

Supporting Information for:

Design and synthesis of a tetradentate '3-amine-1-carboxylate' ligand to mimic the metal binding environment at the non-heme iron(II) oxidase active site

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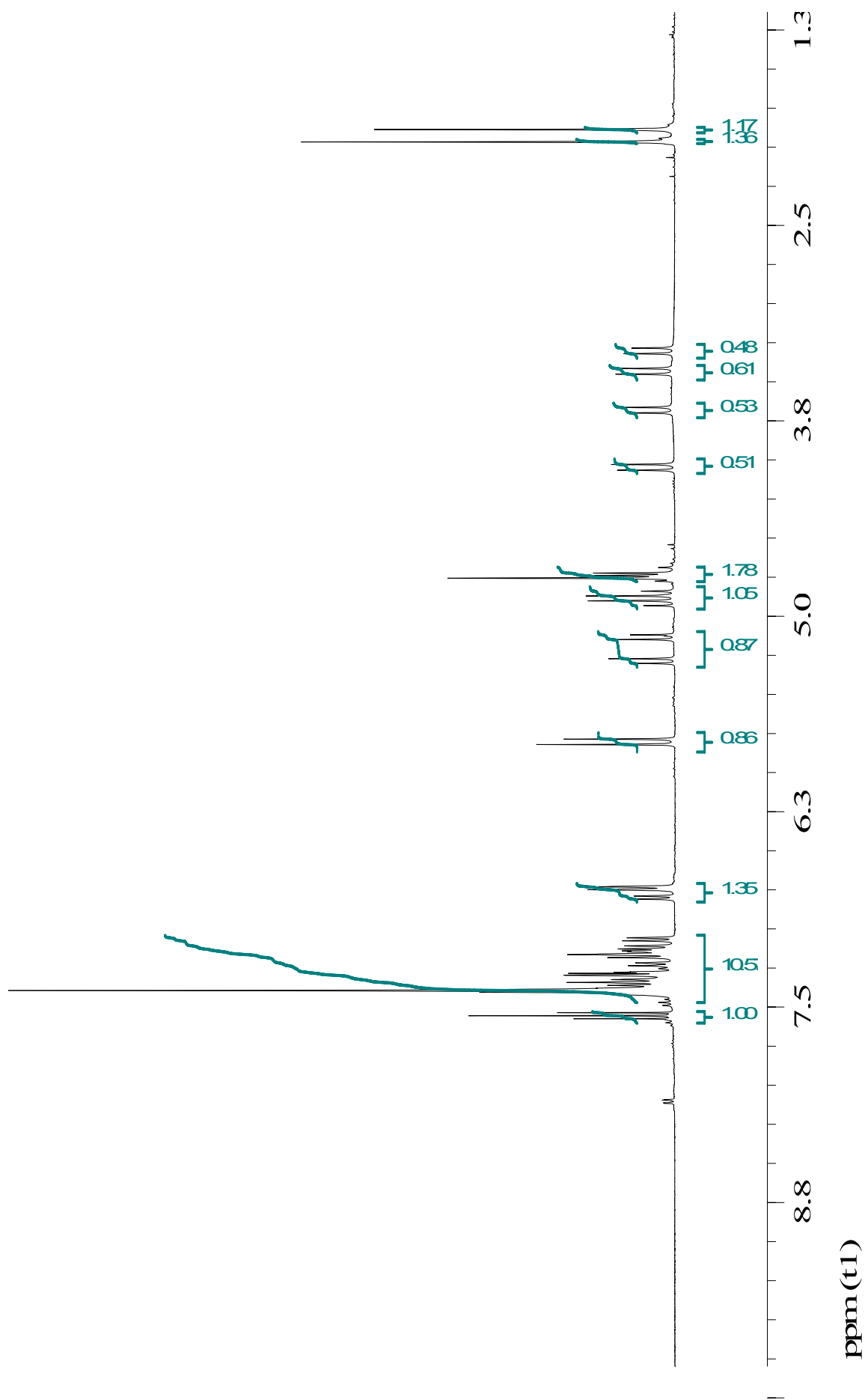
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¹ H NMR spectrum of Compound 11	S2
¹³ C NMR spectrum of Compound 11	S3
¹ H NMR spectrum of Compound 12	S4
¹³ C NMR spectrum of Compound 12	S5
¹ H NMR spectrum of Compound 13	S6
¹³ C NMR spectrum of Compound 13	S7
¹ H NMR spectrum of Compound 14	S8
¹³ C NMR spectrum of Compound 14	S9
¹ H NMR spectrum of Compound 15	S10
¹³ C NMR spectrum of Compound 15	S11
¹ H NMR spectrum of Compound 5	S12
¹³ C NMR spectrum of Compound 5	S13

(2R,4S)-Benzyl 4-((6-(*t*-butyldimethylsilyloxymethyl)pyridine-2-yl)methyl)-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate 11

¹H NMR Spectrum (CDCl₃, 400 MHz)



(2R,4S)-Benzyl 4-((6-(*t*-butyldimethylsilyloxymethyl)pyridine-2-yl)methyl)-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate **11**

