

Supplementary Material

An efficient synthesis of optically active herbicide (**S**)-metolachlor *via* reductive ring opening of 2-methoxymethylaziridine

Viswanadh Nalla,^a Mohammad Mujahid,^{ab} Murugesan Sasikumar,^a Prashant Mujumdar,^a and Murugan Muthukrishnan^{a*}

^a*Division of Organic Chemistry, CSIR-National Chemical Laboratory (NCL), Dr. Homi Bhabha Road, Pune 411 008, India*

^b*Department of Chemistry, Shri. Dr. R. G. Rathod Arts & Science College, Murtizapur, Dist Akola, India*

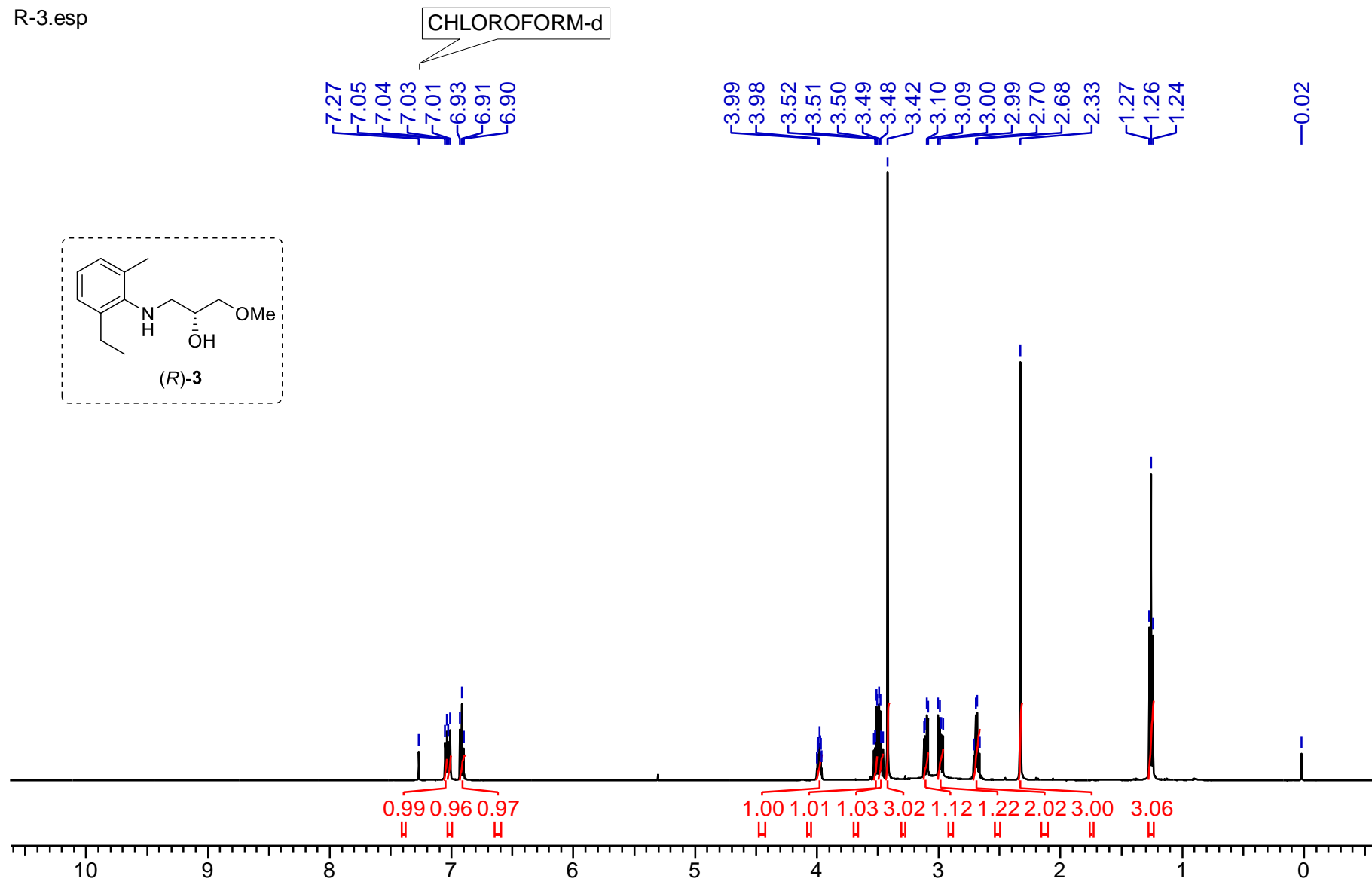
Email: m.muthukrishnan@ncl.res.in

Table of Contents

¹ H NMR of compound (R)-3:	S2
¹³ C NMR of compound (R)-3:	S3
¹ H NMR of compound (S)-4:.....	S4
¹³ C NMR of compound (S)-4:.....	S5
¹ H NMR of compound (S)-5:.....	S6
¹³ C NMR of compound (S)-5:.....	S7
¹ H NMR of compound (S)-1:.....	S8
¹³ C NMR of compound (S)-1:.....	S9
Chiral HPLC analysis of compound (S)-5.....	S10

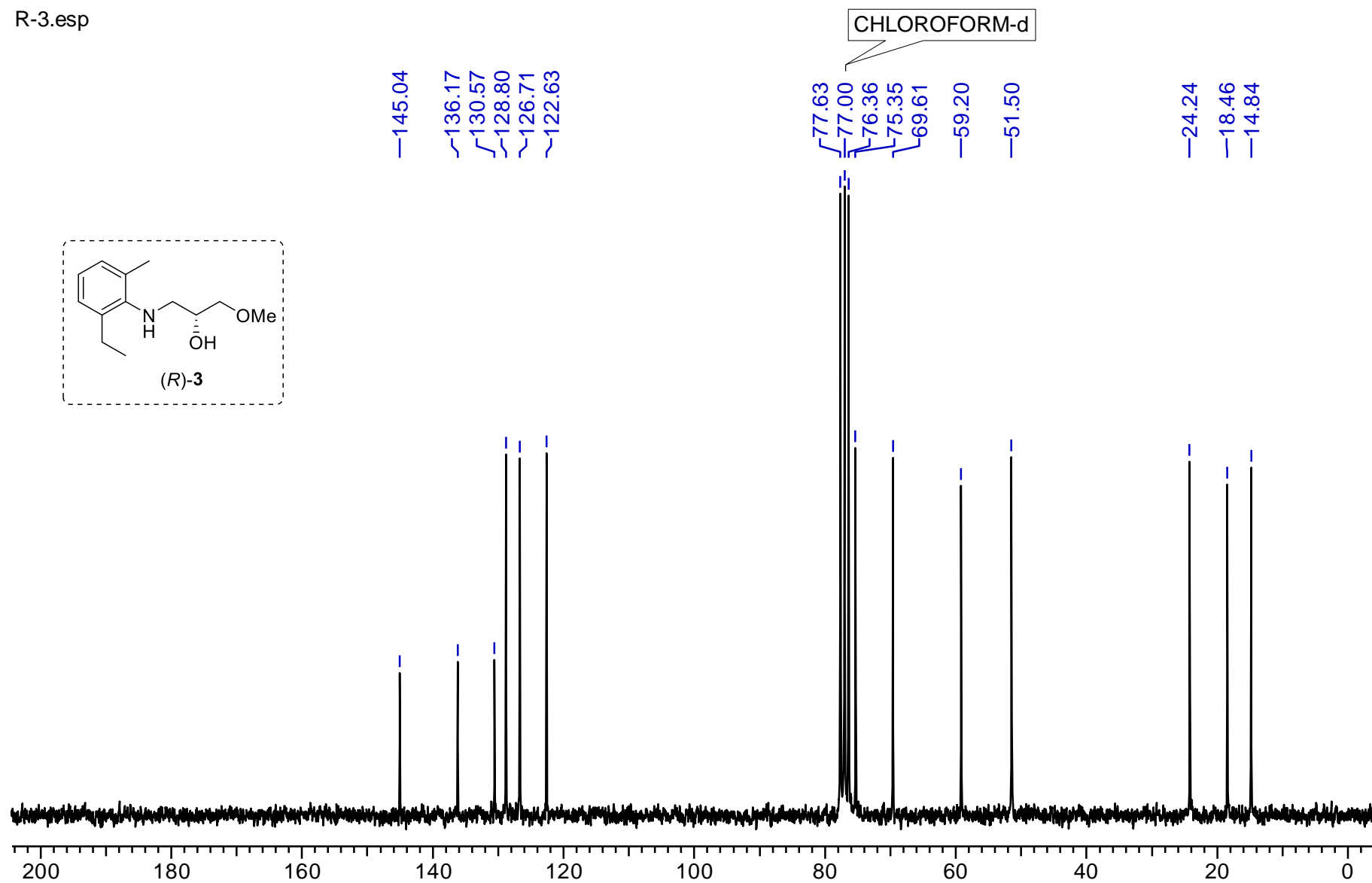
^1H NMR (500 MHz, CDCl_3) of compound (*R*)-3:

