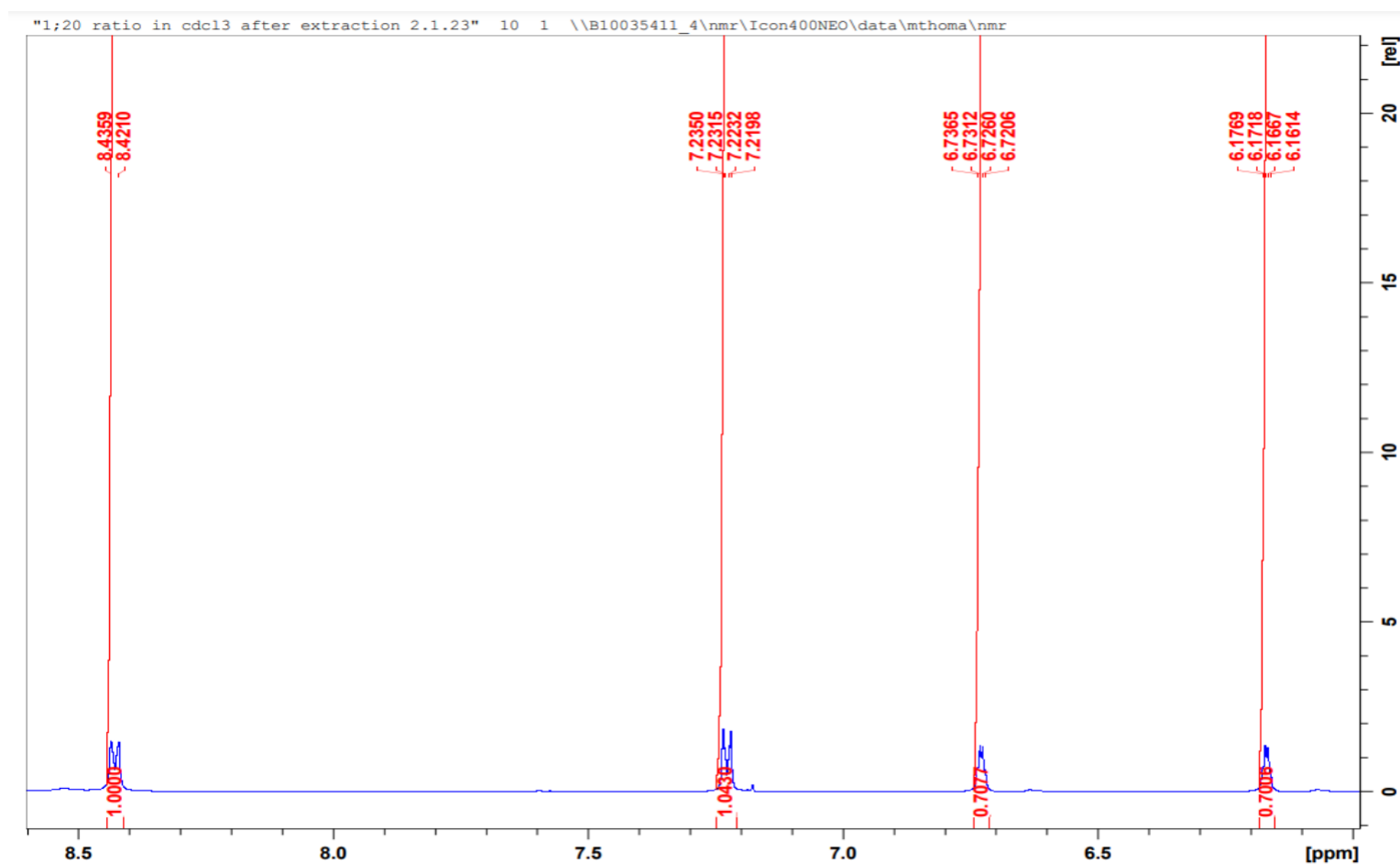


A new, rapid, colorimetric chemodosimeter, 4(pyrrol-1-yl)pyridine, for nitrite detection in aqueous solution

