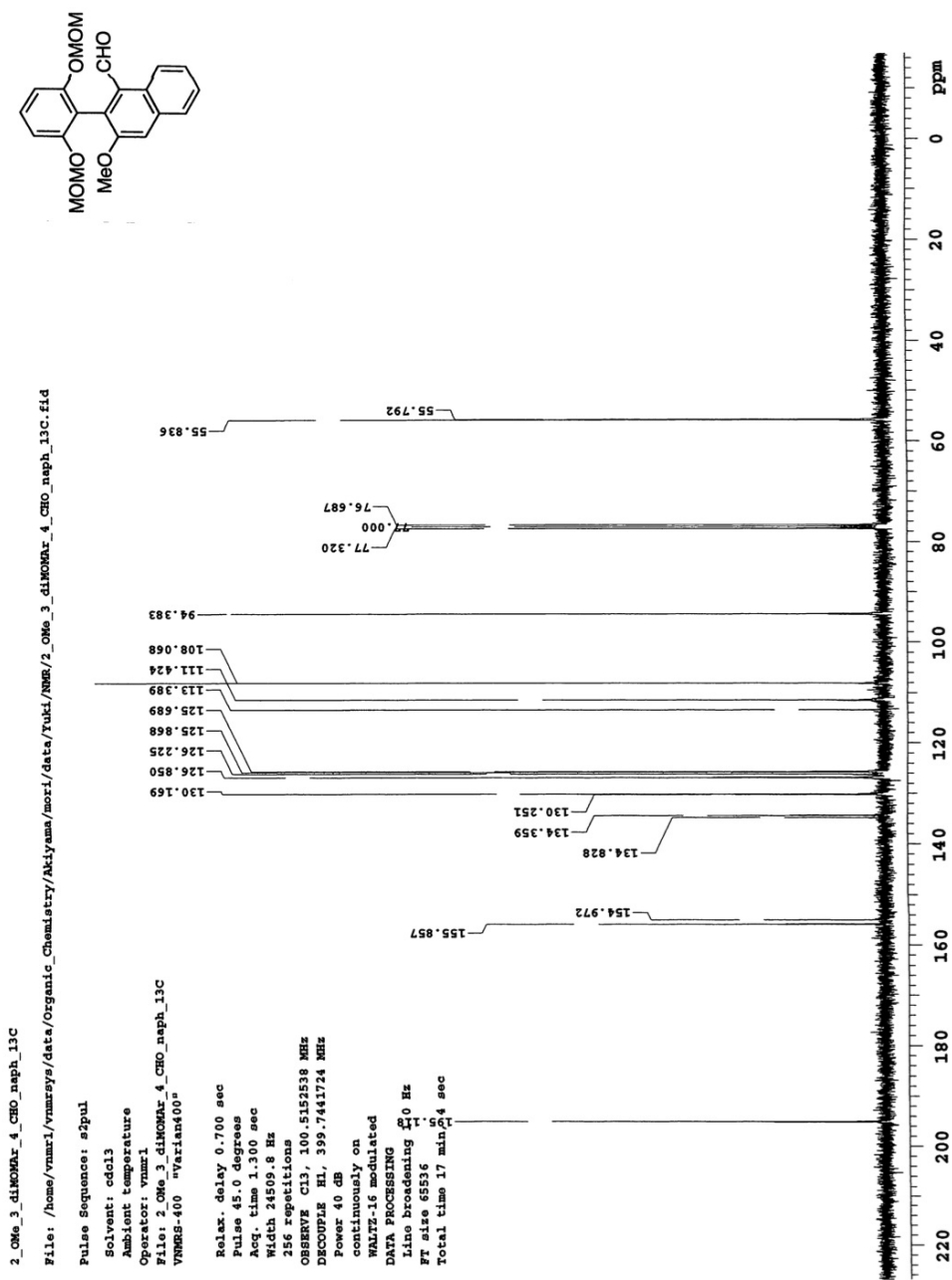
¹³C NMR spectrum of **s25**.



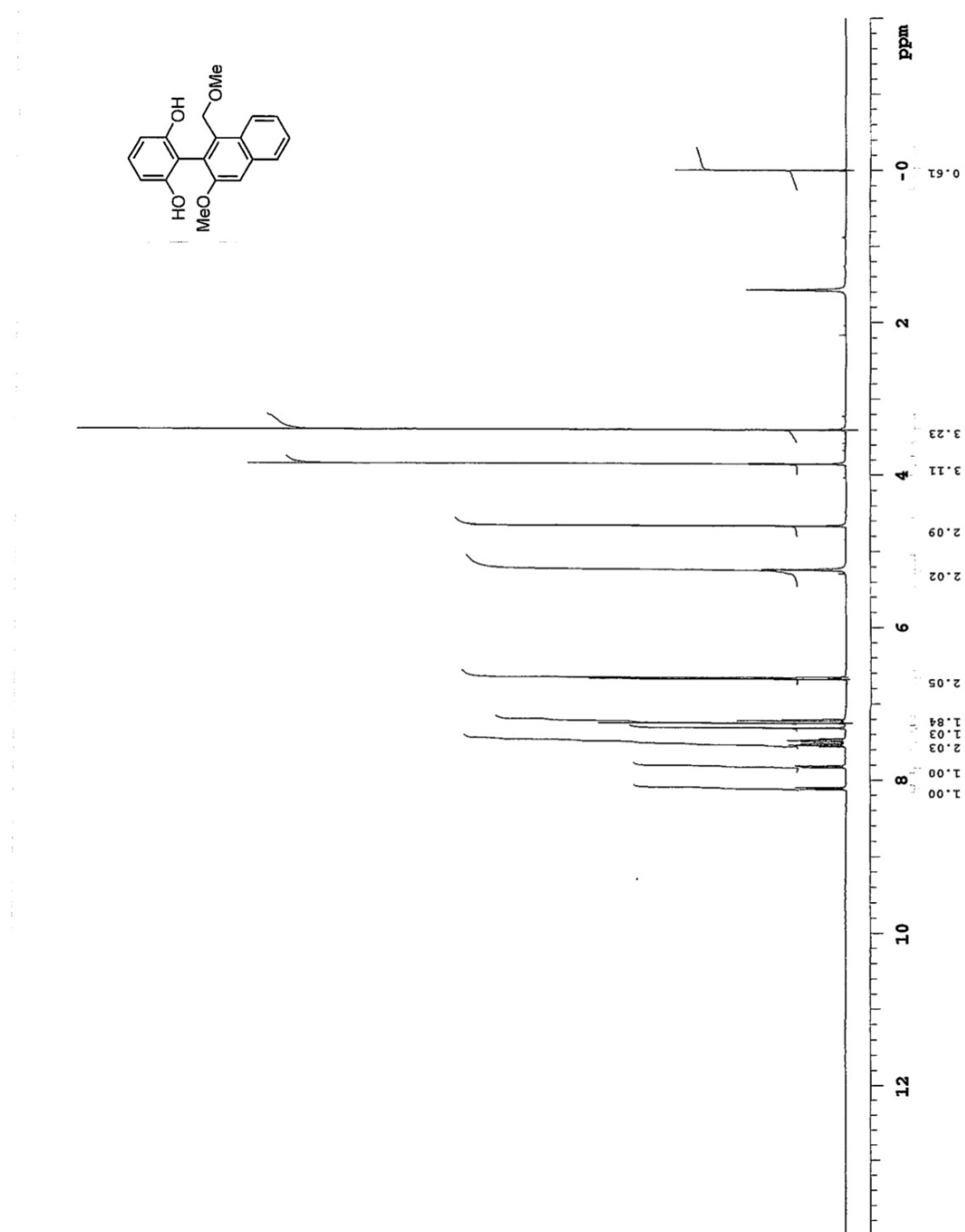
^1H NMR spectrum of **s28**.



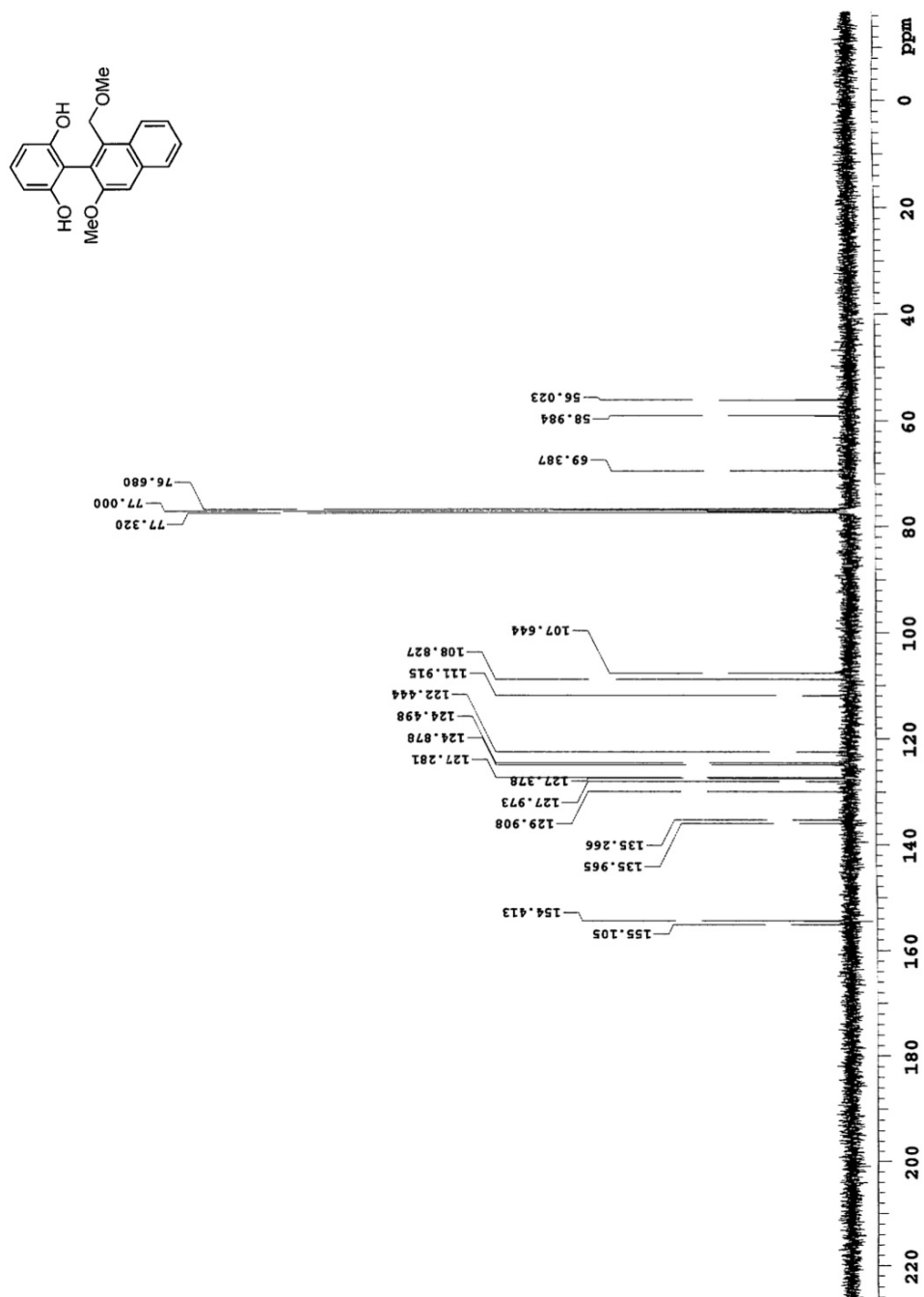
¹³C NMR spectrum of **s28**.



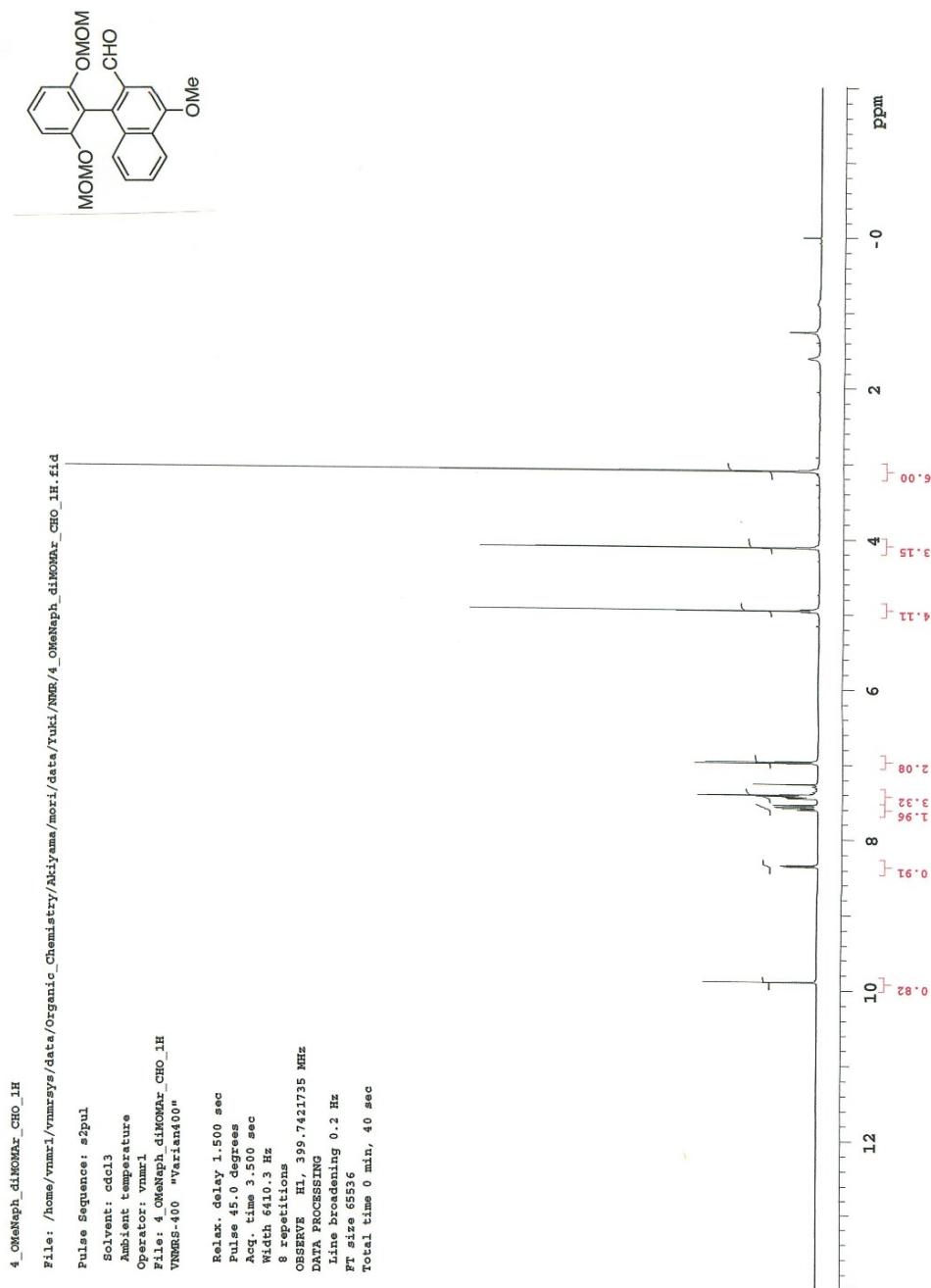
^1H NMR spectrum of **3p**.



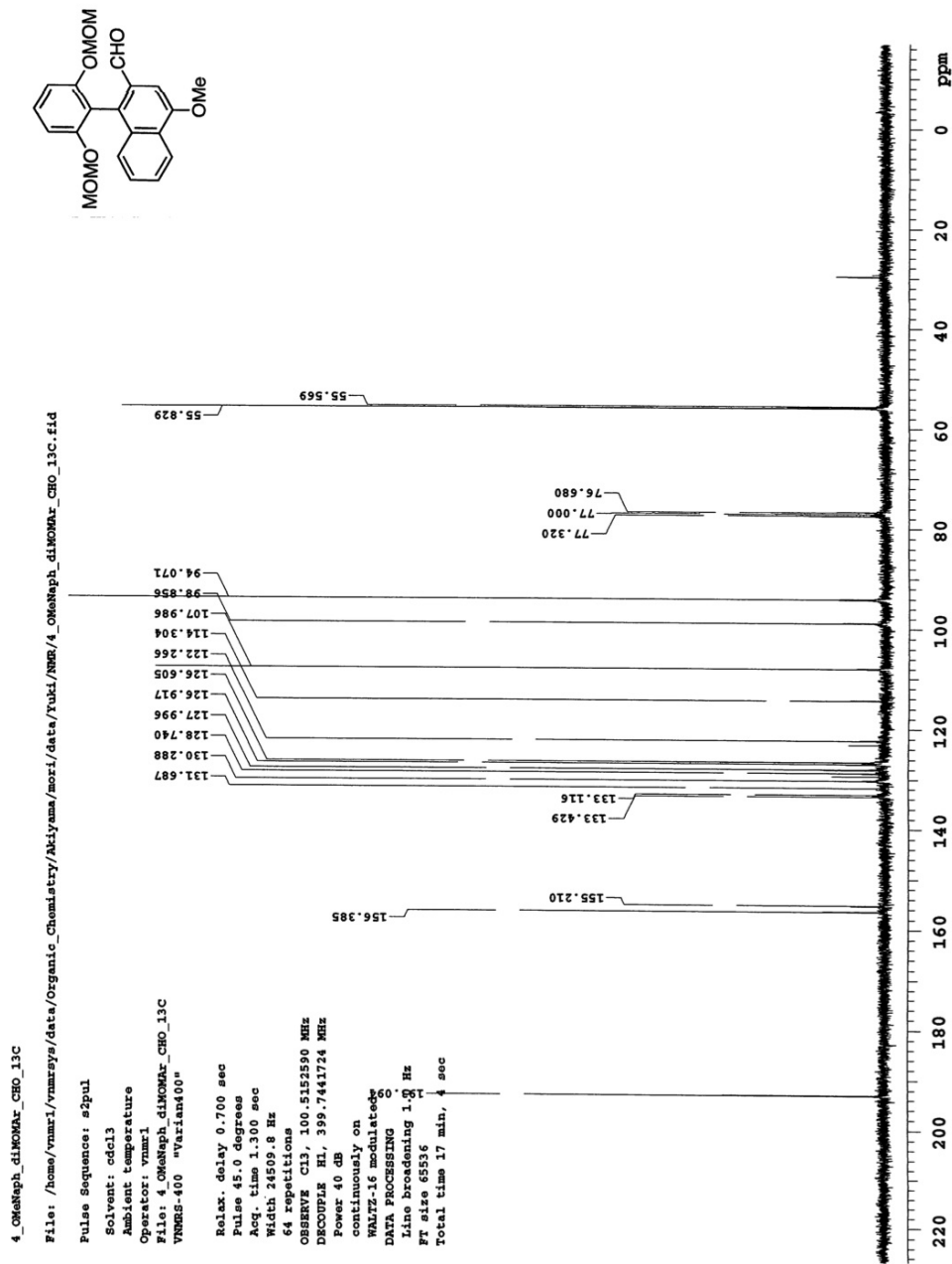
^{13}C NMR spectrum of **3p**.



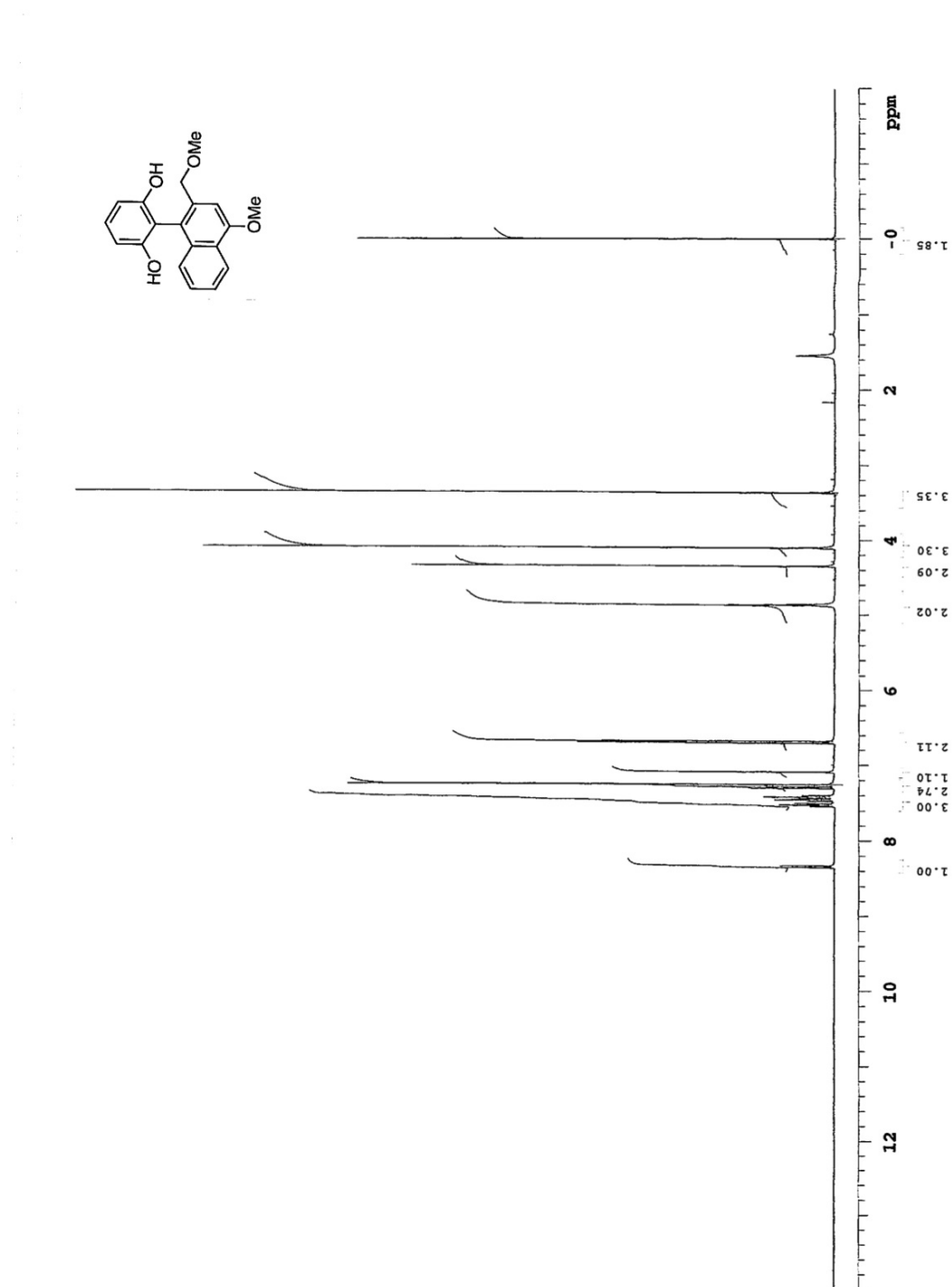
^1H NMR spectrum of **s34**.



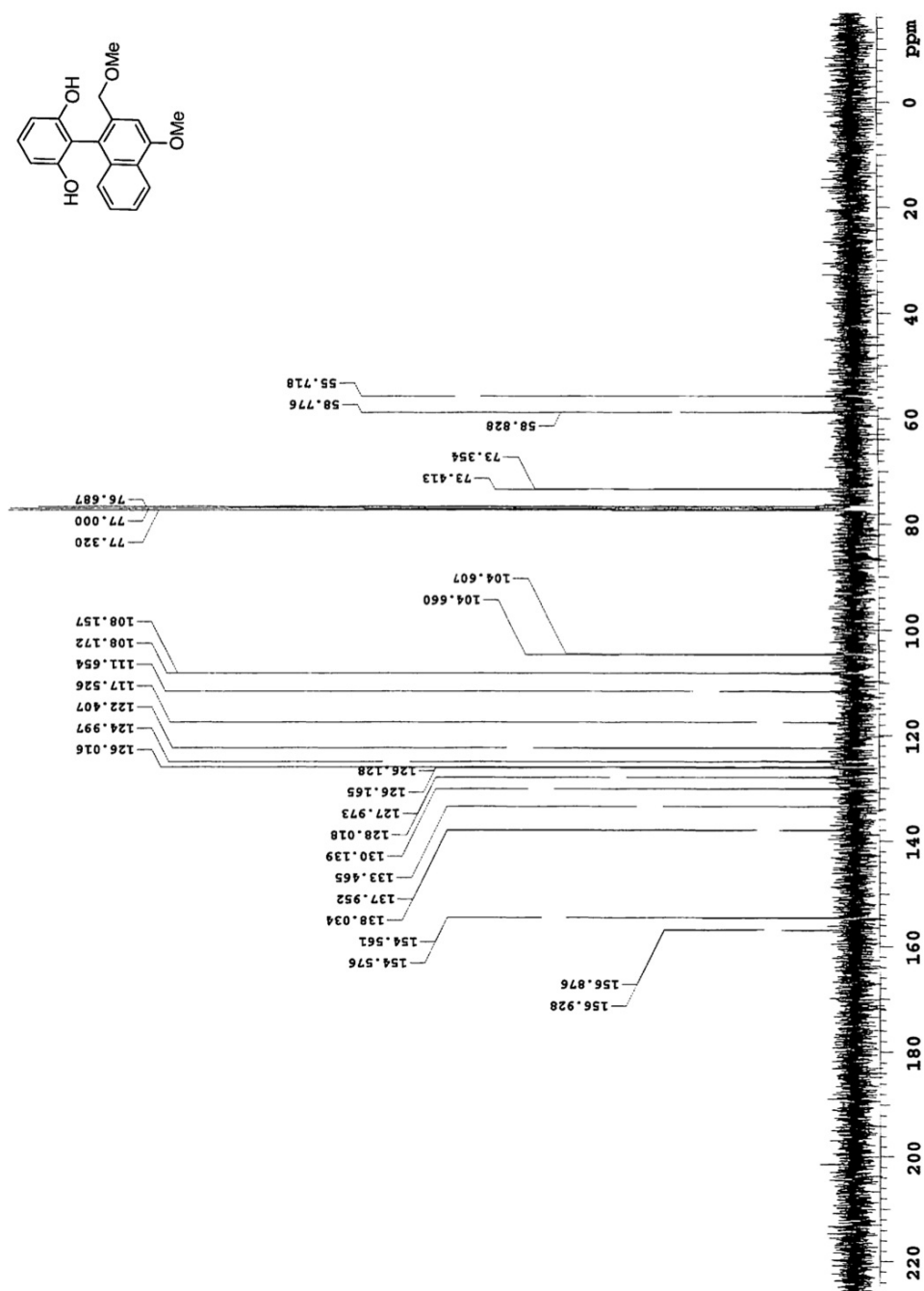
¹³C NMR spectrum of **s34**.



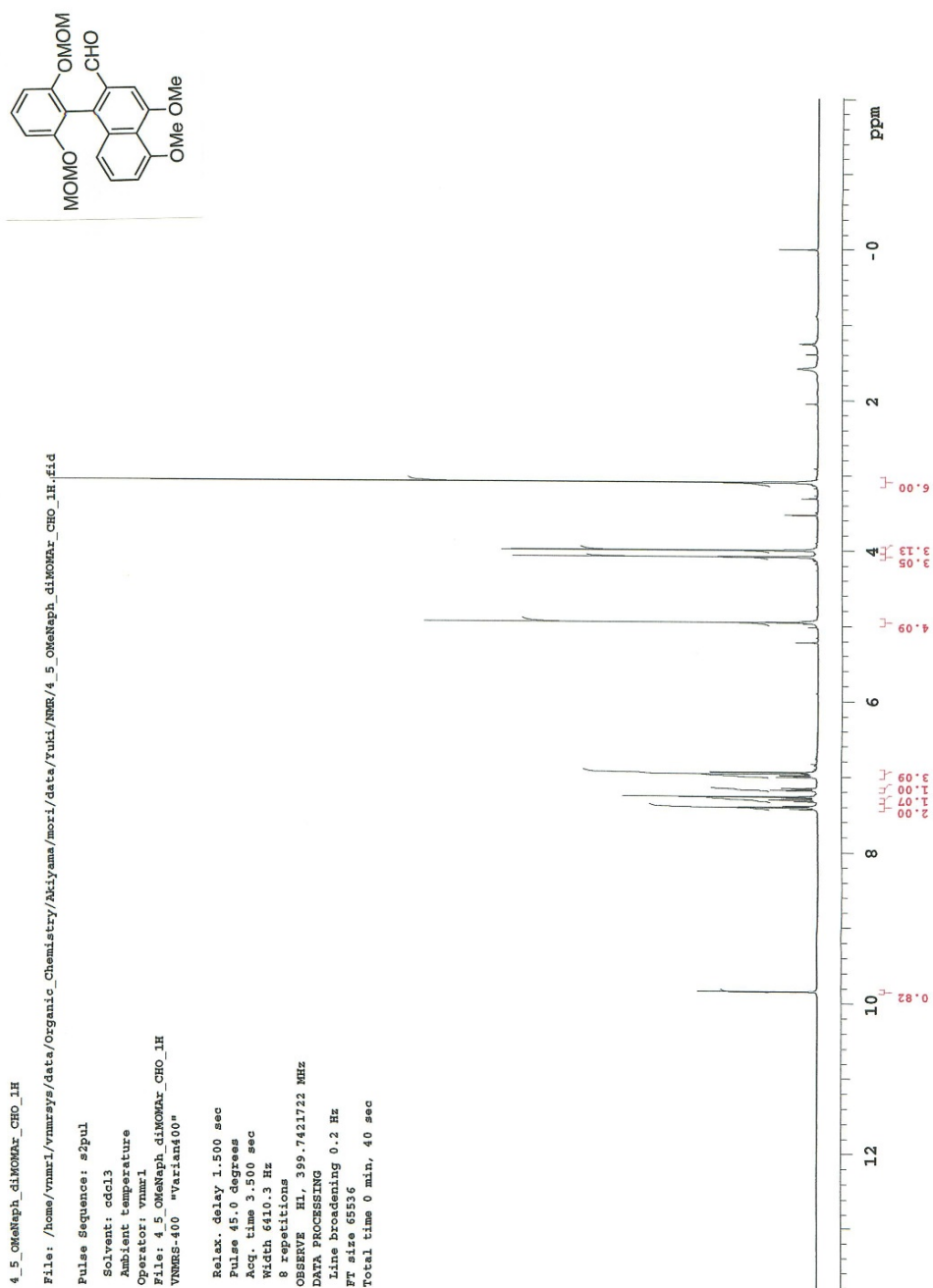
^1H NMR spectrum of **3r**.



