

Supporting information for

**Facile Synthesis and Characterization of a Bromine-Substituted
(Chloromethyl)pyridine Precursor Towards the Immobilization
of Biomimetic Metal Ion Chelates on Functionalized Carbons**

Troy T. Handlovic ¹, Tyler Moreira ¹, Anoshia Khan ¹, Haroon Saeed ¹, Yousuf Khan ¹,
Mohammed R. Elshaer ¹, and Justin A. Bogart ^{1,*}

- 1 Department of Chemistry, Biochemistry and Physics, Becton College of Arts and Sciences, Fairleigh Dickinson University, Madison, NJ 07940, USA;

TABLE OF CONTENTS

NMR SPECTRA OF REACTION MIXTURES AND ISOLATED COMPOUNDS	3
MASS SPECTRA OF REACTION MIXTURES AND ISOLATED COMPOUNDS	10
FT-IR SPECTRA OF ISOLATED PRODUCTS	12

Table of Figures

FIGURE S1. OVERLAY OF THE ¹³ C-NMR SPECTRA OF (A) OIL MIXTURE WITH SOLID, (B) PURE OIL, AND (C) PURE 2,6-DIBROMOPYRIDINE STARTING MATERIAL IN CDCl ₃	3
FIGURE S2. OVERLAY OF THE ¹³ C-NMR SPECTRA FOR THE PRODUCT MIXTURE FROM THE REACTION OF 2-BROMO-6-HYDROXYMETHYLPYRIDINE WITH CYANURIC CHLORIDE•DMF IN DCM AT R.T (TOP) AND SOCl ₂ AT 40 °C (BOTTOM) IN CDCl ₃	3
FIGURE S3. OVERLAY OF THE AROMATIC REGIONS OF THE ¹ H-NMR SPECTRA FOR THE PRODUCT MIXTURES FROM THE REACTION OF 2-BROMO-6-HYDROXYMETHYLPYRIDINE WITH SOCl ₂ (A) NEAT AT 40 °C, (B) NEAT AT R.T., (C) NEAT AT 0 °C, (D) IN DCM AT 0 °C IN CDCl ₃	4
FIGURE S4. ¹ H-NMR SPECTRUM OF THE REACTION MIXTURE CONTAINING 2-BROMO-6-HYDROXYMETHYLPYRIDINE AND 2,6-DIBROMOPYRIDINE IN CDCl ₃	5
FIGURE S5. ¹³ C-NMR SPECTRUM OF THE REACTION MIXTURE CONTAINING 2-BROMO-6-HYDROXYMETHYLPYRIDINE AND 2,6-DIBROMOPYRIDINE IN CDCl ₃	5
FIGURE S6. ¹ H-NMR SPECTRUM OF 2-BROMO-6-HYDROXYMETHYLPYRIDINE IN CDCl ₃	6
FIGURE S7. ¹³ C-NMR SPECTRUM OF 2-BROMO-6-HYDROXYMETHYLPYRIDINE IN CDCl ₃	6
FIGURE S8. ¹ H-NMR SPECTRUM OF 2,6-DIBROMOPYRIDINE IN CDCl ₃	7
FIGURE S9. ¹³ C-NMR SPECTRUM OF 2,6-DIBROMOPYRIDINE IN CDCl ₃	7
FIGURE S10. ¹ H-NMR SPECTRUM OF THE REACTION MIXTURE CONTAINING 2-BROMO-6-CHLOROMETHYLPYRIDINE AND 2-CHLORO-6-CHLOROMETHYLPYRIDINE IN CDCl ₃	8
FIGURE S11. ¹³ C-NMR SPECTRUM OF THE REACTION MIXTURE CONTAINING 2-BROMO-6-CHLOROMETHYLPYRIDINE AND 2-CHLORO-6-CHLOROMETHYLPYRIDINE IN CDCl ₃	8
FIGURE S12. ¹ H-NMR SPECTRUM OF 2-BROMO-6-CHLOROMETHYLPYRIDINE IN CDCl ₃	9
FIGURE S13. ¹³ C-NMR SPECTRUM OF 2-BROMO-6-CHLOROMETHYLPYRIDINE IN CDCl ₃	9
FIGURE S14. MASS SPECTRUM OF THE REACTION MIXTURE CONTAINING 2-BROMO-6-HYDROXYMETHYLPYRIDINE AND 2,6-DIBROMOPYRIDINE.	10
FIGURE S15. MASS SPECTRUM OF 2-BROMO-6-HYDROXYMETHYLPYRIDINE.....	10
FIGURE S16. MASS SPECTRUM OF THE REACTION MIXTURE CONTAINING 2-BROMO-6-CHLOROMETHYLPYRIDINE AND 2-CHLORO-6-CHLOROMETHYLPYRIDINE.	11
FIGURE S17. MASS SPECTRUM OF 2-BROMO-6-CHLOROMETHYLPYRIDINE.	11
FIGURE S18. OVERLAY OF THE FT-IR SPECTRA OF 2-BROMO-6-HYDROXYMETHYLPYRIDINE (RED) AND THE PRODUCT OF THE REACTION WITH CYANURIC CHLORIDE (BLUE).	12

NMR Spectra of Reaction Mixtures and Isolated Compounds

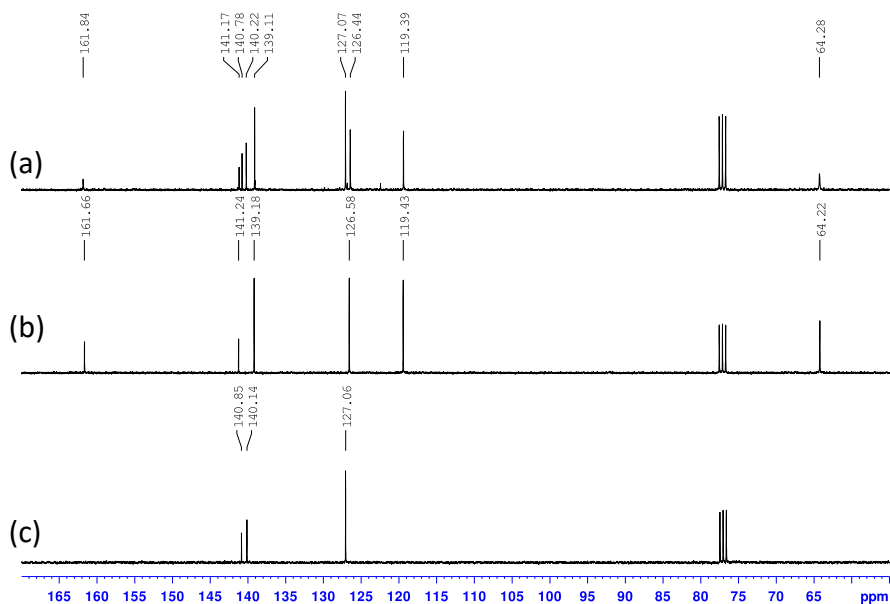


Figure S1. Overlay of the ^{13}C -NMR spectra of (a) oil mixture with solid, (b) pure oil, and (c) pure 2,6-dibromopyridine starting material in CDCl_3 .