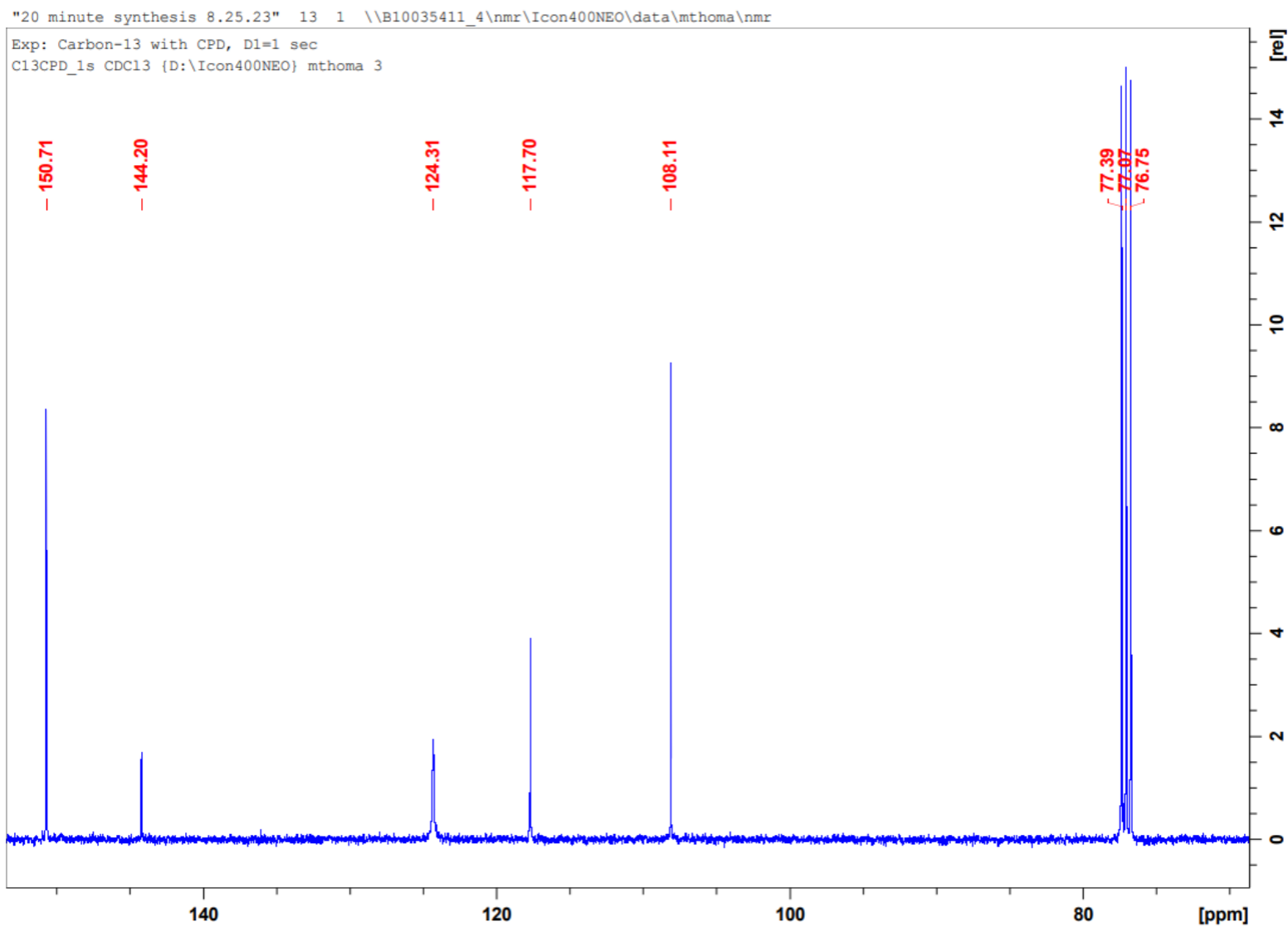
Mallory E. Thomas, Lynn D. Schmitt, Alistair J. Lees

