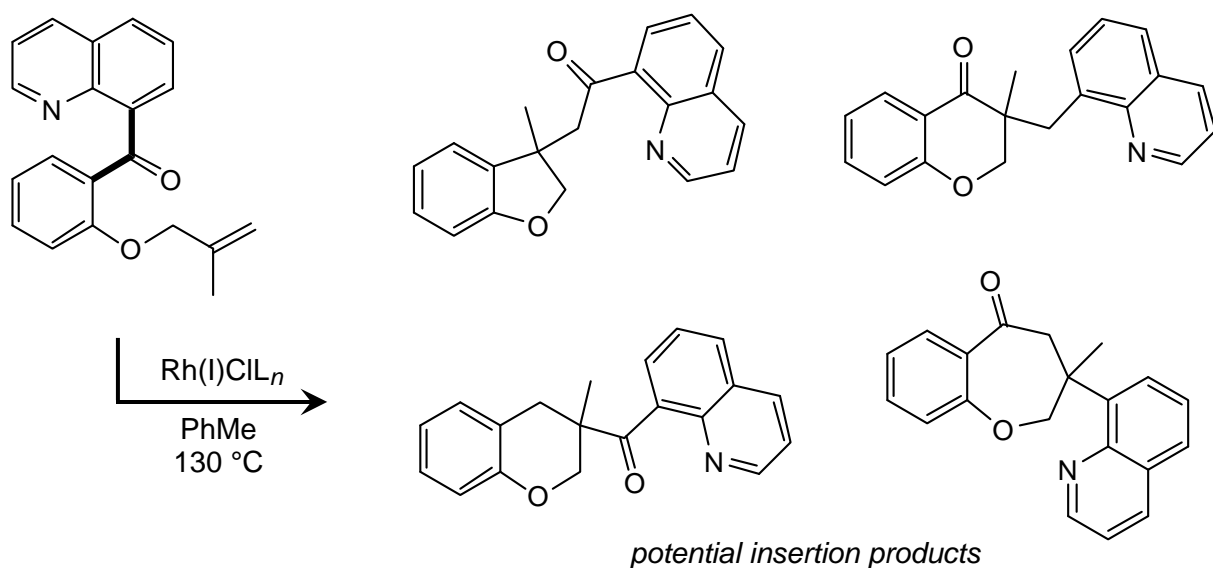


Workshop 4

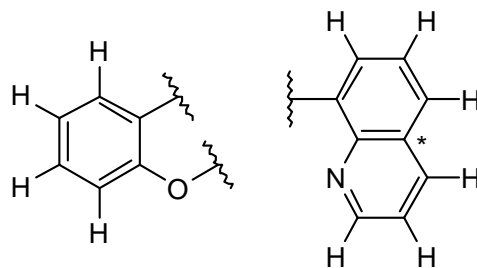
Heteronuclear Correlations

Ashley Dreis (Douglas group) investigated a series of rhodium(I) complexes as catalysts for the intramolecular insertion of an alkene into an arylketone carbon-carbon bond. In the starting material below, there are two arylketone C-C bonds (highlighted in bold), and two directions that the alkene might insert, meaning that Ashley might have found as many as four insertion products from this reaction. Fortunately for her, she isolated only one. In this problem, you will use 2D NMR (as she did) to determine which product she made selectively.



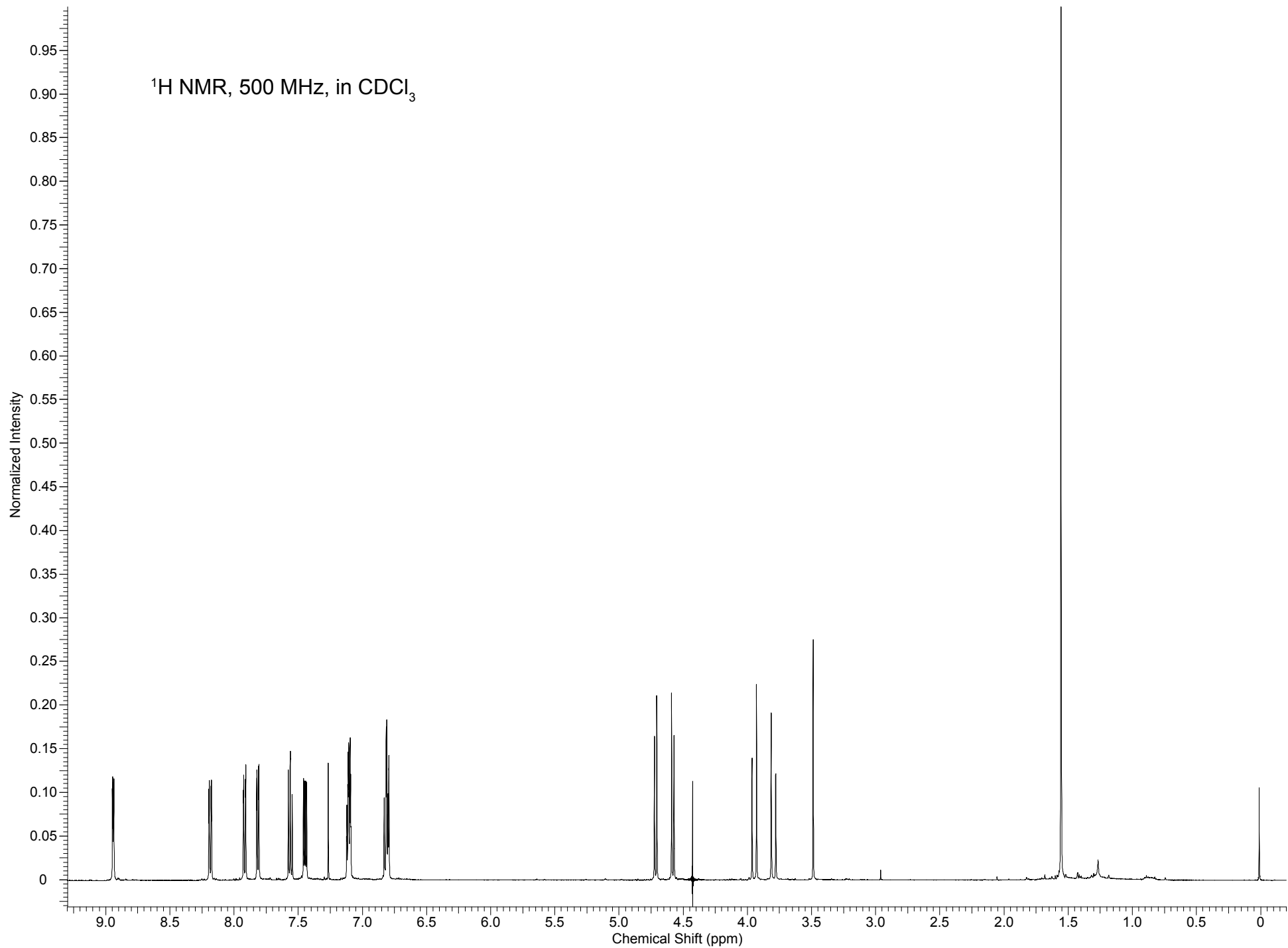
^1H , ^{13}C , ^1H - ^1H COSY, ^1H - ^{13}C HMQC and HMBC spectra of Ashley's product are shown on the following pages.