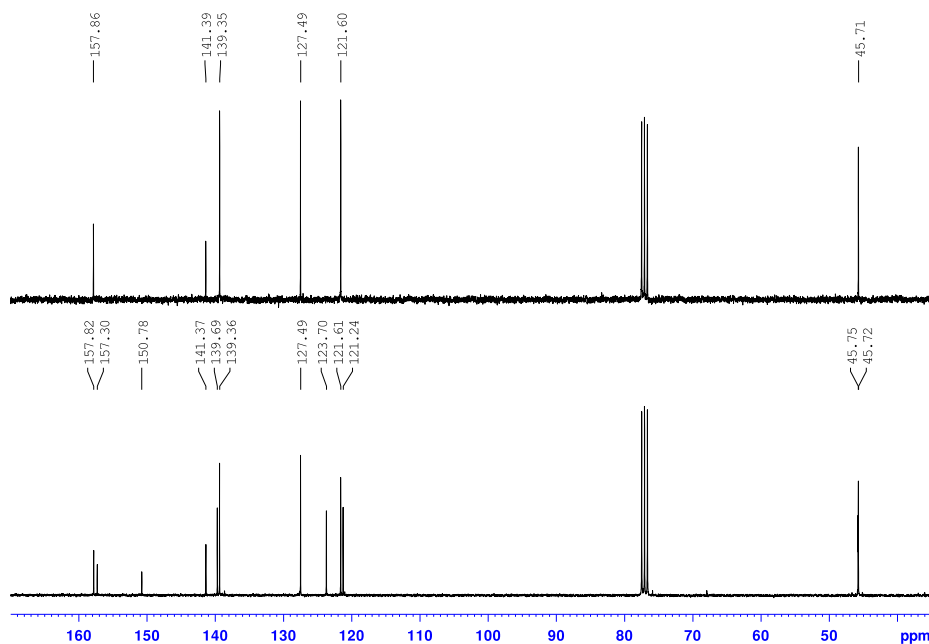


Figure S2. Overlay of the ^{13}C -NMR spectra for the product mixture from the reaction of 2-bromo-6-hydroxymethylpyridine with cyanuric chloride•DMF in DCM at r.t (top) and SOCl_2 at 40 °C (bottom) in CDCl_3 .

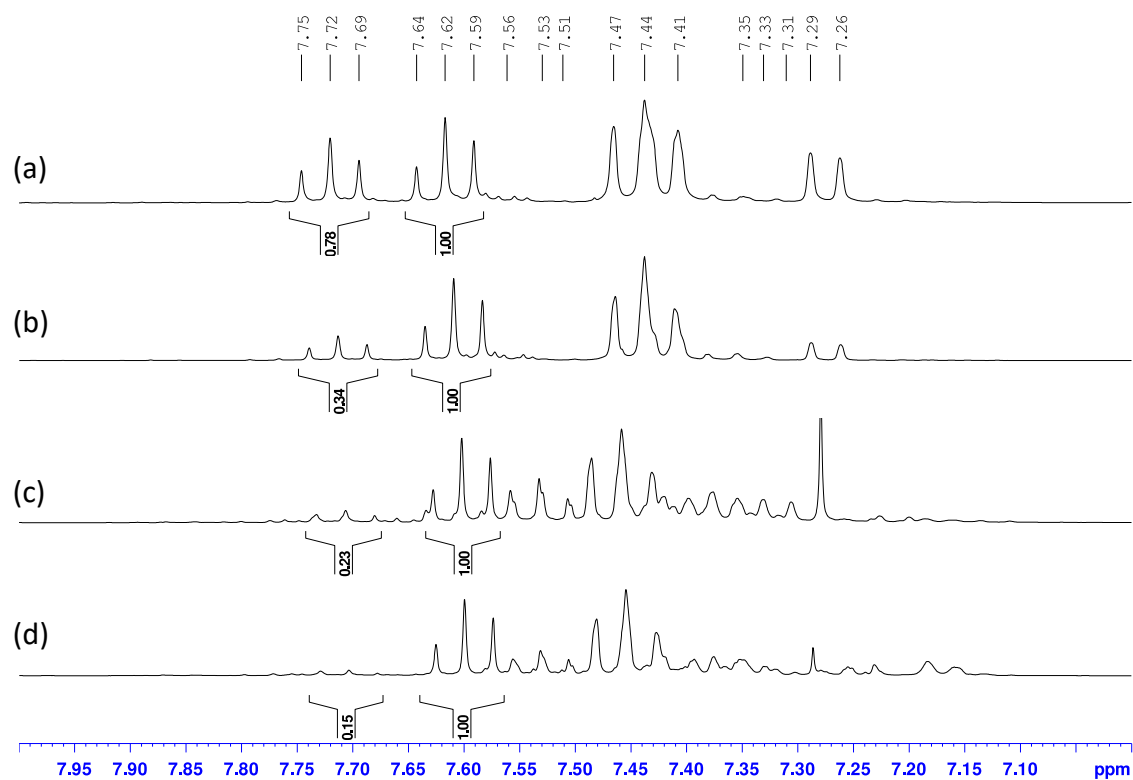


Figure S3. Overlay of the aromatic regions of the ^1H -NMR spectra for the product mixtures from the reaction of 2-bromo-6-hydroxymethylpyridine with SOCl_2 (a) neat at 40 $^\circ\text{C}$, (b) neat at r.t., (c) neat at 0 $^\circ\text{C}$, (d) in DCM at 0 $^\circ\text{C}$ in CDCl_3 .