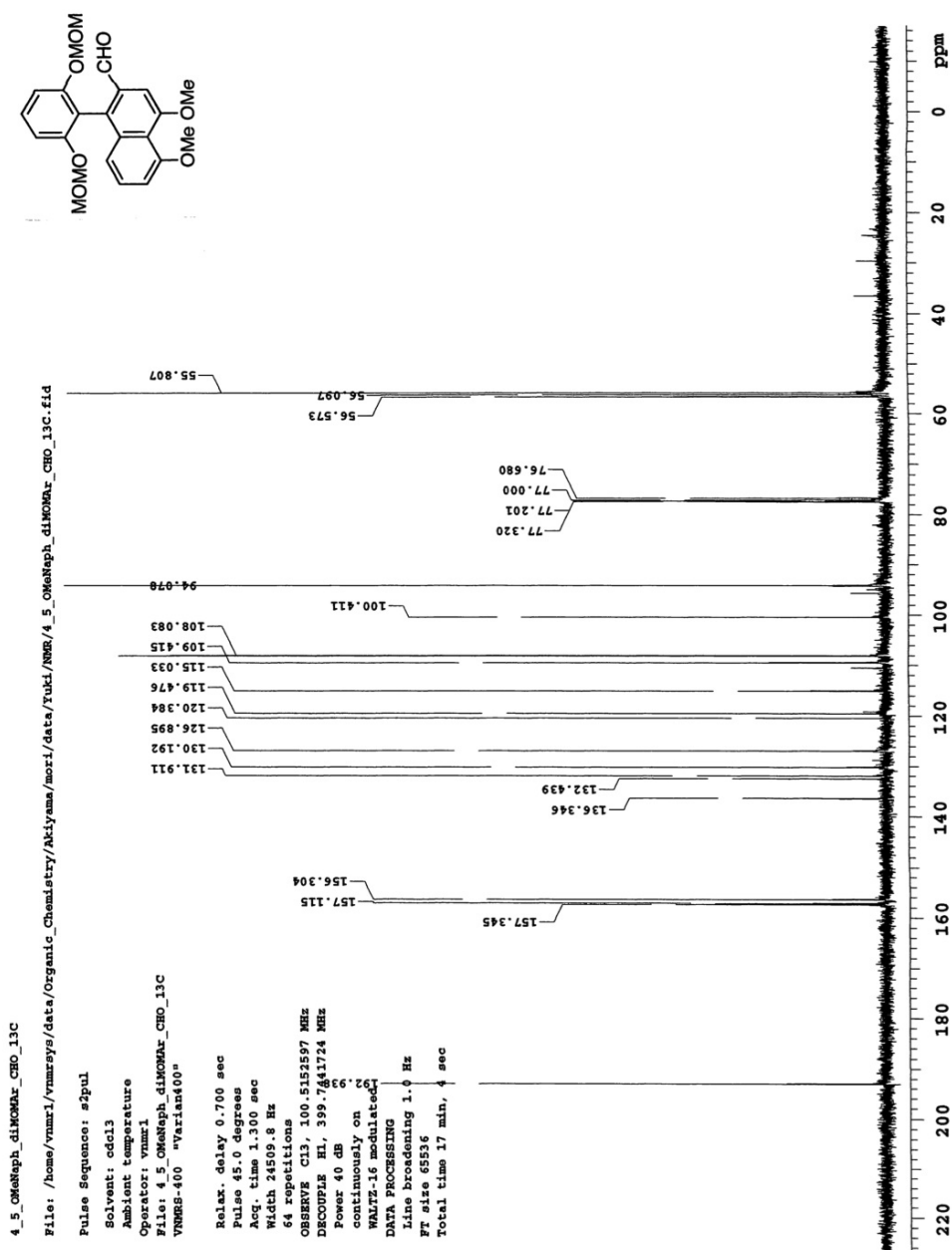
^{13}C NMR spectrum of **3r**.



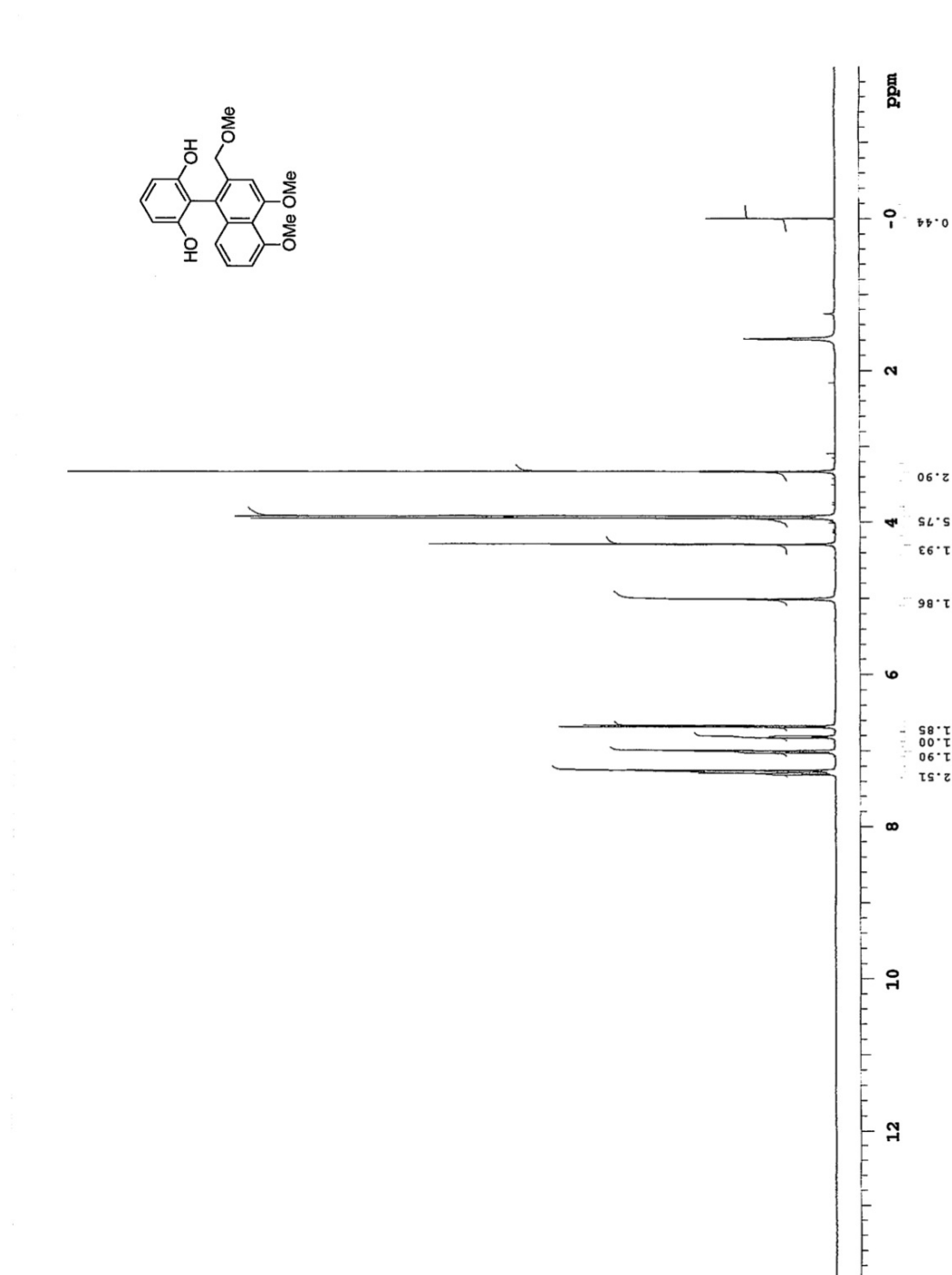
^1H NMR spectrum of **s37**.



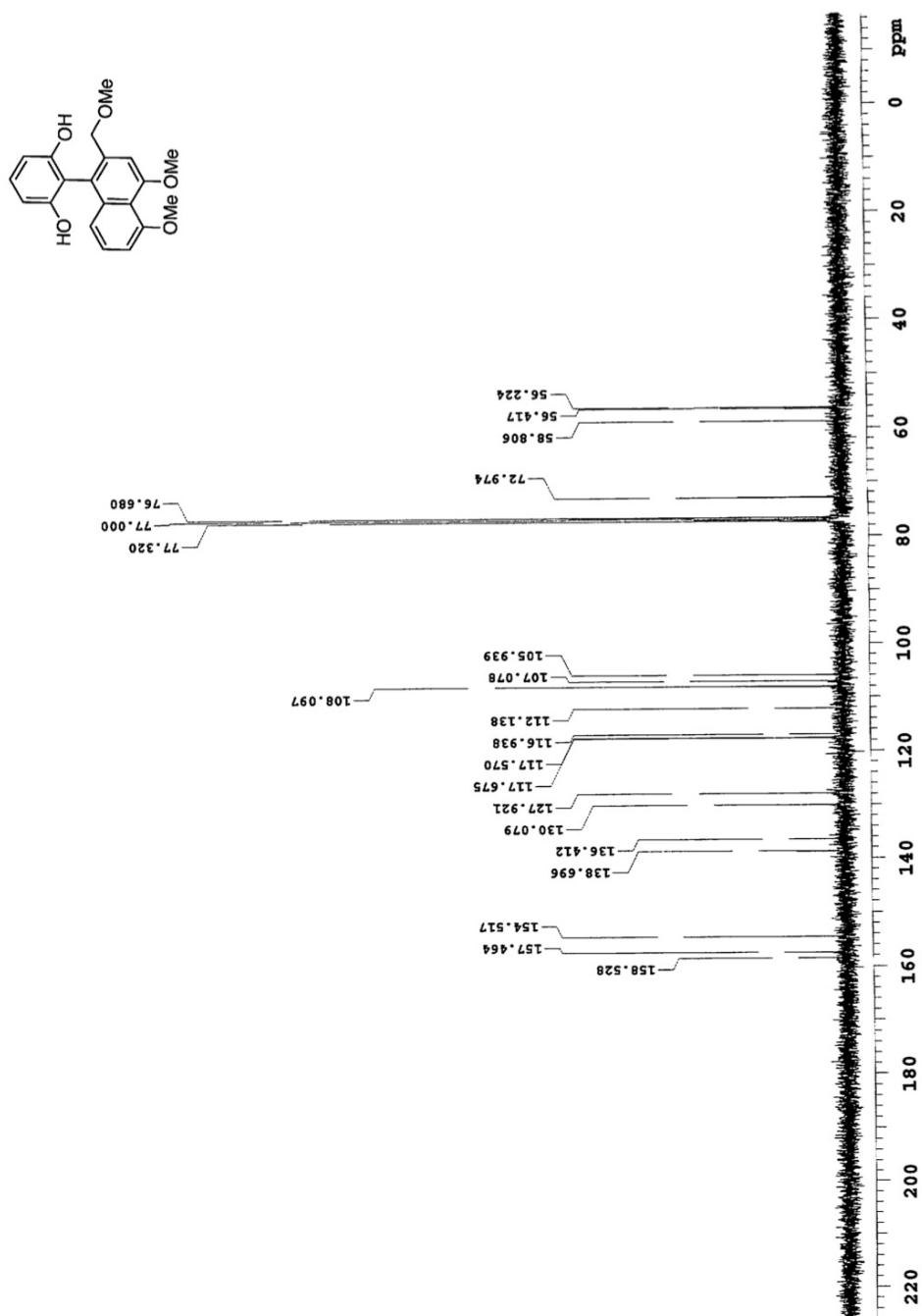
¹³C NMR spectrum of **s37**.



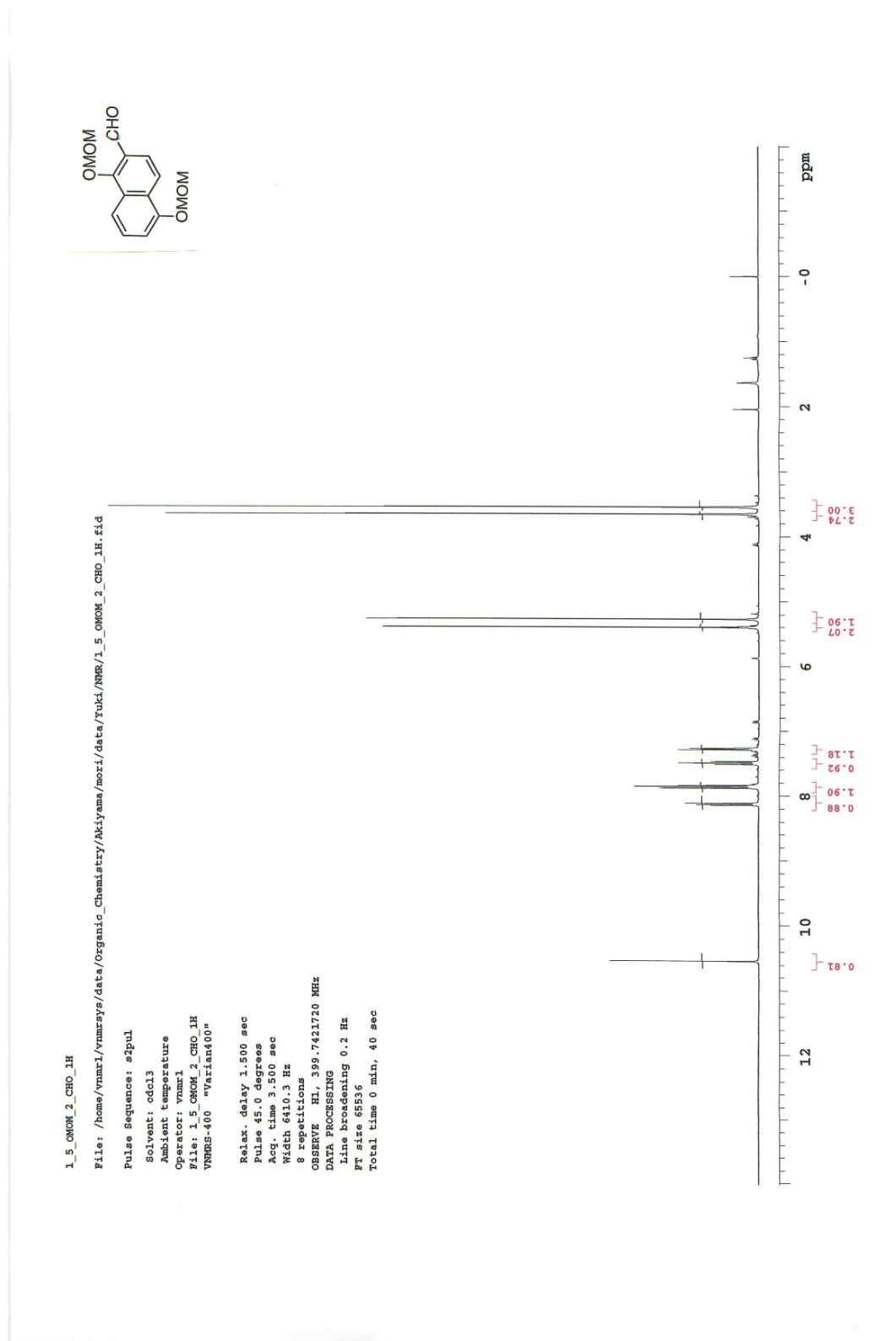
^1H NMR spectrum of **3t**.



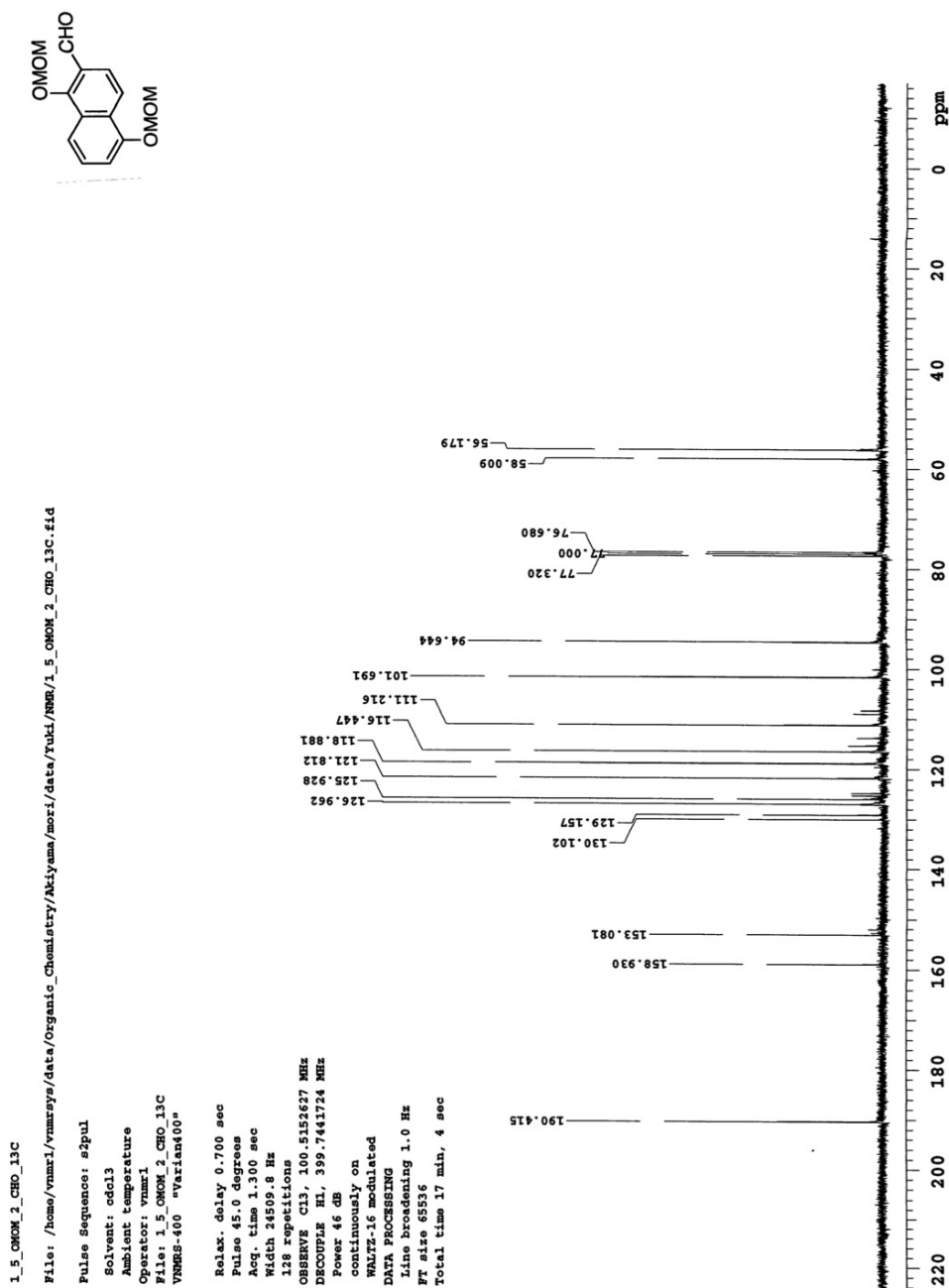
^{13}C NMR spectrum of **3t**.



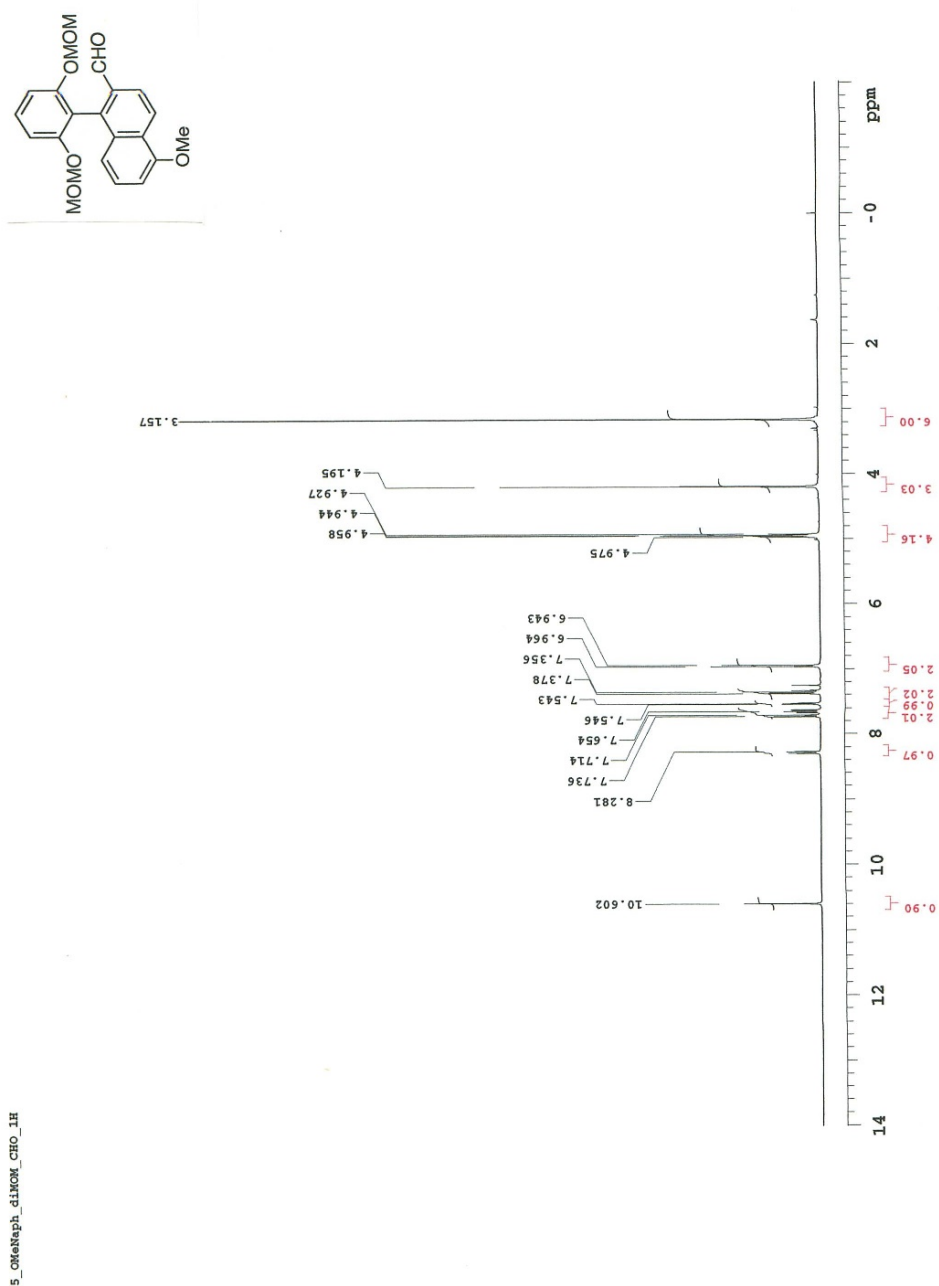
^1H NMR spectrum of **s40**.



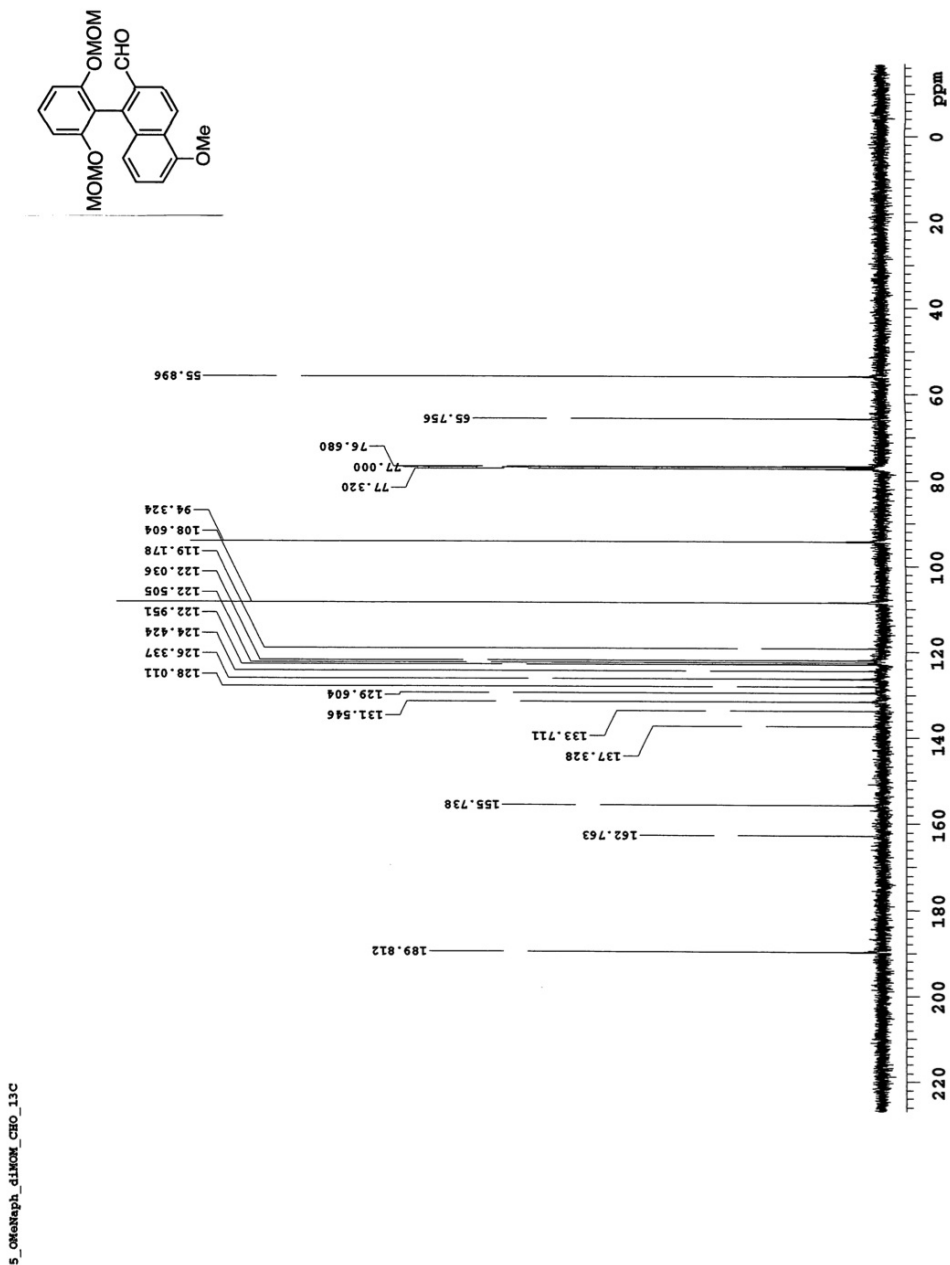
¹³C NMR spectrum of **s40**.



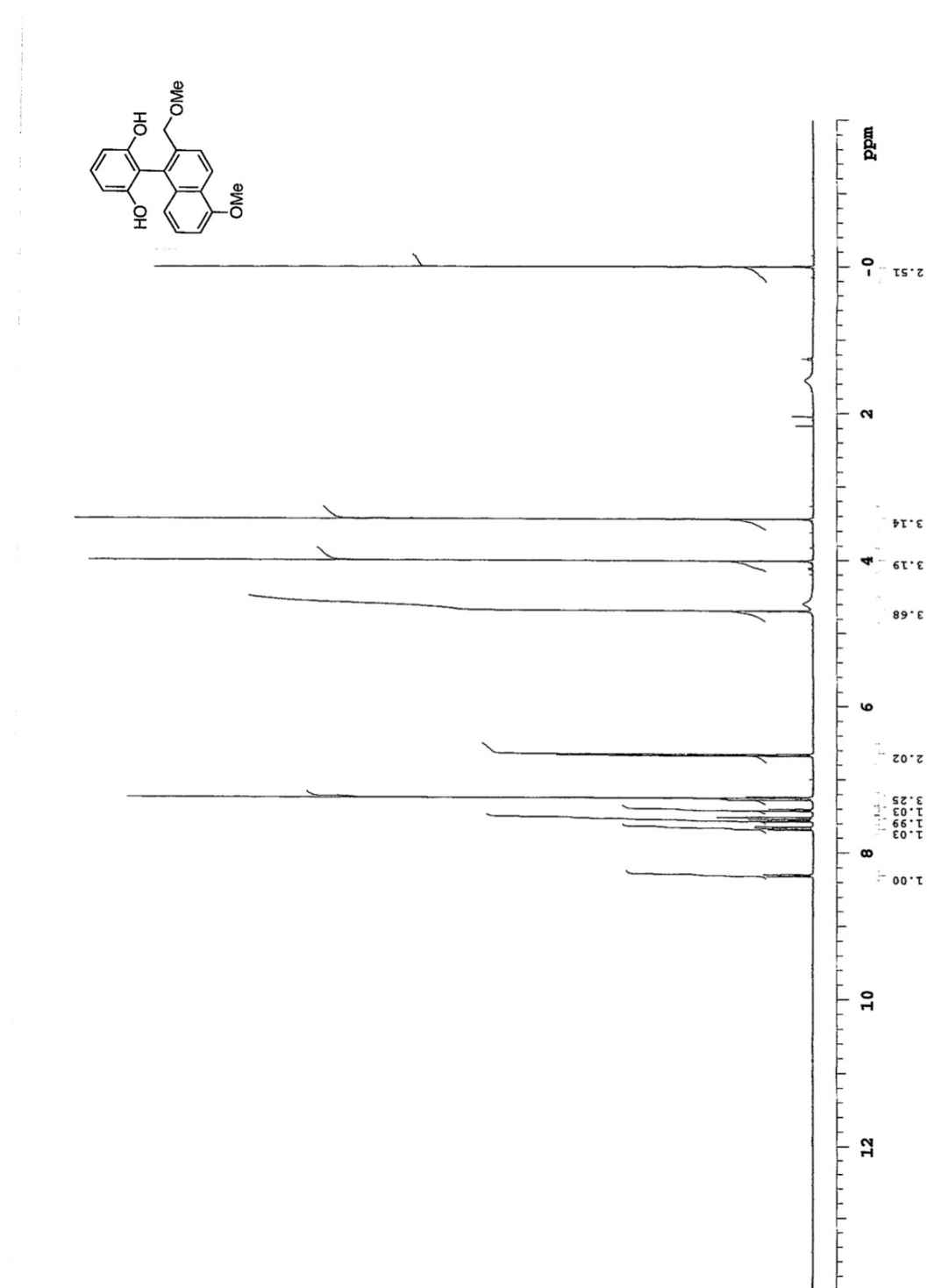
^1H NMR spectrum of **s45**.