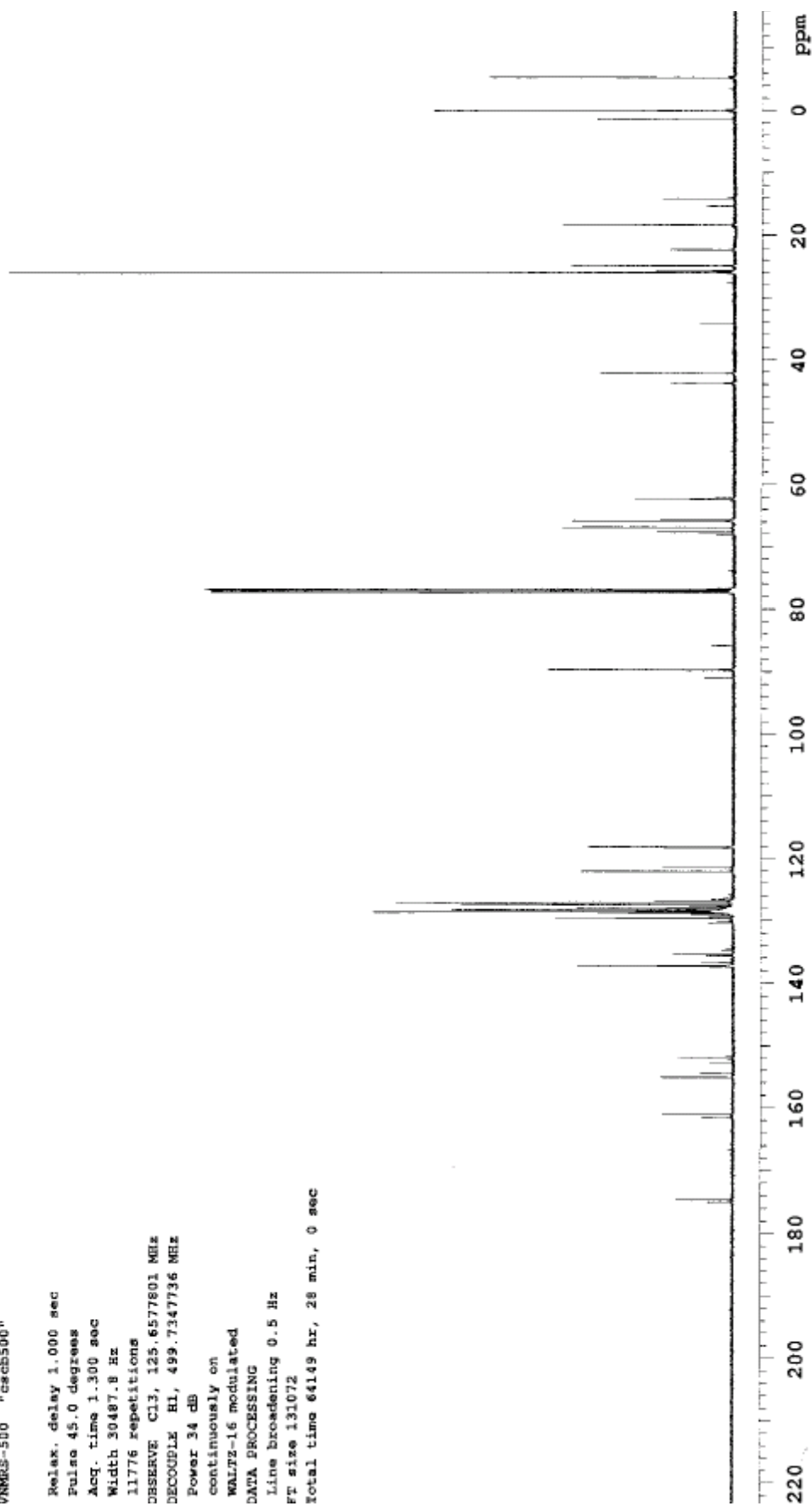
¹³C NMR Spectrum (CDCl₃, 125 MHz)

VD-TBDM
(With added TMS)

Solvent: cdcl3
Temp. 30.0 C / 303.1 K
Operator: vnmr1
VNMR5-500 "csqb500"

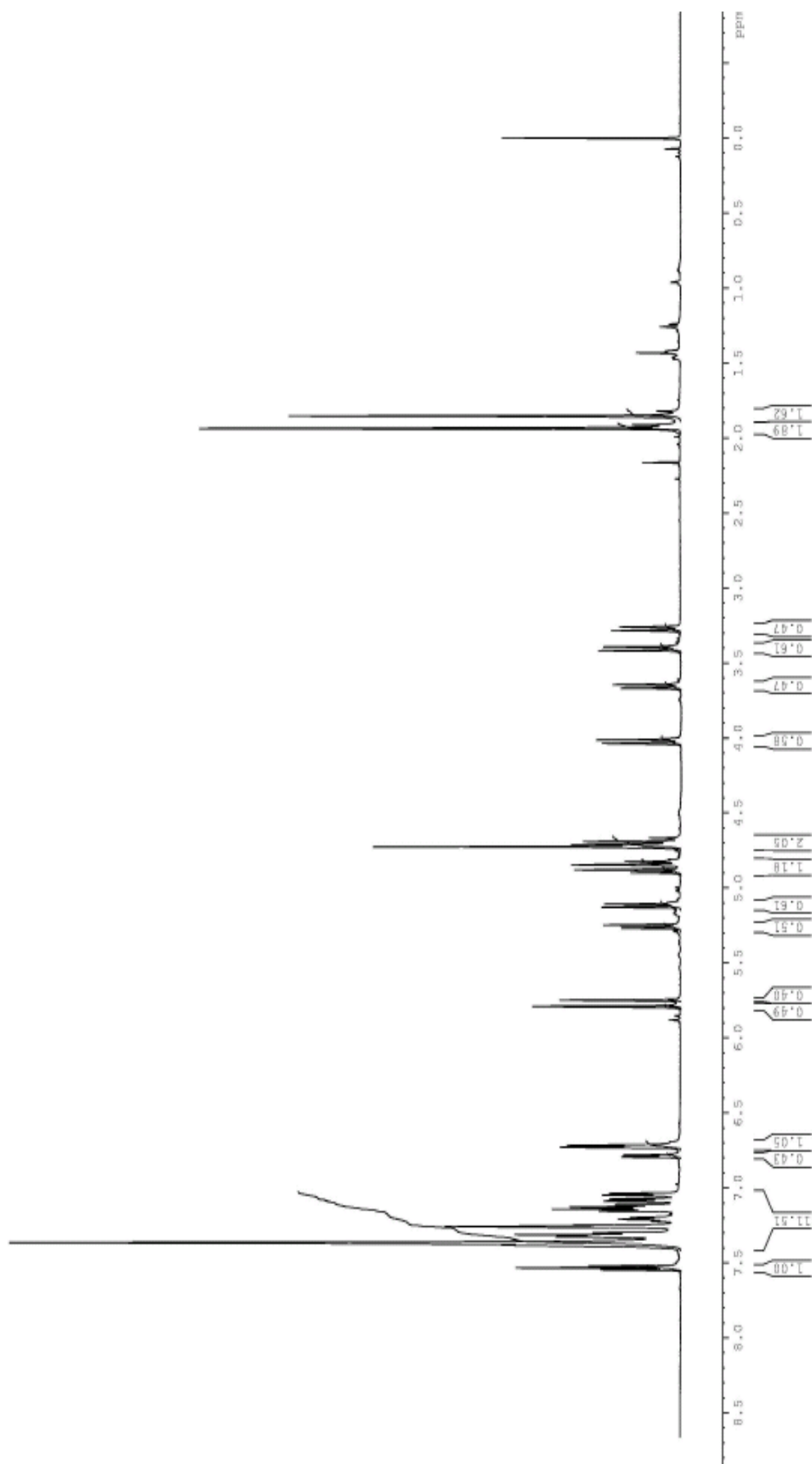
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
11776 repetitions
OBSERVE C13, 125.6577801 MHz
DECOUPLE H1, 499.7347736 MHz
Power 34 dB

continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 64149 hr, 28 min, 0 sec



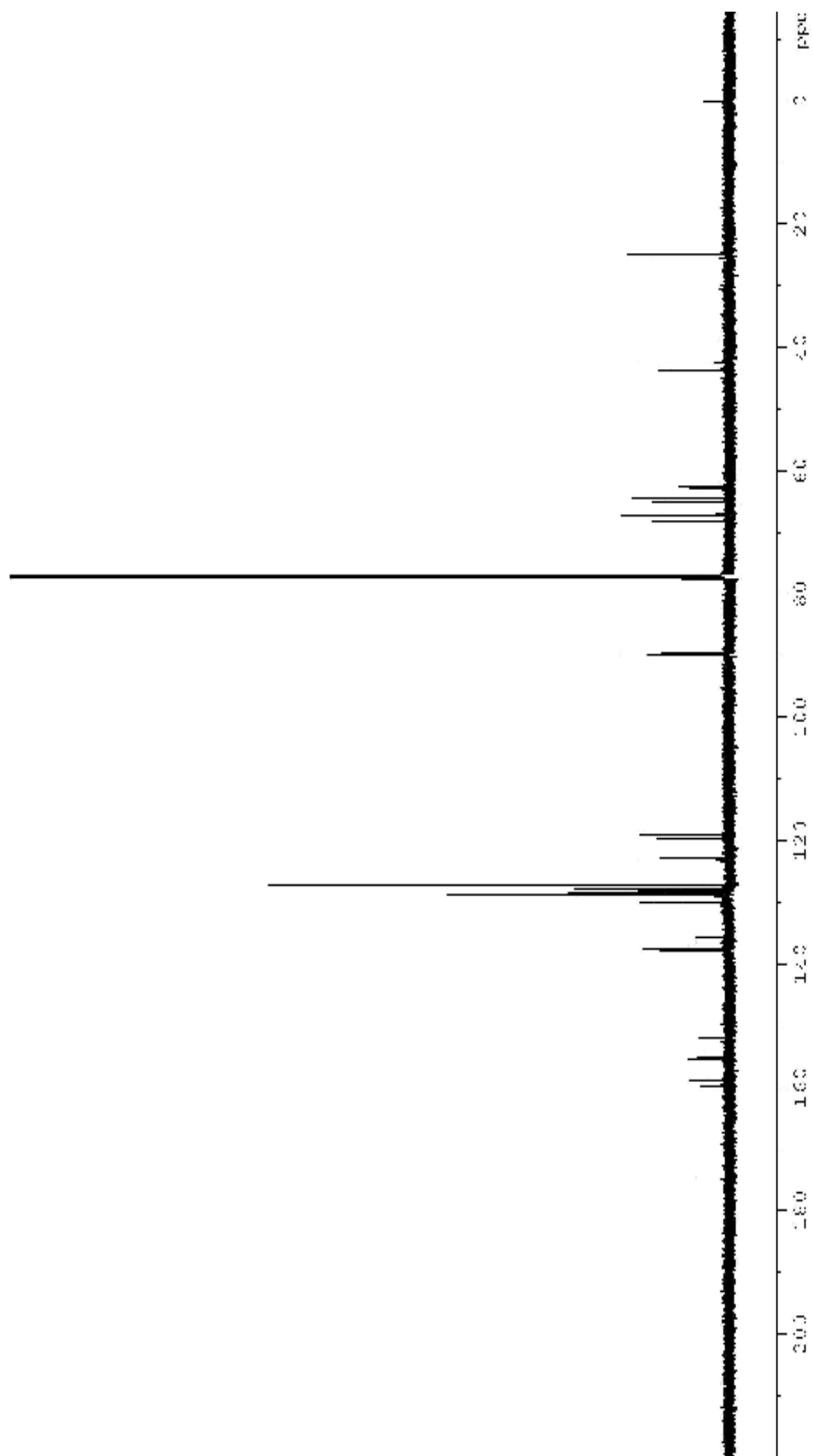
(2R,4S)-Benzyl-4-((6-(hydroxymethyl)pyridine-2-yl)methyl)-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate **12**