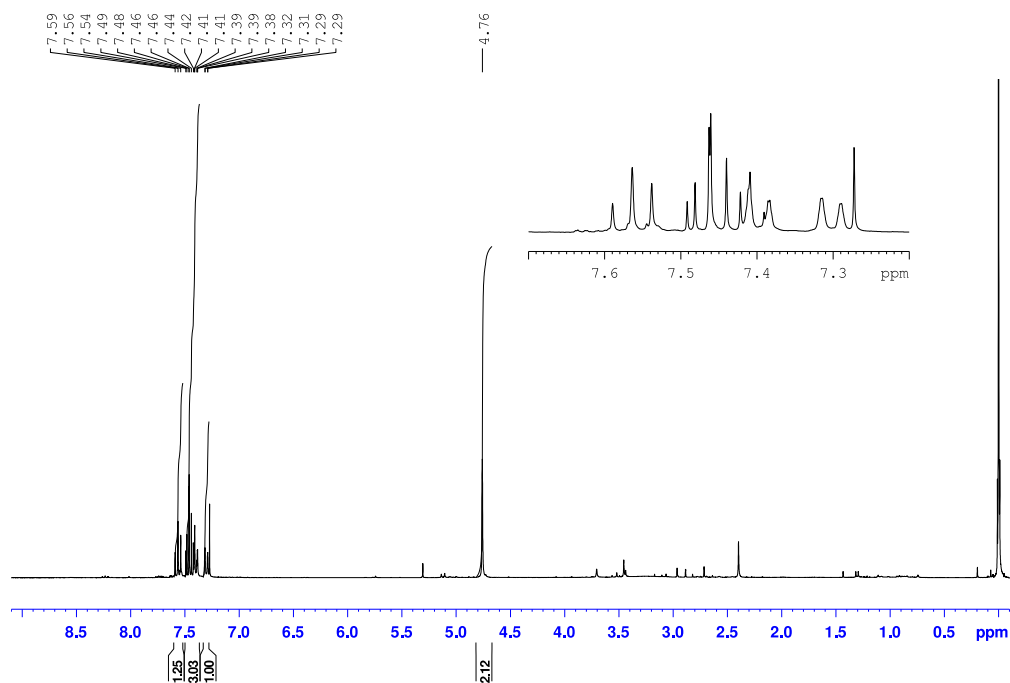


Figure S4. ^1H -NMR Spectrum of the reaction mixture containing 2-bromo-6-hydroxymethylpyridine and 2,6-dibromopyridine in CDCl_3 .

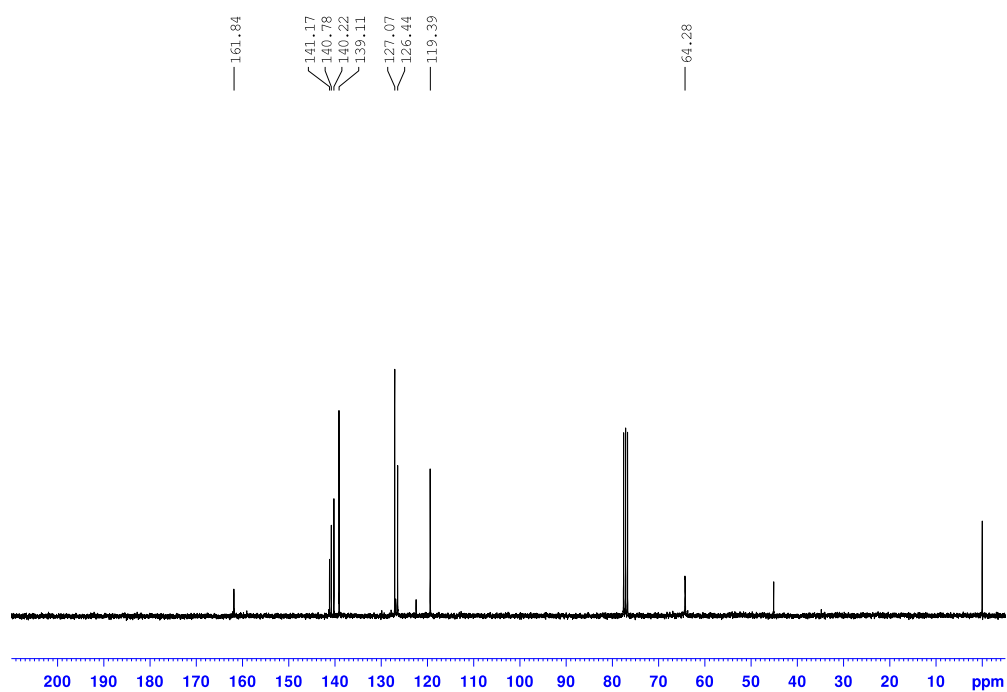


Figure S5. ^{13}C -NMR Spectrum of the reaction mixture containing 2-bromo-6-hydroxymethylpyridine and 2,6-dibromopyridine in CDCl_3 .