- a. All of the structures above have a phenyl group and a quinoline group in common, and it will be helpful to analyze this problem if you first roughly assign chemical shifts to some of the protons and carbons of these groups. *Note:* I think the resonance for the asterisked carbon is too weak to be observed by ^{13}C NMR or HMBC.

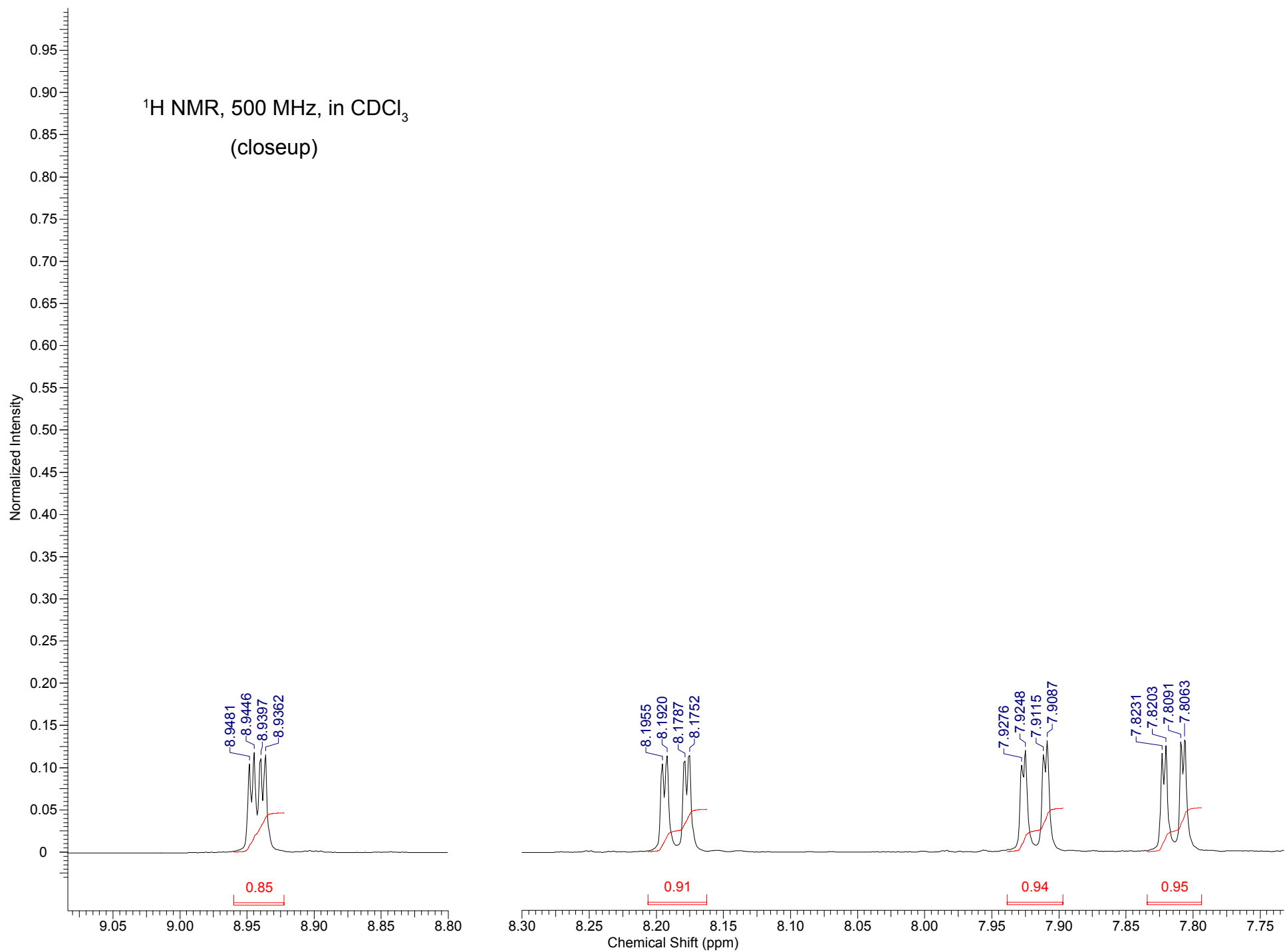


- b. HMBC is a great tool for identifying two- and three-bond C-H correlations that pass through carbons without attached protons. What HMBC correlations do you observe that help you identify the correct product structure? What is the correct structure?