¹H NMR Spectrum (CDCl₃, 600 MHz)



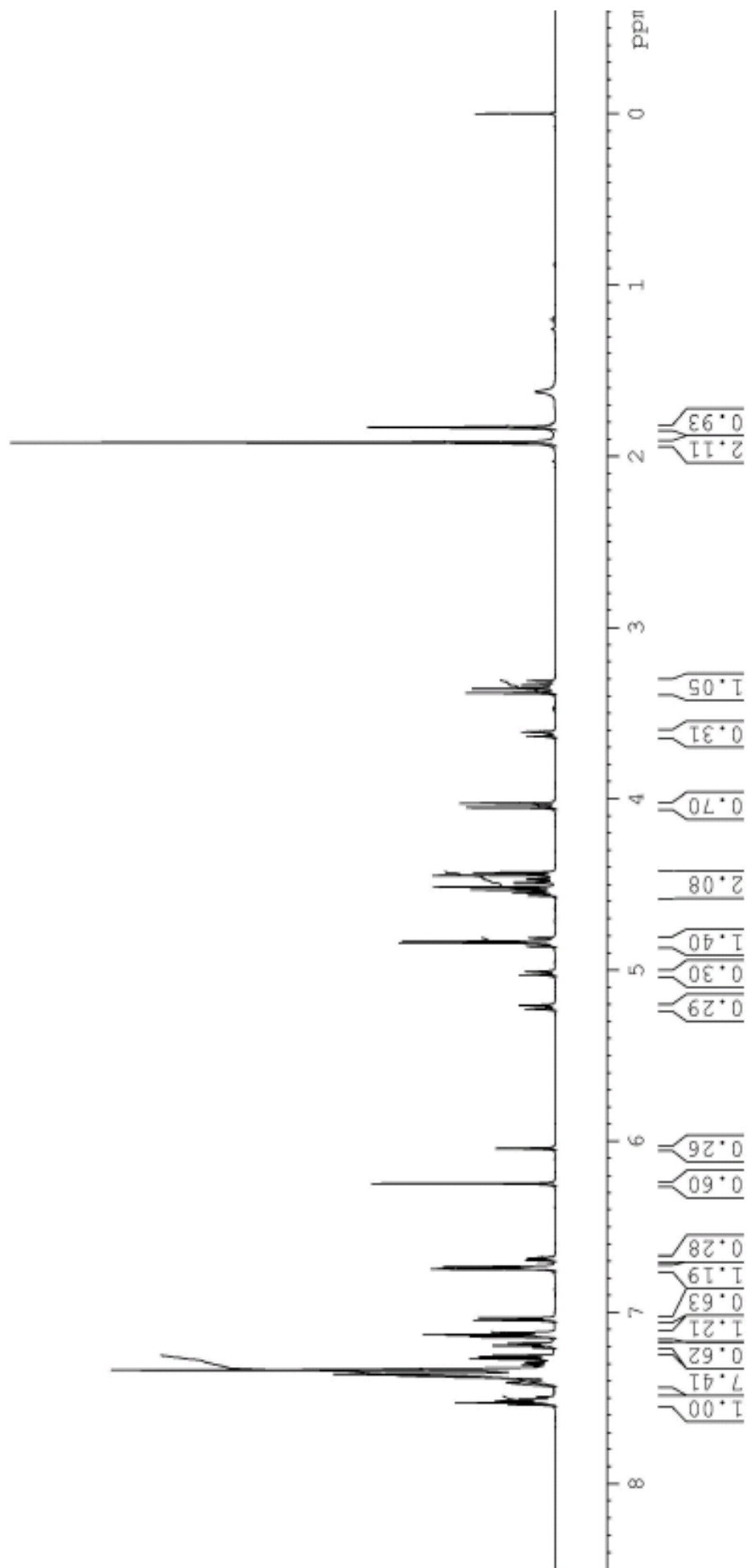
(2R,4S)-Benzyl-4-((6-(hydroxymethyl)pyridine-2-yl)methyl)-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate **12**

¹³C NMR Spectrum (CDCl₃, 125 MHz)