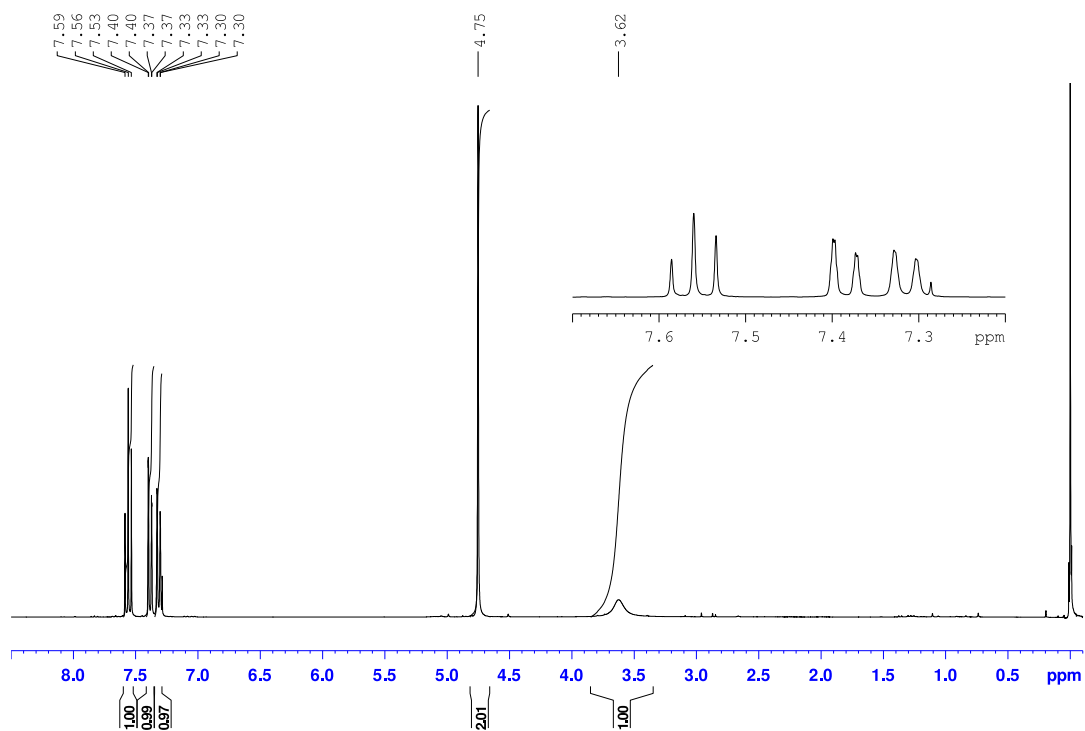


Figure S6. ¹H-NMR Spectrum of 2-bromo-6-hydroxymethylpyridine in CDCl₃.

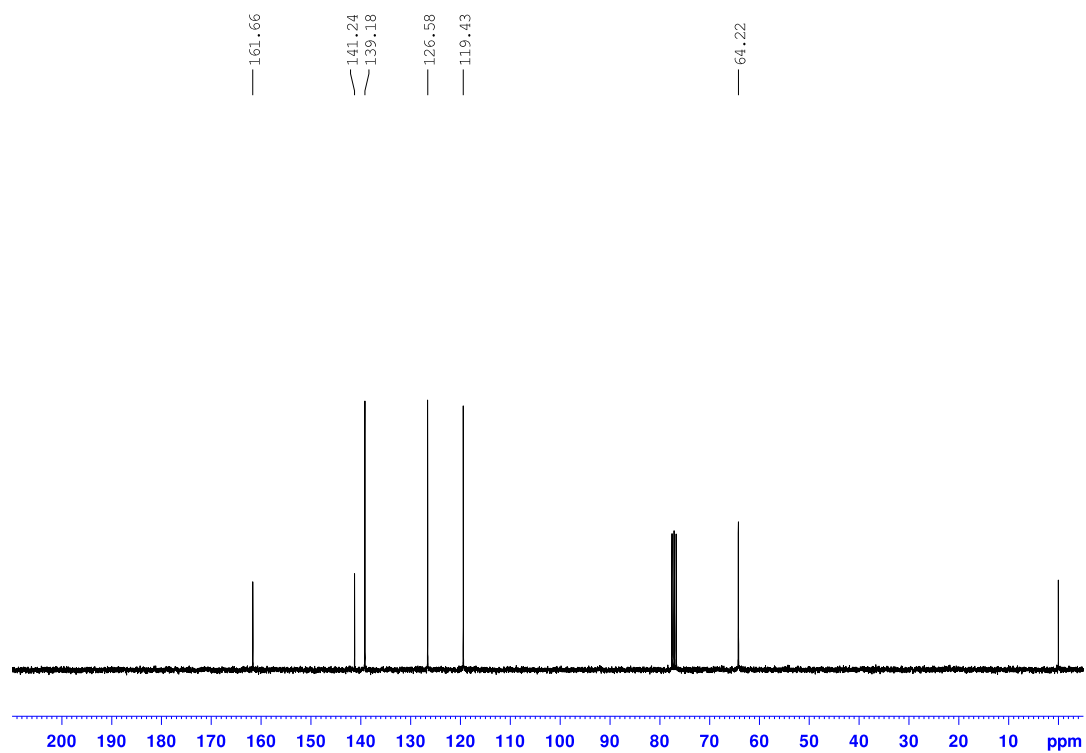


Figure S7. ¹³C-NMR Spectrum of 2-bromo-6-hydroxymethylpyridine in CDCl₃.

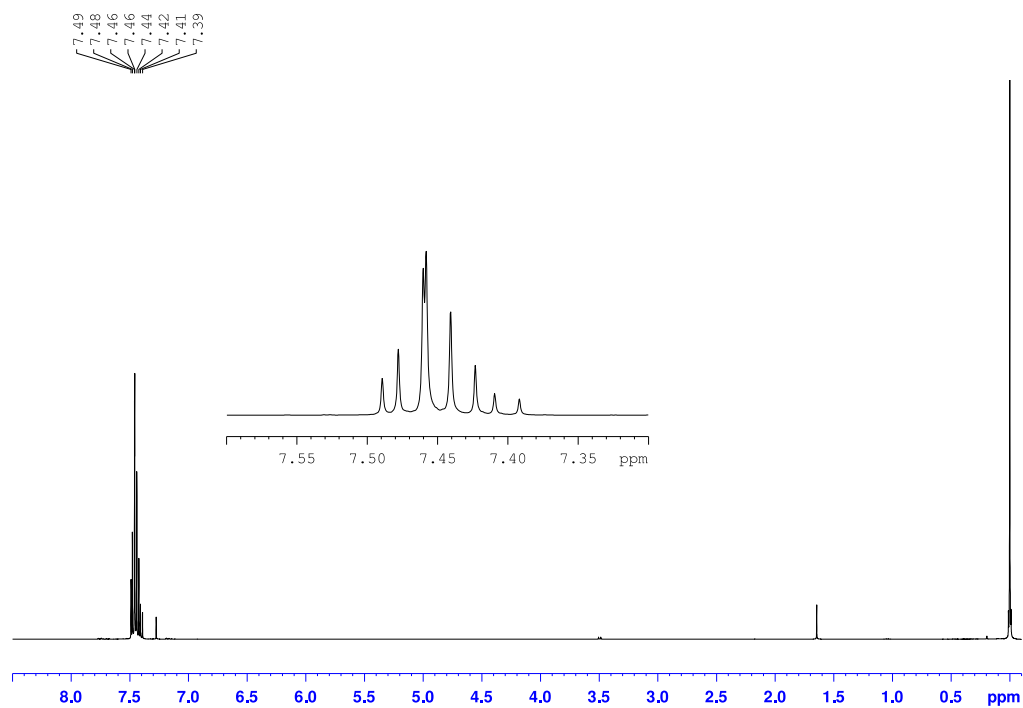


Figure S8. ^1H -NMR Spectrum of 2,6-dibromopyridine in CDCl_3 .