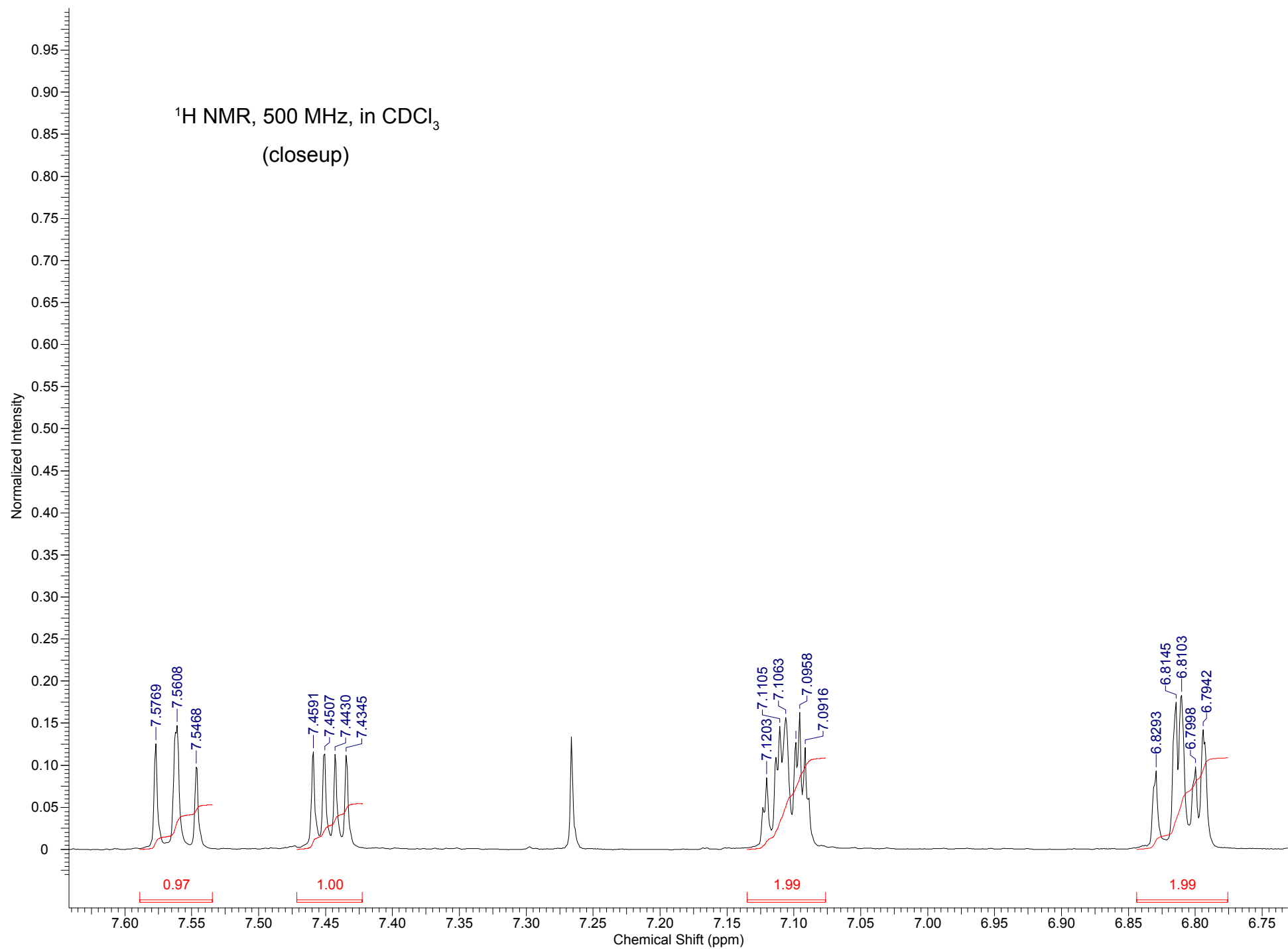
^1H NMR, 500 MHz, in CDCl_3



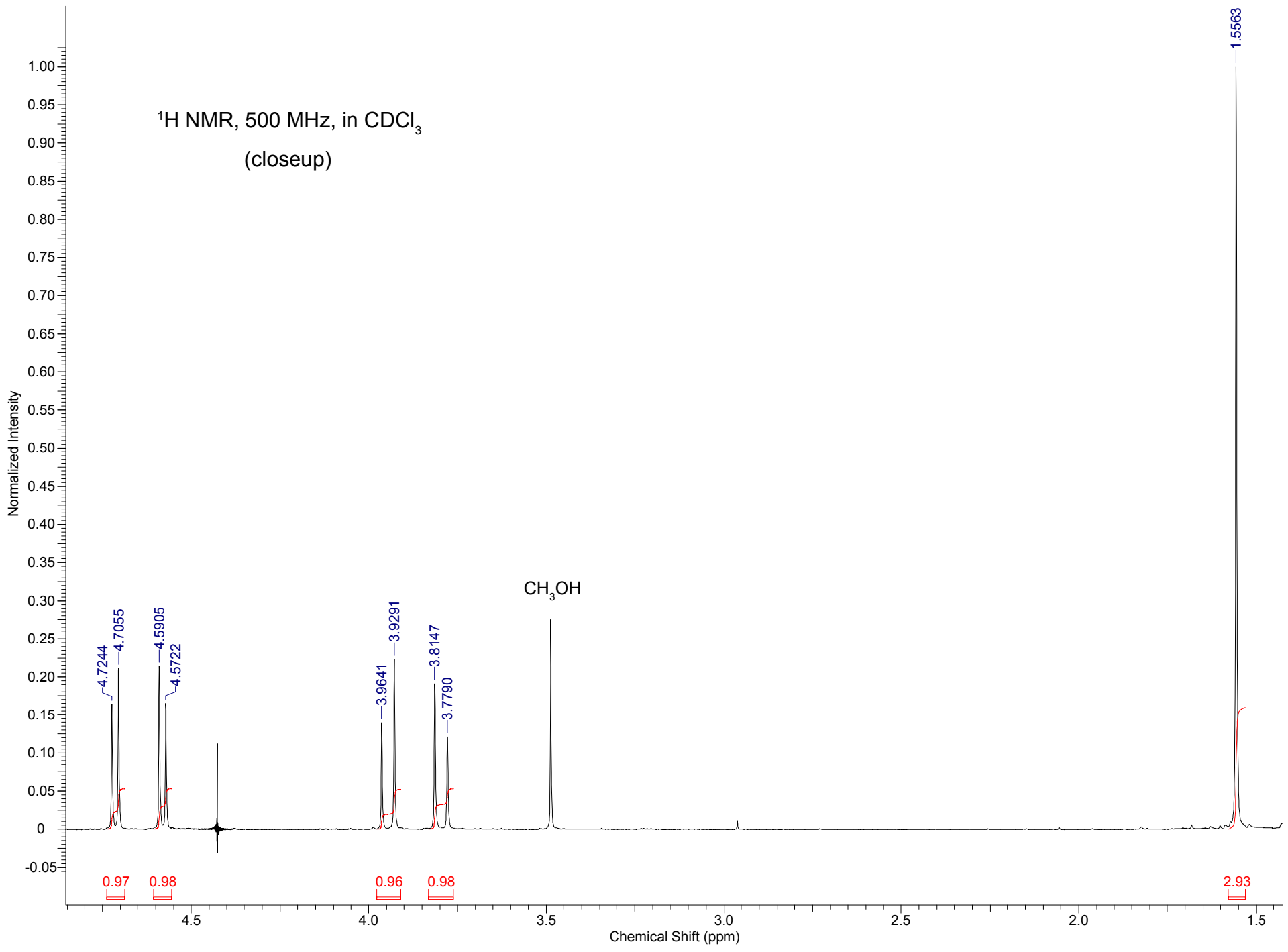
^1H NMR, 500 MHz, in CDCl_3
(closeup)