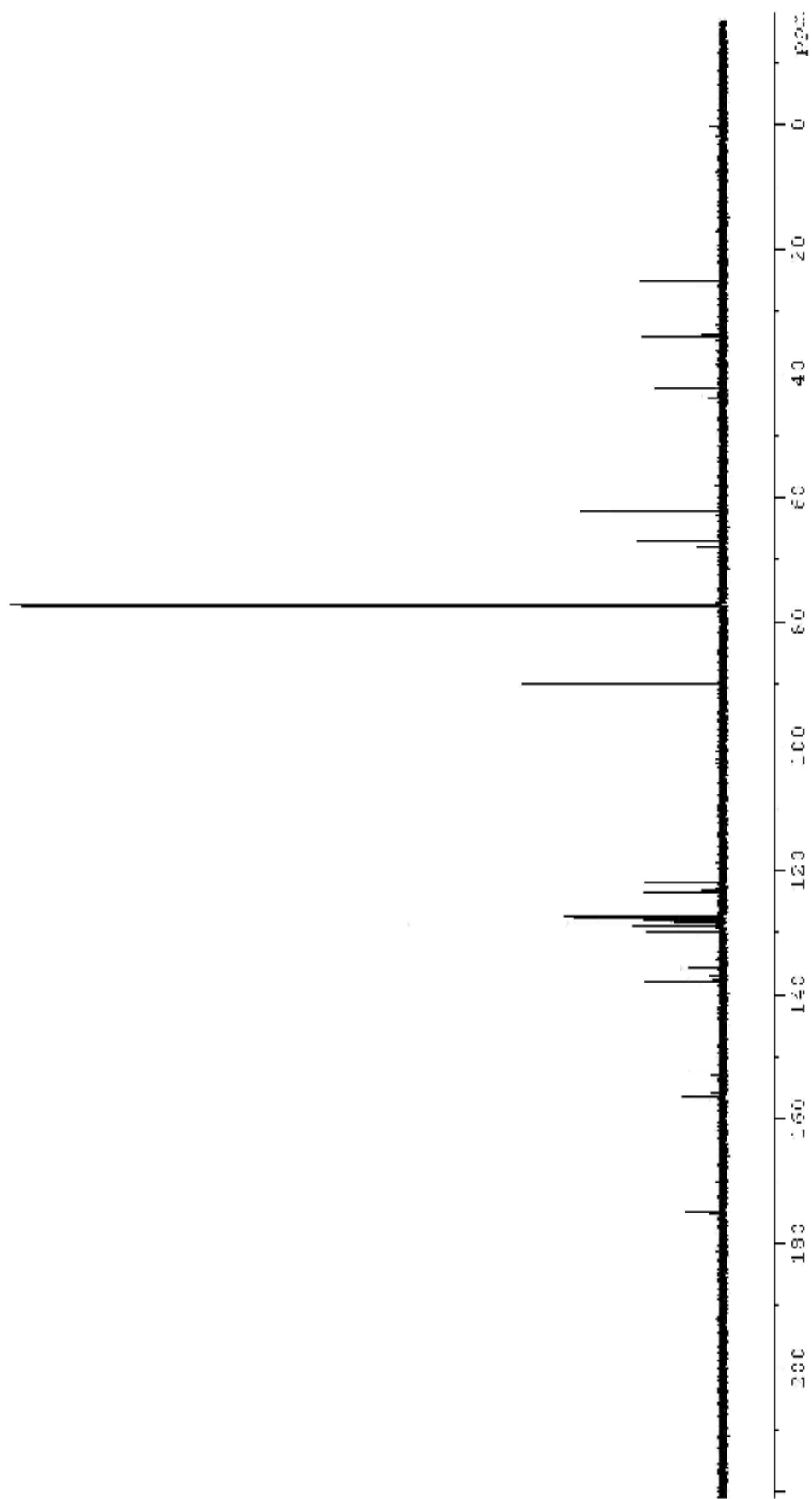
(2R,4S)-Benzyl 4((6-(bromomethyl)pyridine-2-yl)methyl)-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate **13**

¹H NMR Spectrum (CDCl₃, 600 MHz)



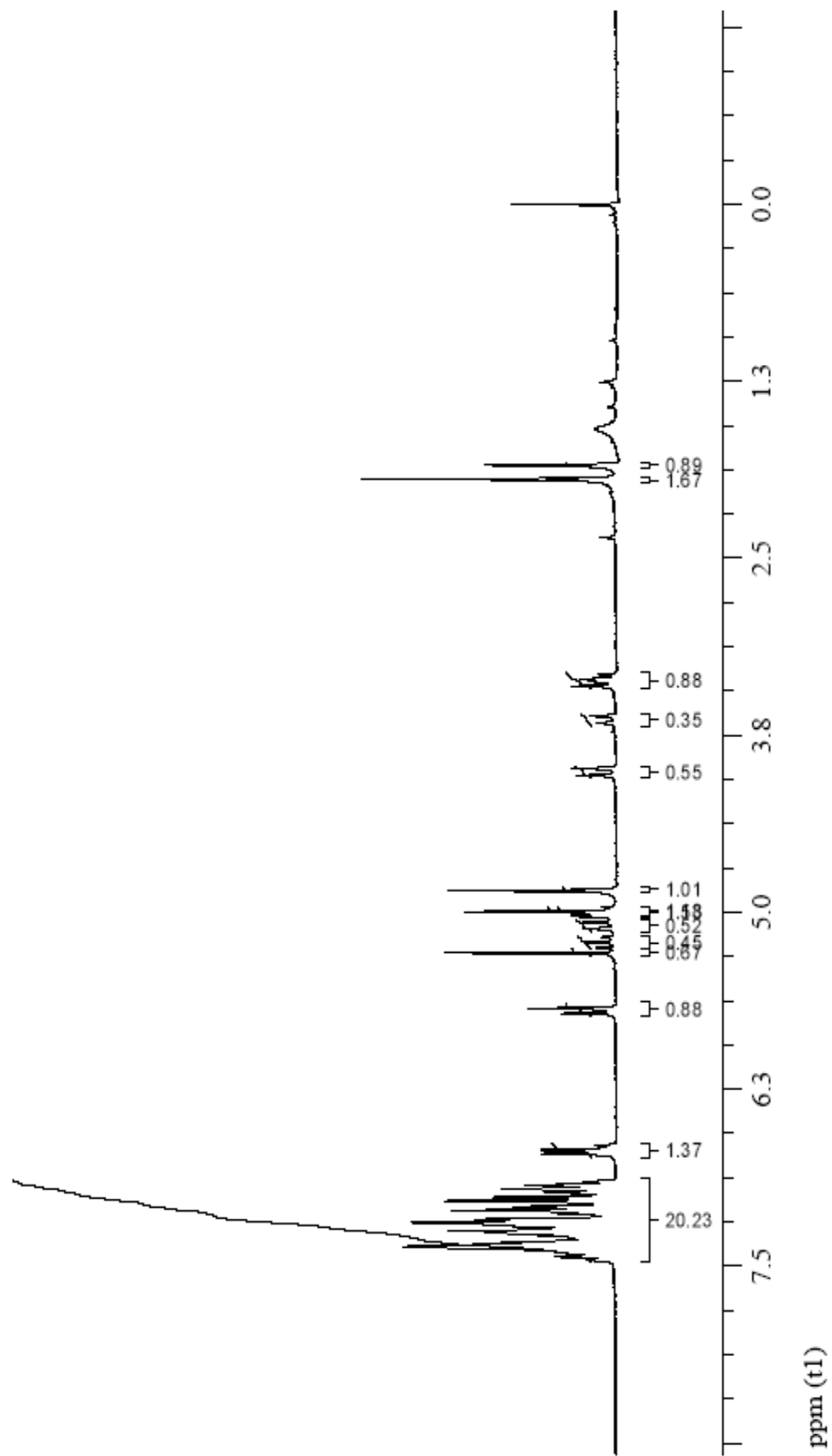
(2R,4S)-Benzyl 4((6-(bromomethyl)pyridine-2-yl)methyl)-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate **13**