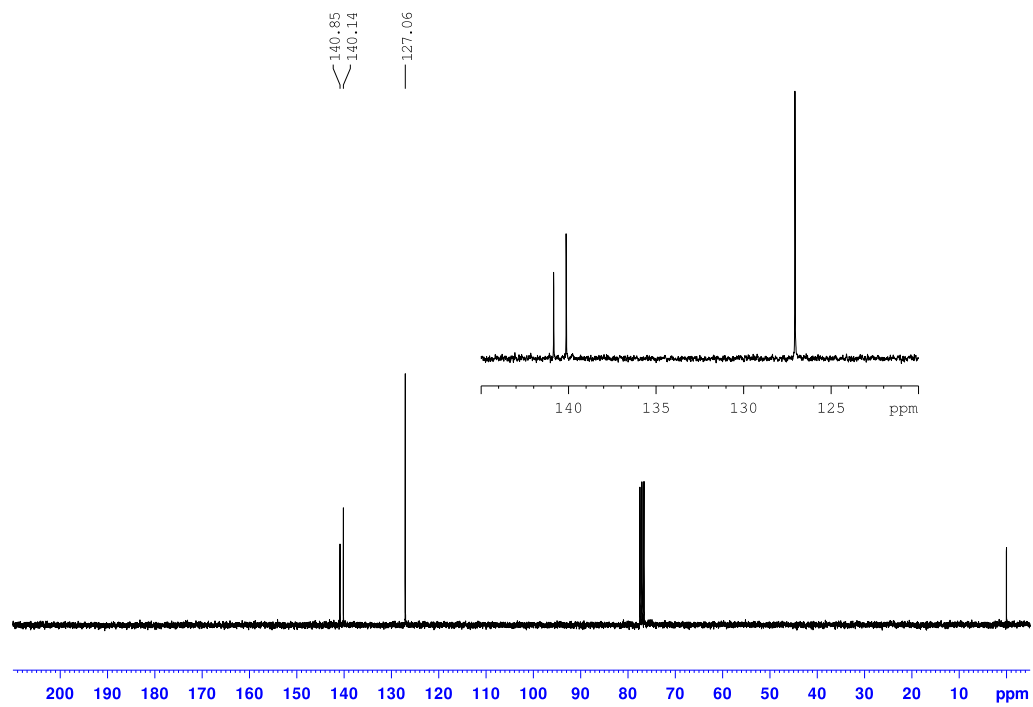


Figure S9. ^{13}C -NMR Spectrum of 2,6-dibromopyridine in CDCl_3 .

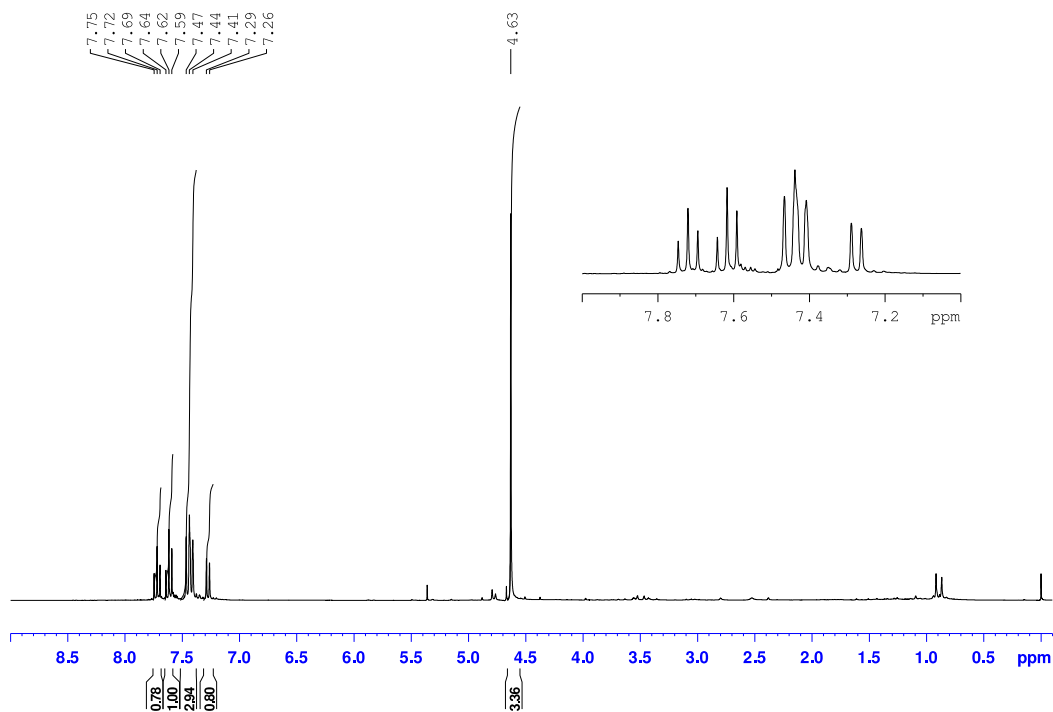


Figure S10. ¹H-NMR Spectrum of the reaction mixture containing 2-bromo-6-chloromethylpyridine and 2-chloro-6-chloromethylpyridine in CDCl₃.