^1H NMR, 500 MHz, in CDCl_3
(closeup)

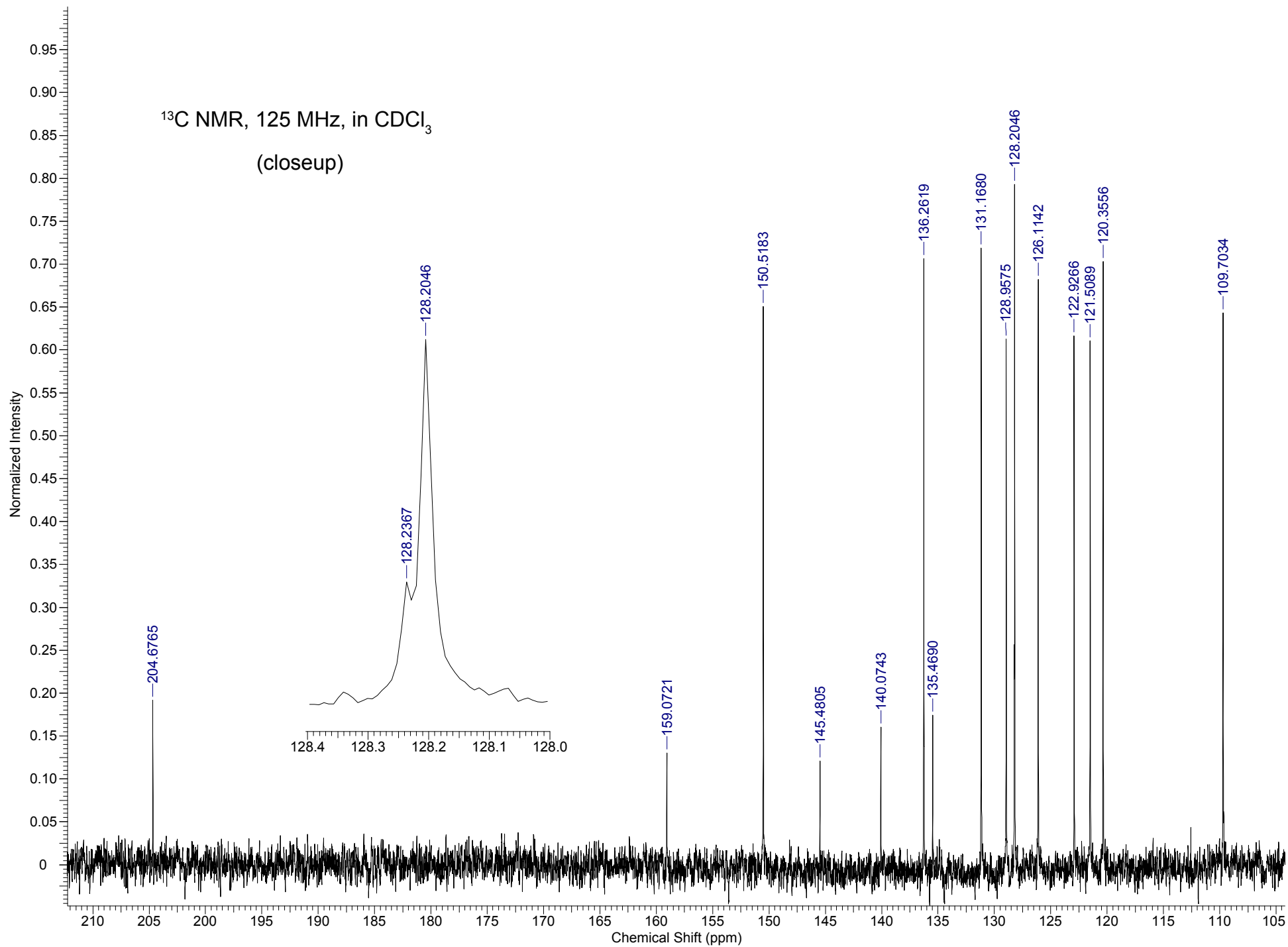


¹H NMR, 500 MHz, in CDCl₃
(closeup)