Supplementary Information

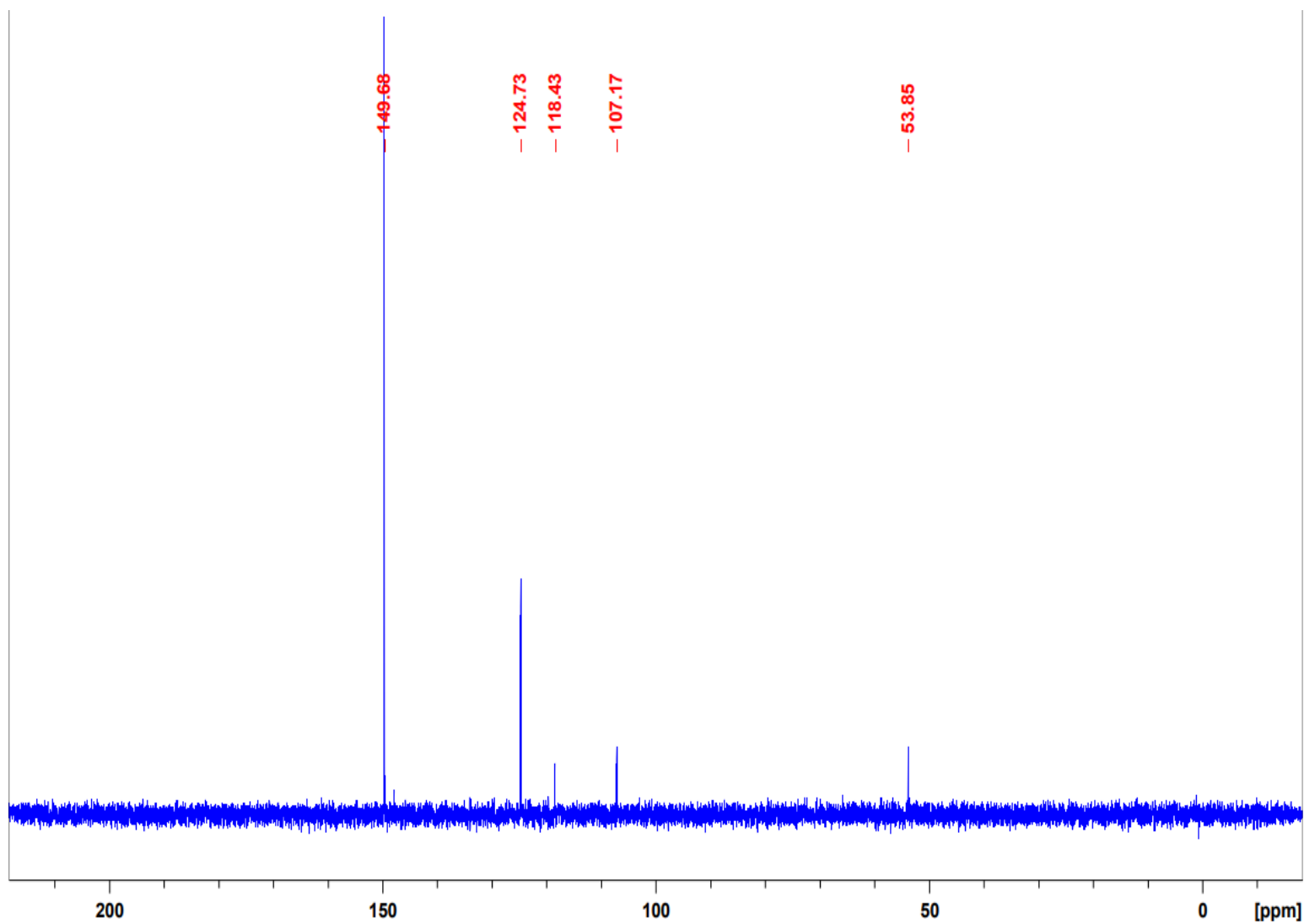
S1: ^1H NMR of dilute (<10% v/v) 4(pyrrol-1-yl)pyridine in CDCl_3 with integrations