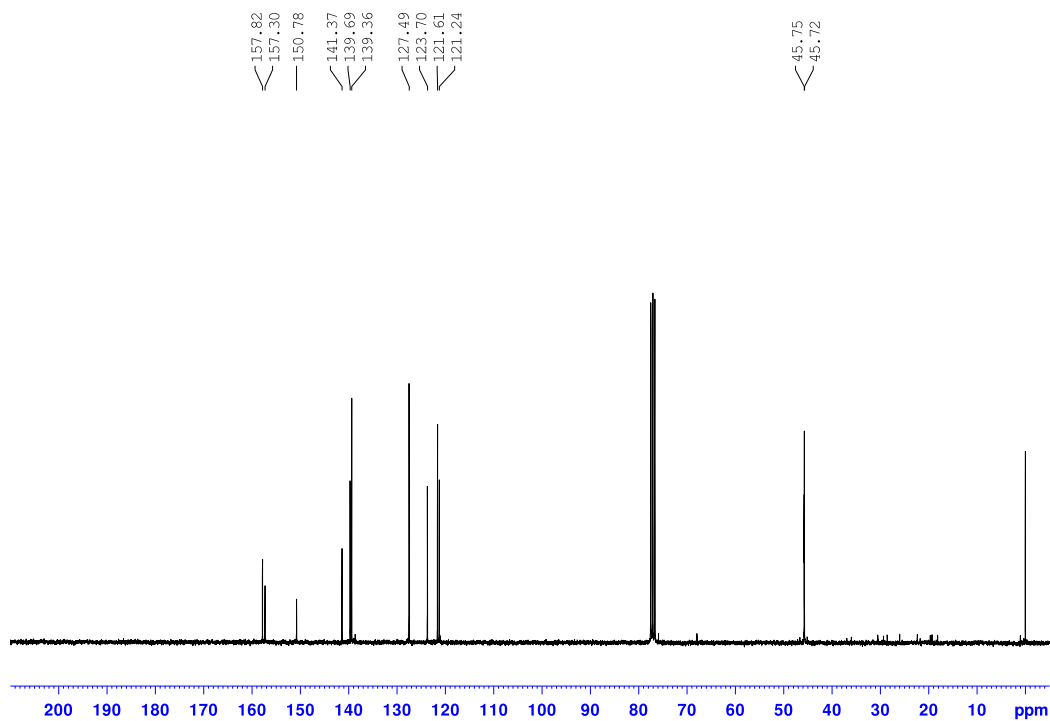


Figure S11. ¹³C-NMR Spectrum of the reaction mixture containing 2-bromo-6-chloromethylpyridine and 2-chloro-6-chloromethylpyridine in CDCl₃.

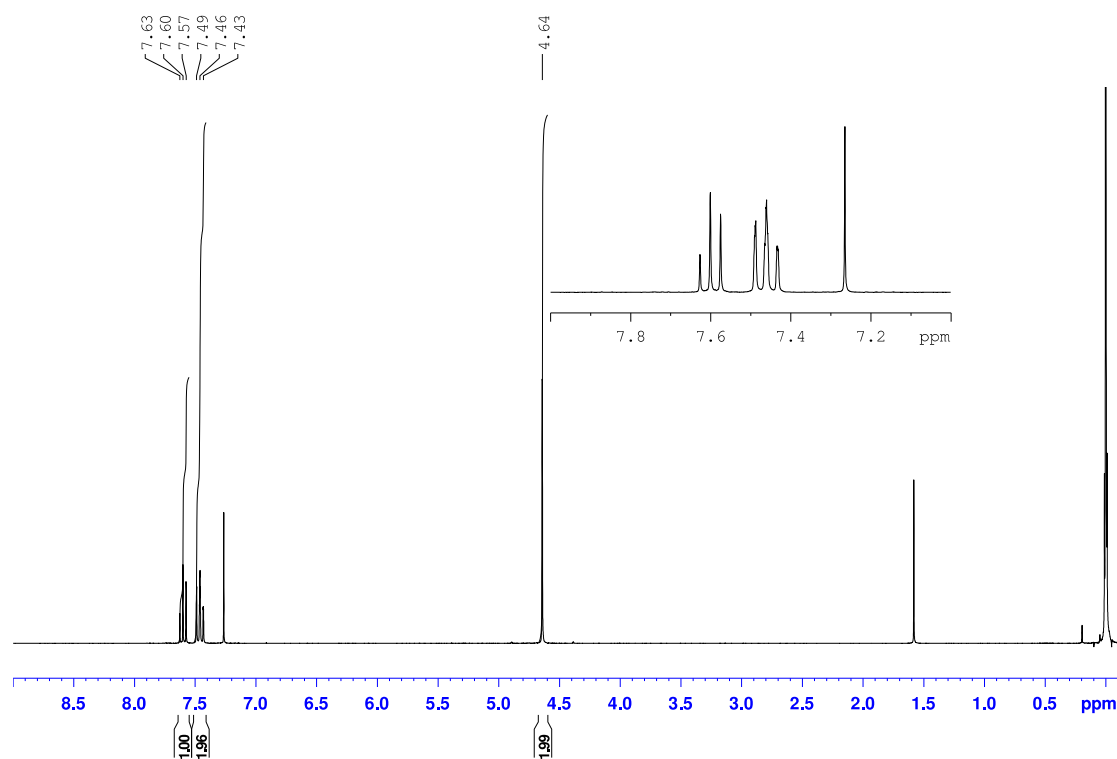


Figure S12. ¹H-NMR Spectrum of 2-bromo-6-chloromethylpyridine in CDCl₃.

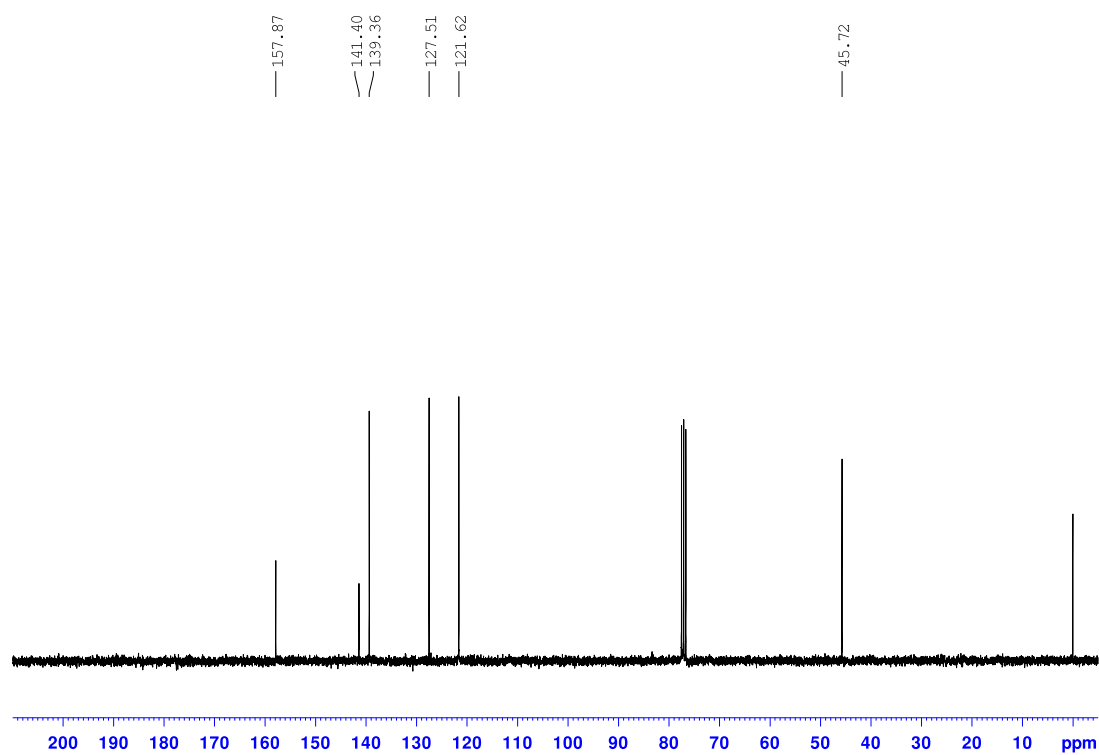


Figure S13. ¹³C-NMR Spectrum of 2-bromo-6-chloromethylpyridine in CDCl₃.