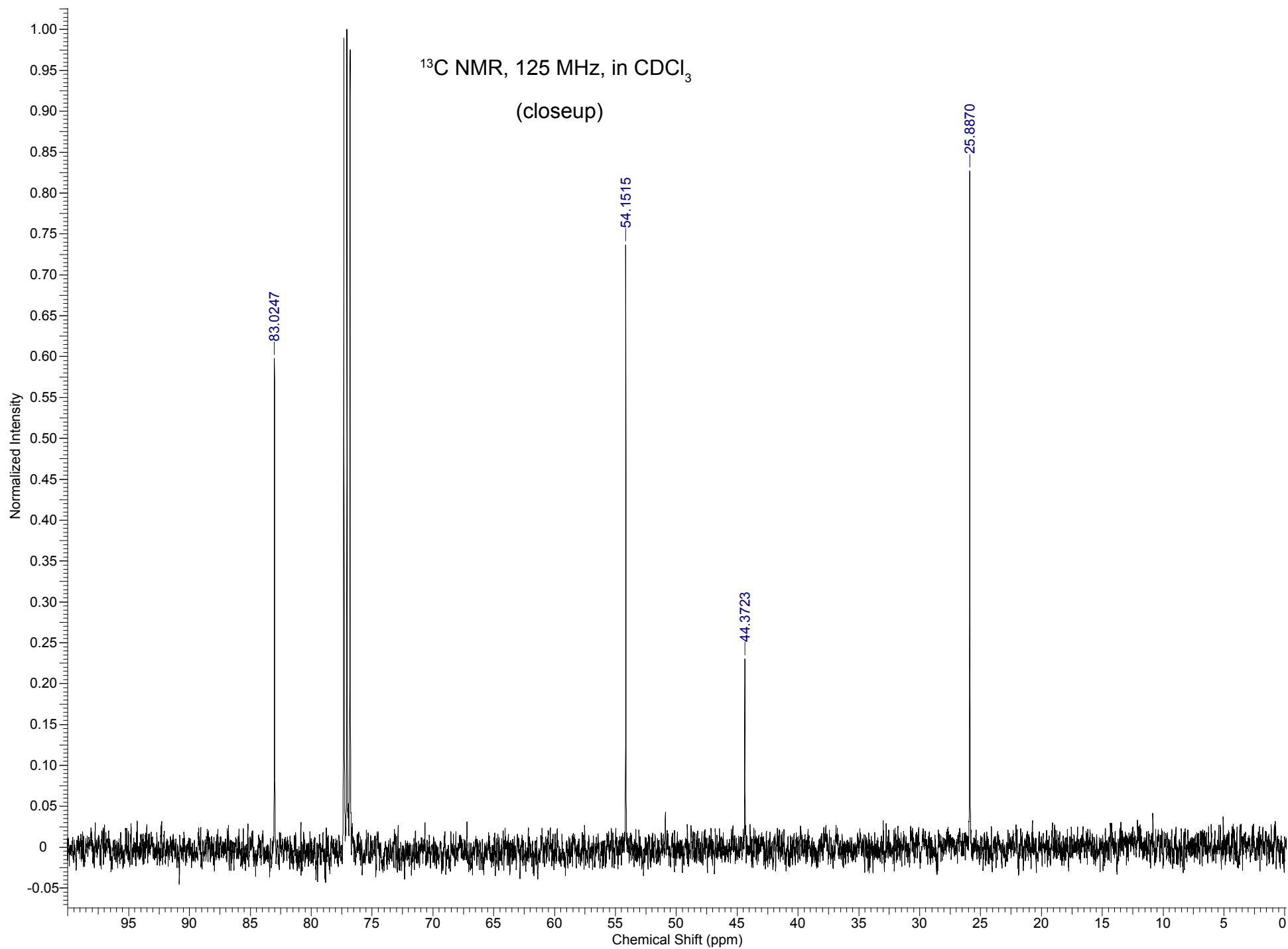


CH₃OH

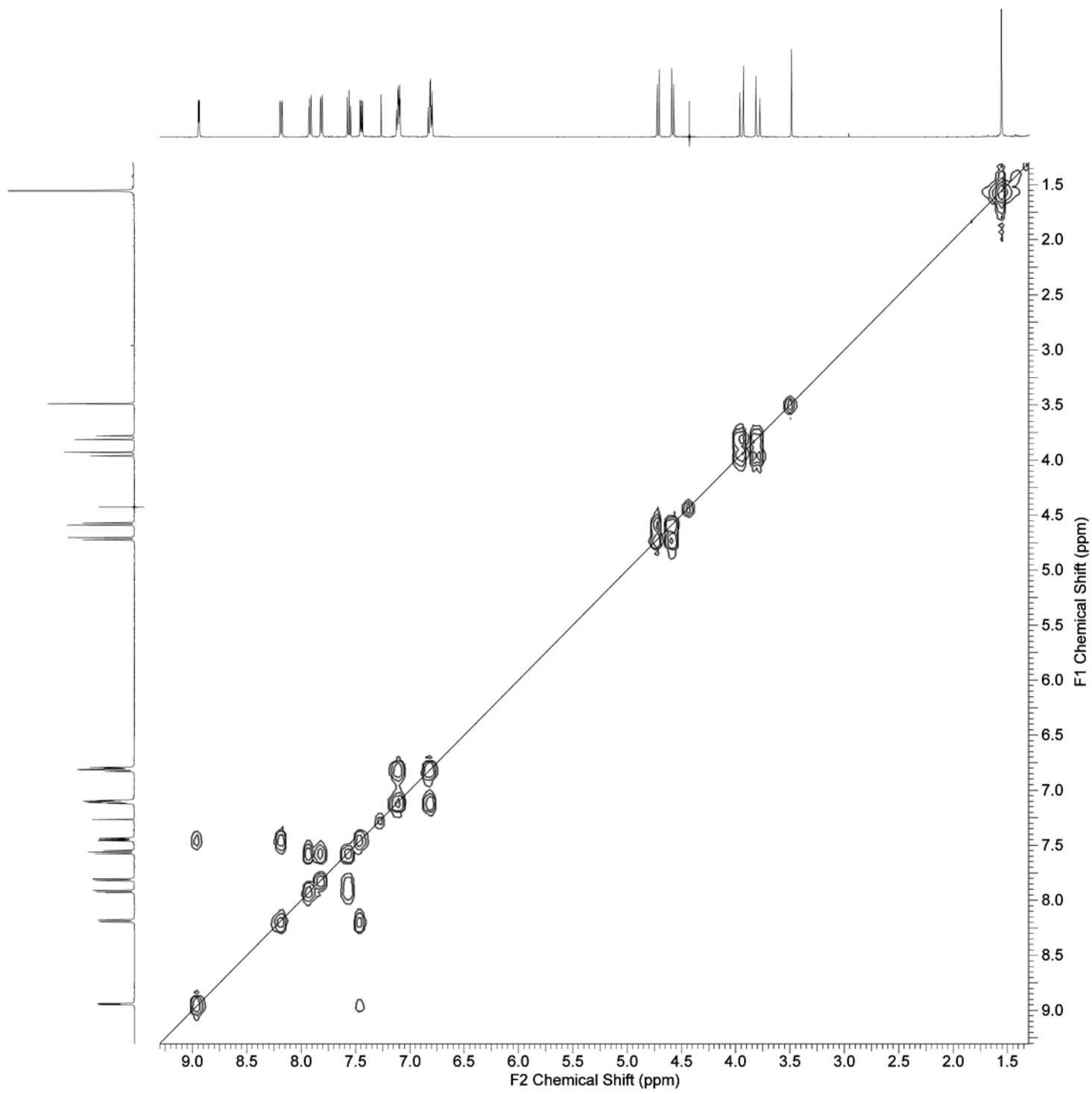
^{13}C NMR, 125 MHz, in CDCl_3
(closeup)