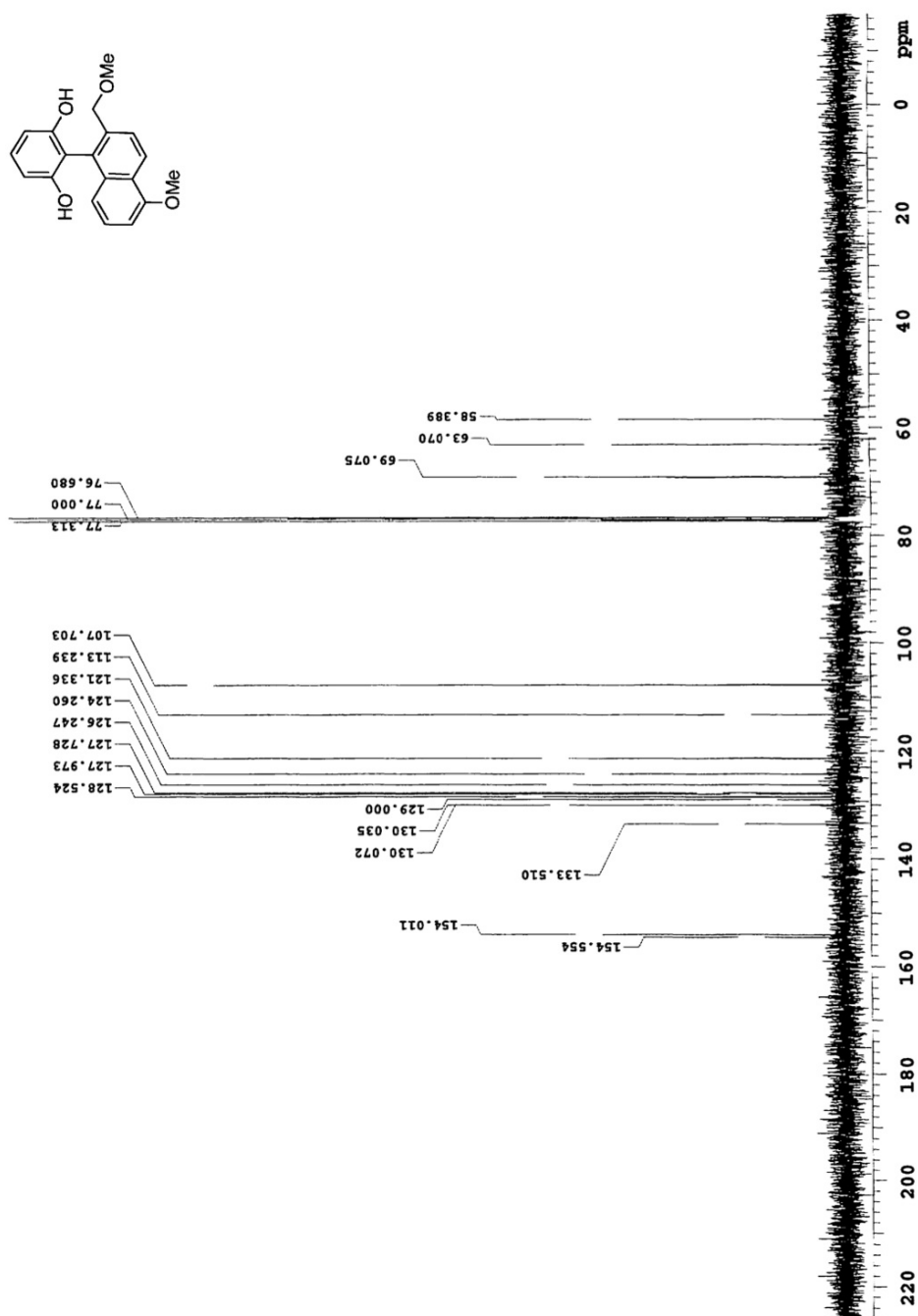
¹³C NMR spectrum of **s45**.



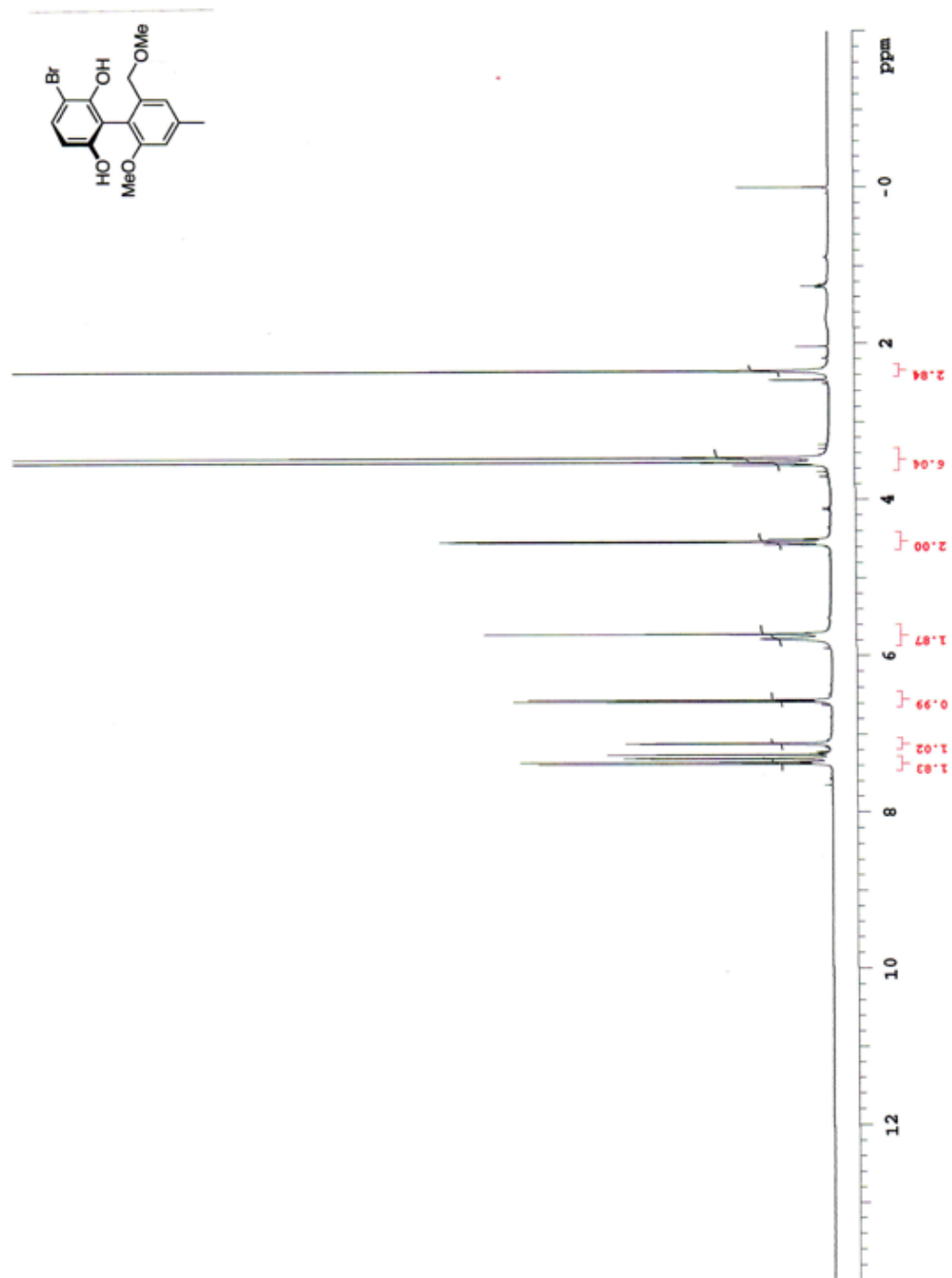
^1H NMR spectrum of **3s**.



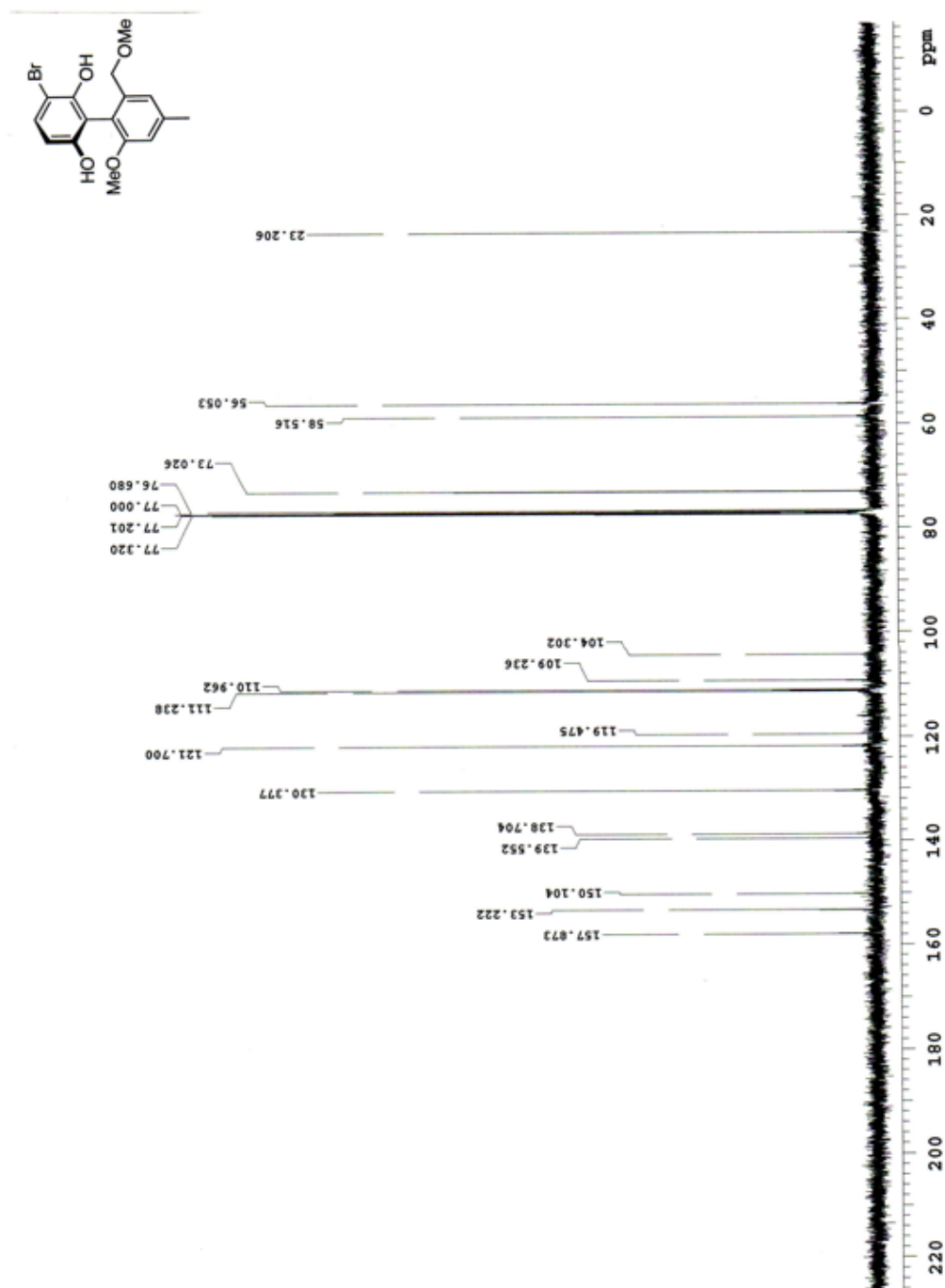
^{13}C NMR spectrum of **3s**.



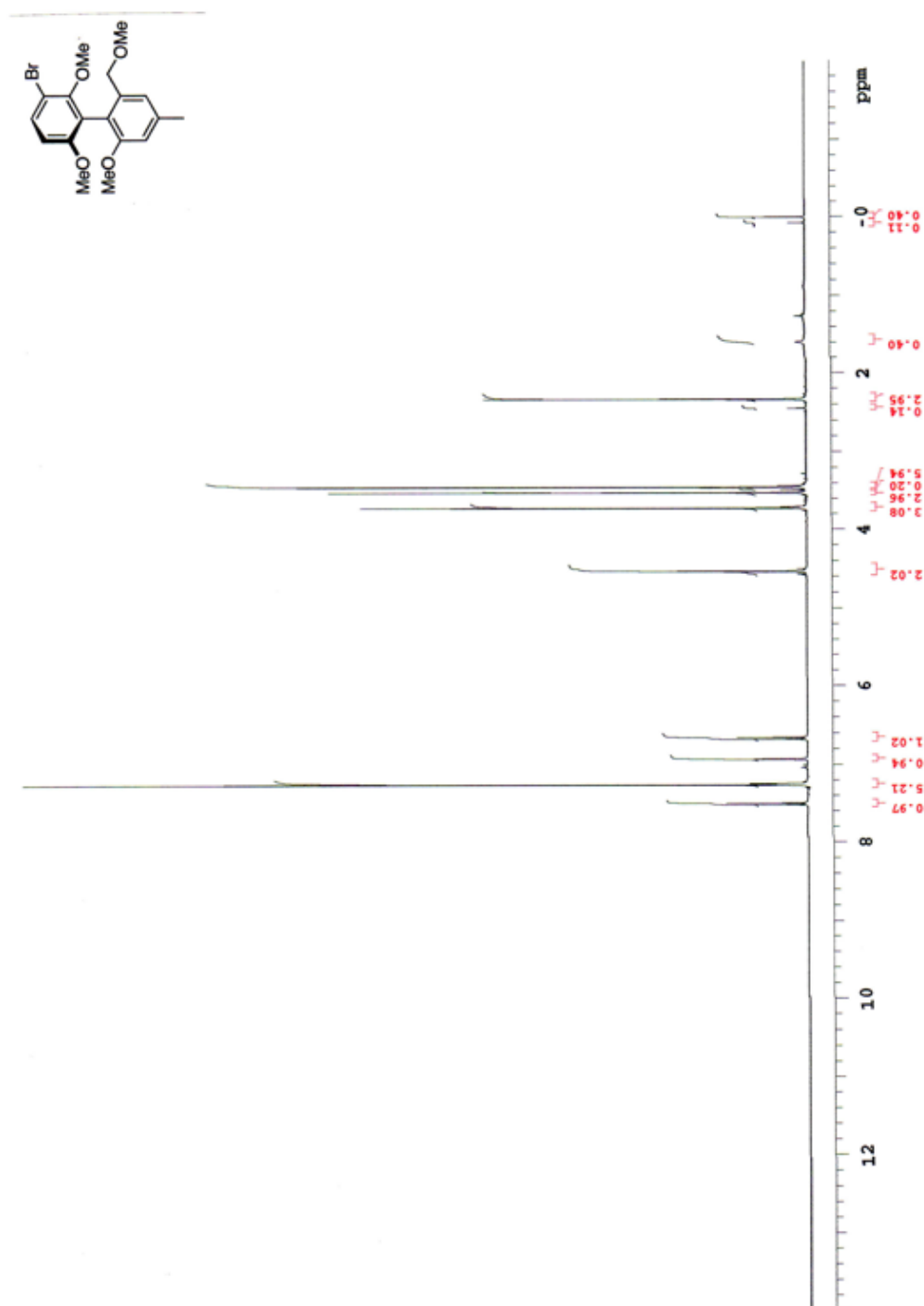
^1H NMR spectrum of **4n**.



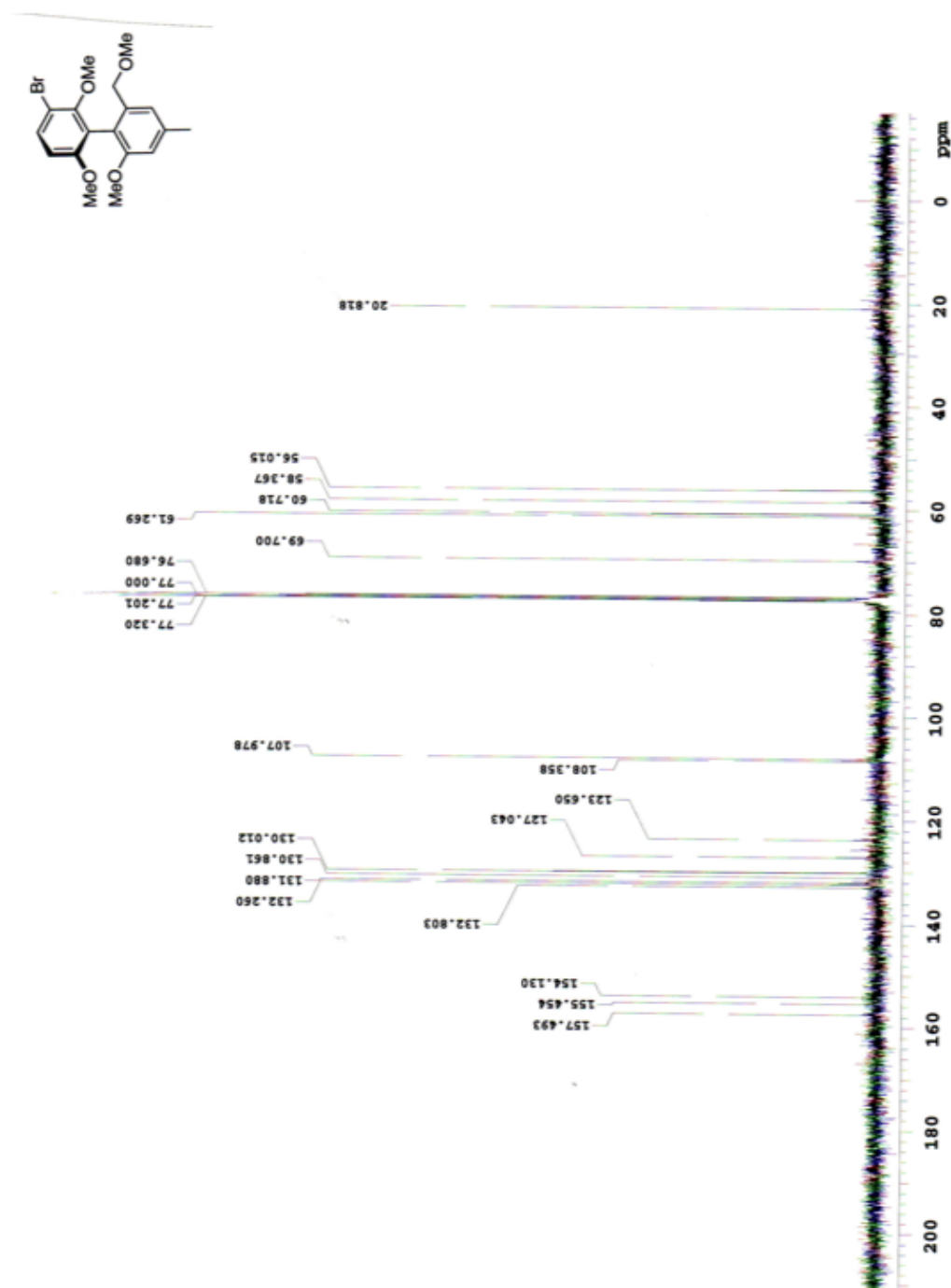
^{13}C NMR spectrum of **4n**.



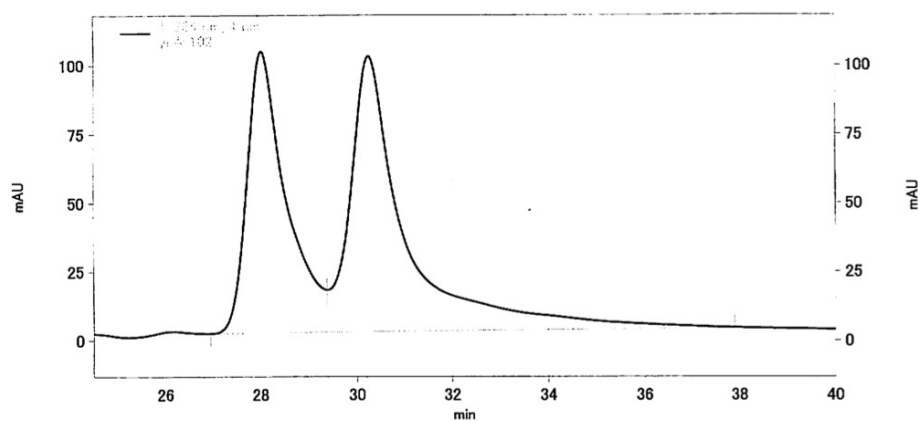
^1H NMR spectrum of **s8**.



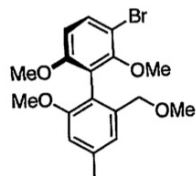
^{13}C NMR spectrum of **s8**.



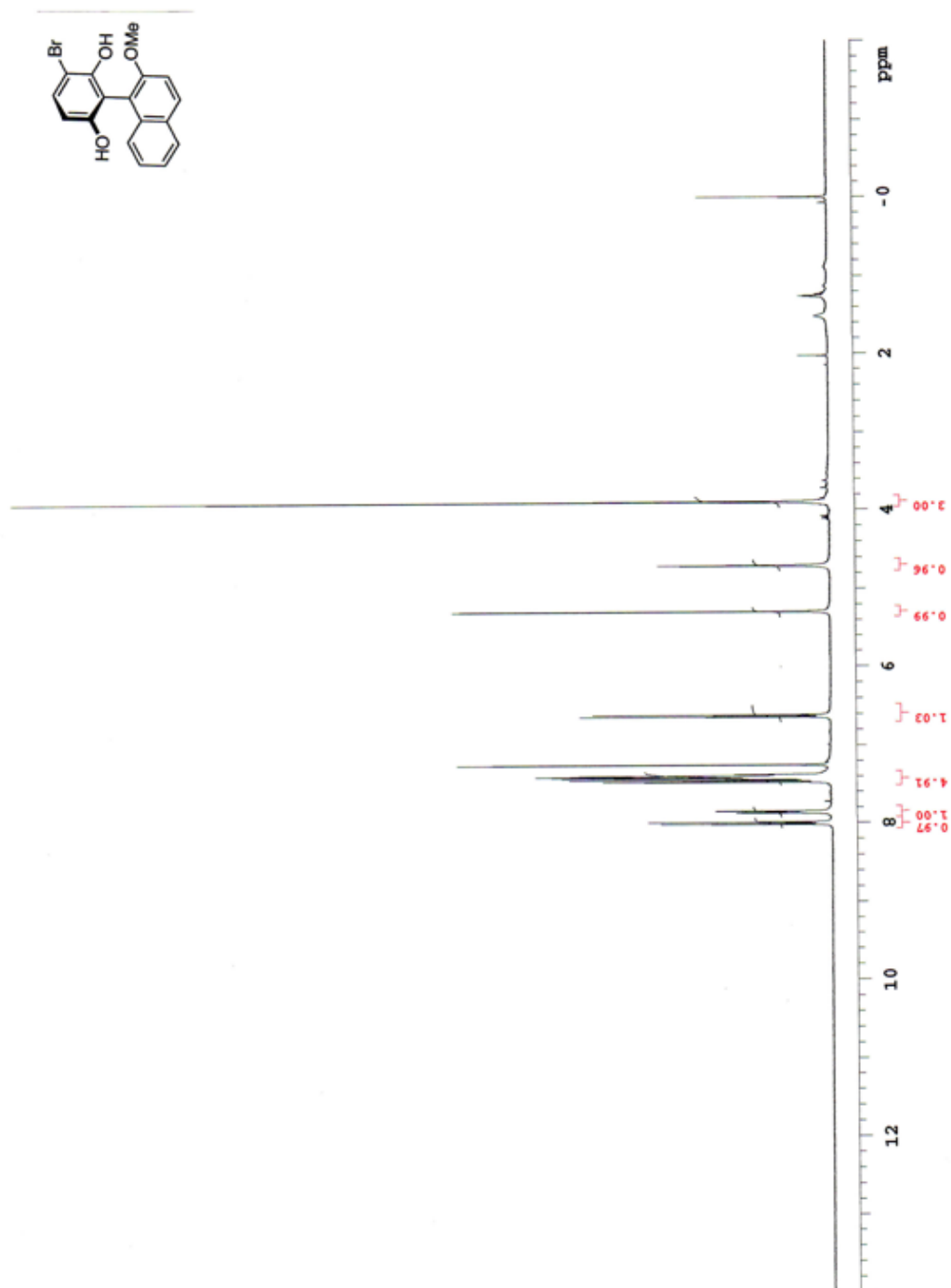
HPLC chart of **s8**.



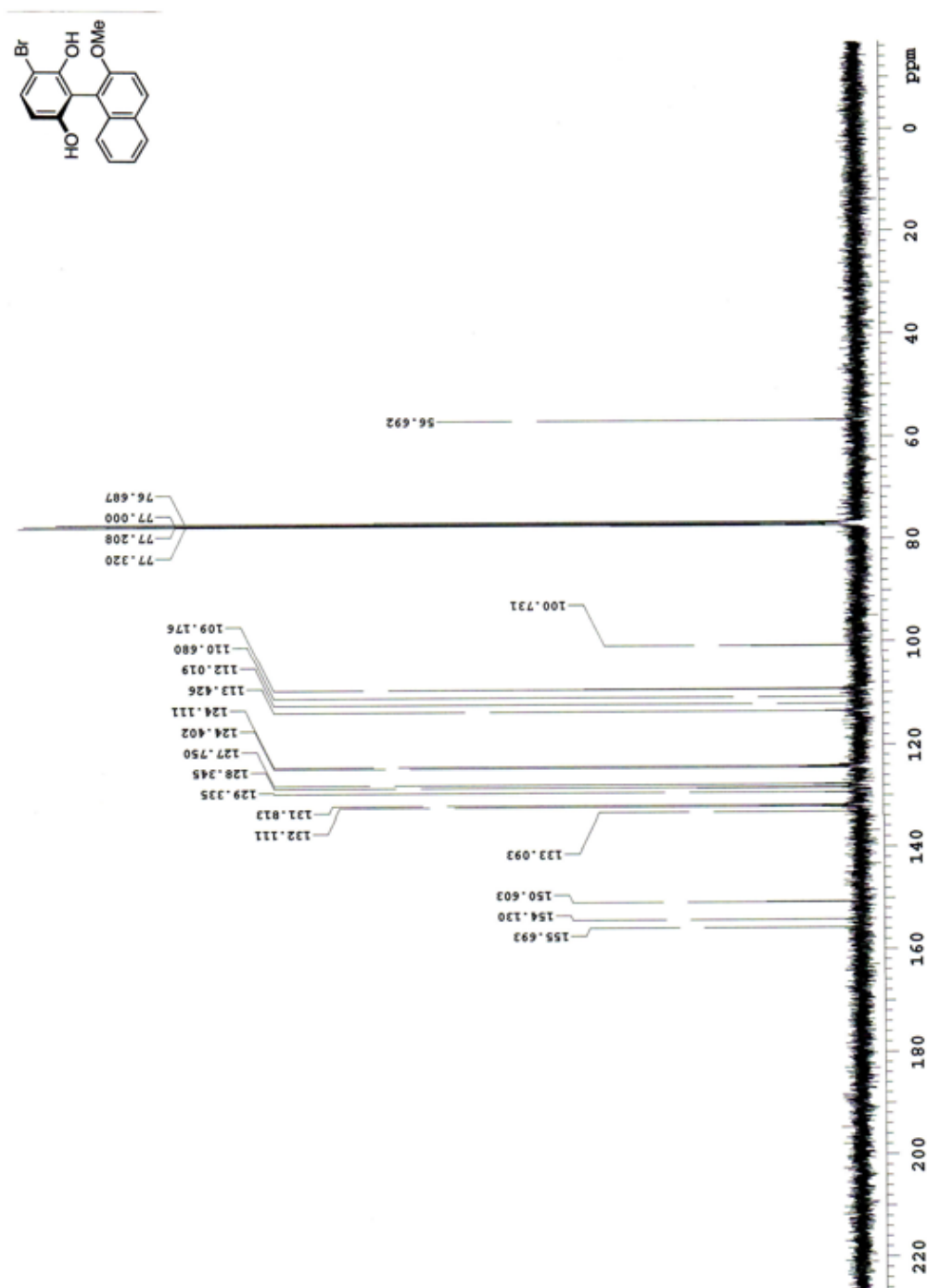
Peak #	Retention time	Type	Area	Area %
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2	30.25	VB	32610497	58.432



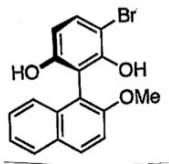
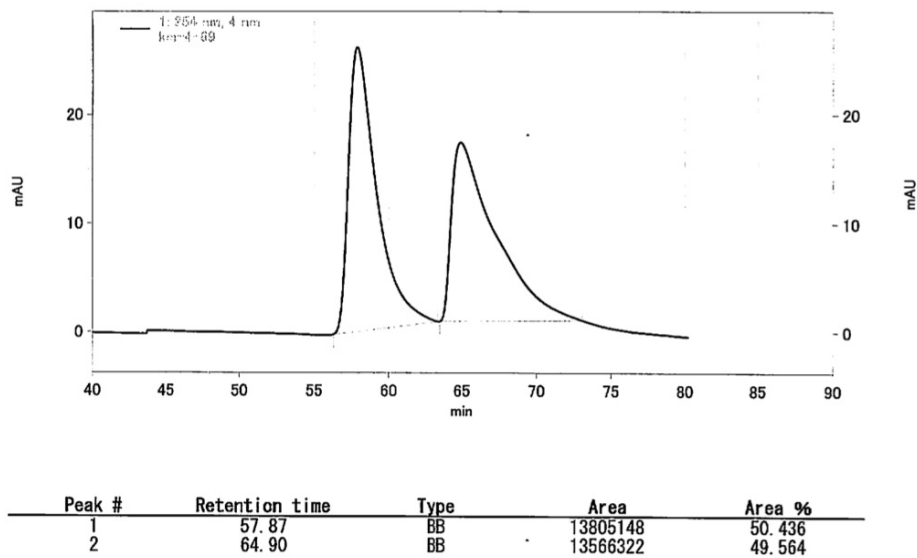
^1H NMR spectrum of **4o**.