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



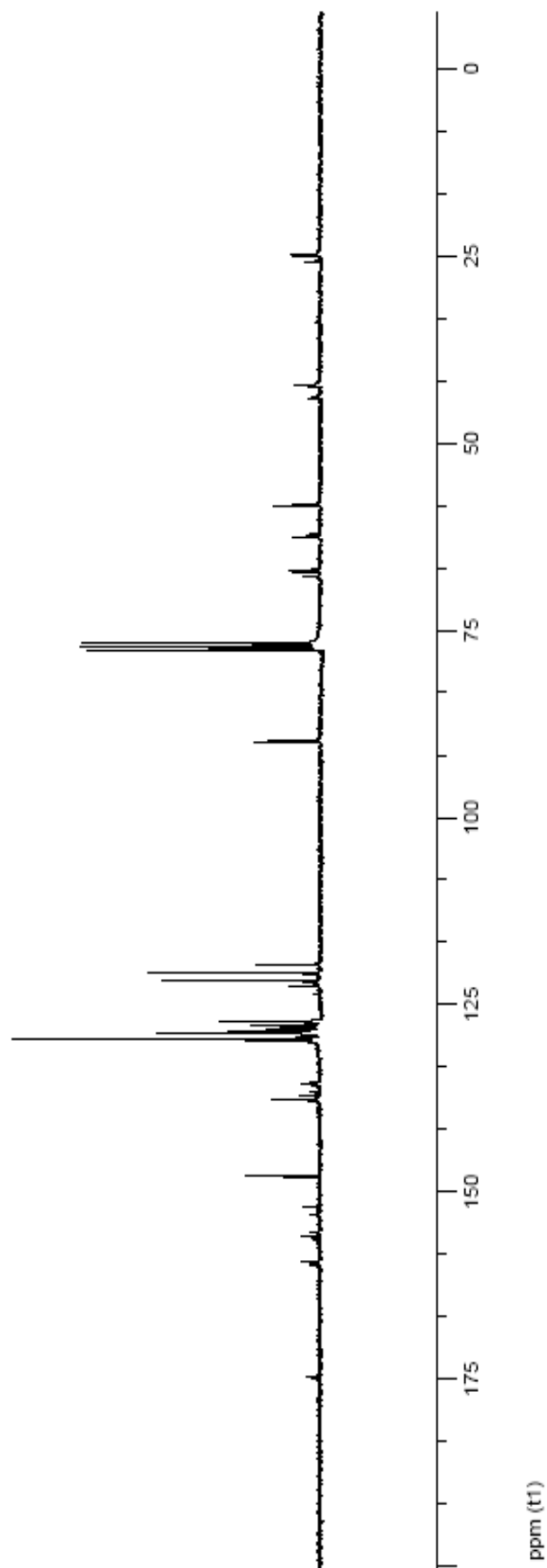
(2R,4S)-Benzyl 4-((6-((diphenylamino)-methyl)-pyridin-2-yl)-methyl-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate **14**

¹H NMR Spectrum (CDCl₃, 600 MHz)