Mass Spectra of Reaction Mixtures and Isolated Compounds

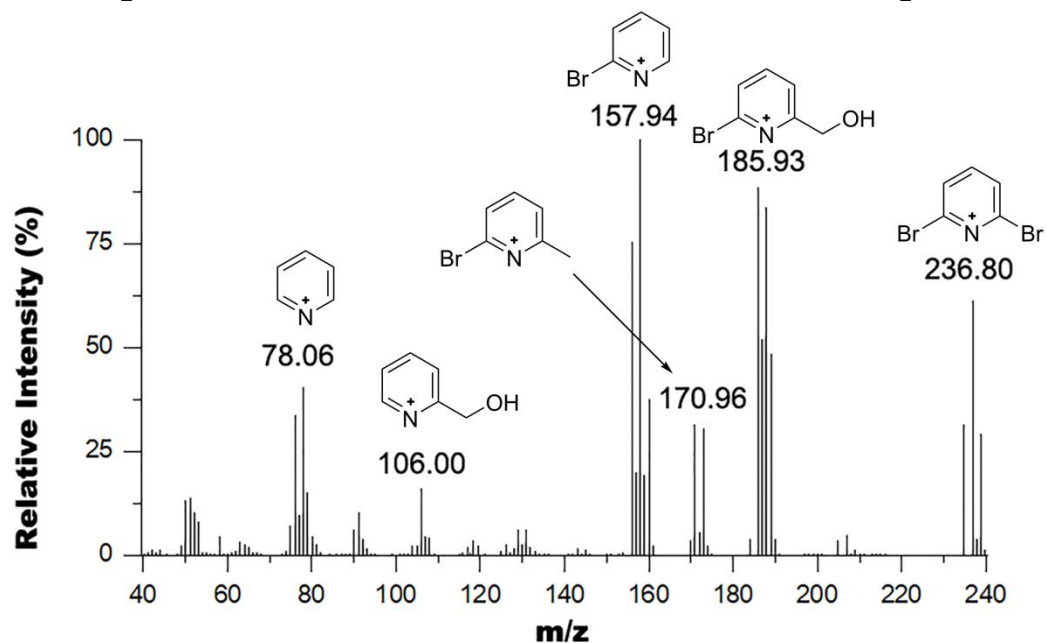


Figure S14. Mass spectrum of the reaction mixture containing 2-bromo-6-hydroxymethylpyridine and 2,6-dibromopyridine.

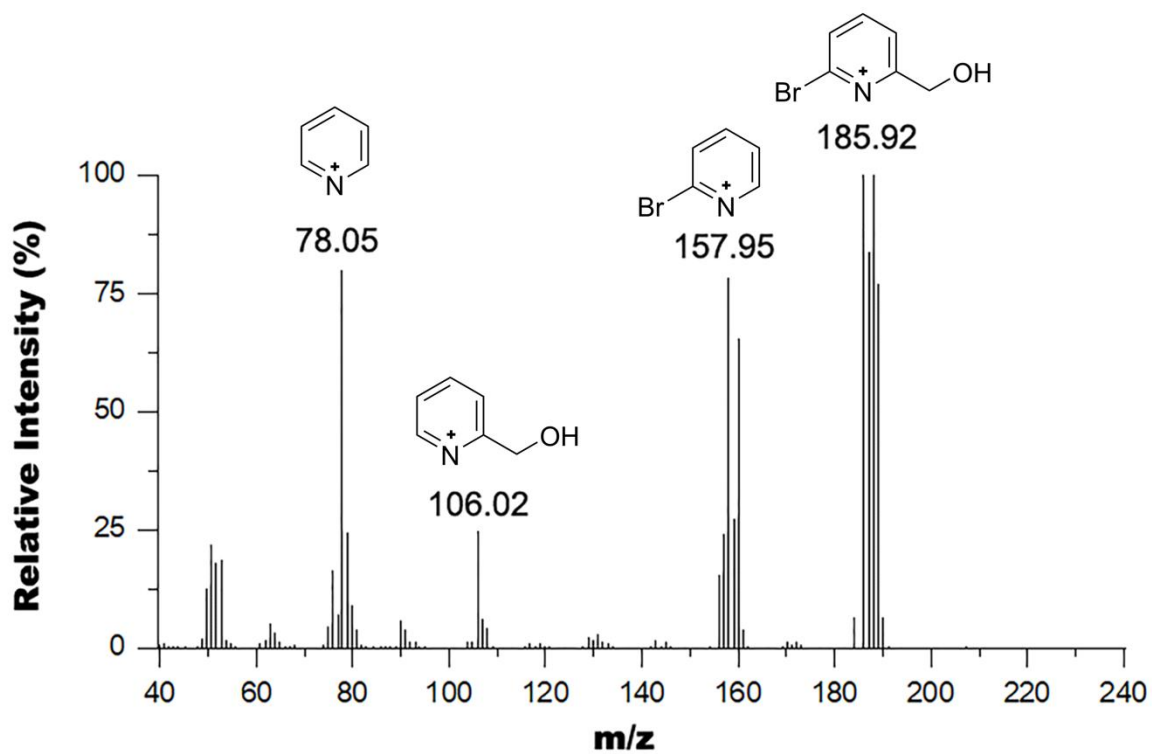


Figure S15. Mass spectrum of 2-bromo-6-hydroxymethylpyridine.