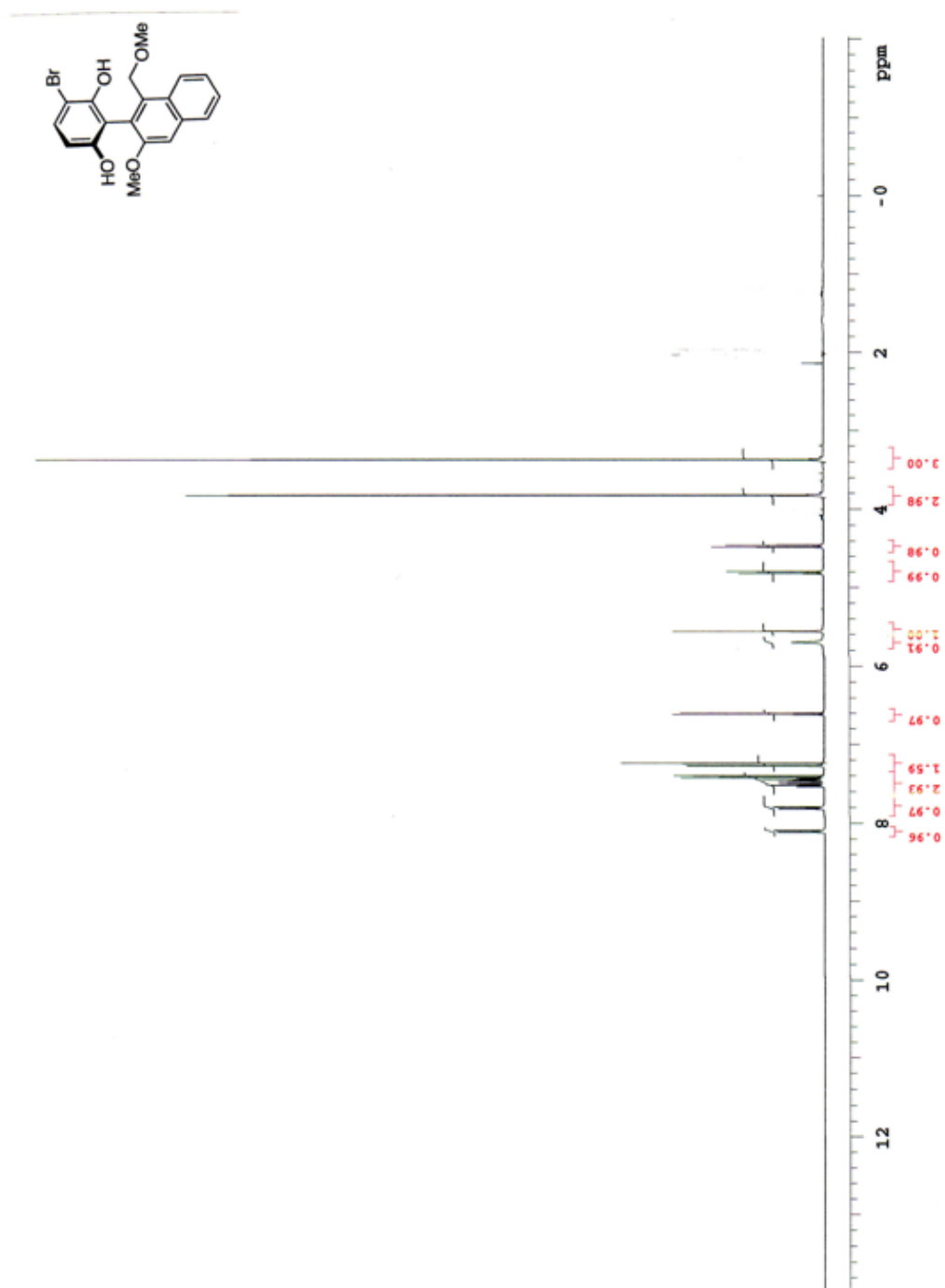
^{13}C NMR spectrum of **40**.



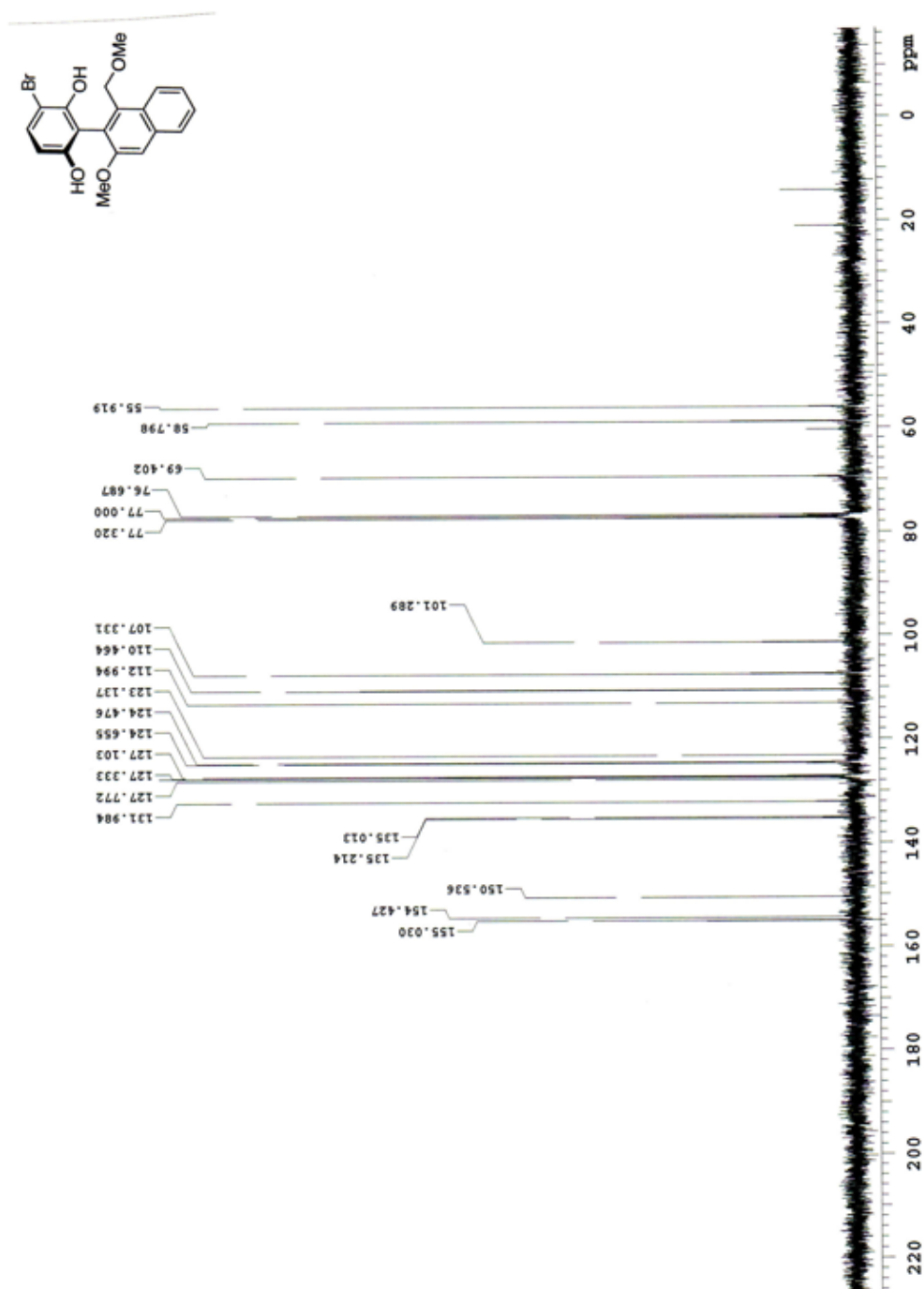
HPLC chart of **4o**.



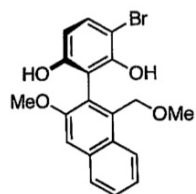
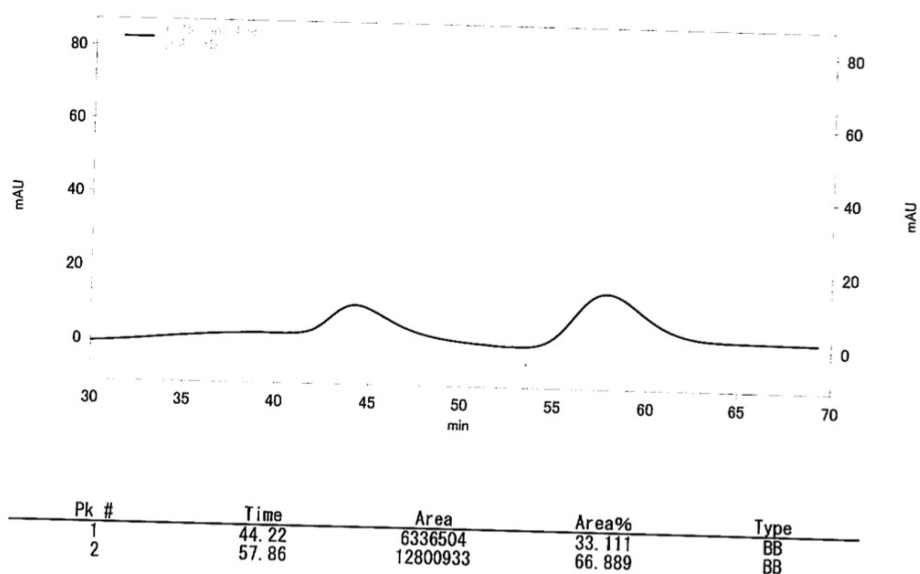
^1H NMR spectrum of **4p**.



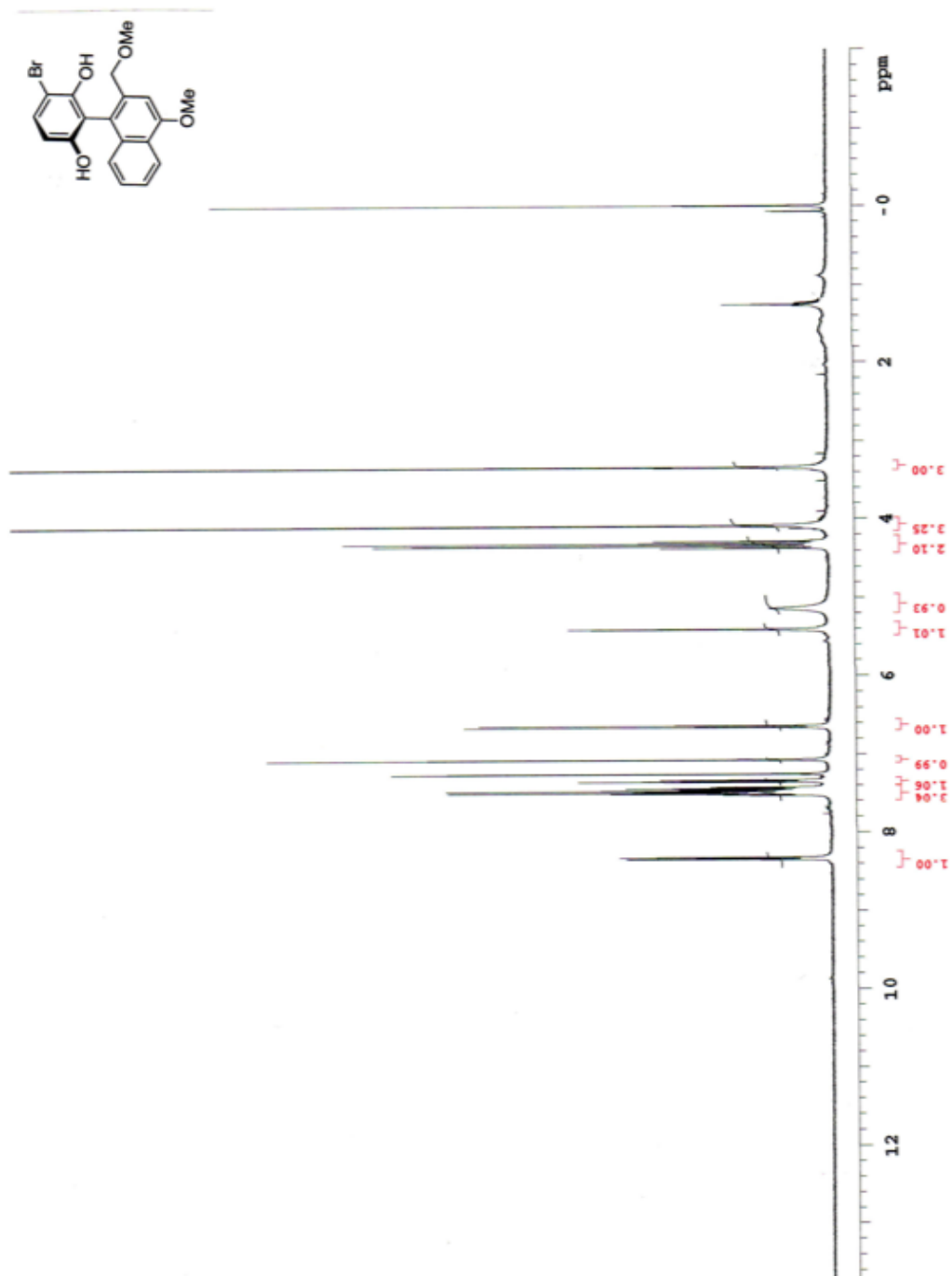
^{13}C NMR spectrum of **4p**.



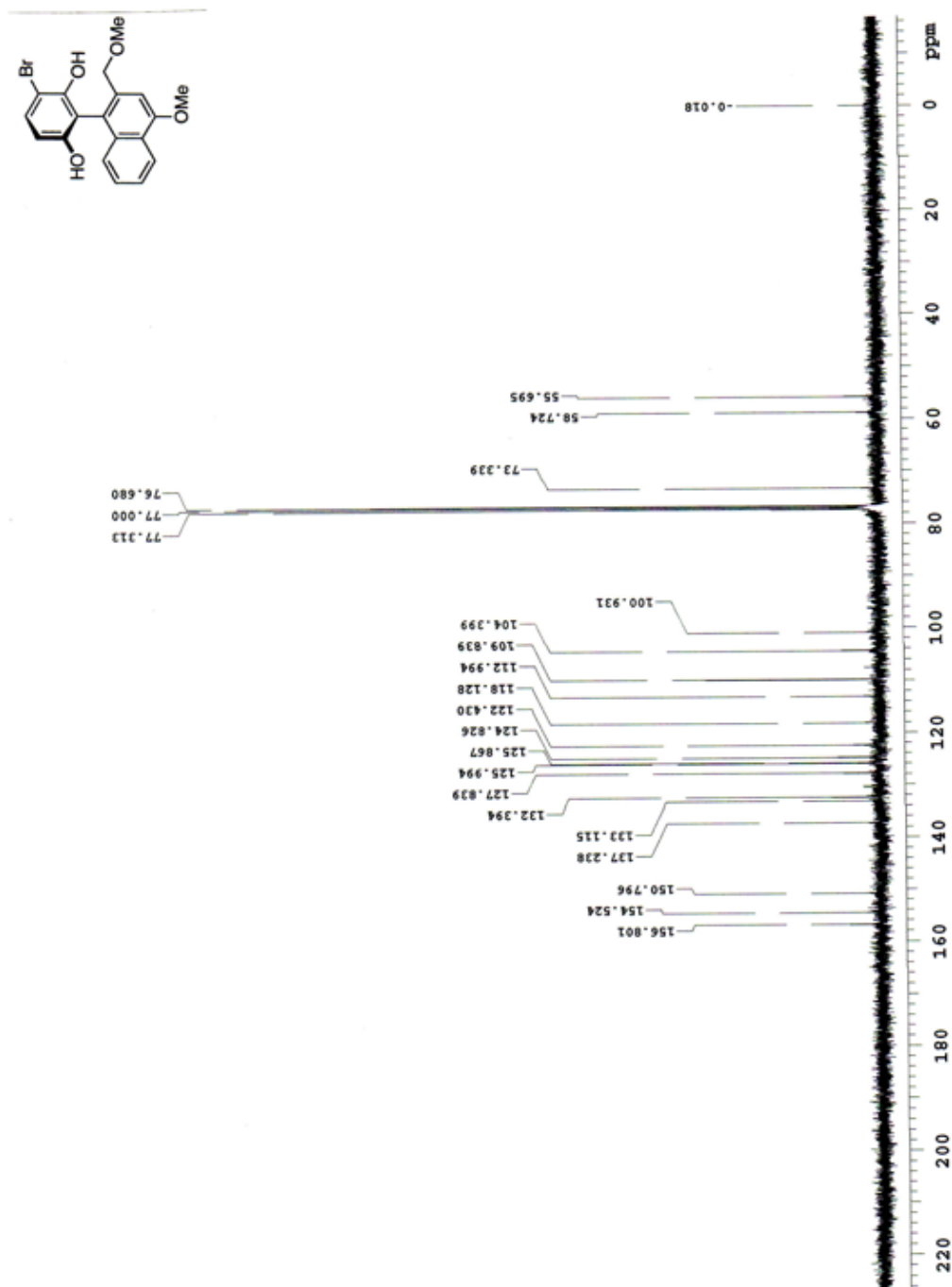
HPLC chart of **4p**.



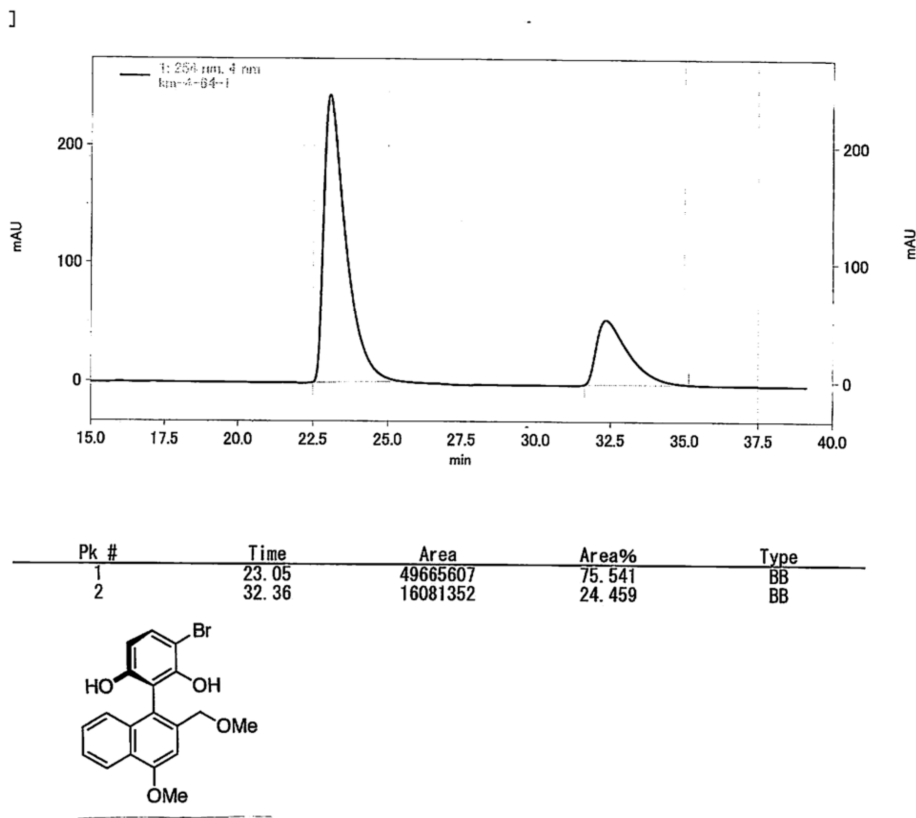
^1H NMR spectrum of **4r**.



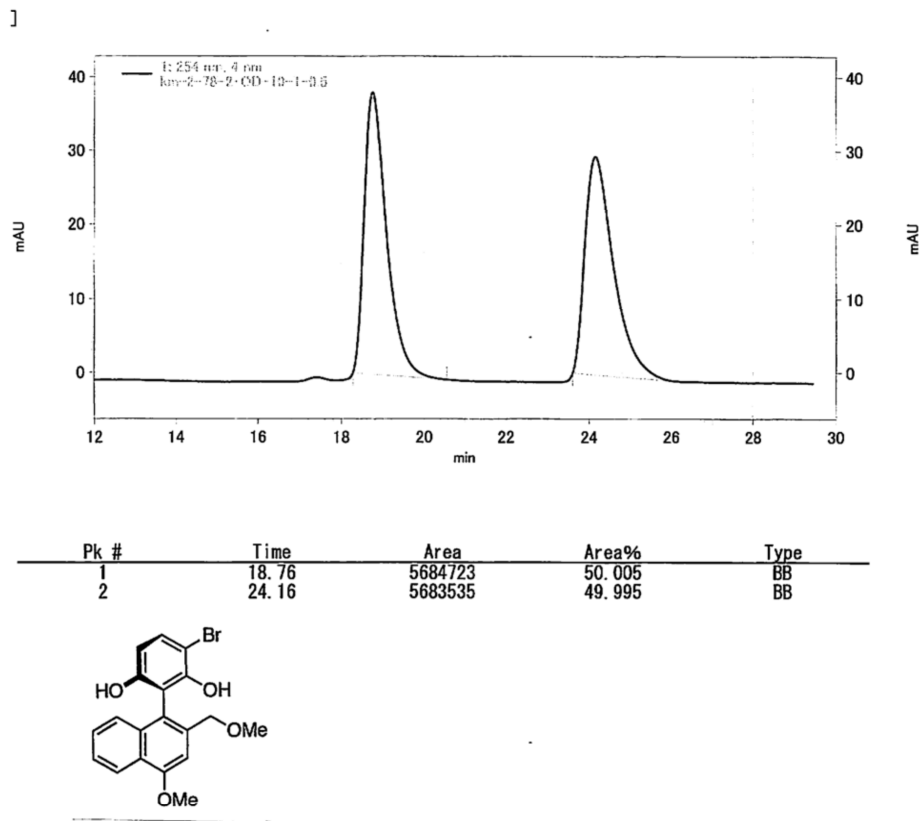
^{13}C NMR spectrum of **4r**.



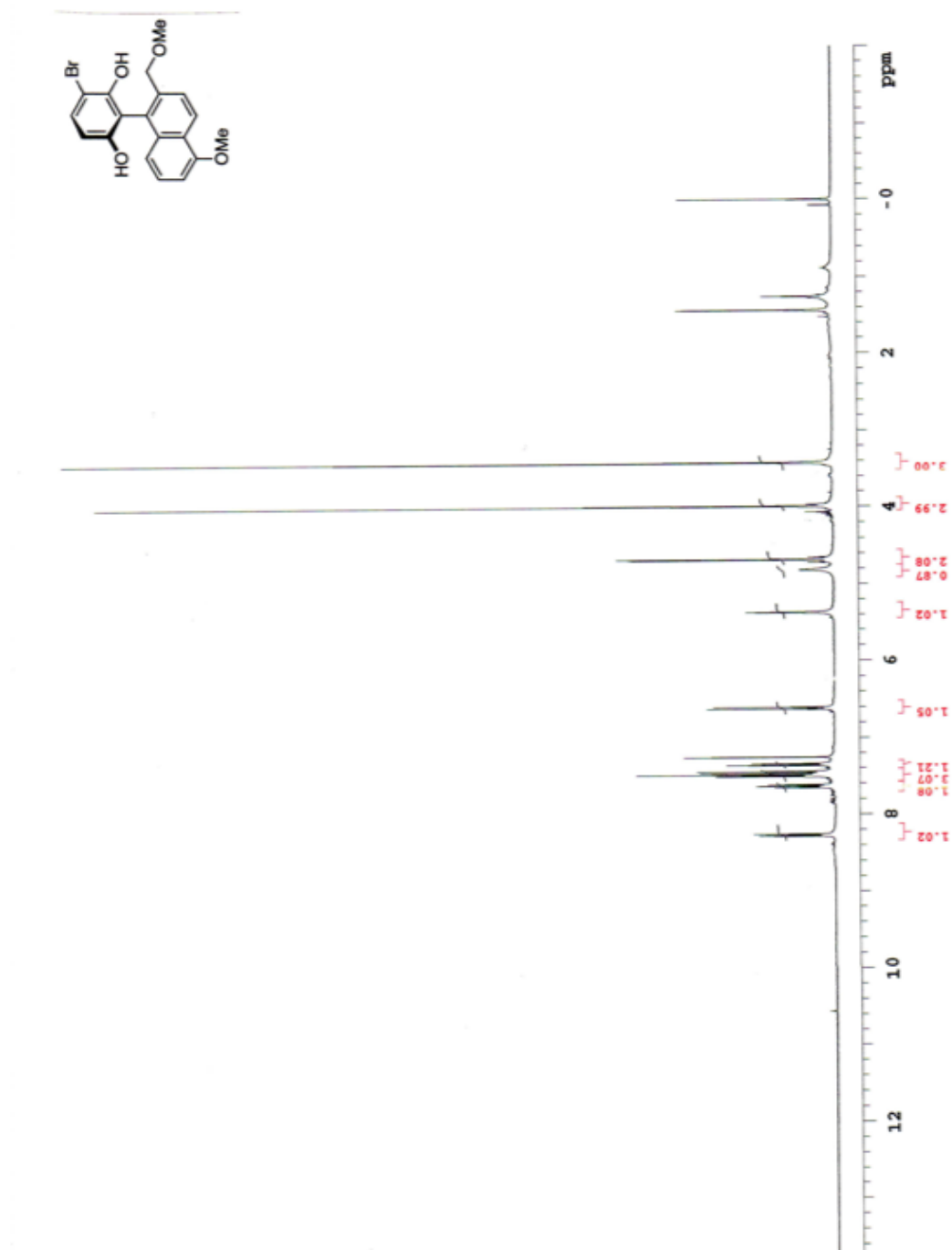
HPLC chart of **4r**.



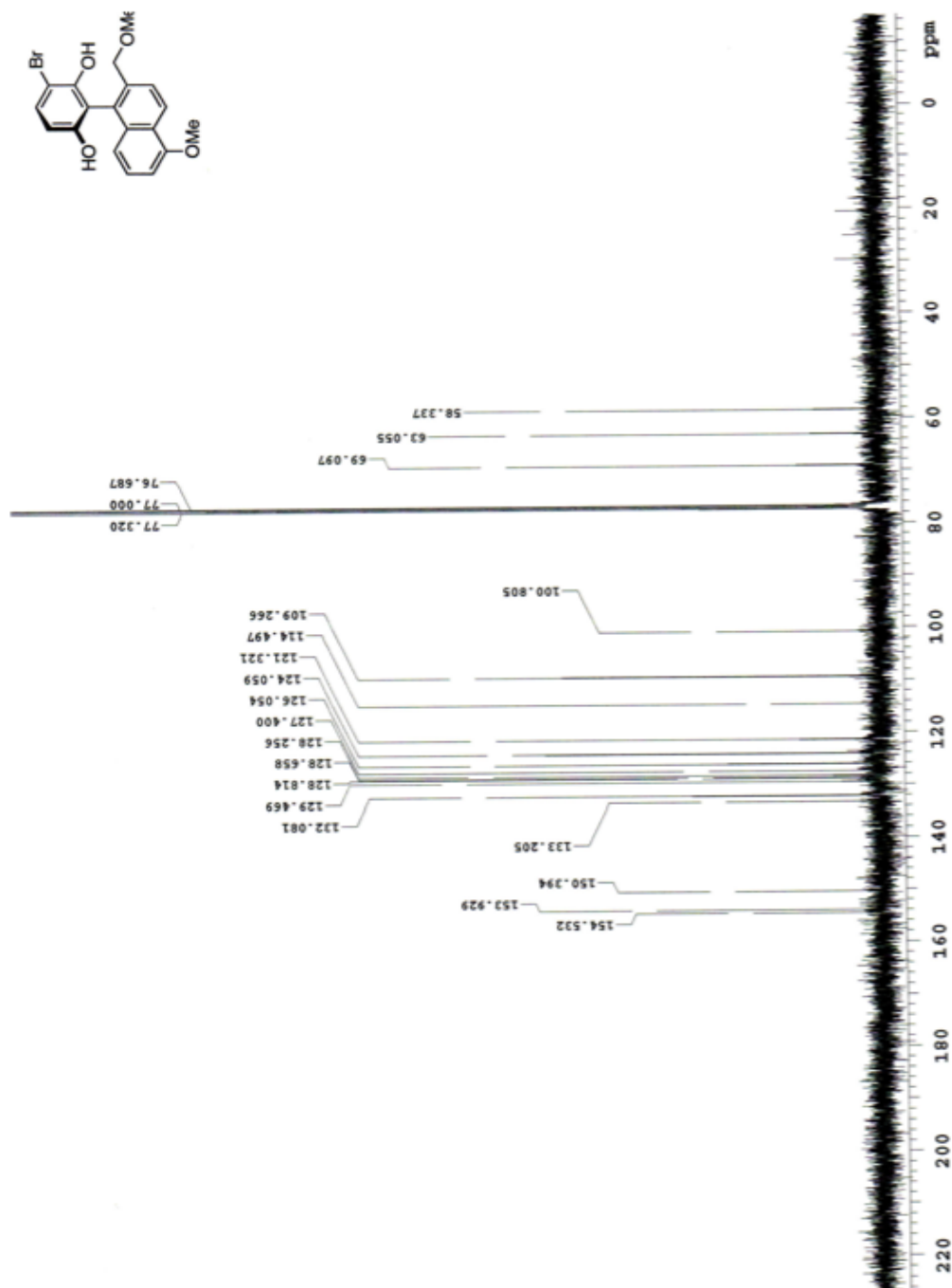
HPLC chart of **4r** (racemic).