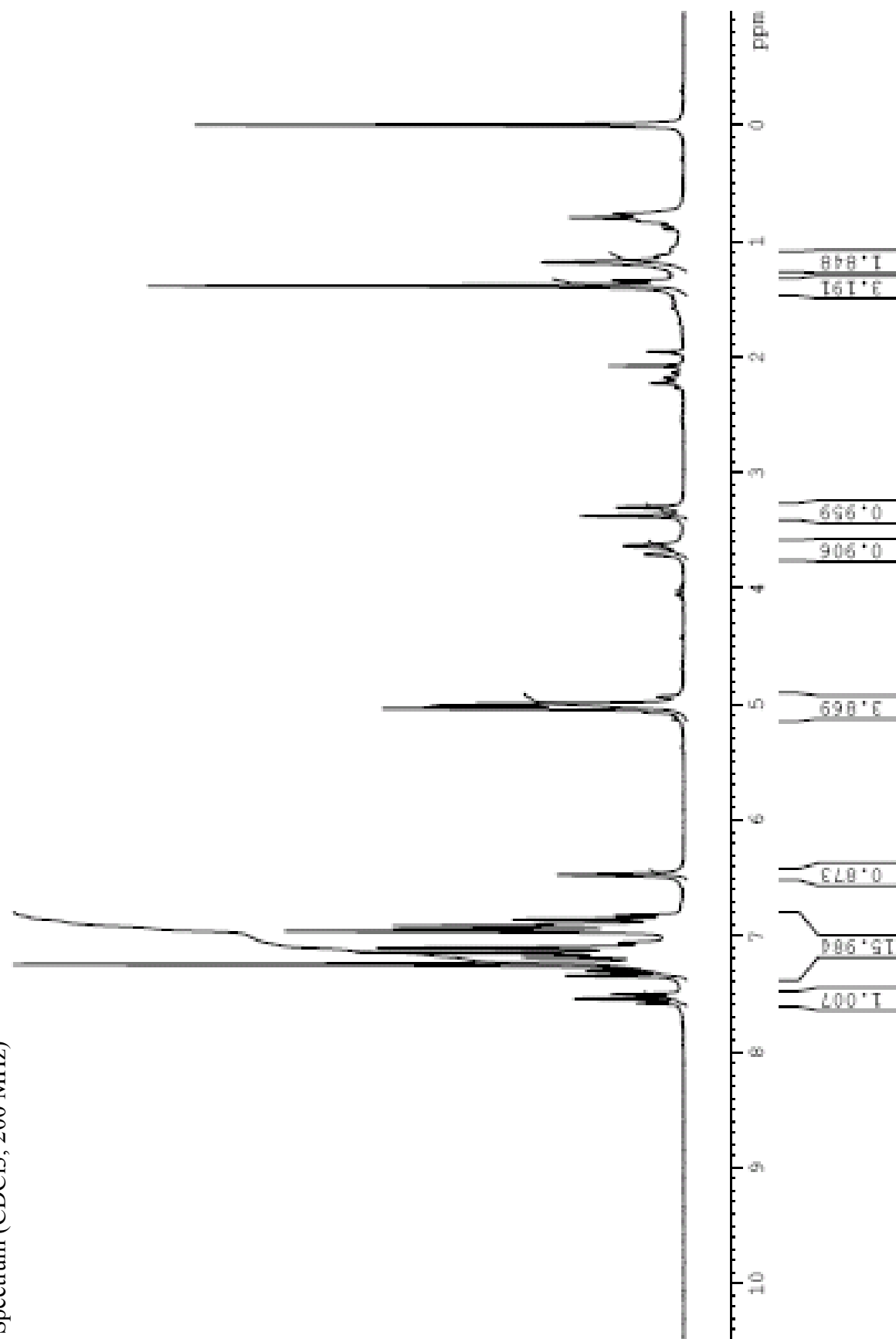
(2R,4S)-Benzyl 4-((6-((diphenylamino)-methyl)-pyridin-2-yl)-methyl-4-methyl-5-oxo-2-phenyloxazolidine-3-carboxylate **14**

^{13}C NMR Spectrum (CDCl_3 , 150 MHz)



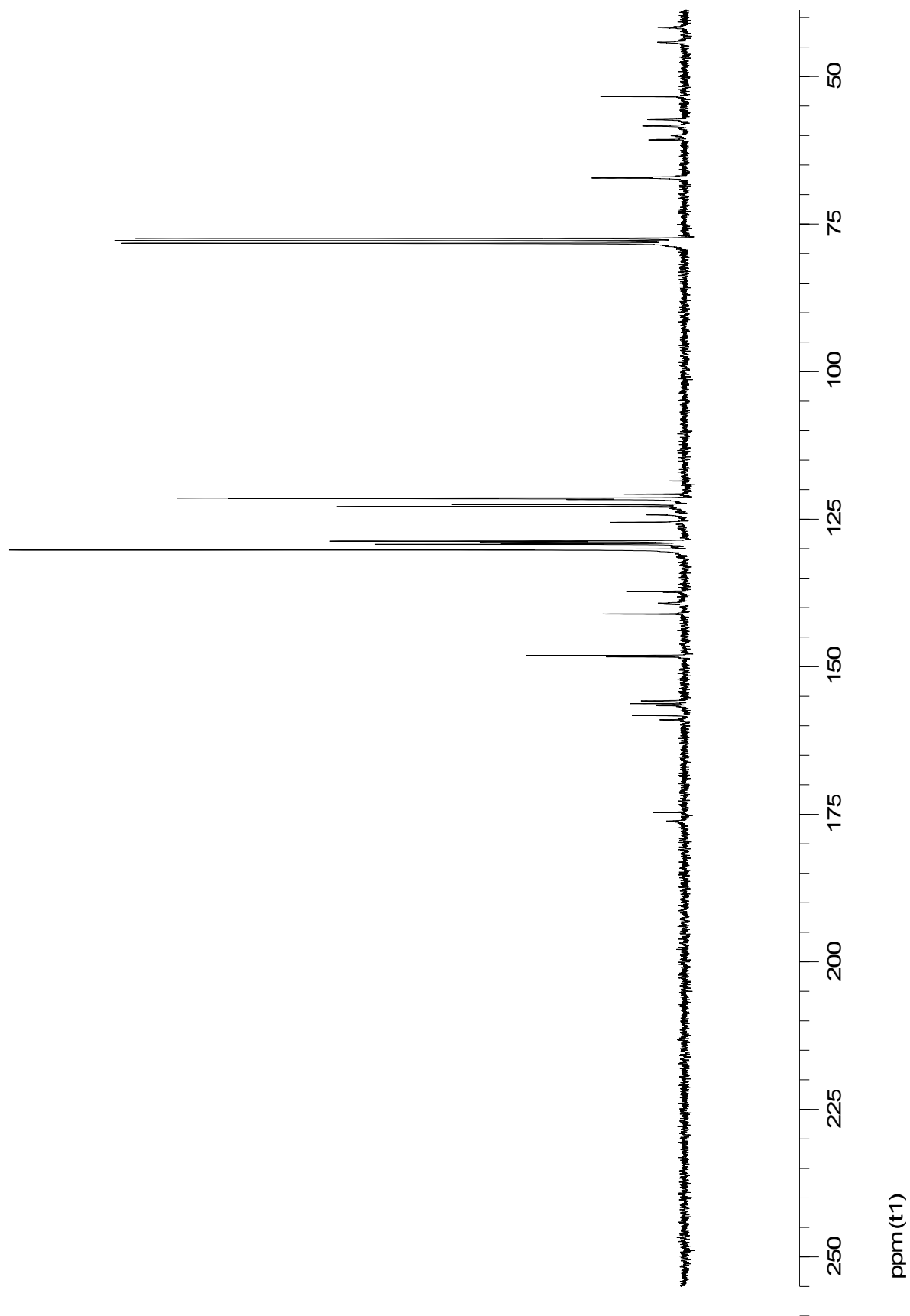
(R)-2-(Benzoyloxycarbonylamino)-3-(6-((diphenylamino)methyl)pyridin-2-yl)-2-methylpropanoic acid **15**