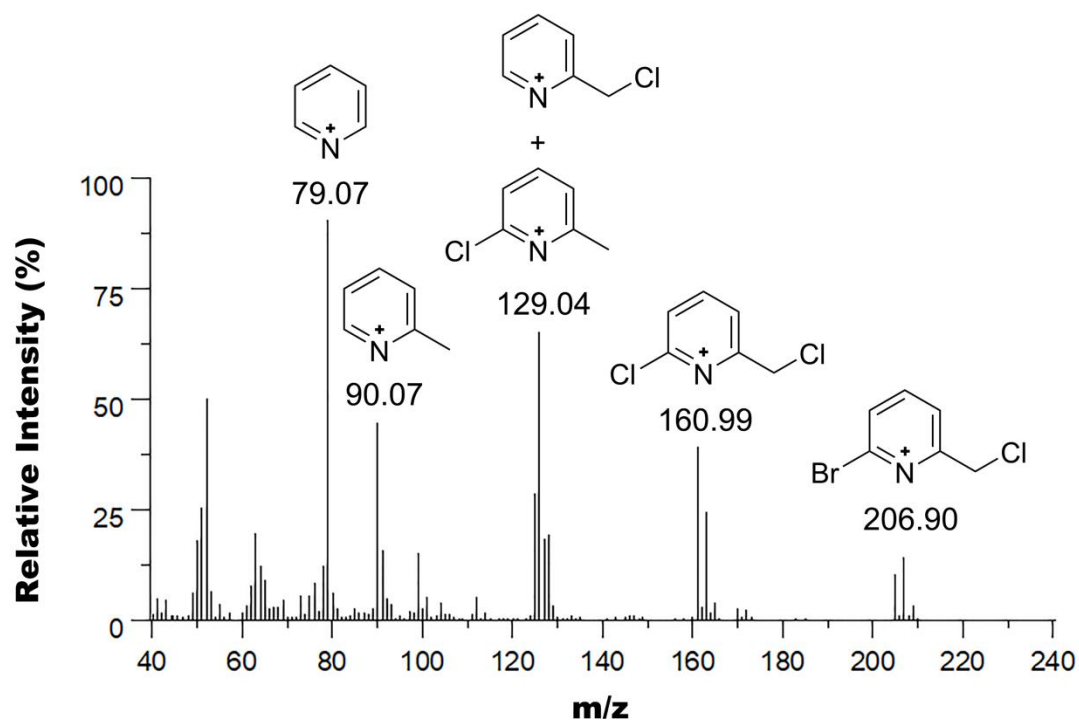


Figure S16. Mass spectrum of the reaction mixture containing 2-bromo-6-chloromethylpyridine and 2-chloro-6-chloromethylpyridine.

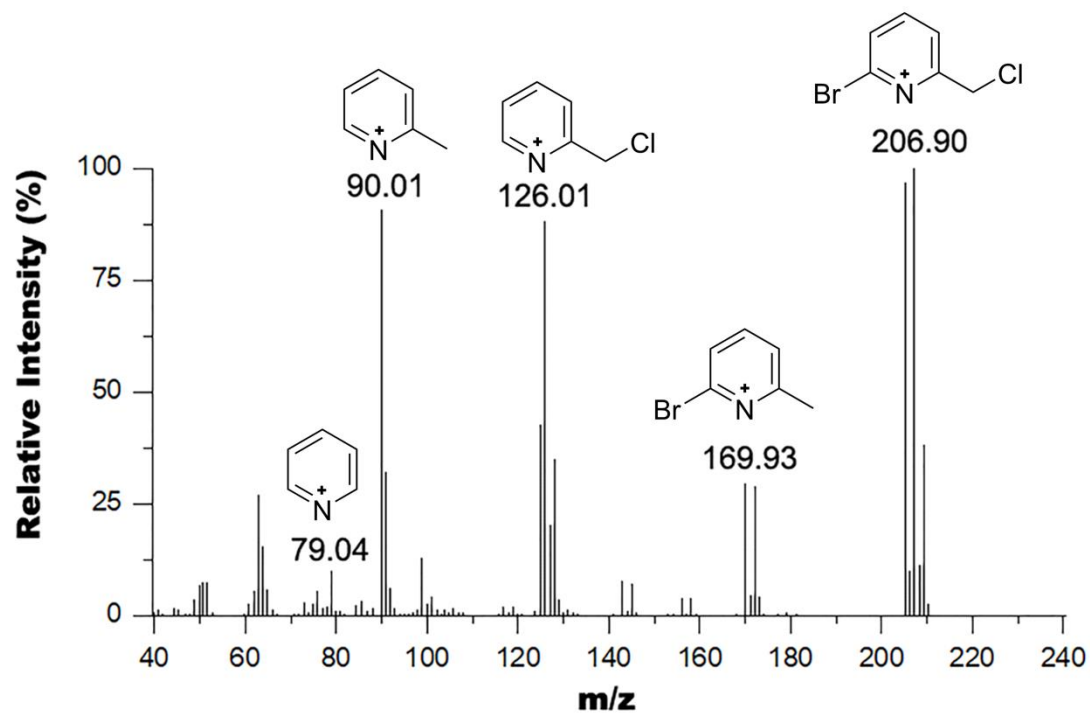


Figure S17. Mass spectrum of 2-bromo-6-chloromethylpyridine.

FT-IR Spectra of Isolated Products

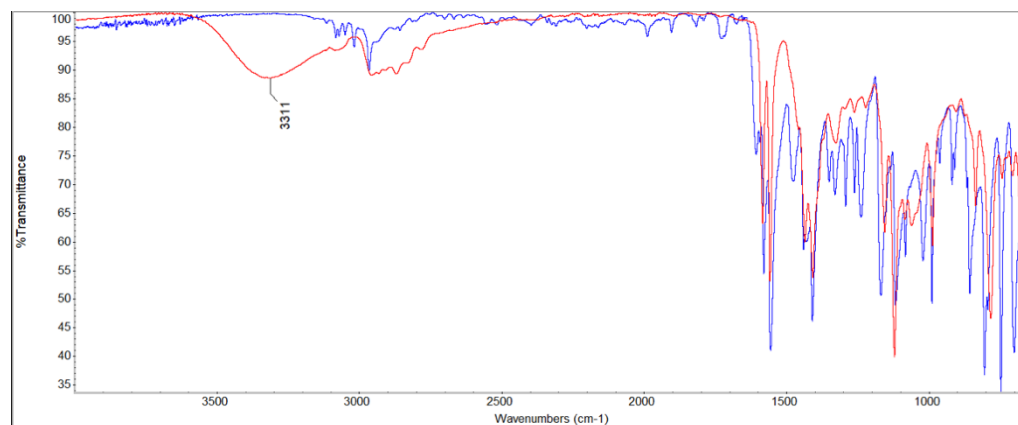


Figure S18. Overlay of the FT-IR spectra of 2-bromo-6-hydroxymethylpyridine (red) and the product of the reaction with cyanuric chloride (blue).