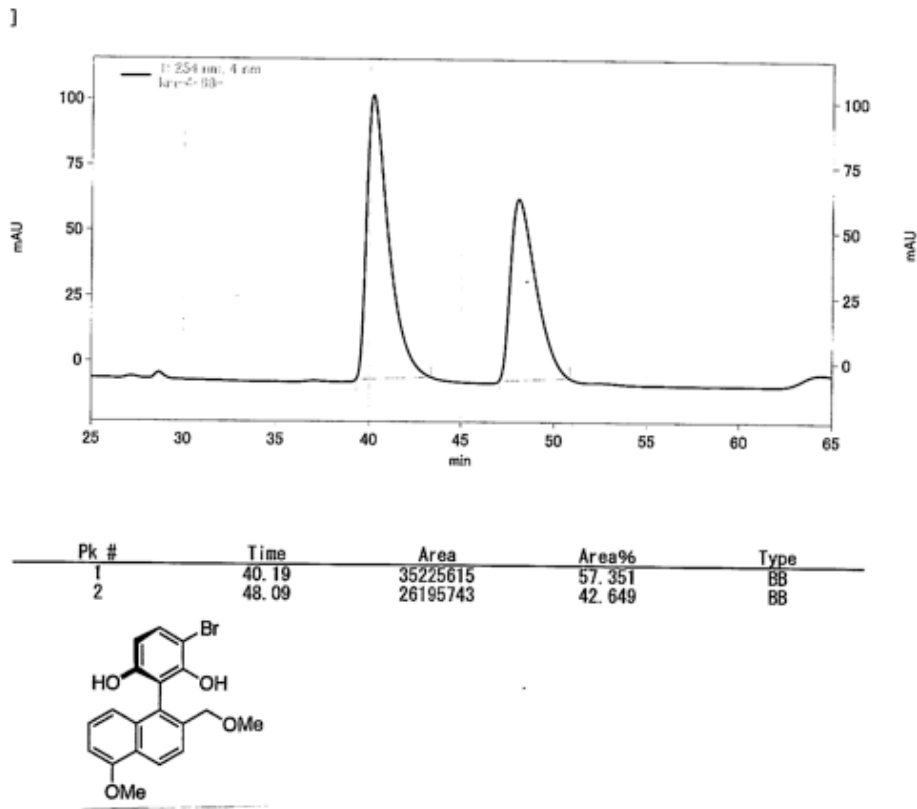
^1H NMR spectrum of **4s**.



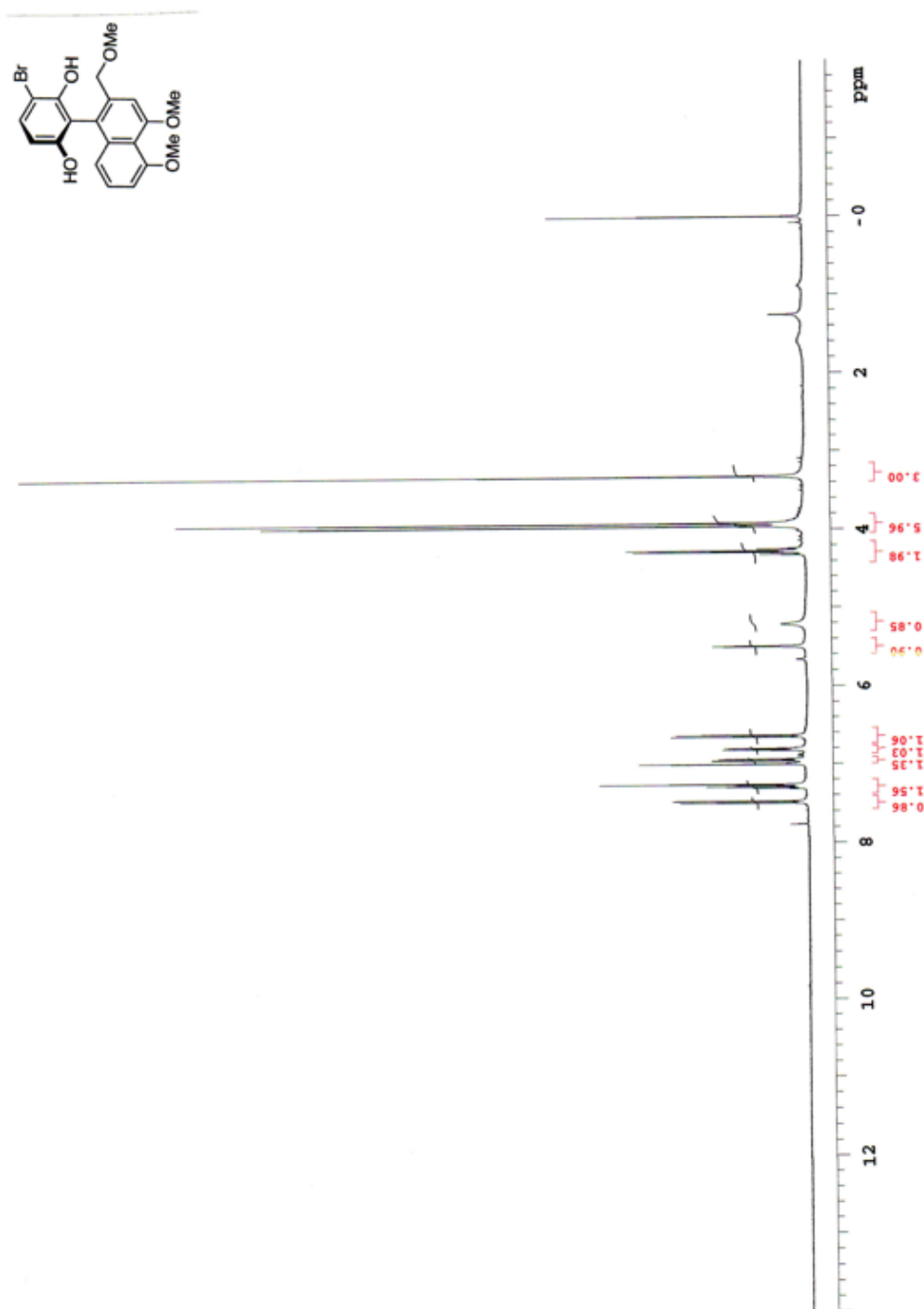
^{13}C NMR spectrum of **4s**.



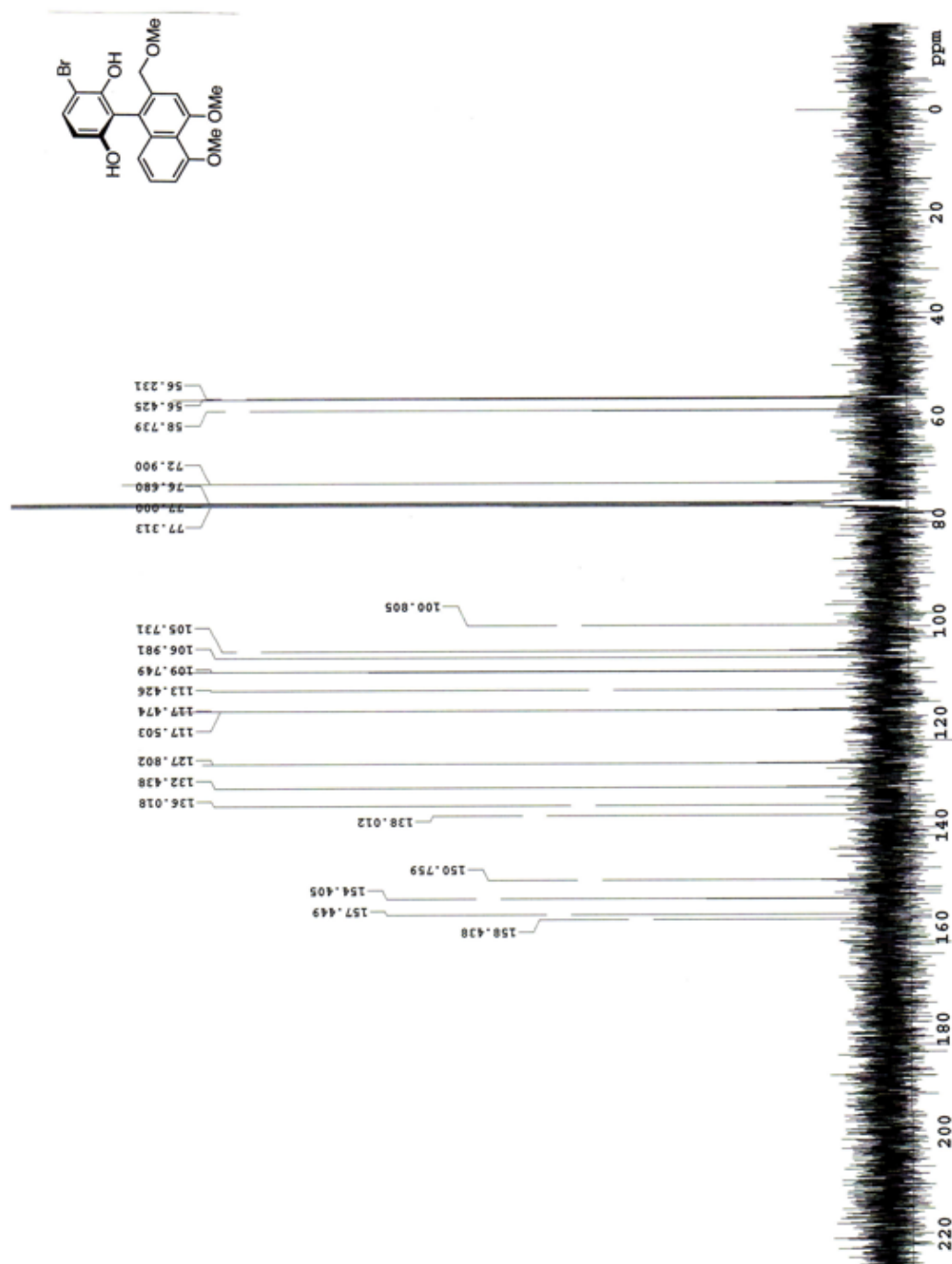
HPLC chart of **4s**.



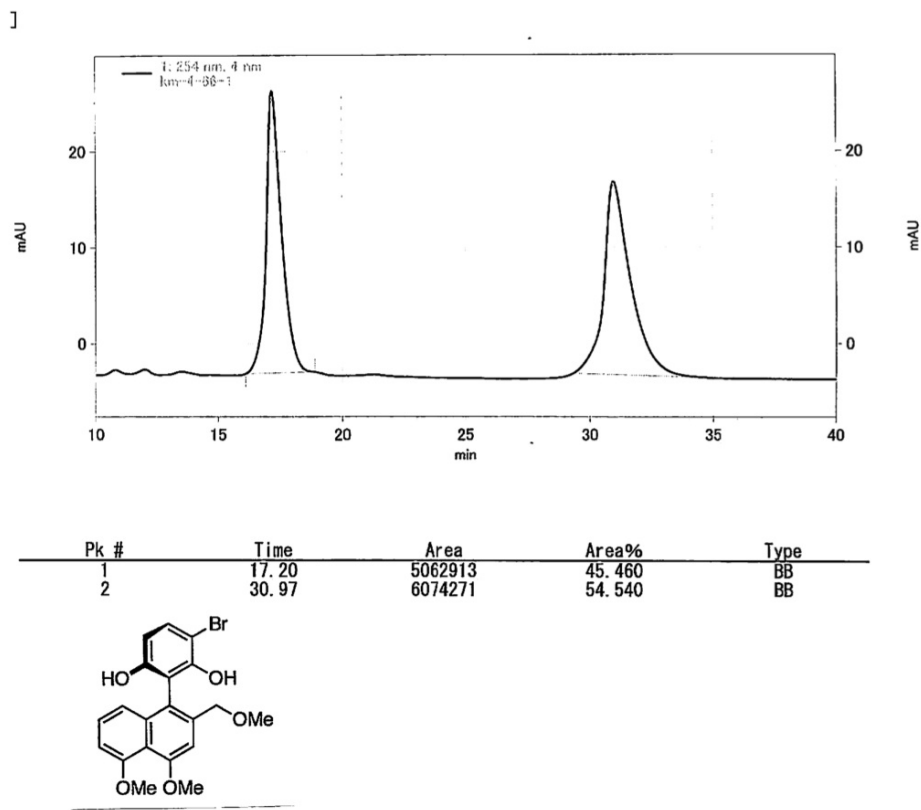
^1H NMR spectrum of **4t**.



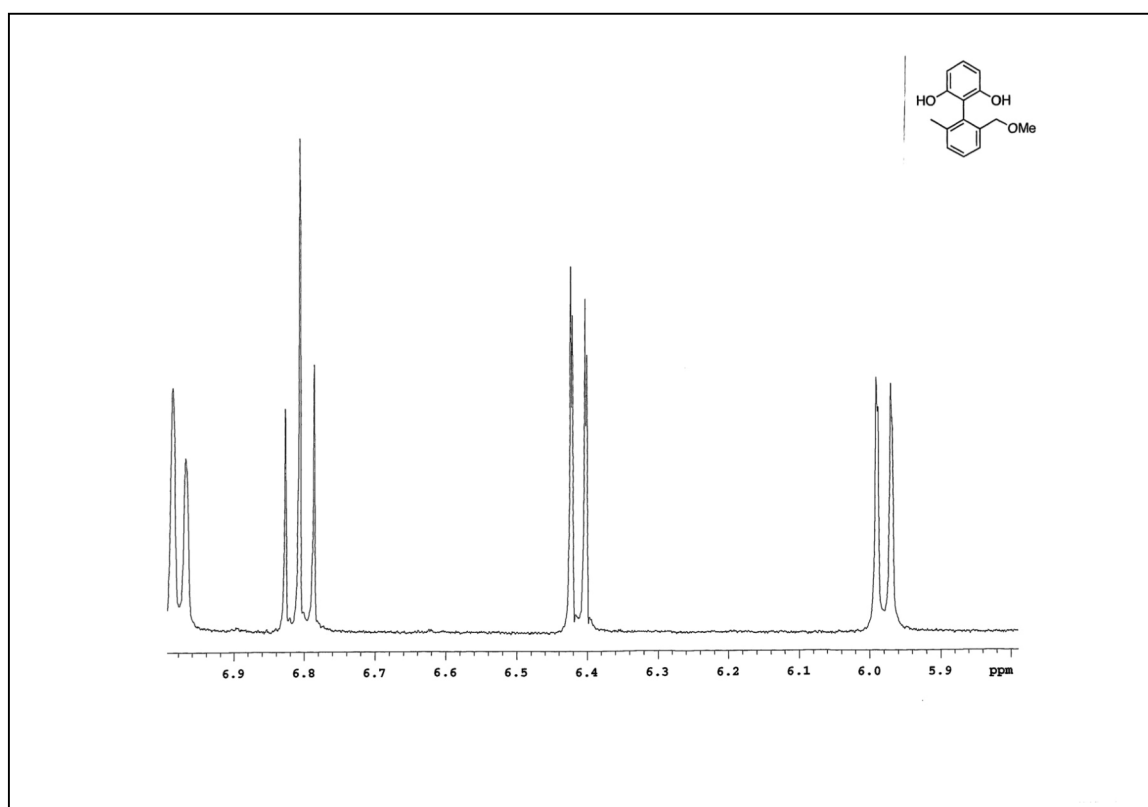
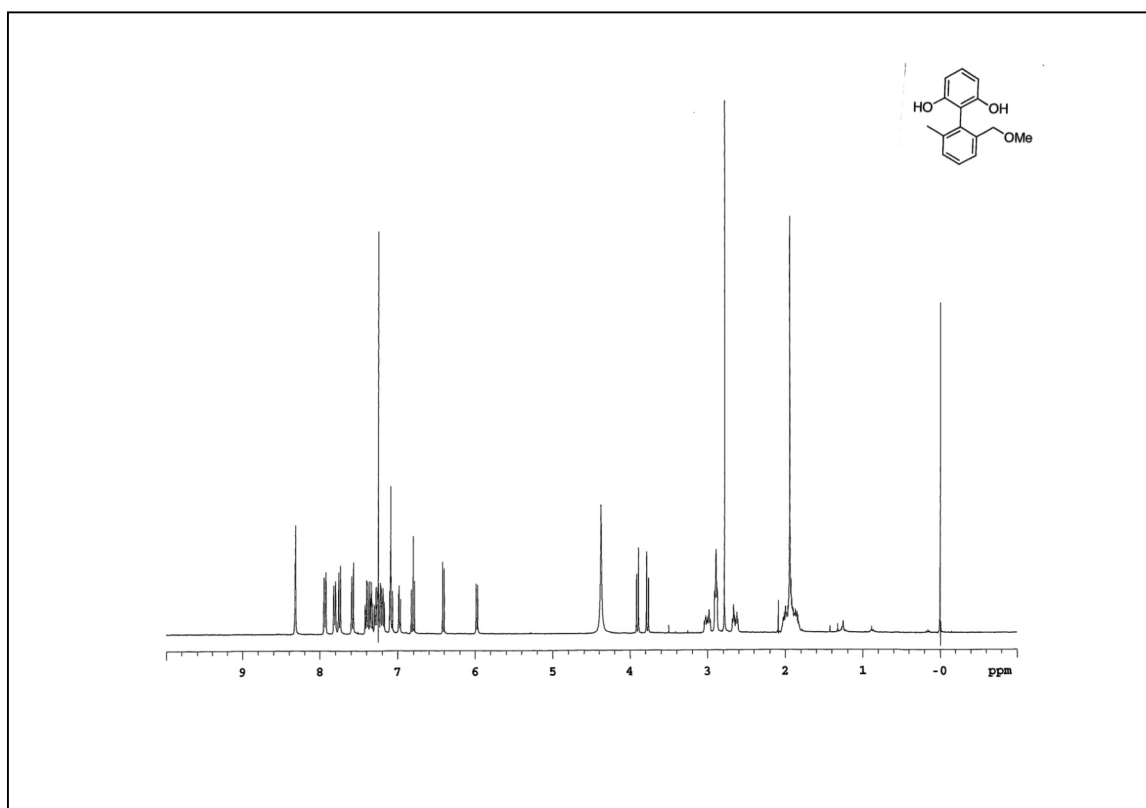
^{13}C NMR spectrum of **4t**.



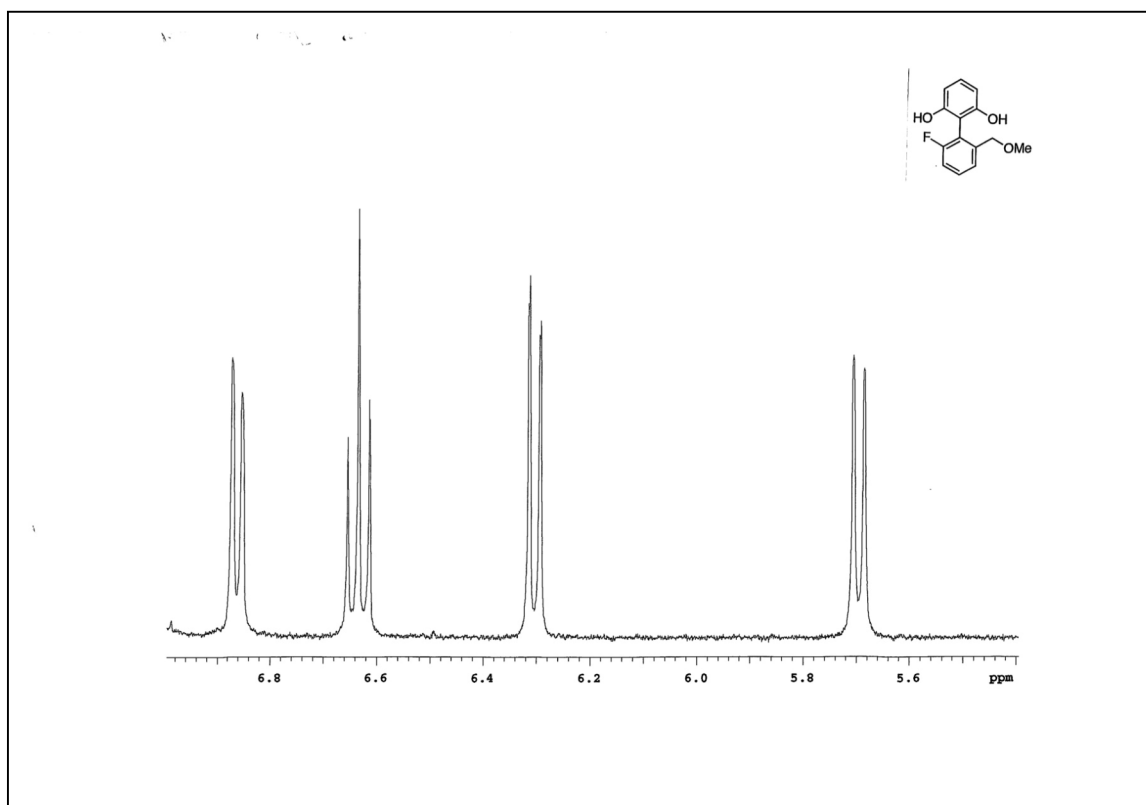
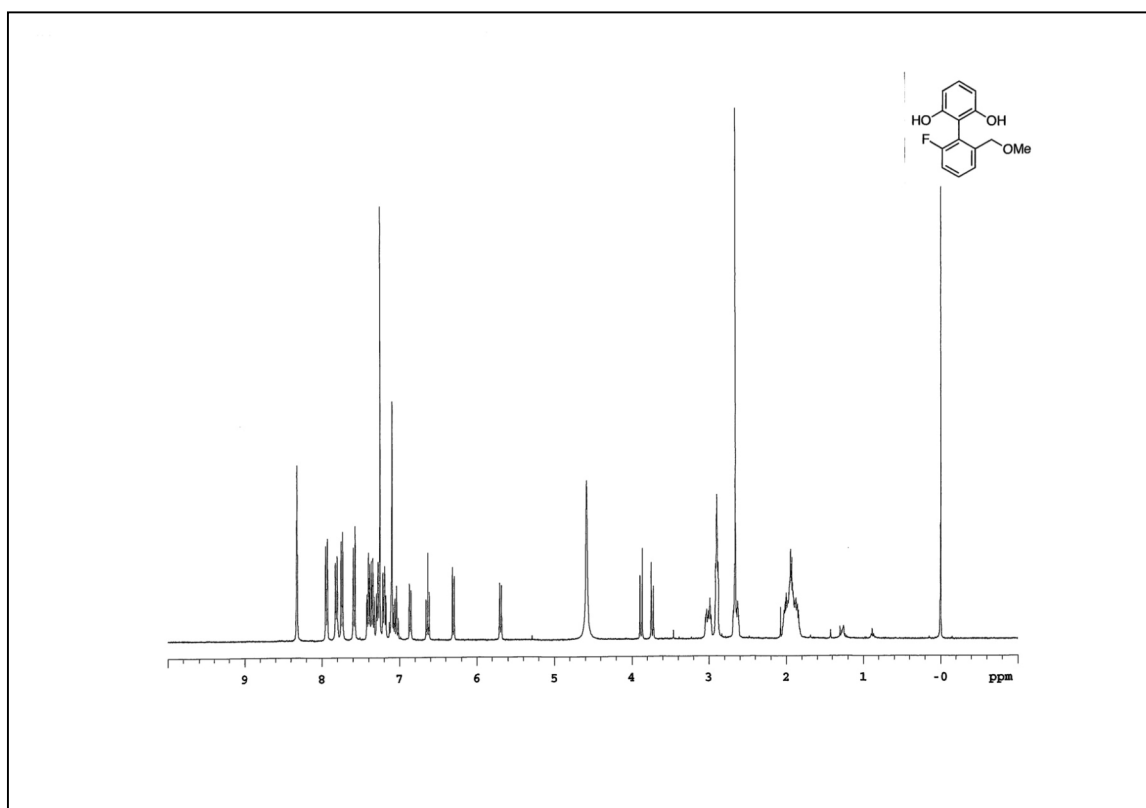
HPLC chart of **4t**.



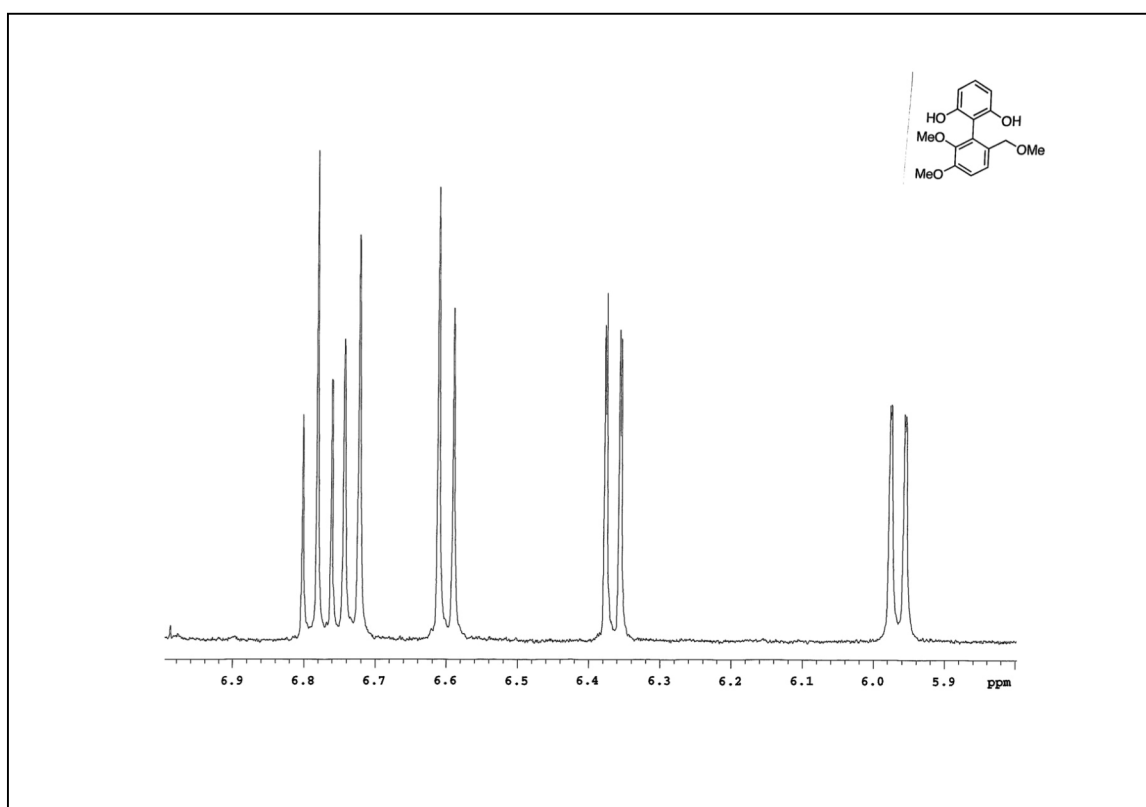
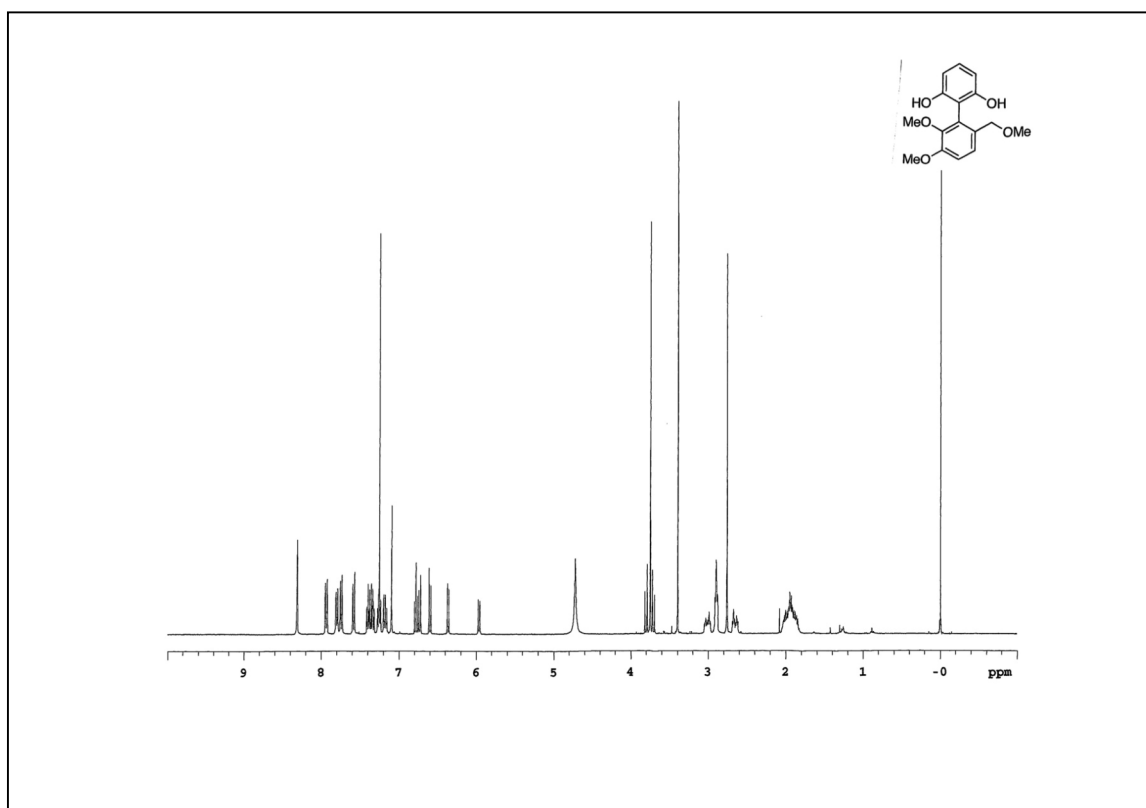
^1H NMR spectrum of the mixture of **3b** and **2j** (X = 9-anthryl).