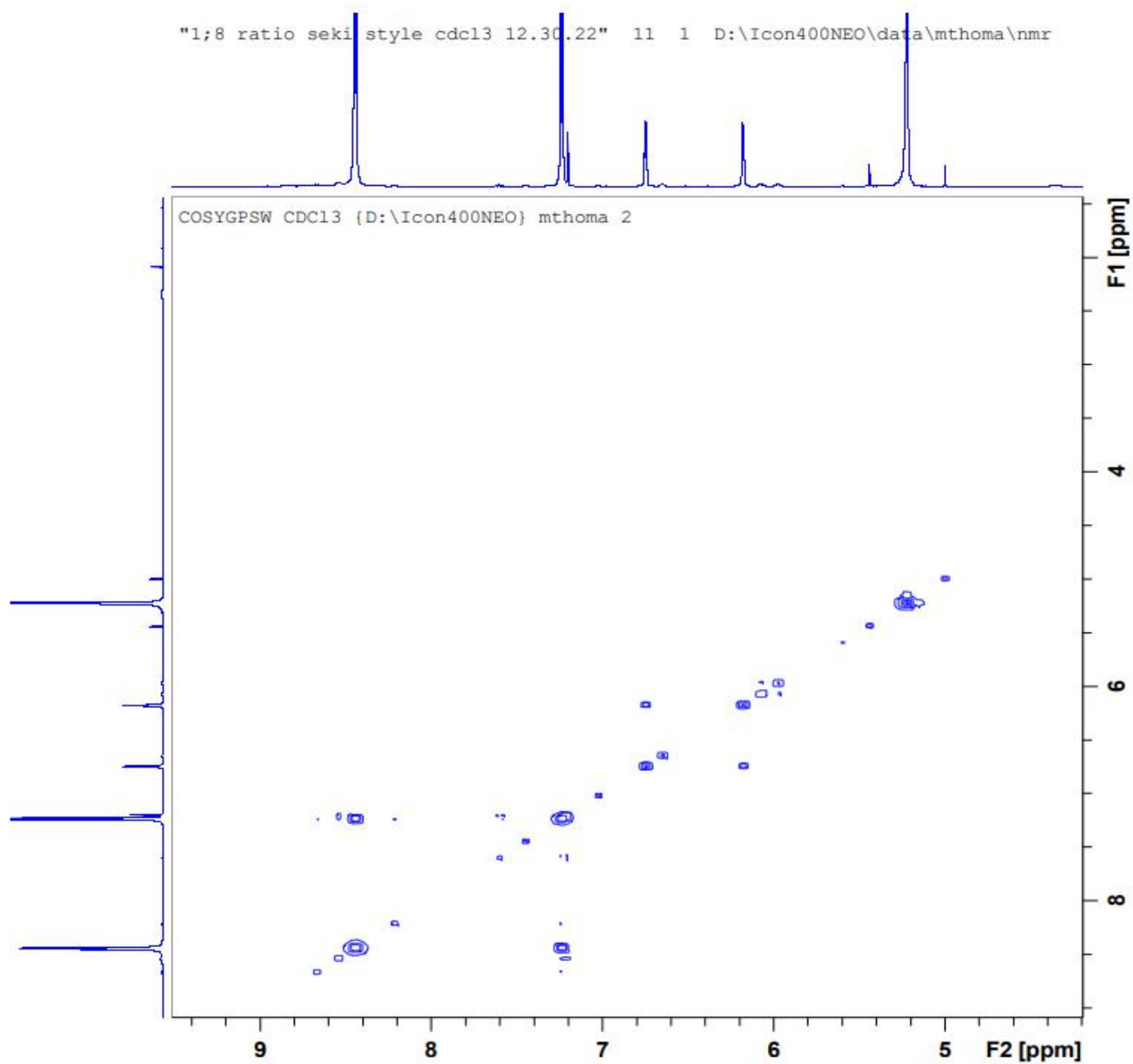
S2: ^{13}C NMR of 4(pyrrol-1-yl)pyridine in CDCl_3 with peak locations from NMR solvent