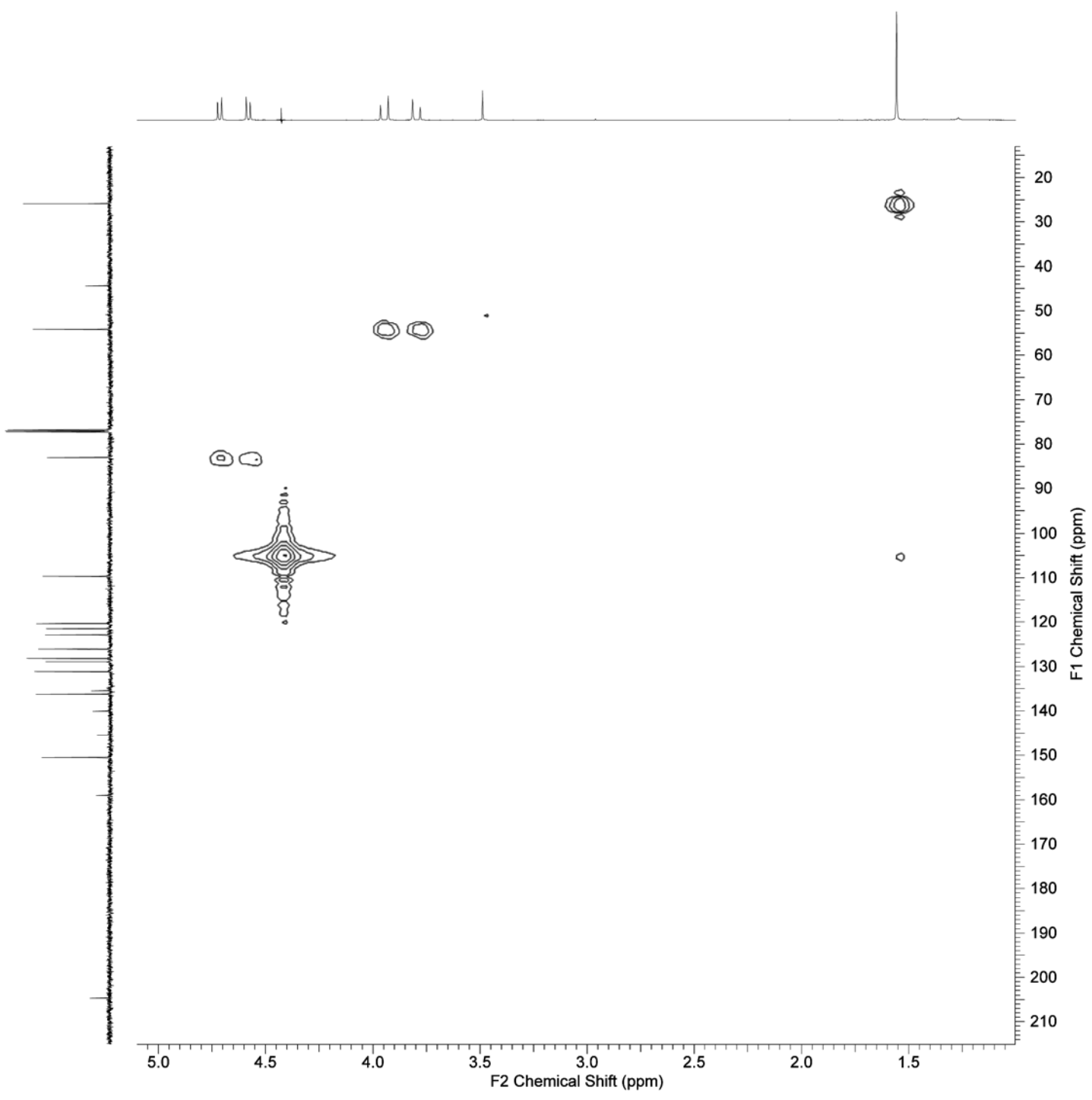
^{13}C NMR, 125 MHz, in CDCl_3
(closeup)