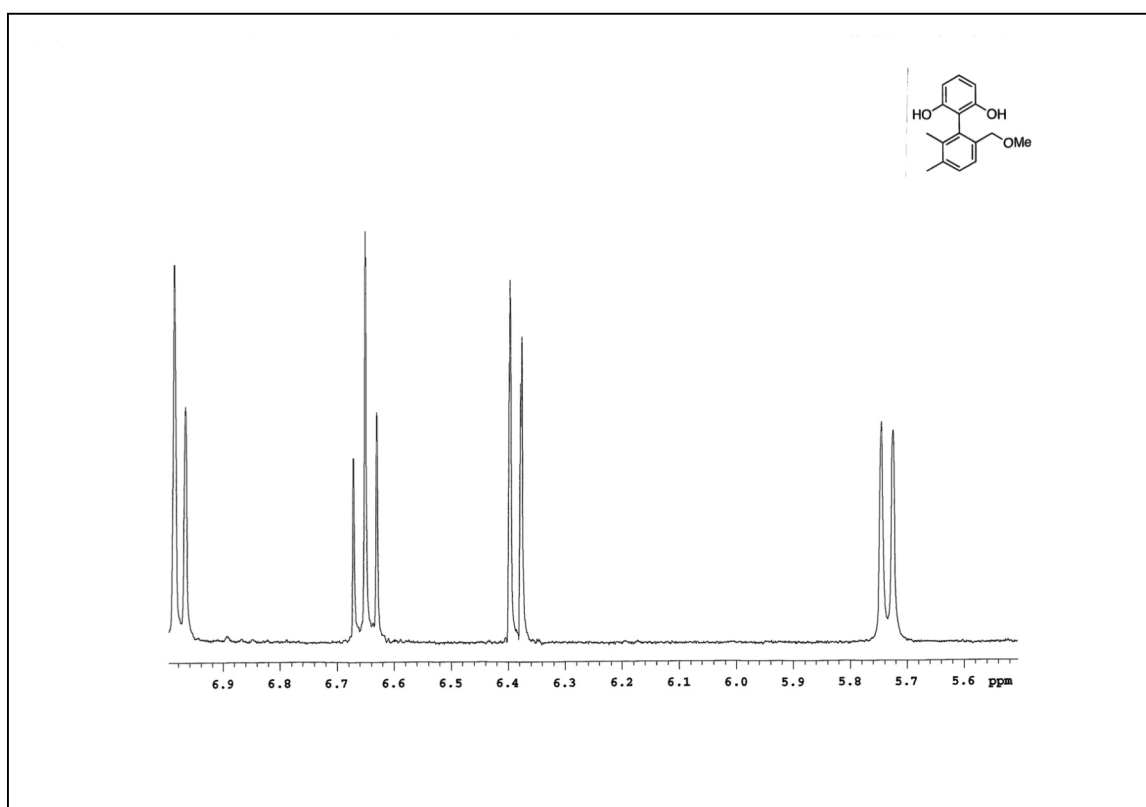
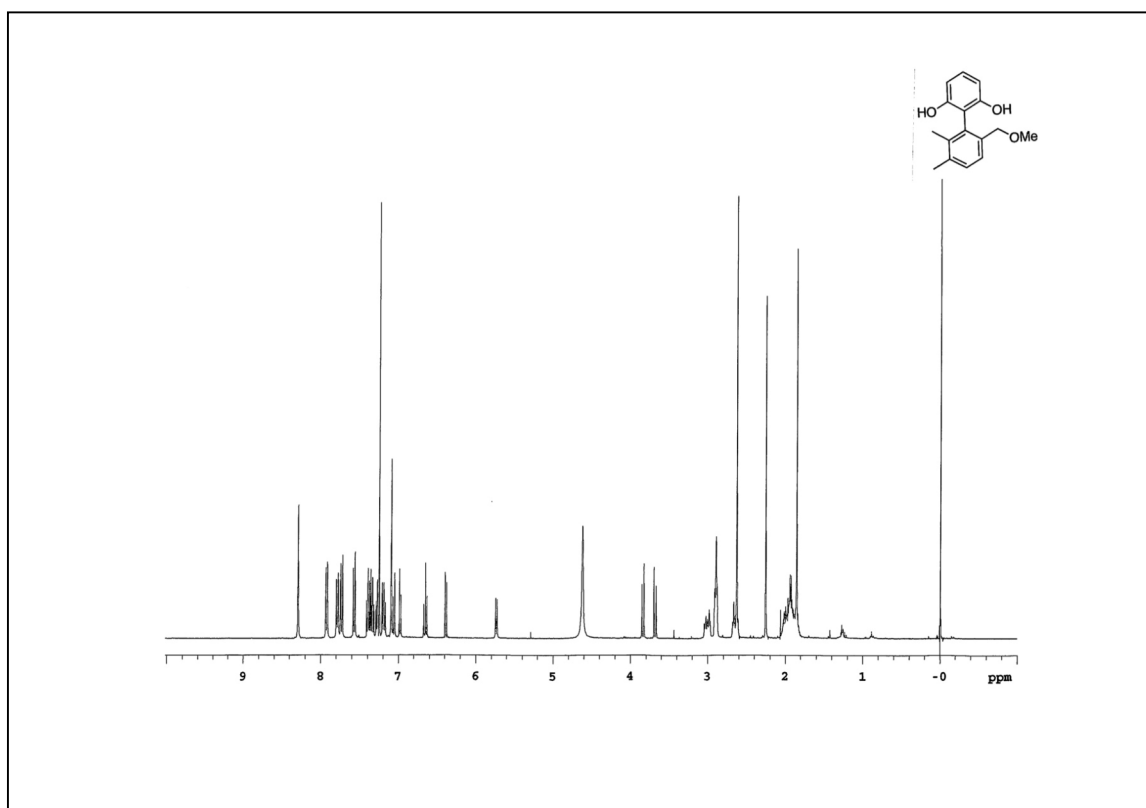
^1H NMR spectrum of the mixture of **3c** and **2j** (X = 9-anthryl).



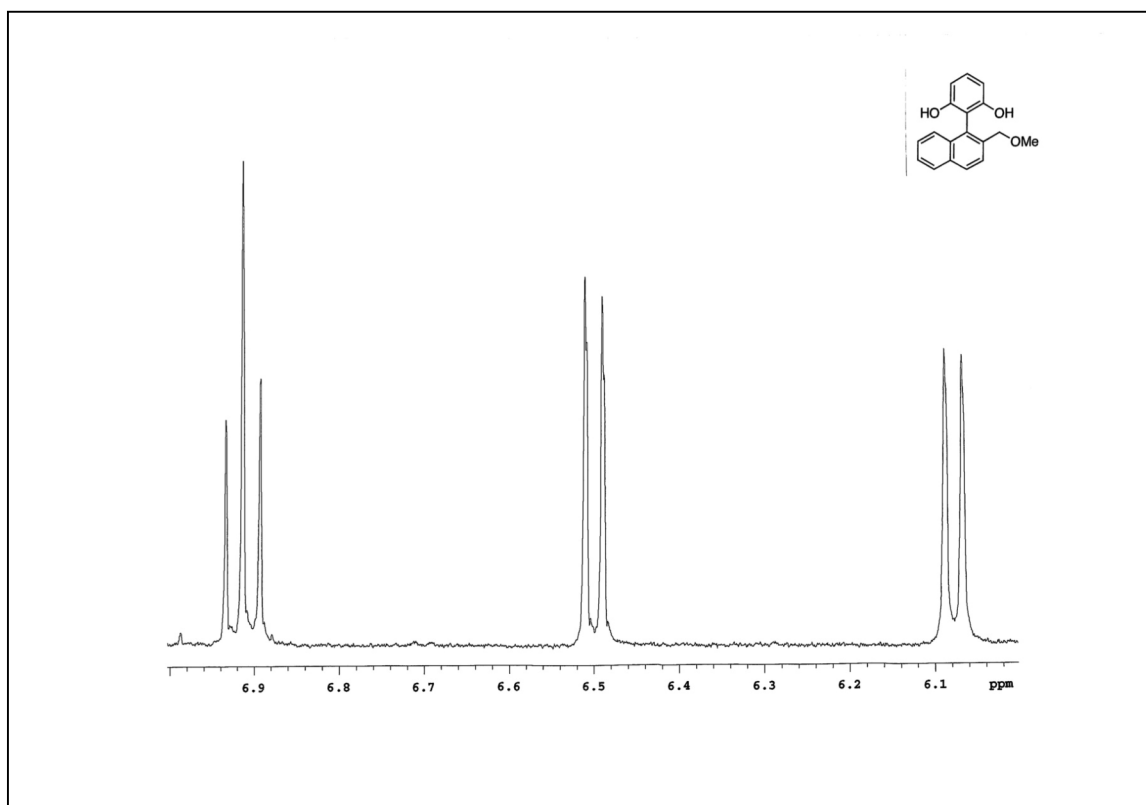
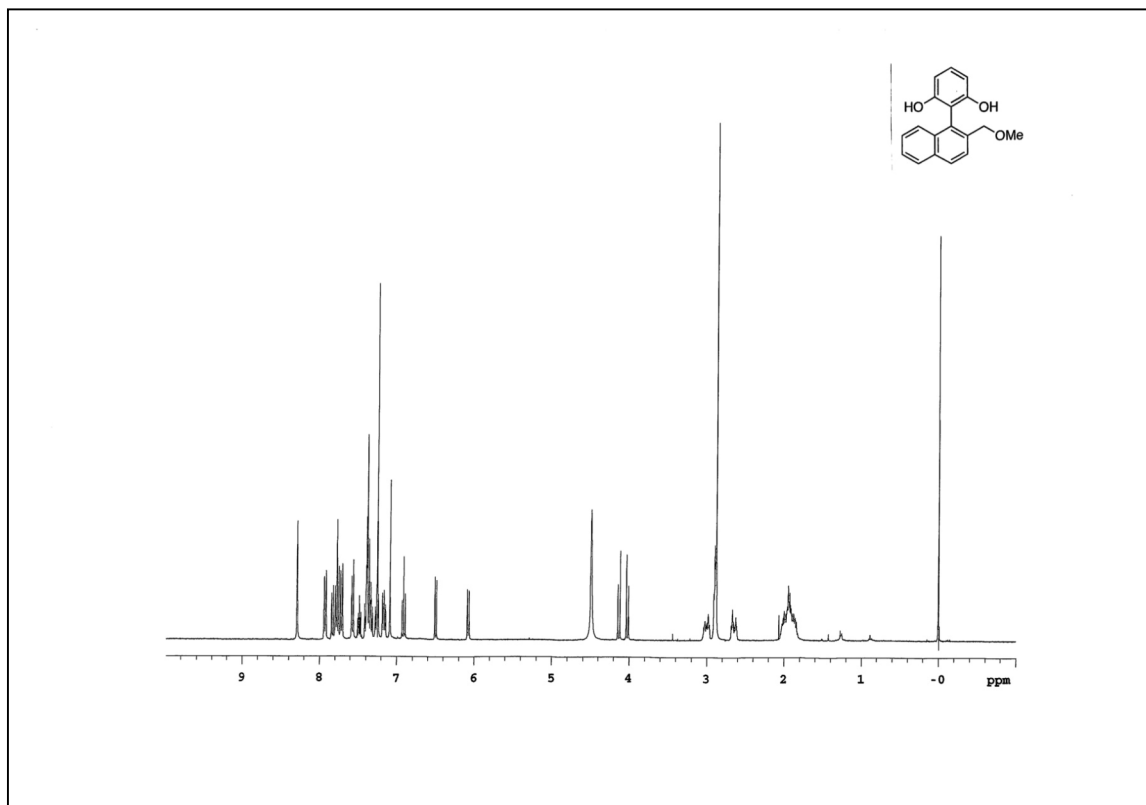
^1H NMR spectrum of the mixture of **3d** and **2j** (X = 9-anthryl).



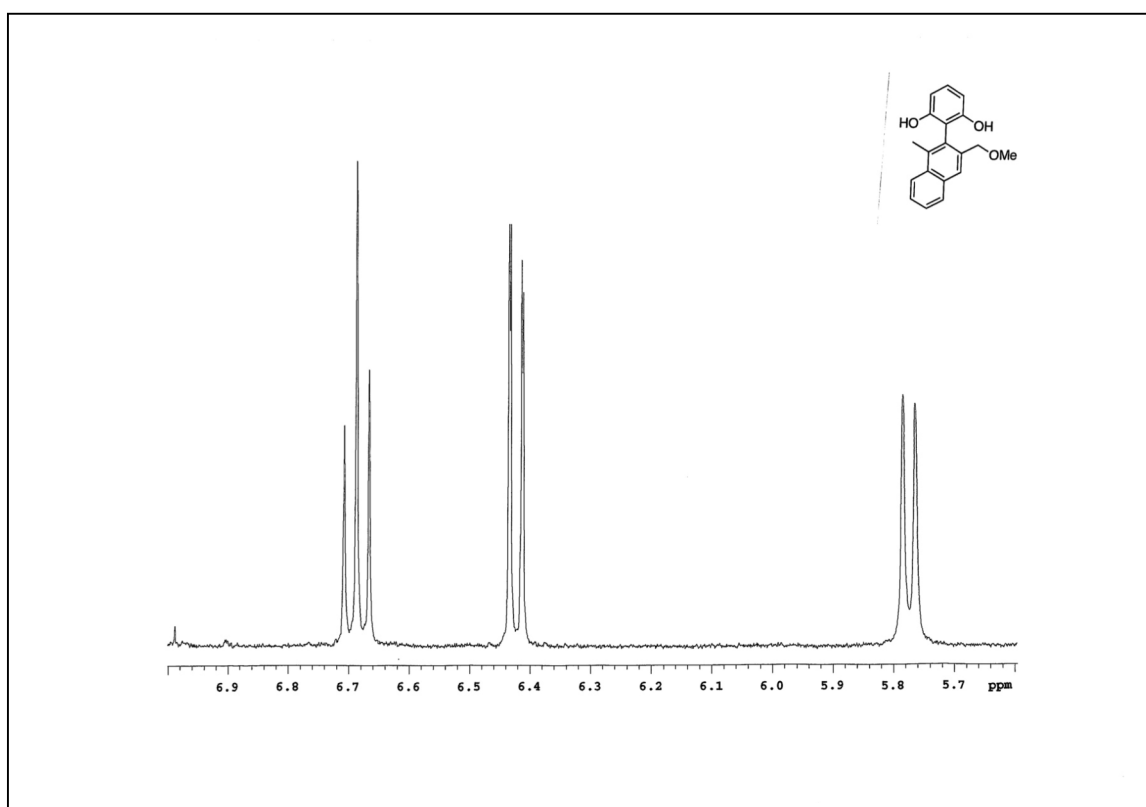
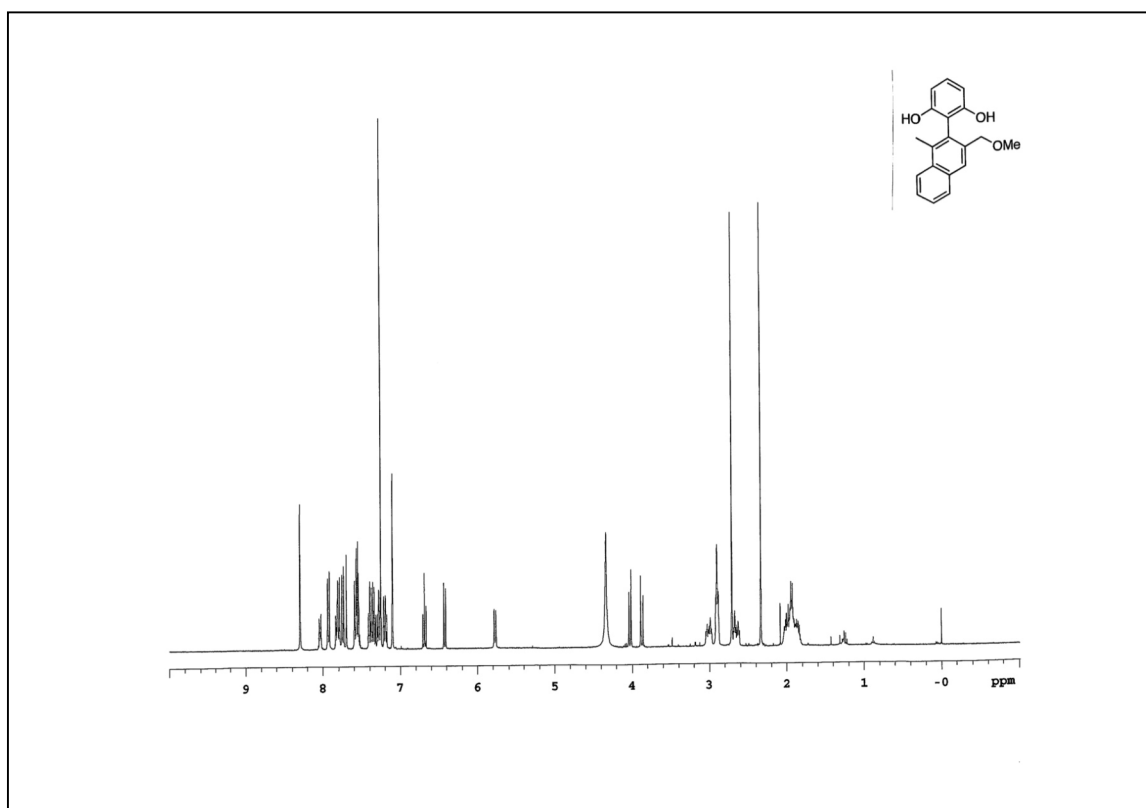
^1H NMR spectrum of the mixture of **3e** and **2j** (X = 9-anthryl).



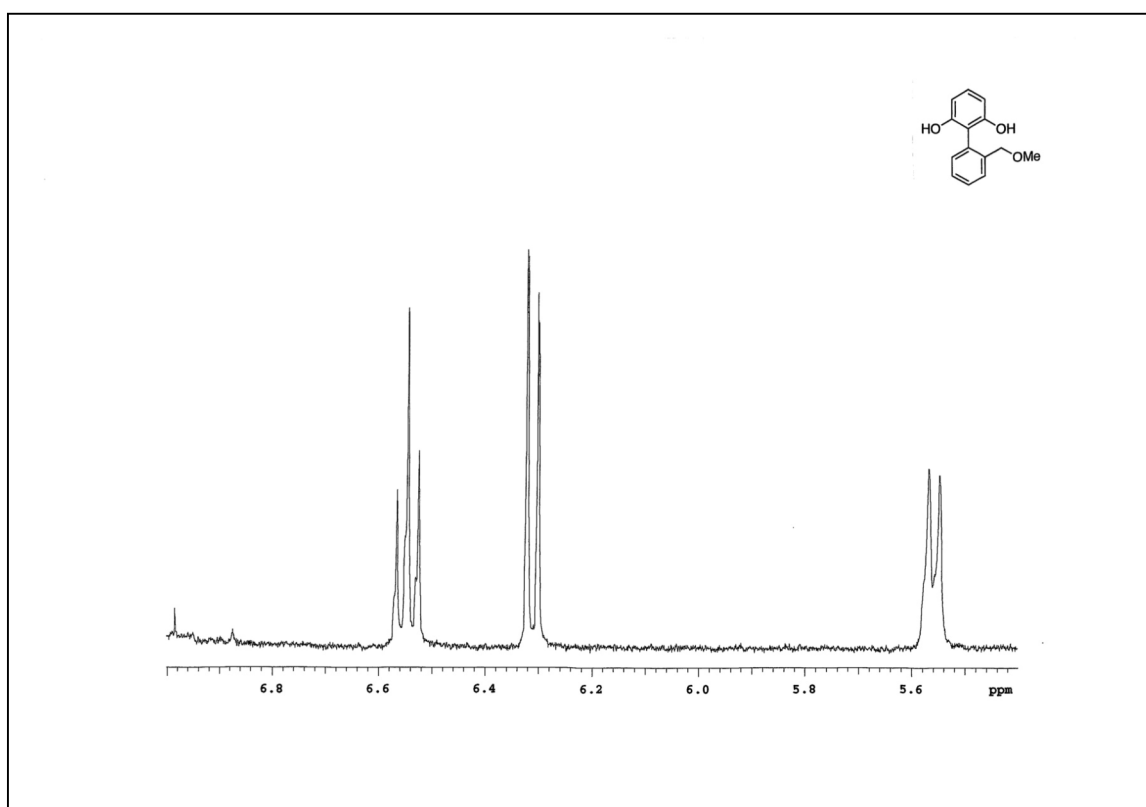
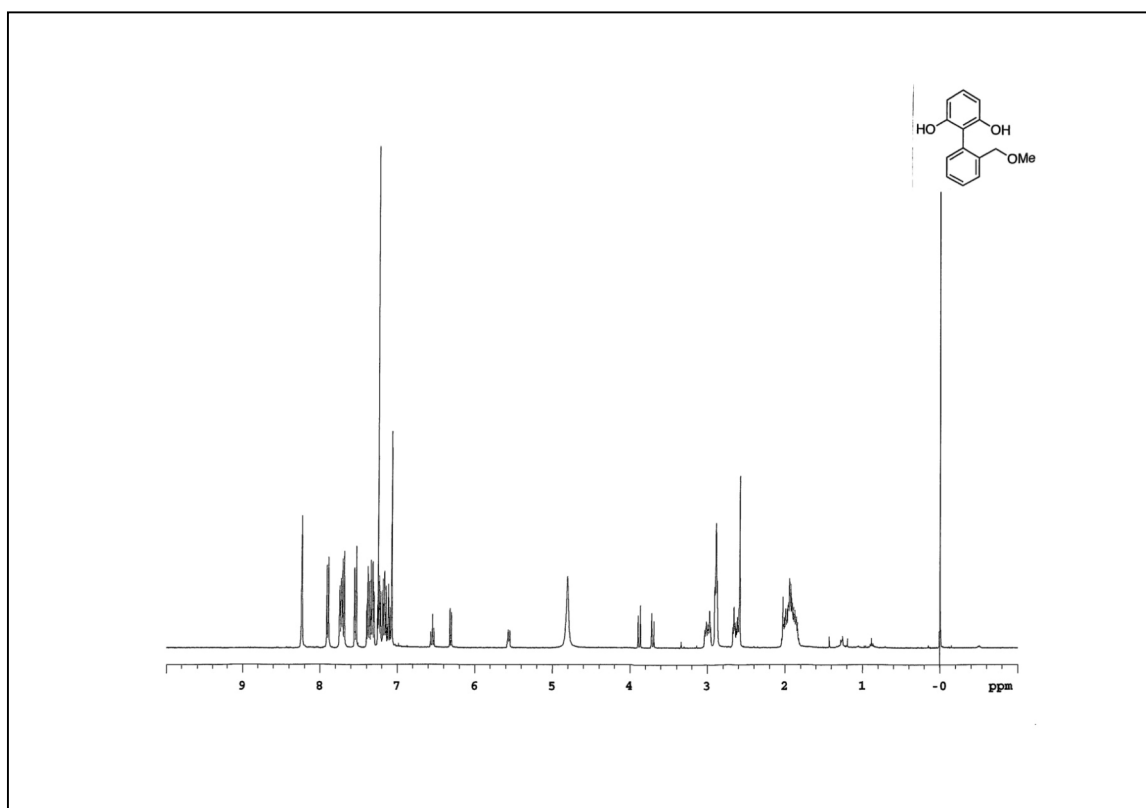
^1H NMR spectrum of the mixture of **3f** and **2j** (X = 9-anthryl).



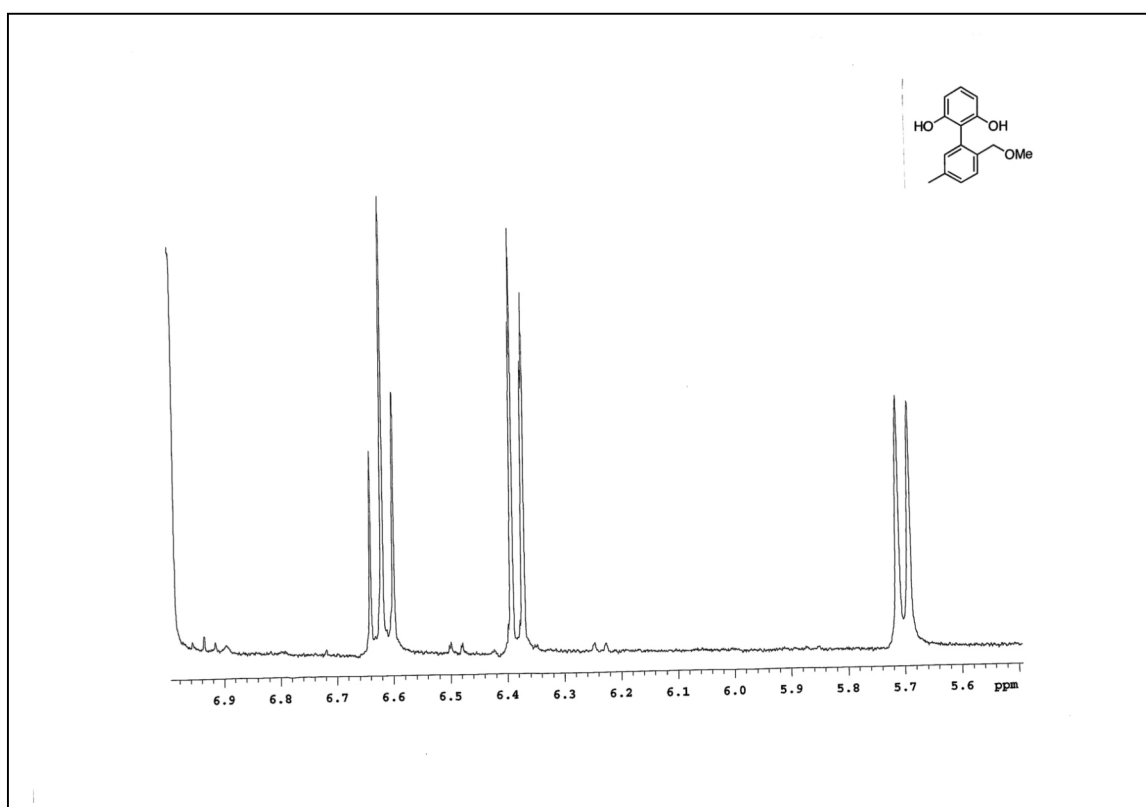
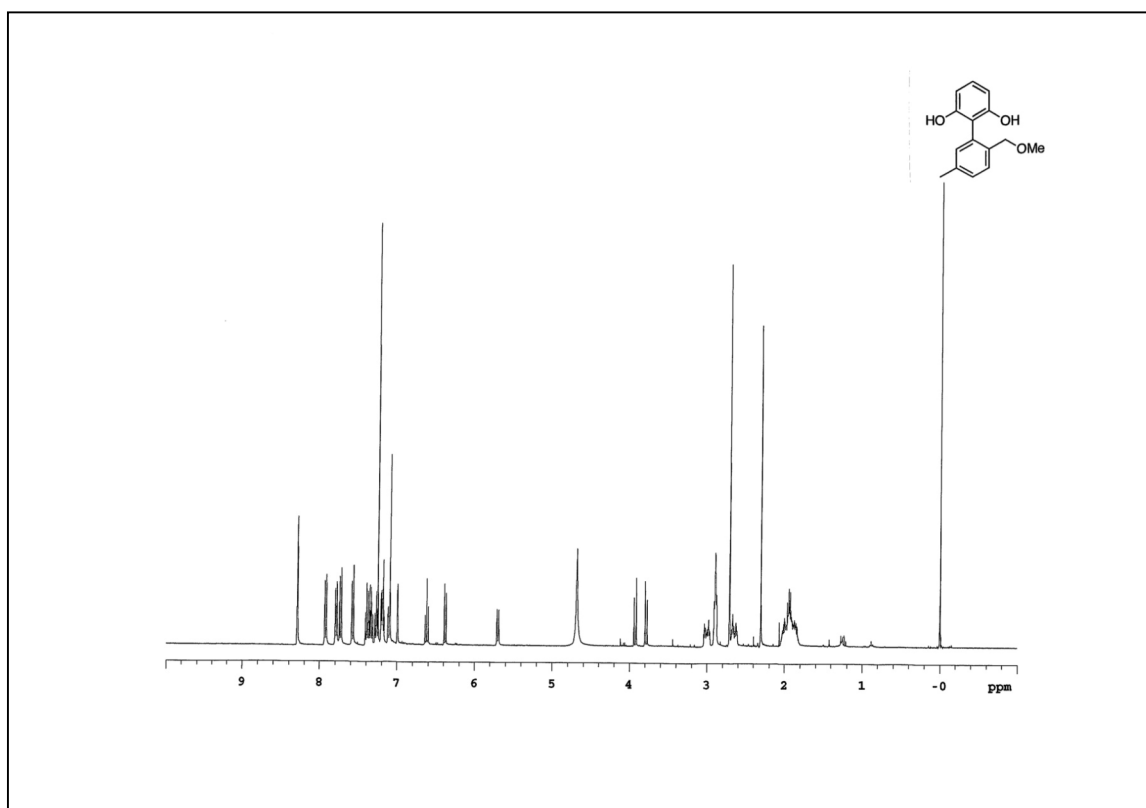
^1H NMR spectrum of the mixture of **3g** and **2j** (X = 9-anthryl).