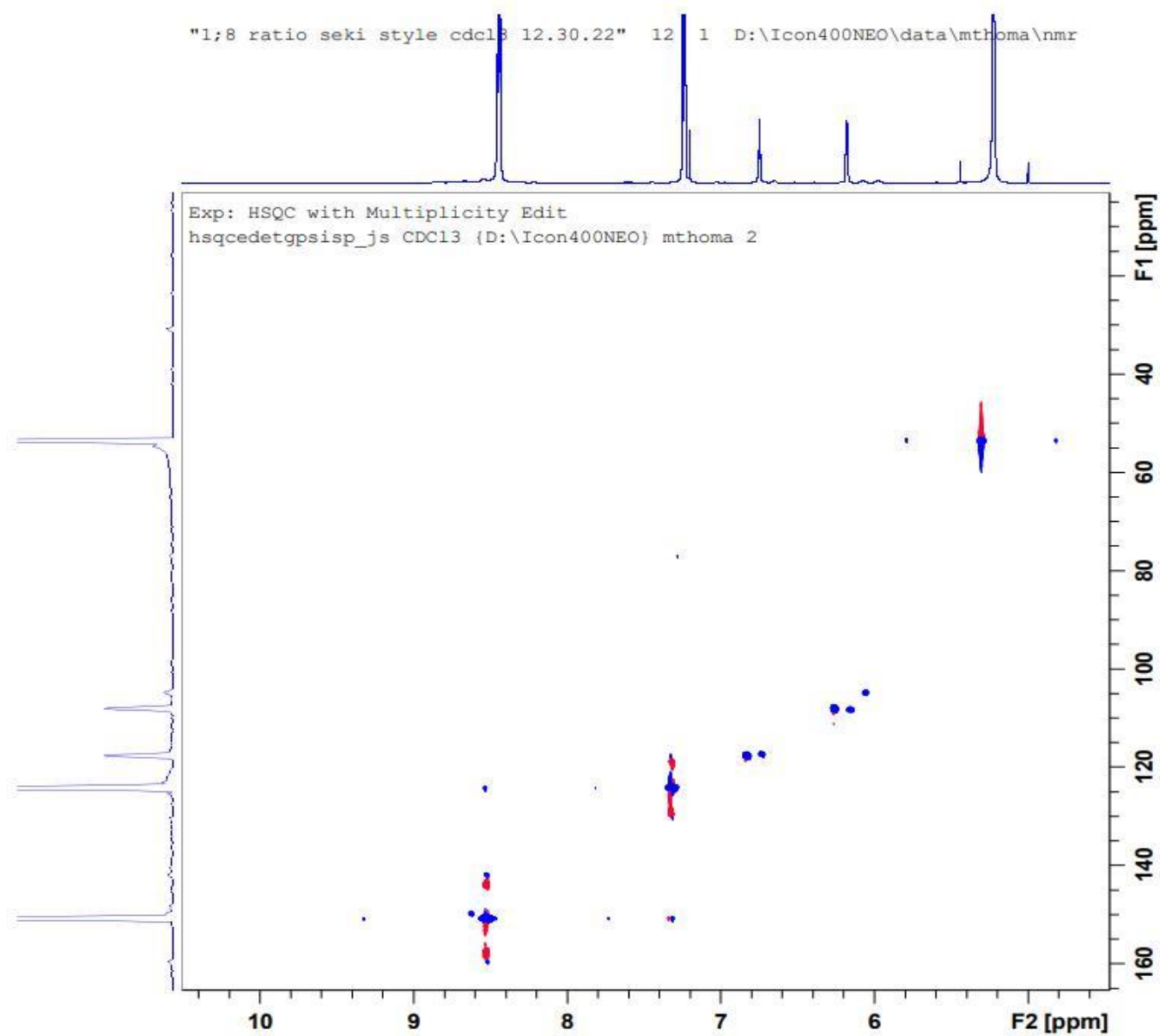
S3: DEPT 90 ^{13}C NMR of 4(pyrrol-1-yl)pyridine in CDCl_3 . Peak observed at 53.85 ppm is indicative of residual dichloromethane following extraction. Quaternary carbons do not appear in the spectrum.



S4: HSQC NMR of dilute (<10% v/v) 4(pyrrol-1-yl)pyridine in CDCl₃. Peak observed at 5.2 ppm is indicative of residual dichloromethane following extraction.