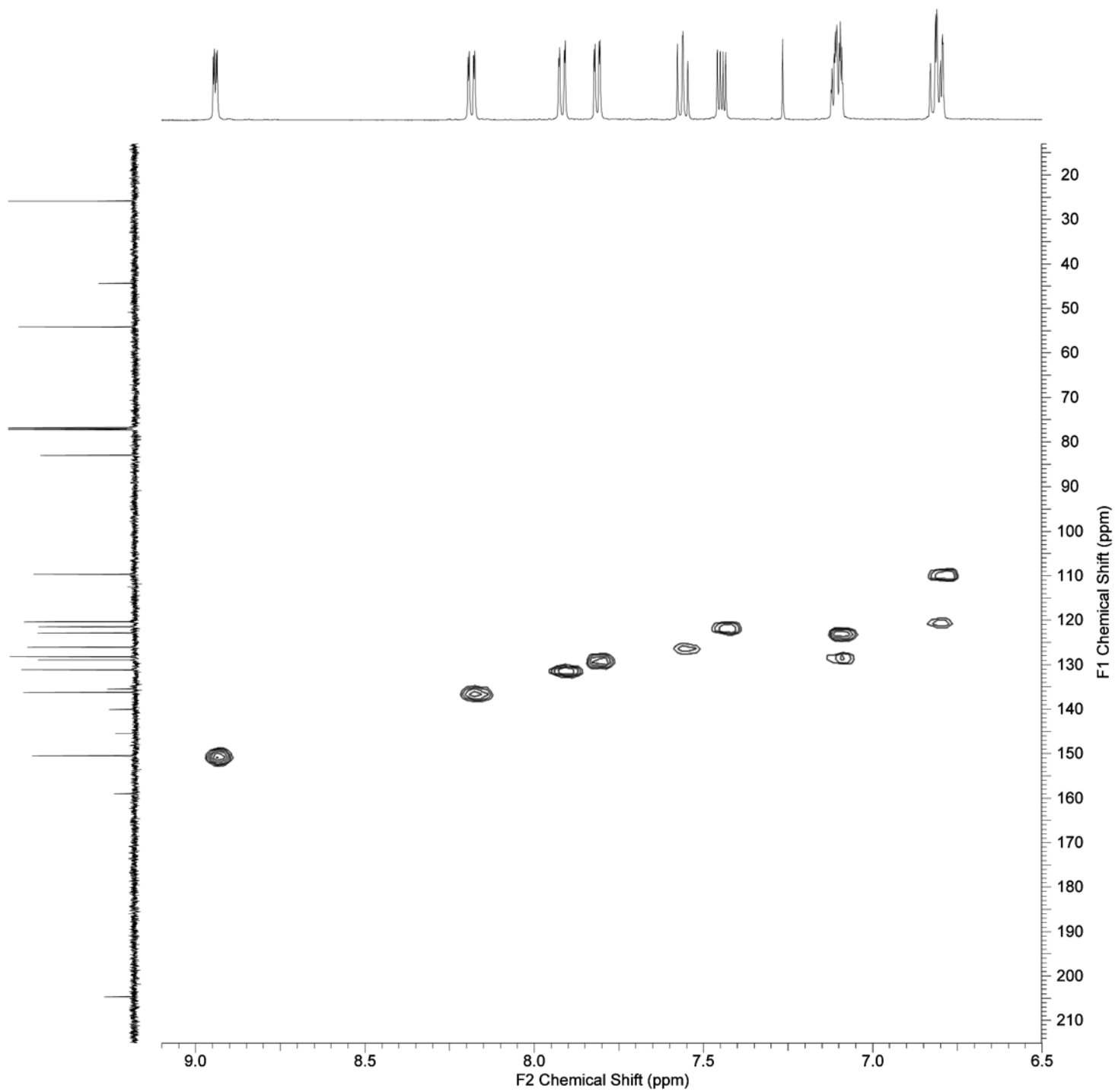
^1H - ^1H COSY, 500 MHz, in CDCl_3



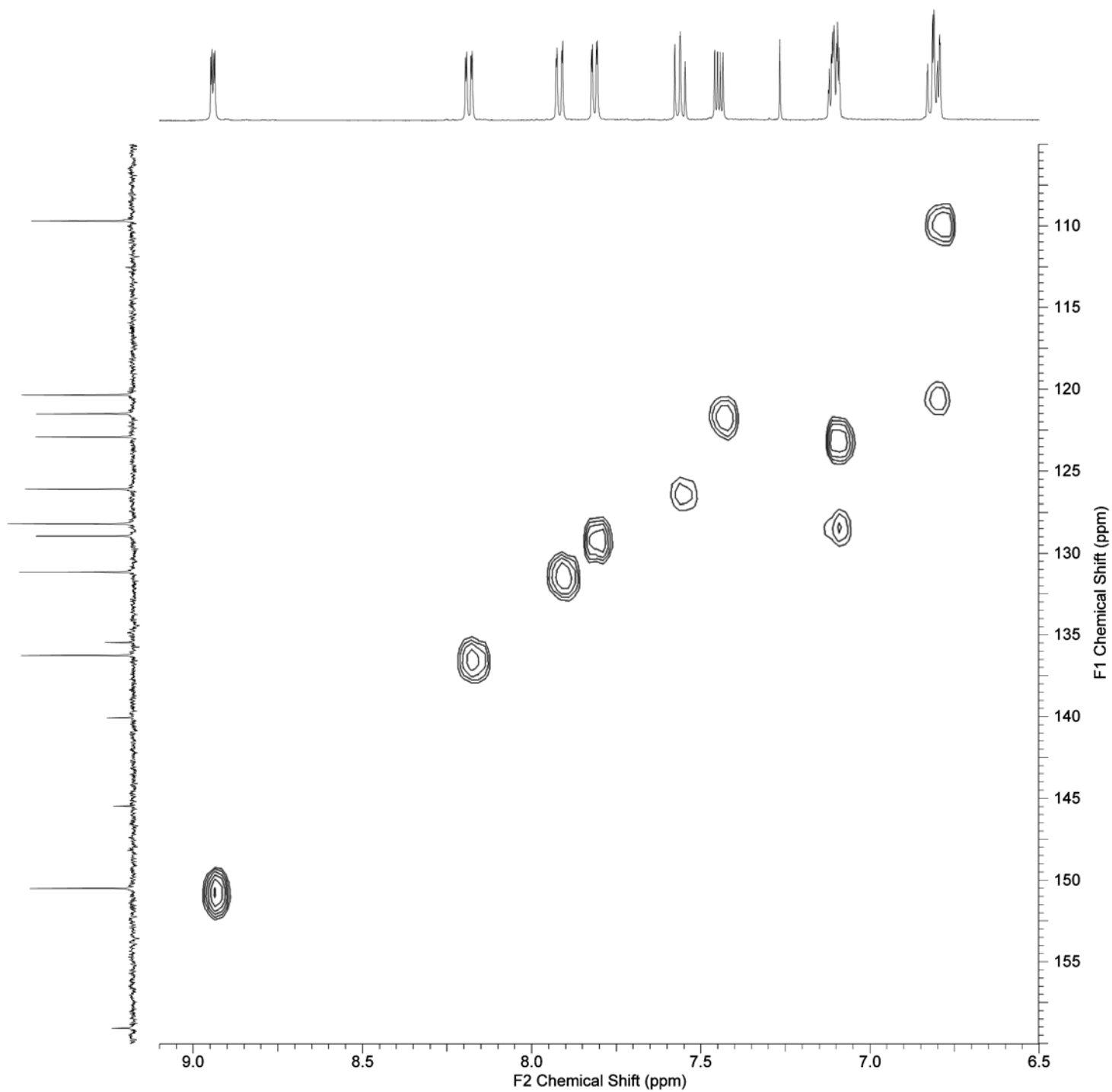
^1H - ^{13}C HMQC, in CDCl_3
(closeup)