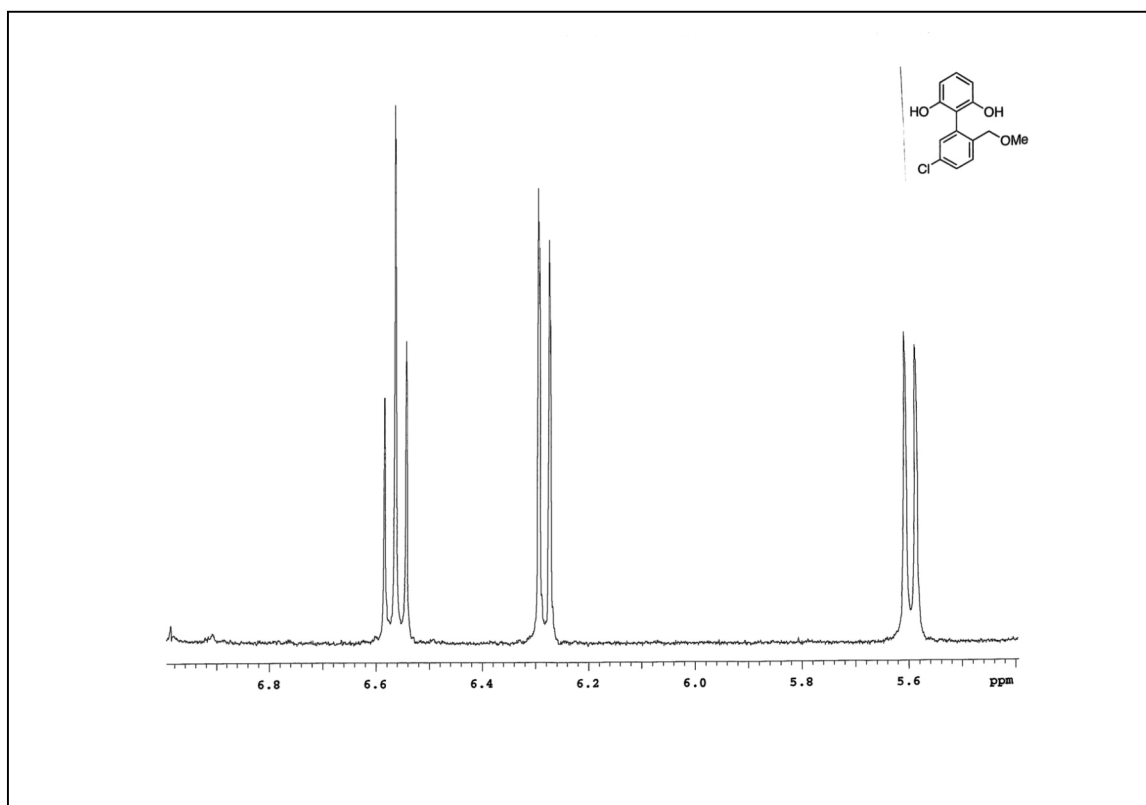
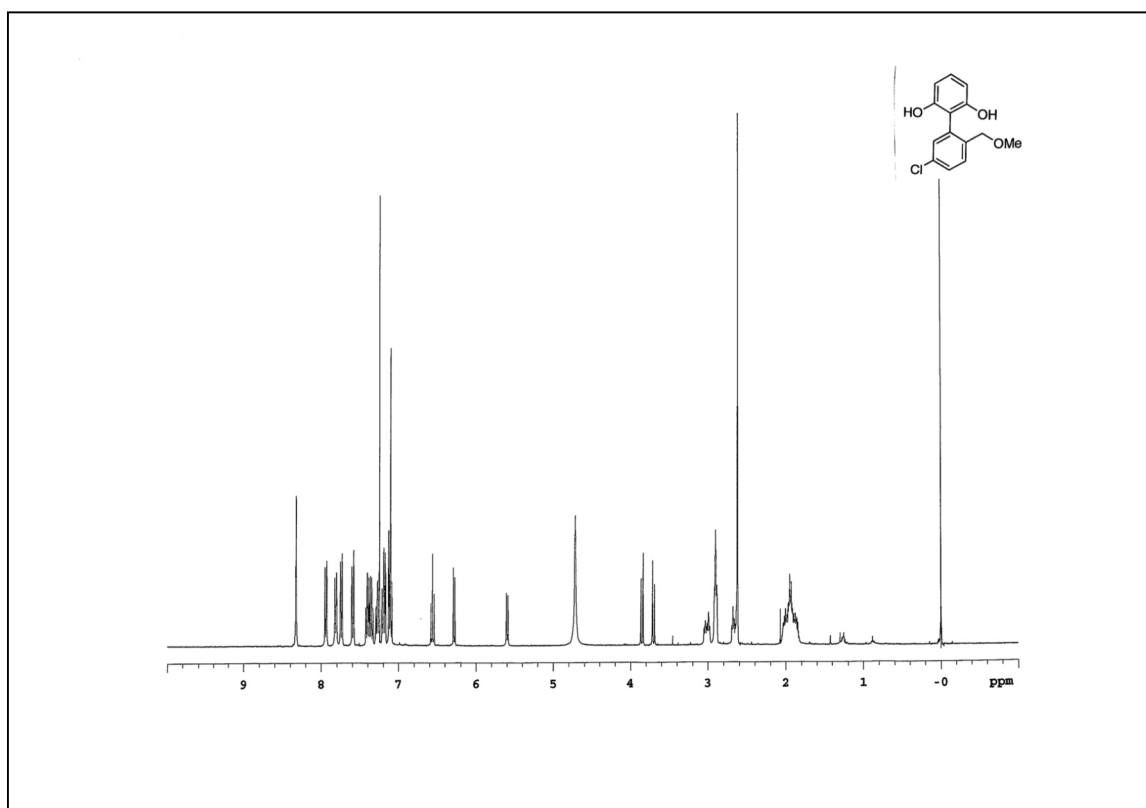
^1H NMR spectrum of the mixture of **3h** and **2j** (X = 9-anthryl).



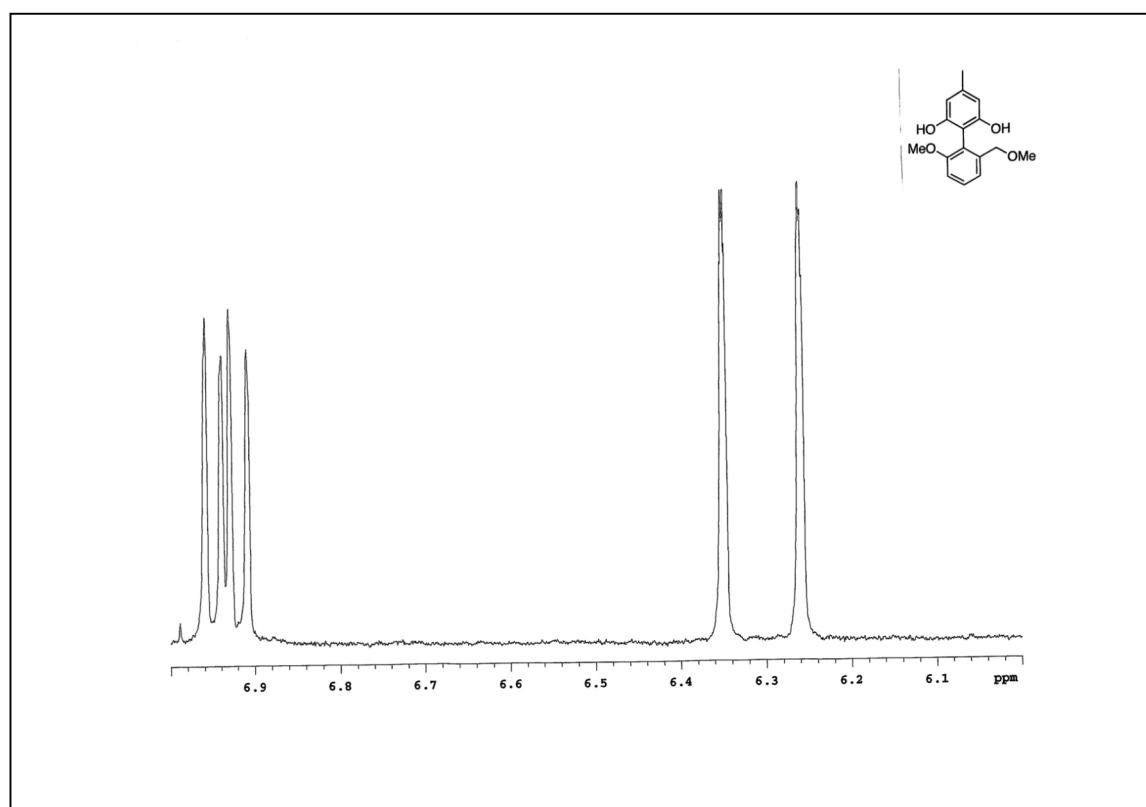
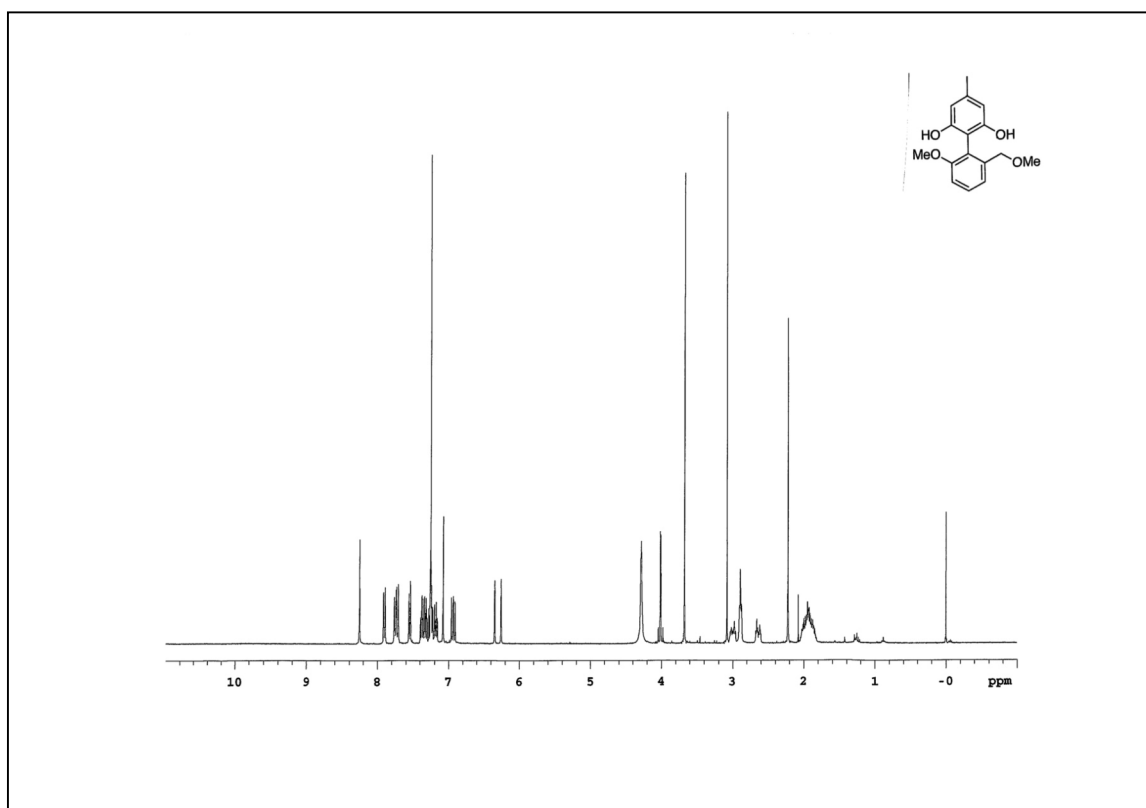
^1H NMR spectrum of the mixture of **3i** and **2j** (X = 9-anthryl).



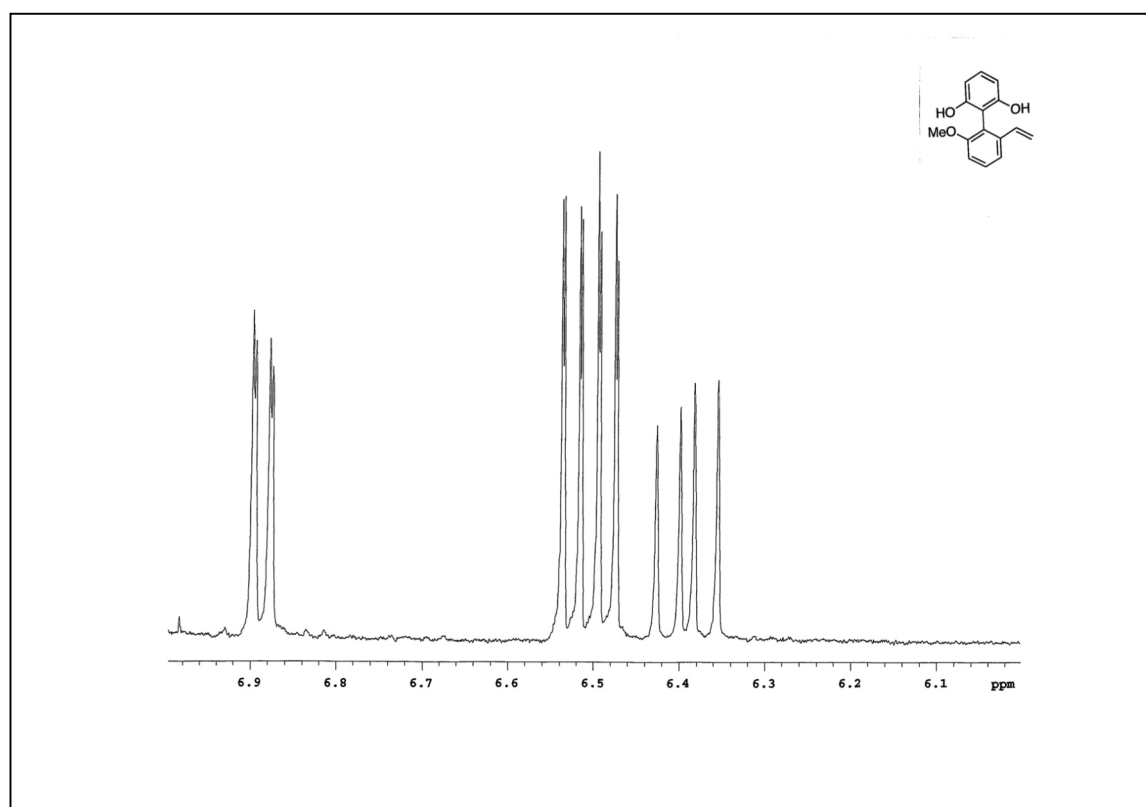
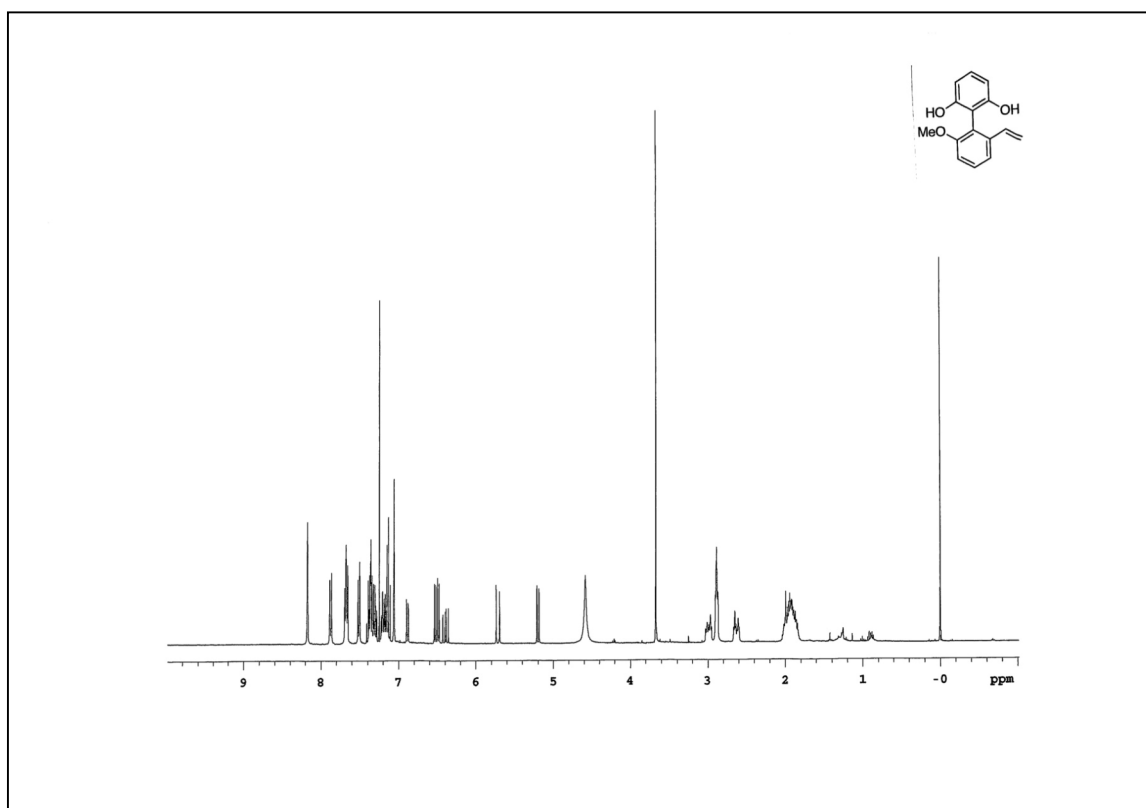
^1H NMR spectrum of the mixture of **3j** and **2j** (X = 9-anthryl).



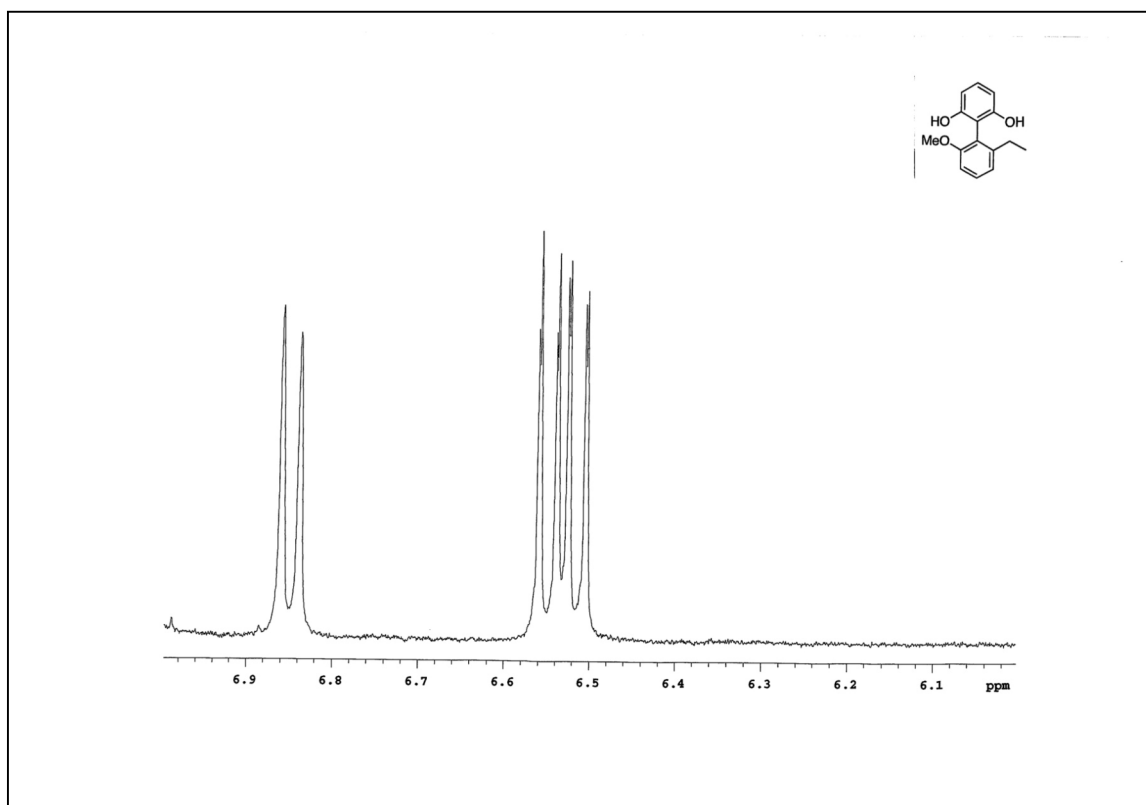
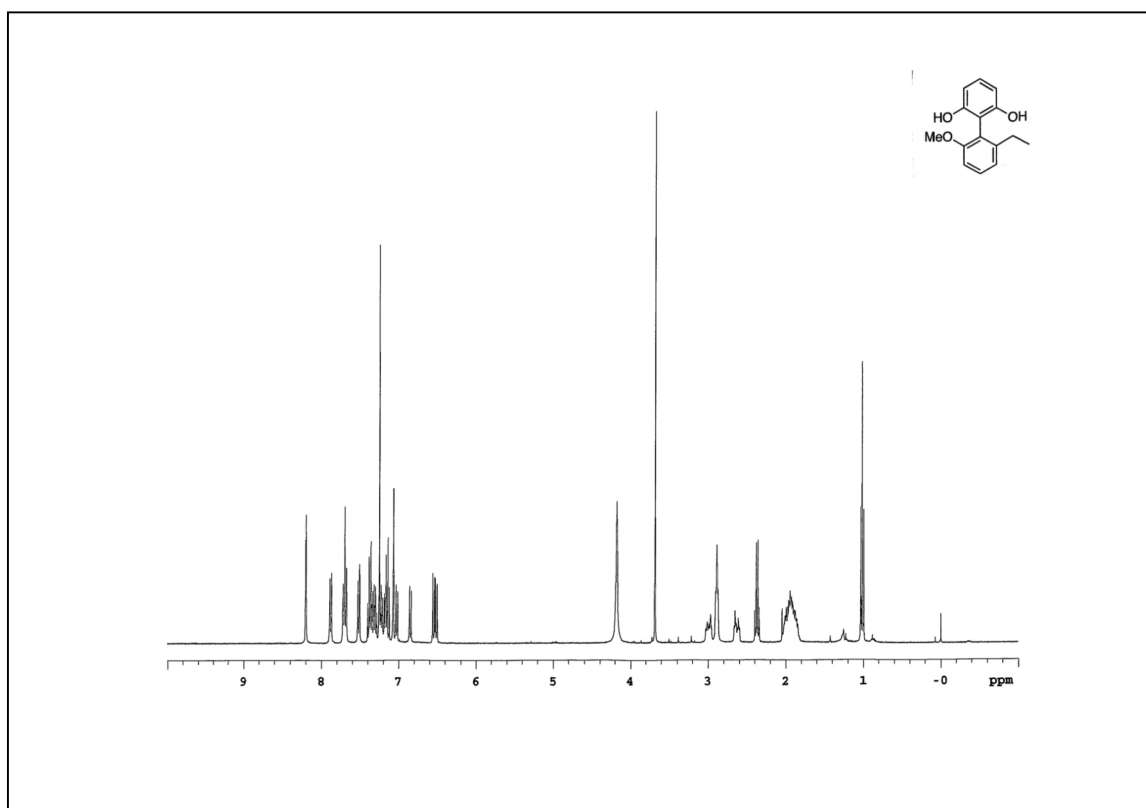
^1H NMR spectrum of the mixture of **3k** and **2j** (X = 9-anthryl).



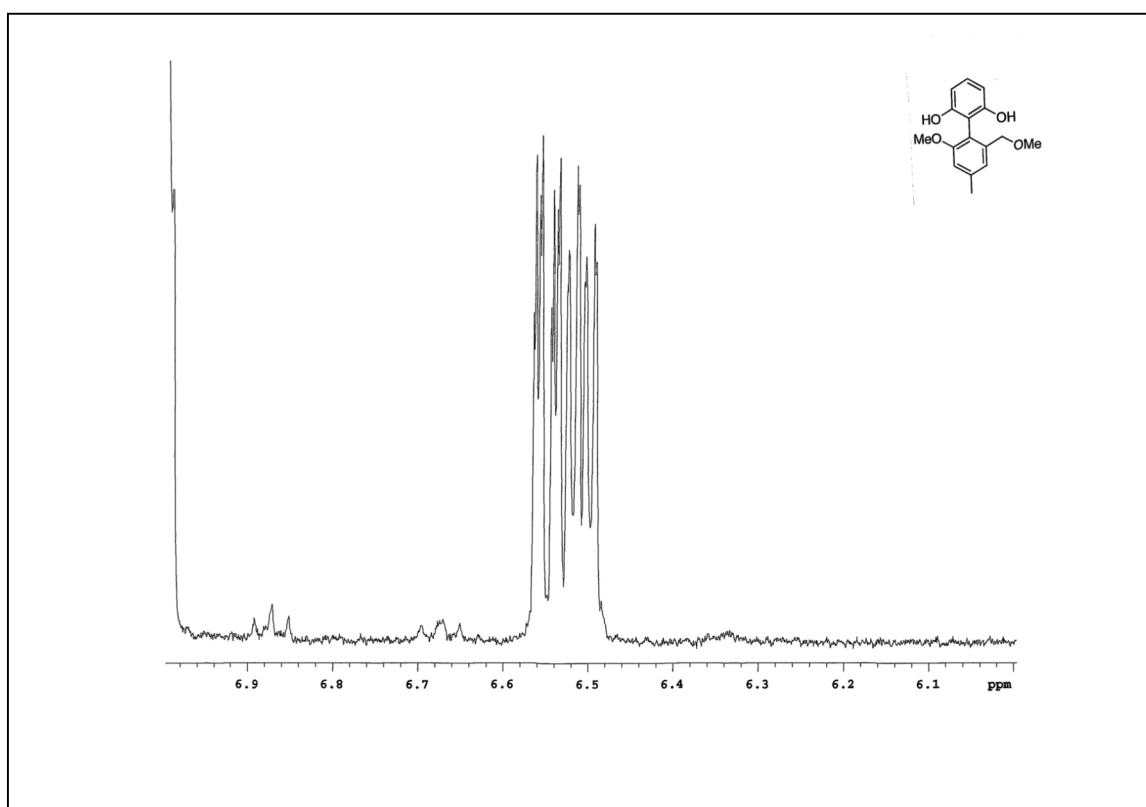
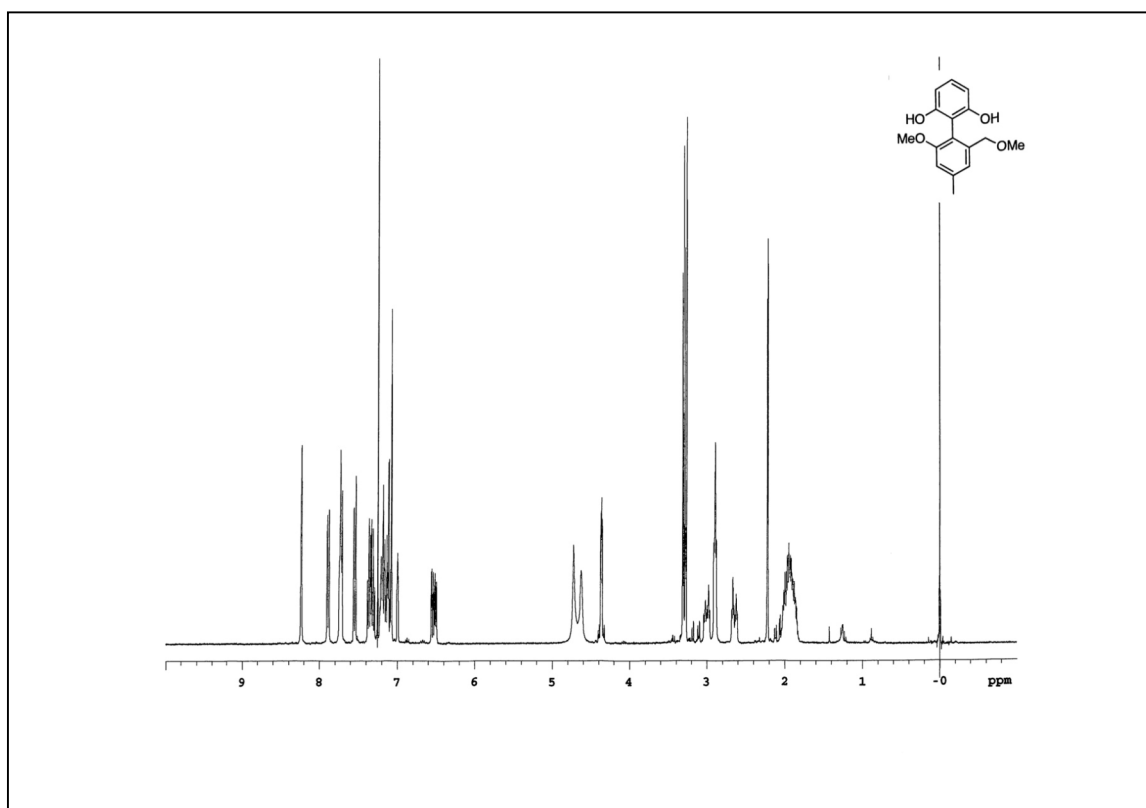
^1H NMR spectrum of the mixture of **3l** and **2j** (X = 9-anthryl).