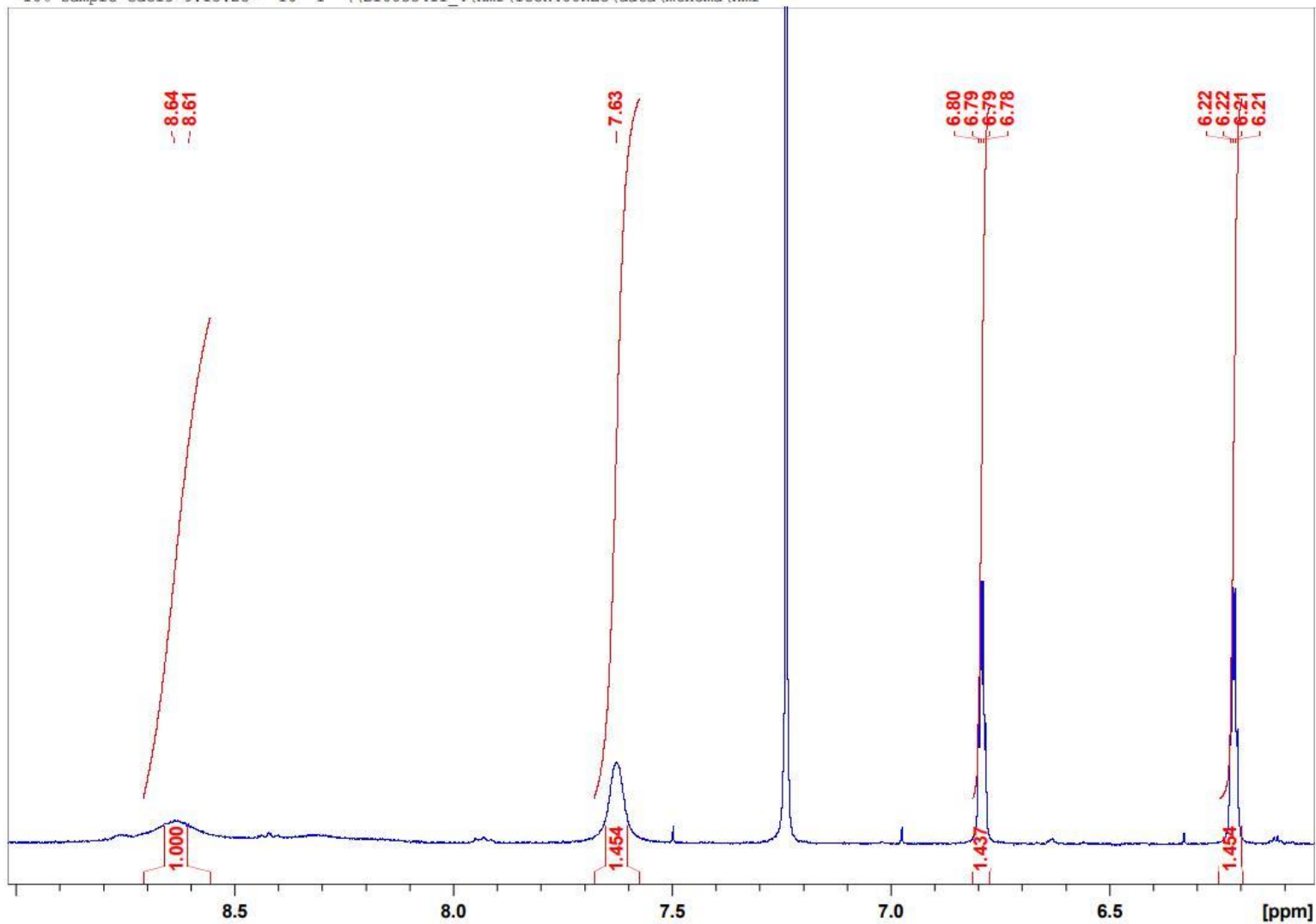


S5: COSY NMR of dilute (<10% v/v) 4(pyrrol-1-yl)pyridine in CDCl₃. Peak observed at 5.2 ppm is indicative of residual dichloromethane following extraction