¹H NMR Spectrum (CDCl₃, 200 MHz)



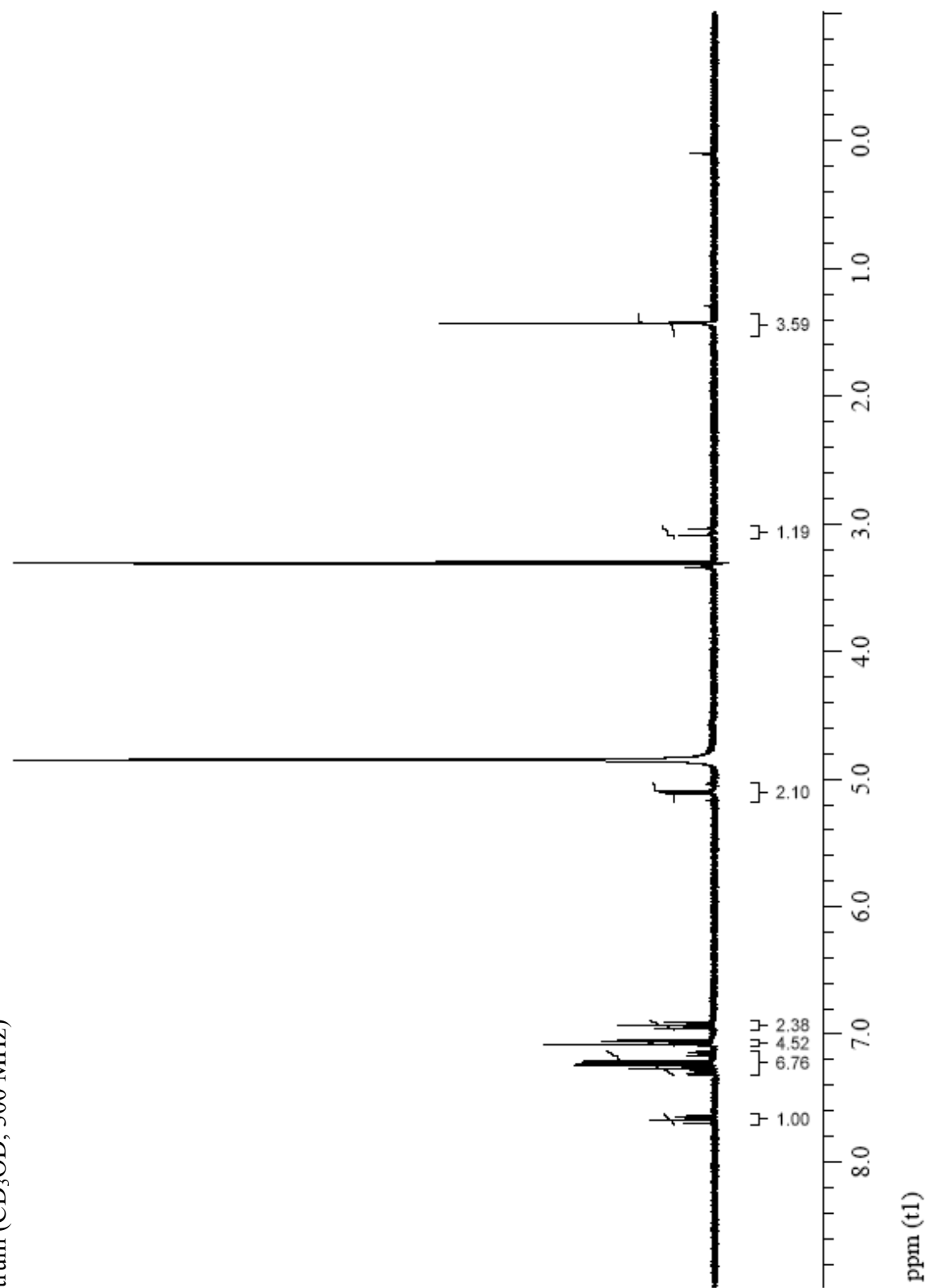
(R)-2-(Benzoyloxycarbonylamino)-3-(6-((diphenylamino)methyl)pyridin-2-yl)-2-methylpropanoic acid **15**

^{13}C NMR Spectrum (CDCl_3 , 75 MHz)



(R)-2-((6-((Diphenylamino)methyl)pyridine-2-yl)methyl)-2-aminopropanoic acid **5**

¹H NMR Spectrum (CD₃OD, 300 MHz)



(R)-2-((6-((Diphenylamino)methyl)pyridine-2-yl)methyl)-2-aminopropanoic acid **5**

¹³C NMR Spectrum (CD₃OD, 75 MHz)