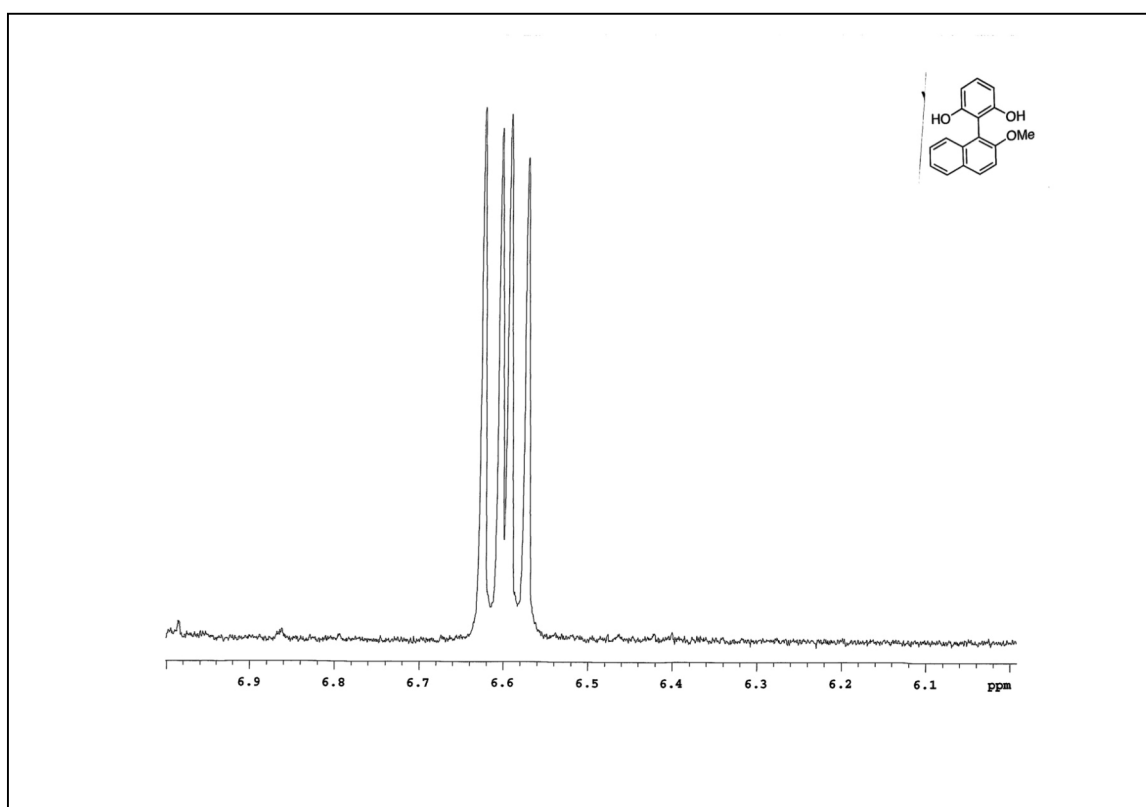
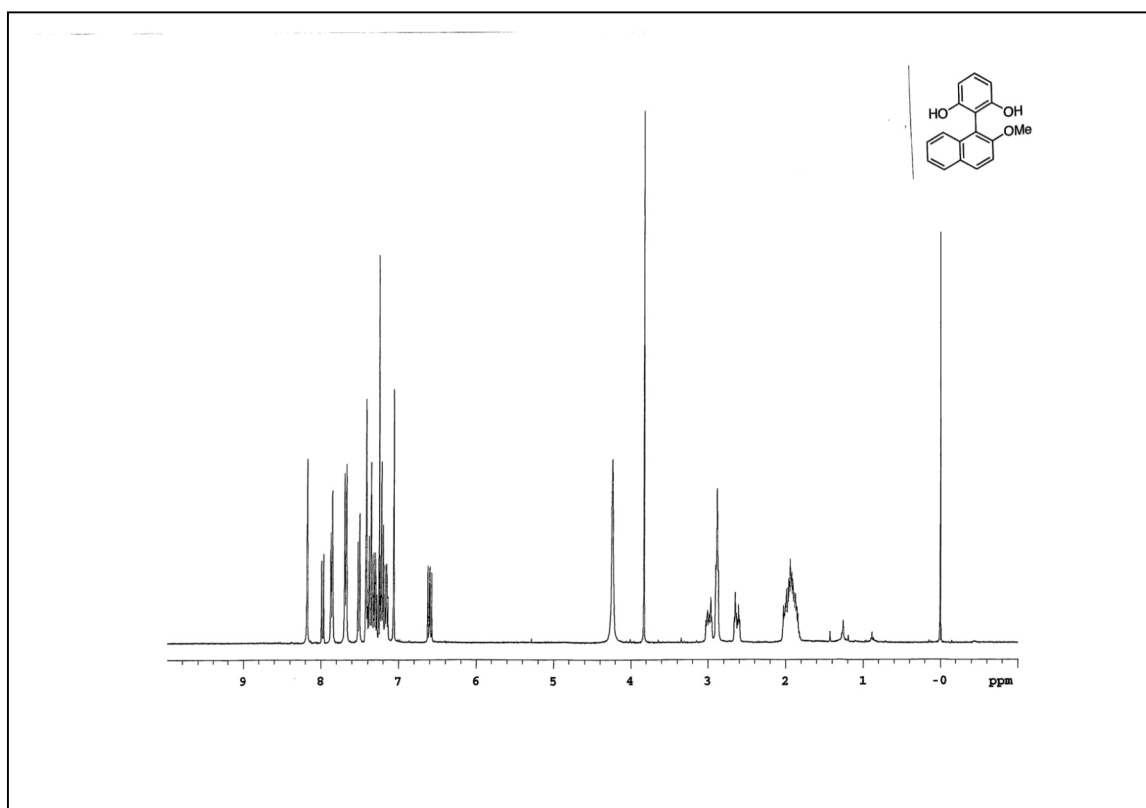
^1H NMR spectrum of the mixture of **3m** and **2j** (X = 9-anthryl).



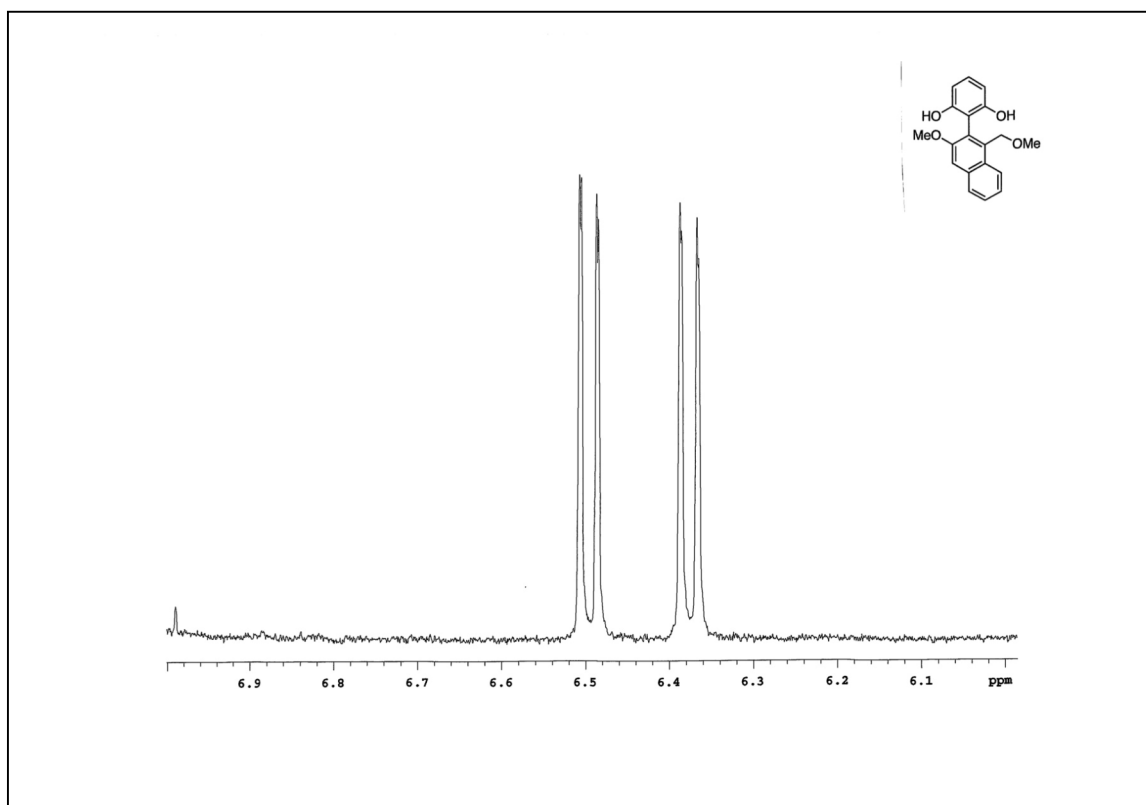
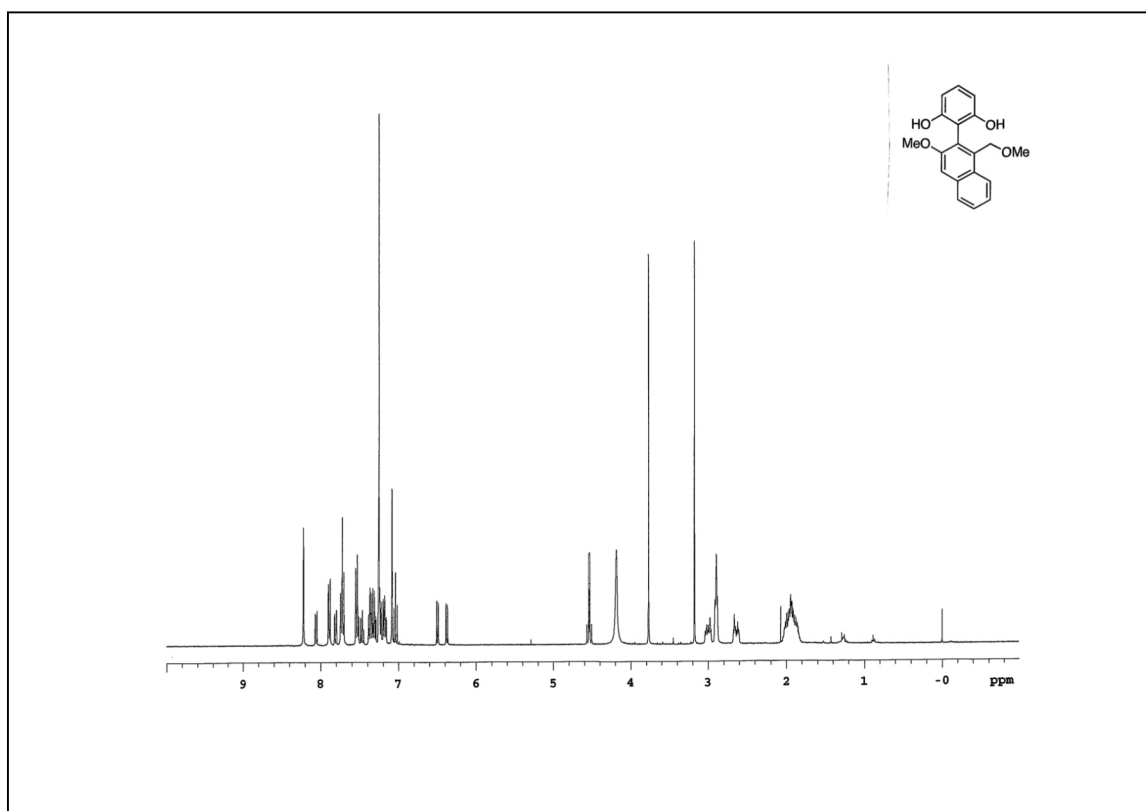
^1H NMR spectrum of the mixture of **3n** and **2j** (X = 9-anthryl).



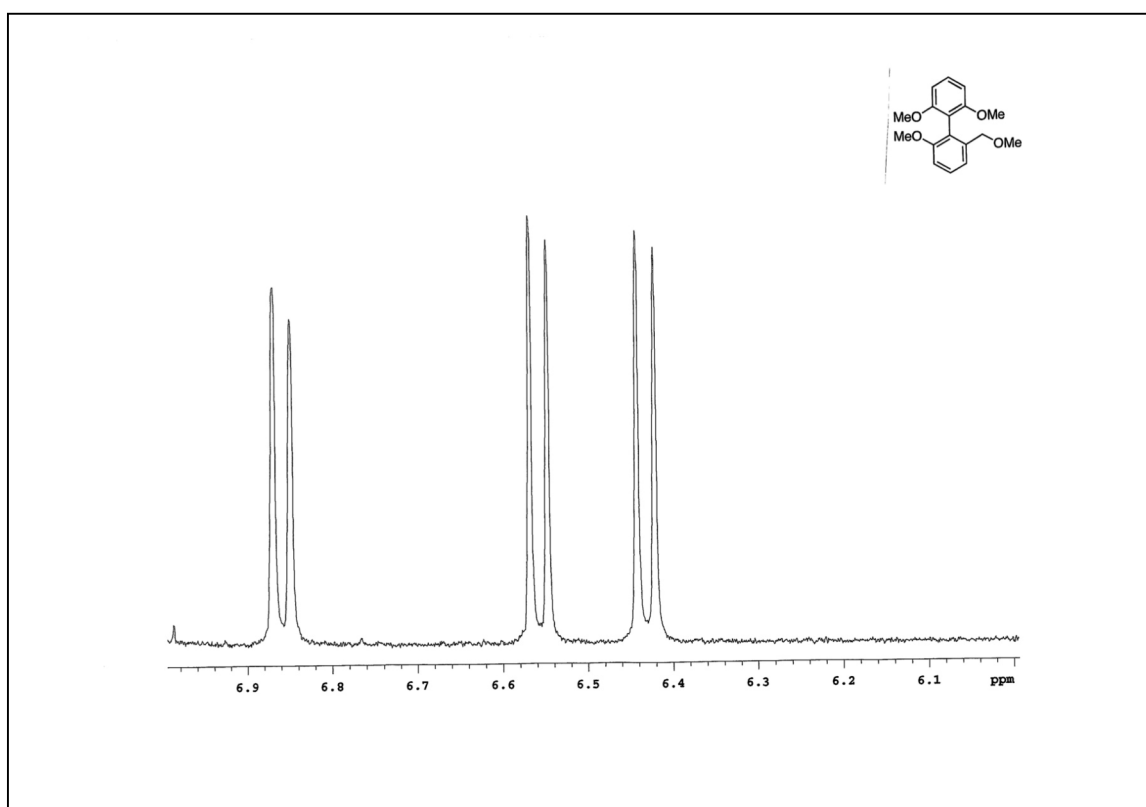
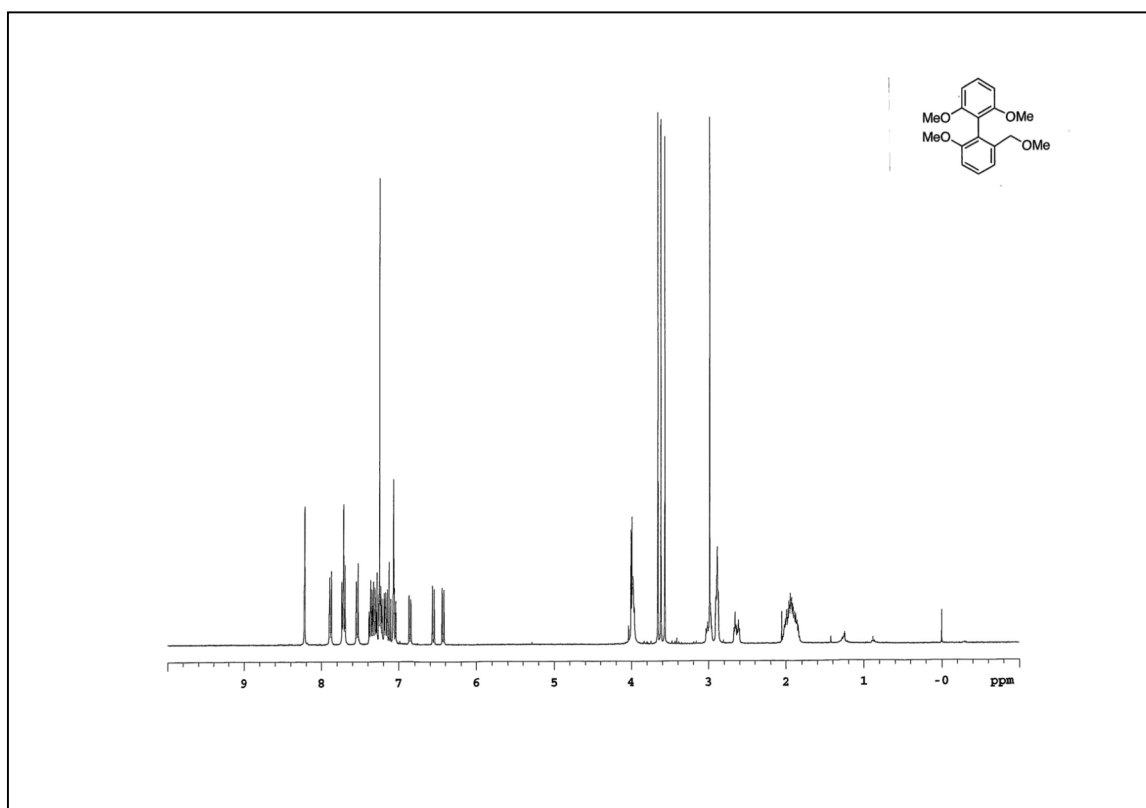
^1H NMR spectrum of the mixture of **3o** and **2j** (X = 9-anthryl).



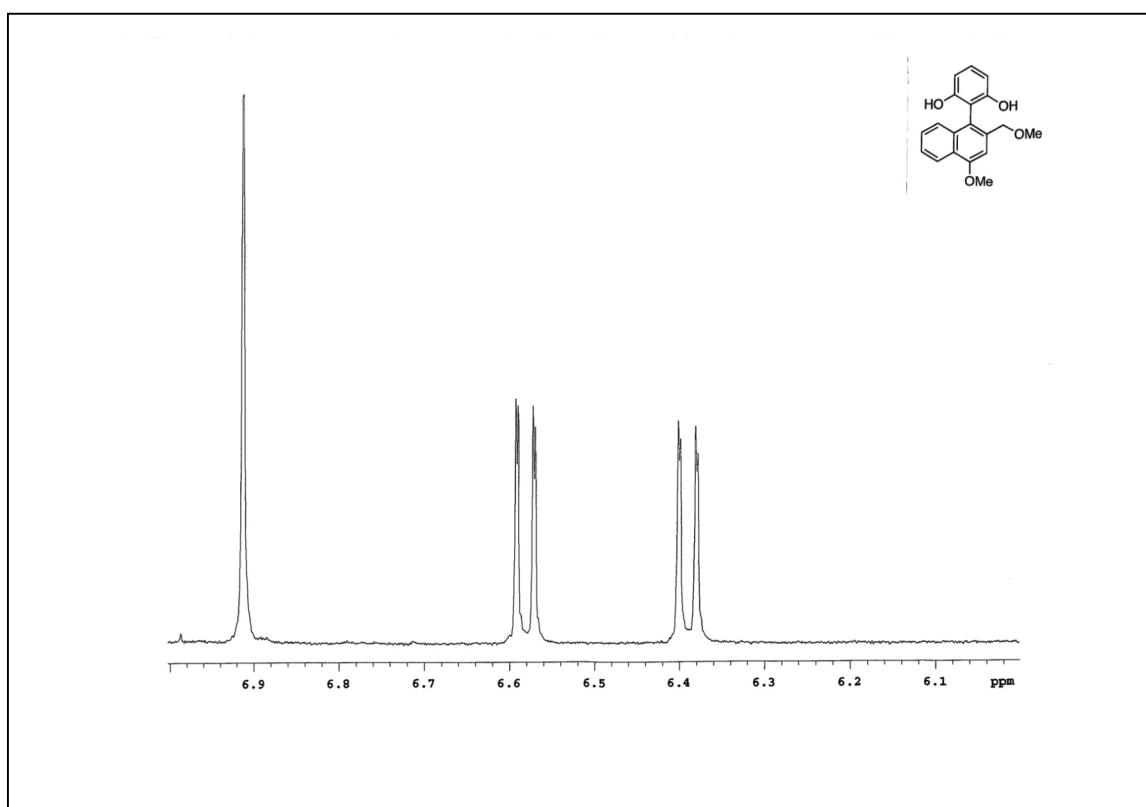
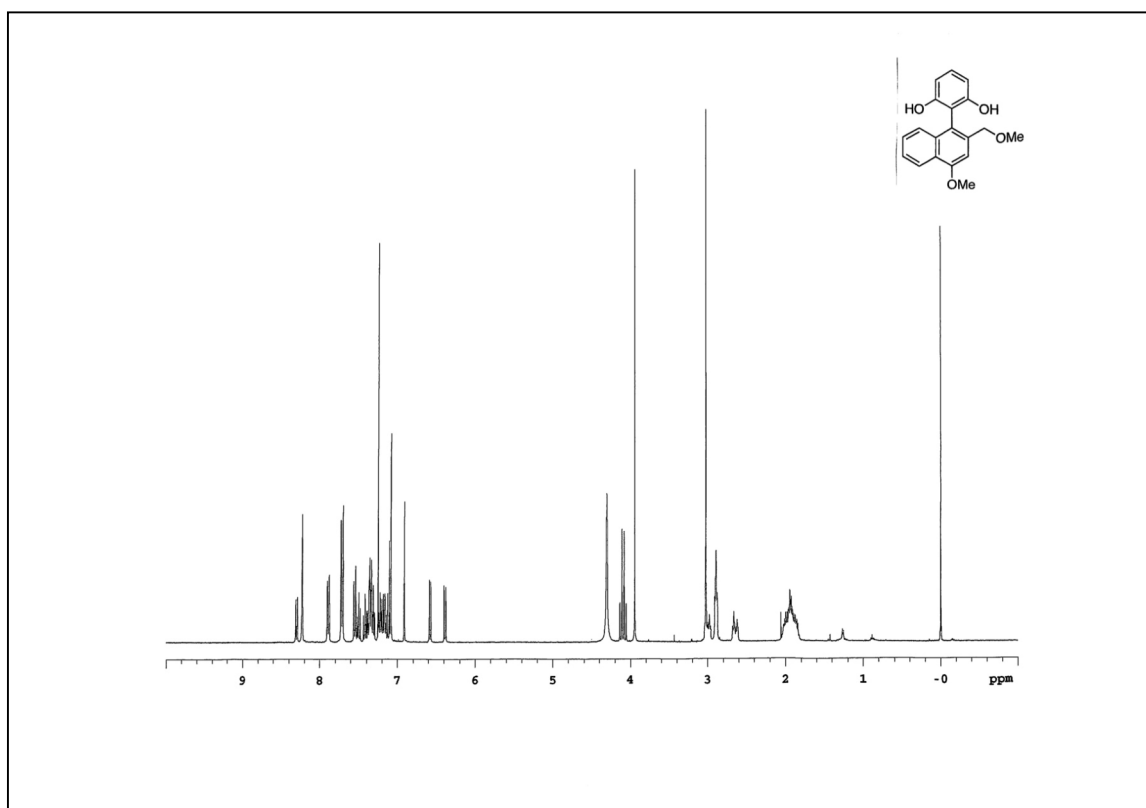
^1H NMR spectrum of the mixture of **3p** and **2j** (X = 9-anthryl).



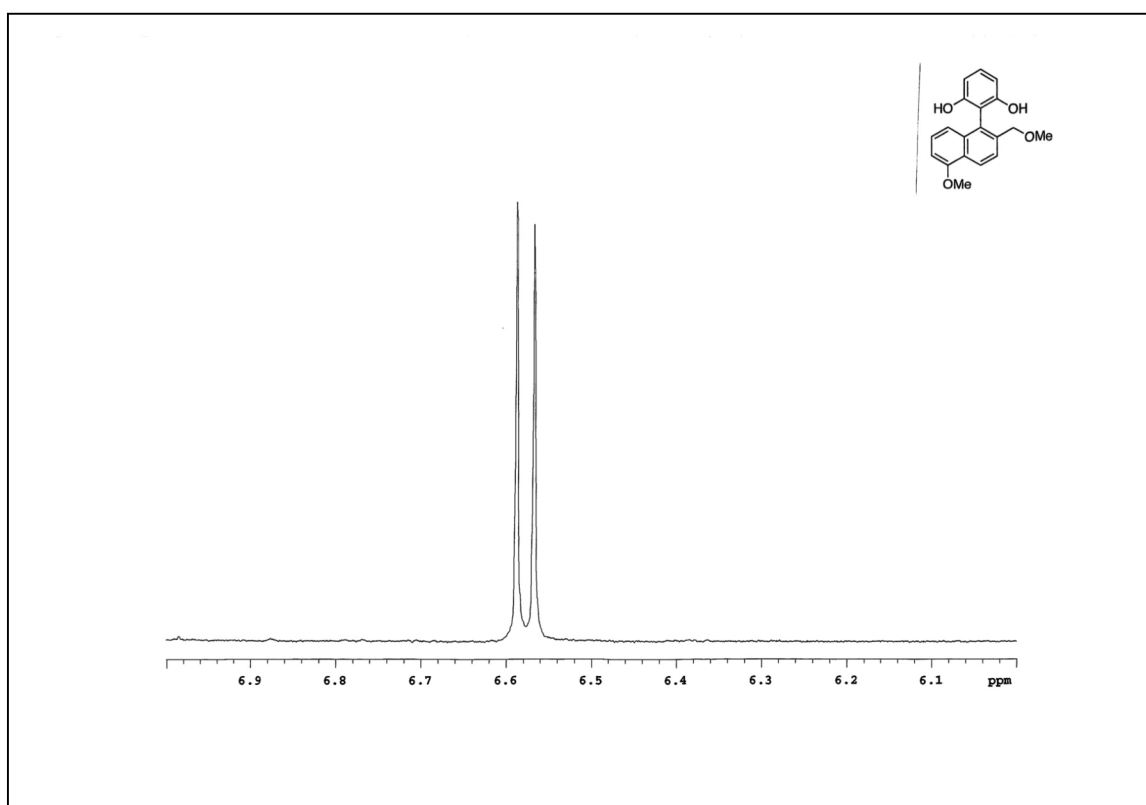
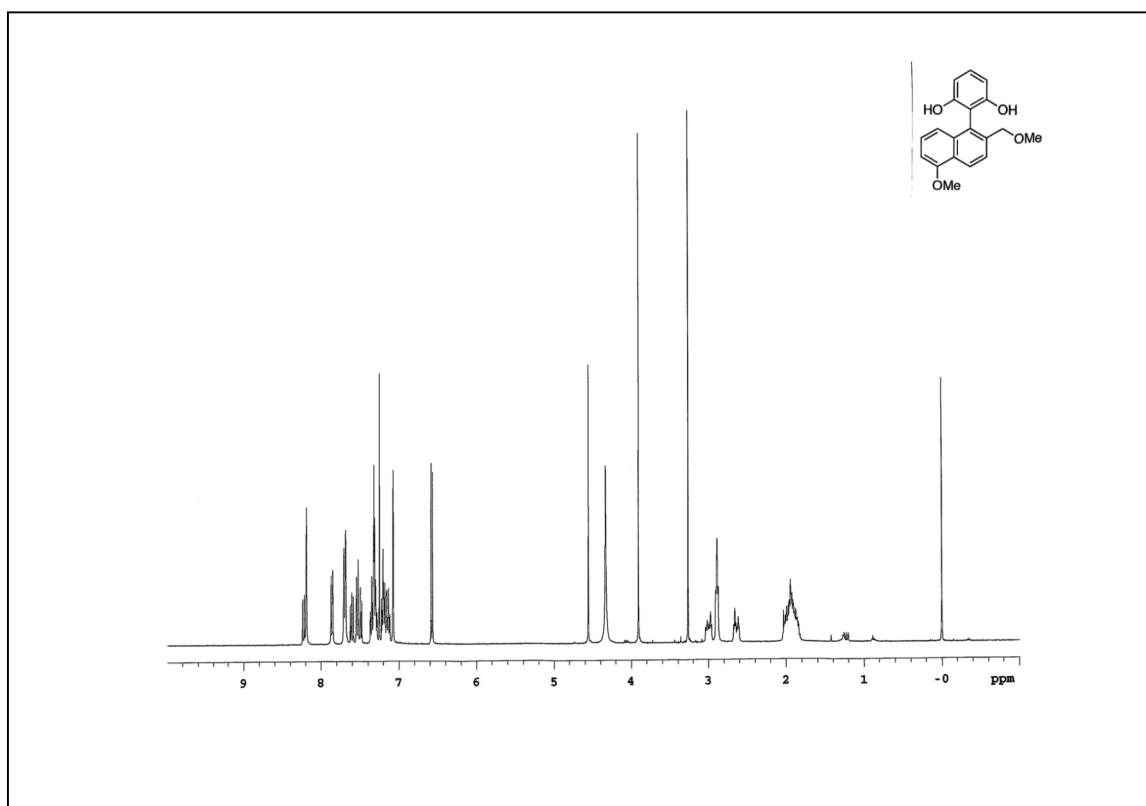
^1H NMR spectrum of the mixture of **3q** and **2j** (X = 9-anthryl).



^1H NMR spectrum of the mixture of **3r** and **2j** (X = 9-anthryl).



^1H NMR spectrum of the mixture of **3s** and **2j** (X = 9-anthryl).



^1H NMR spectrum of the mixture of **3t** and **2j** (X = 9-anthryl).