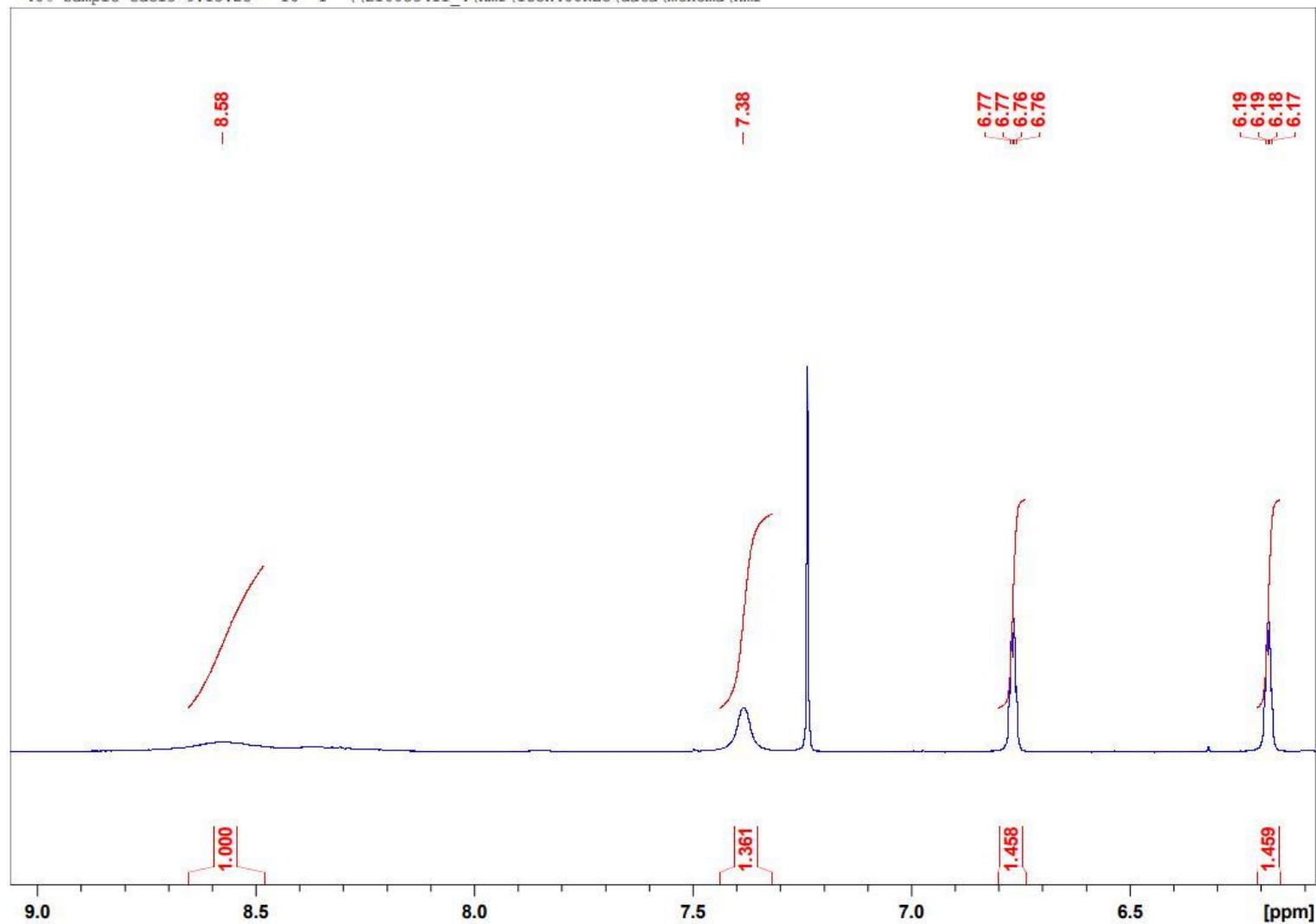
S6: ^1H NMR of 10% (v/v) 4(pyrrol-1-yl)pyridine in CDCl_3 . Solvent peak observed at 7.24ppm.