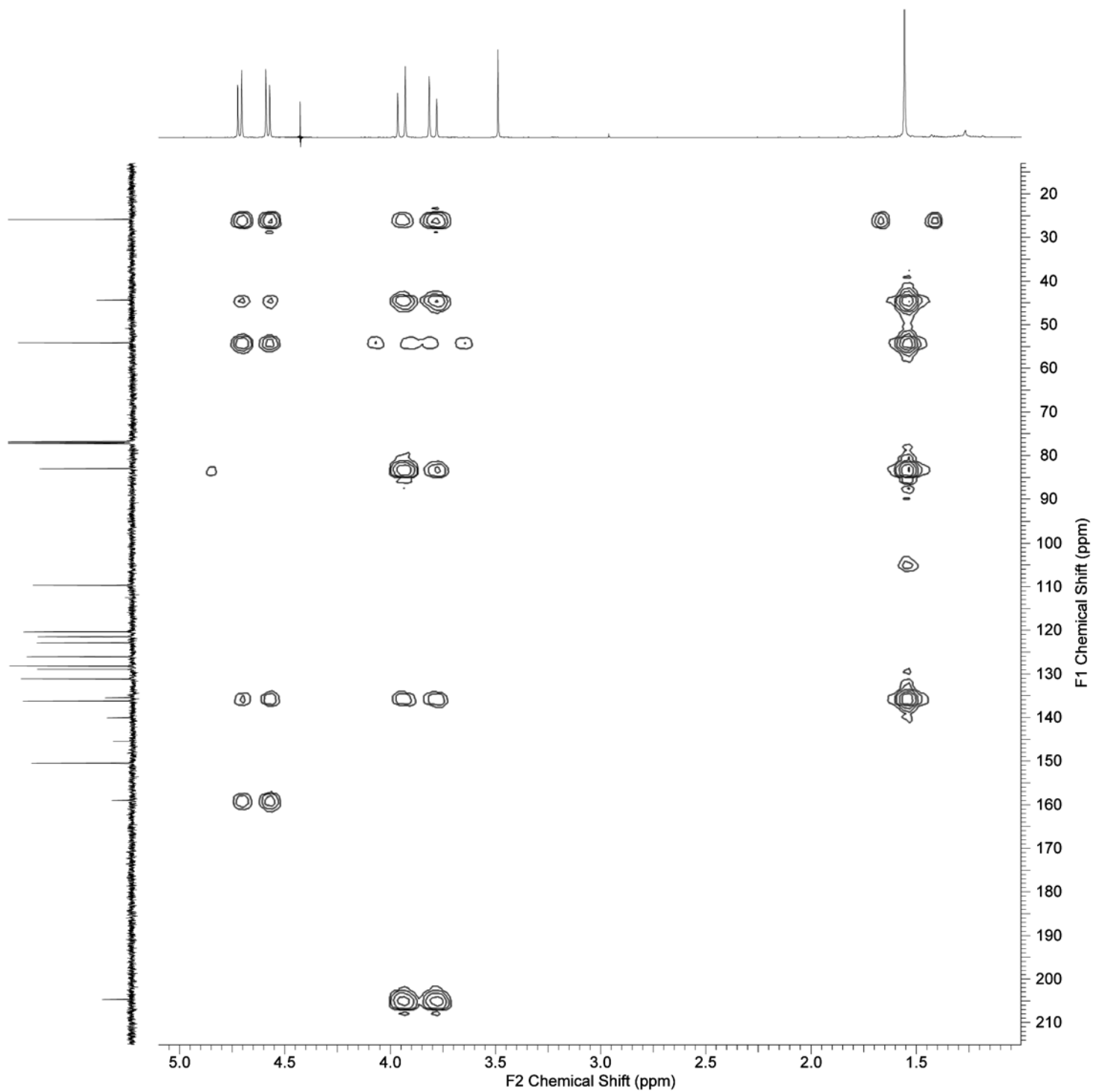
^1H - ^{13}C HMQC, in CDCl_3
(closeup)



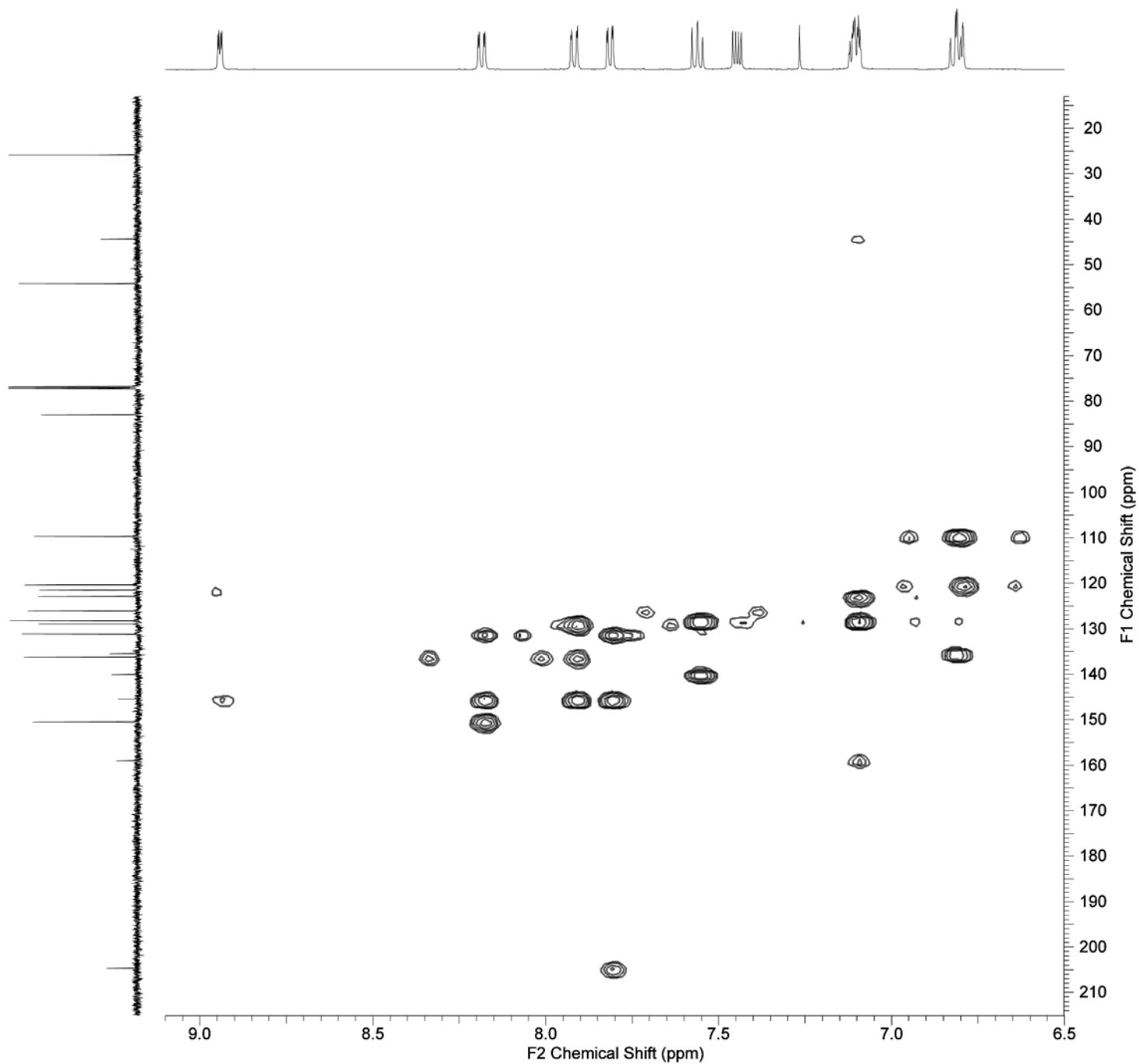
^1H - ^{13}C HMQC, in CDCl_3
(closeup)



^1H - ^{13}C HMBC, in CDCl_3
(closeup)



^1H - ^{13}C HMBC, in CDCl_3
(closeup)



^1H - ^{13}C HMBC, in CDCl_3
(closeup)