"10% sample cdc13 9.15.23" 10 1 \\B10035411_4\nmr\Icon400NEO\data\mthoma\nmr

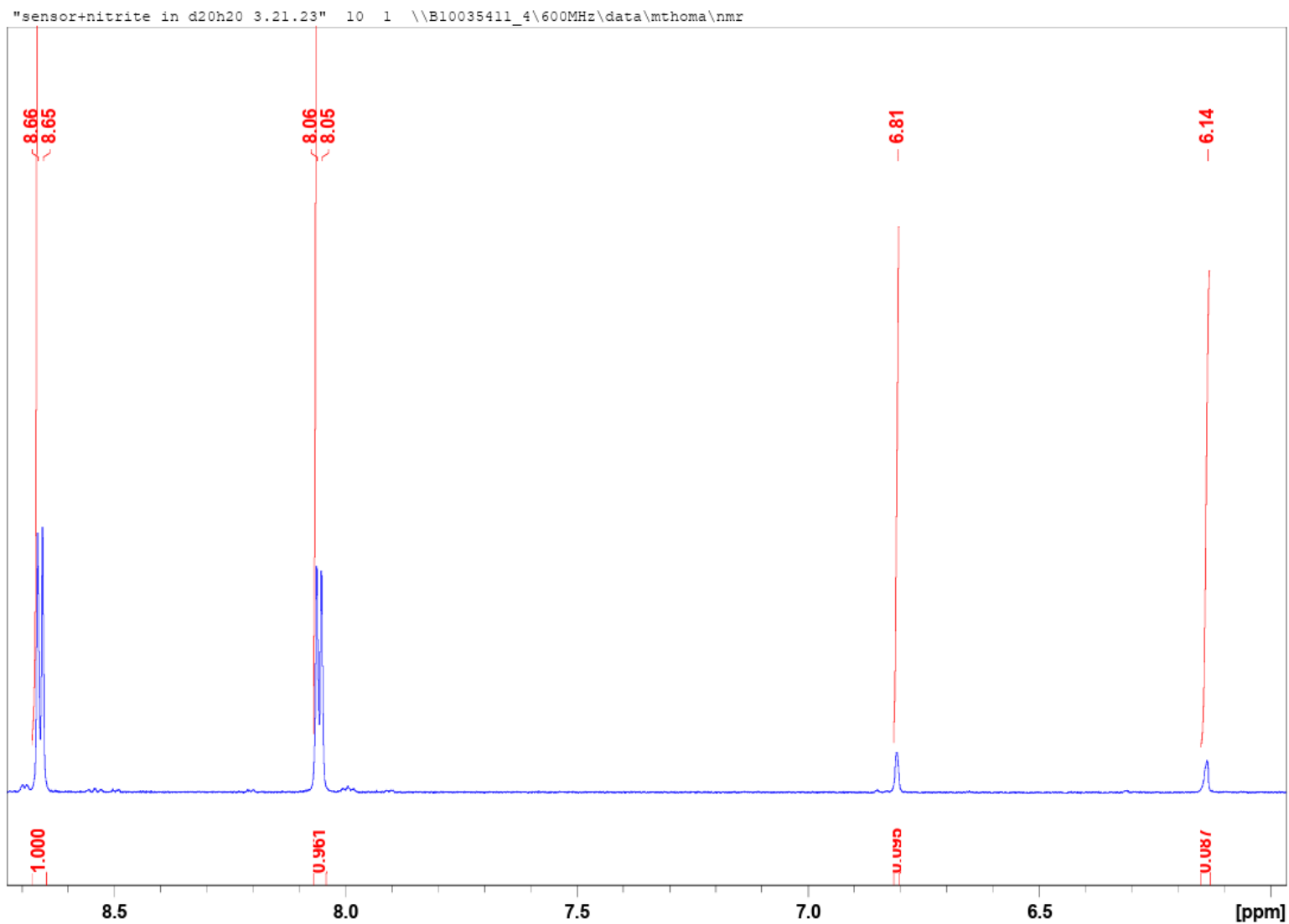


S7: ^1H NMR of 40% (v/v) 4(pyrrol-1-yl)pyridine in CDCl_3 . Solvent peak observed at 7.24ppm.

"40% sample cdc13 9.15.23" 10 1 \\B10035411_4\nmr\Icon400NEO\data\mthoma\nmr



S8: ^1H NMR of dilute 4(pyrrol-1-yl)pyridine and nitrite final product in $\text{D}_2\text{O}/\text{H}_2\text{O}$. Solvent peak observed at 4.80 ppm.



S9: COSY NMR for dilute 4(pyrrol-1-yl)pyridine and nitrite final product in D₂O/H₂O. Solvent peak appearing at 4.80 ppm.