R-3.esp



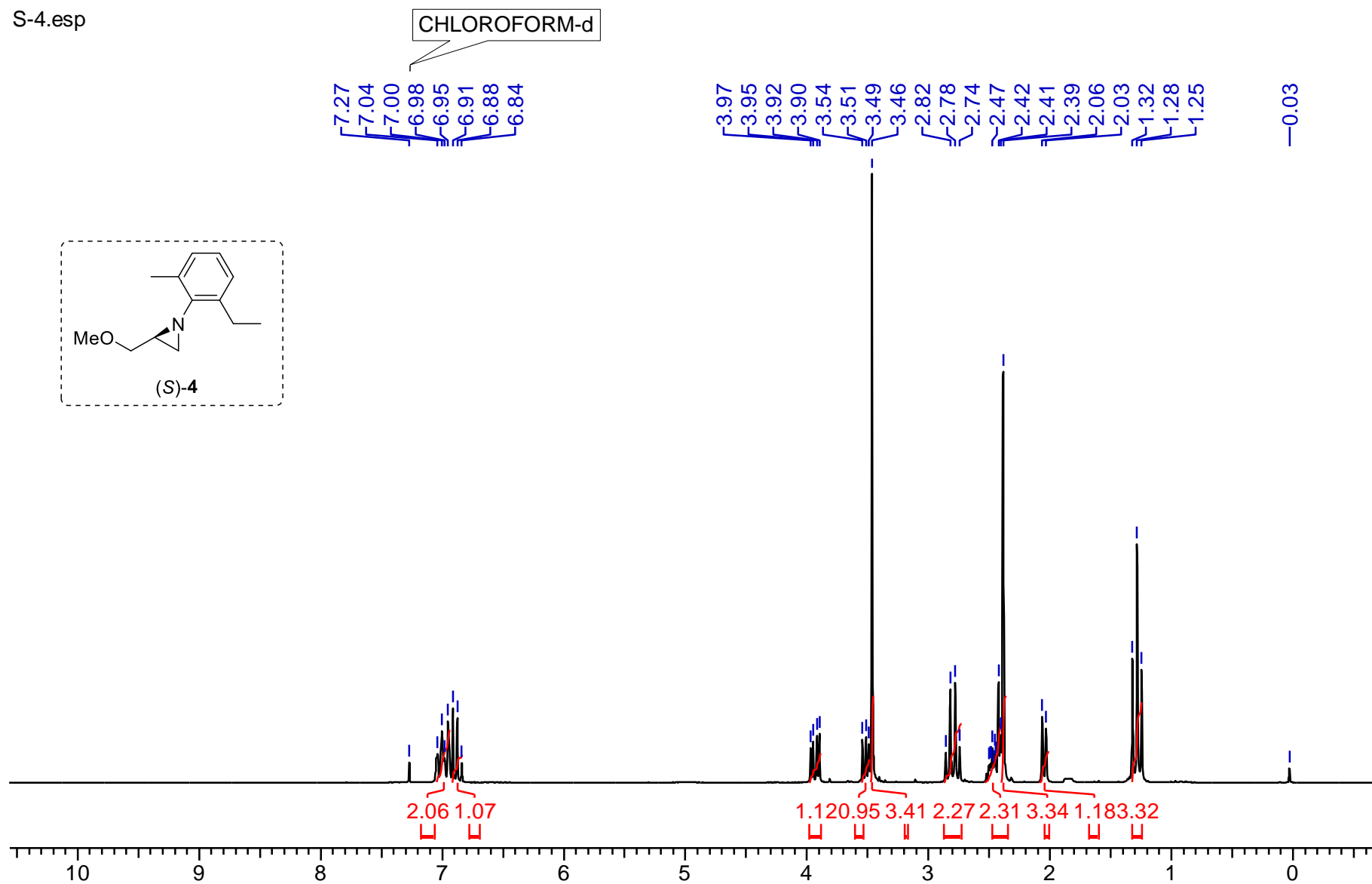
^{13}C NMR (50 MHz, CDCl_3) of compound (*R*)-3:

R-3.esp



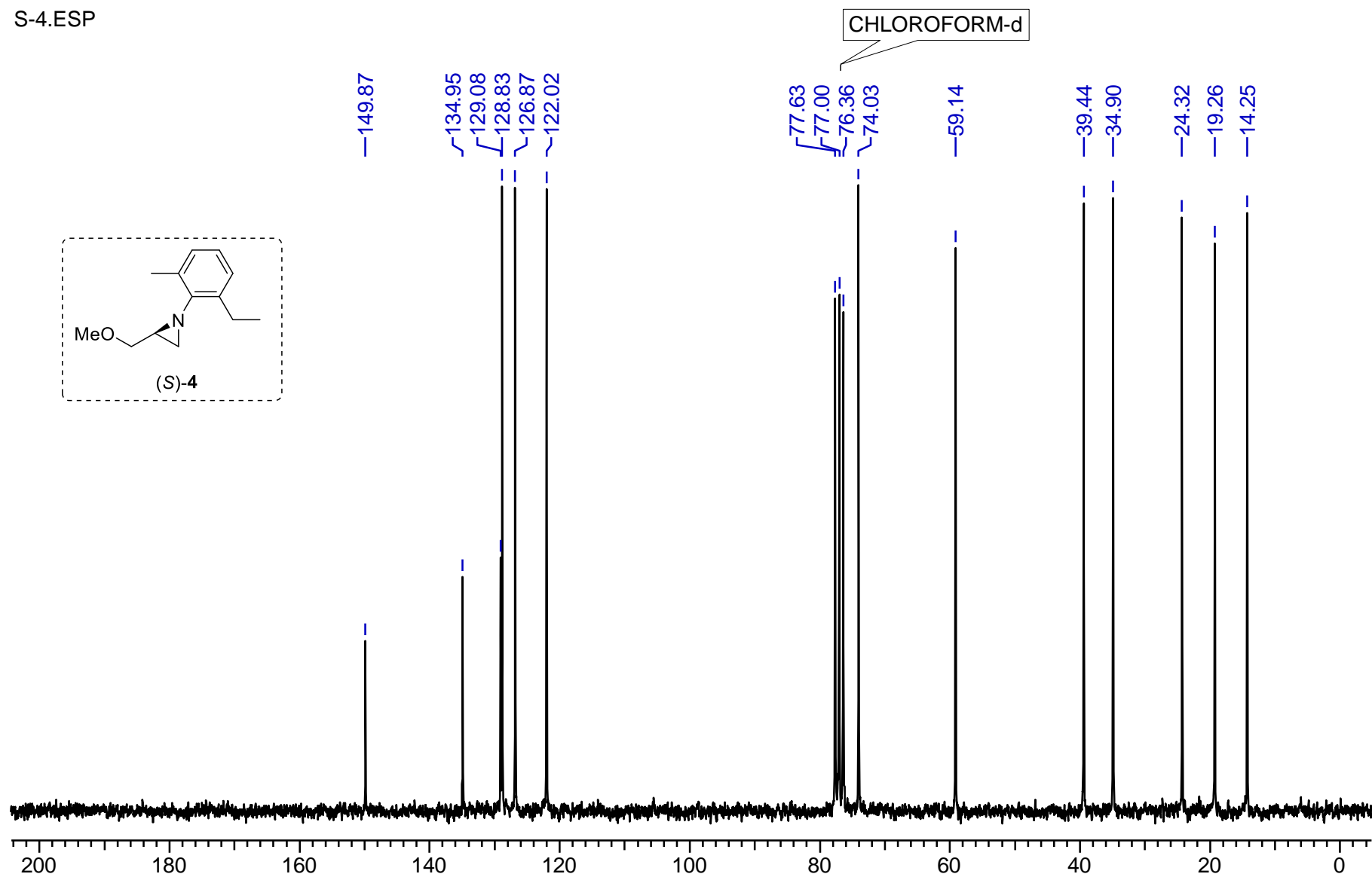
^1H NMR (200 MHz, CDCl_3) of compound (S)-4:

S-4.esp



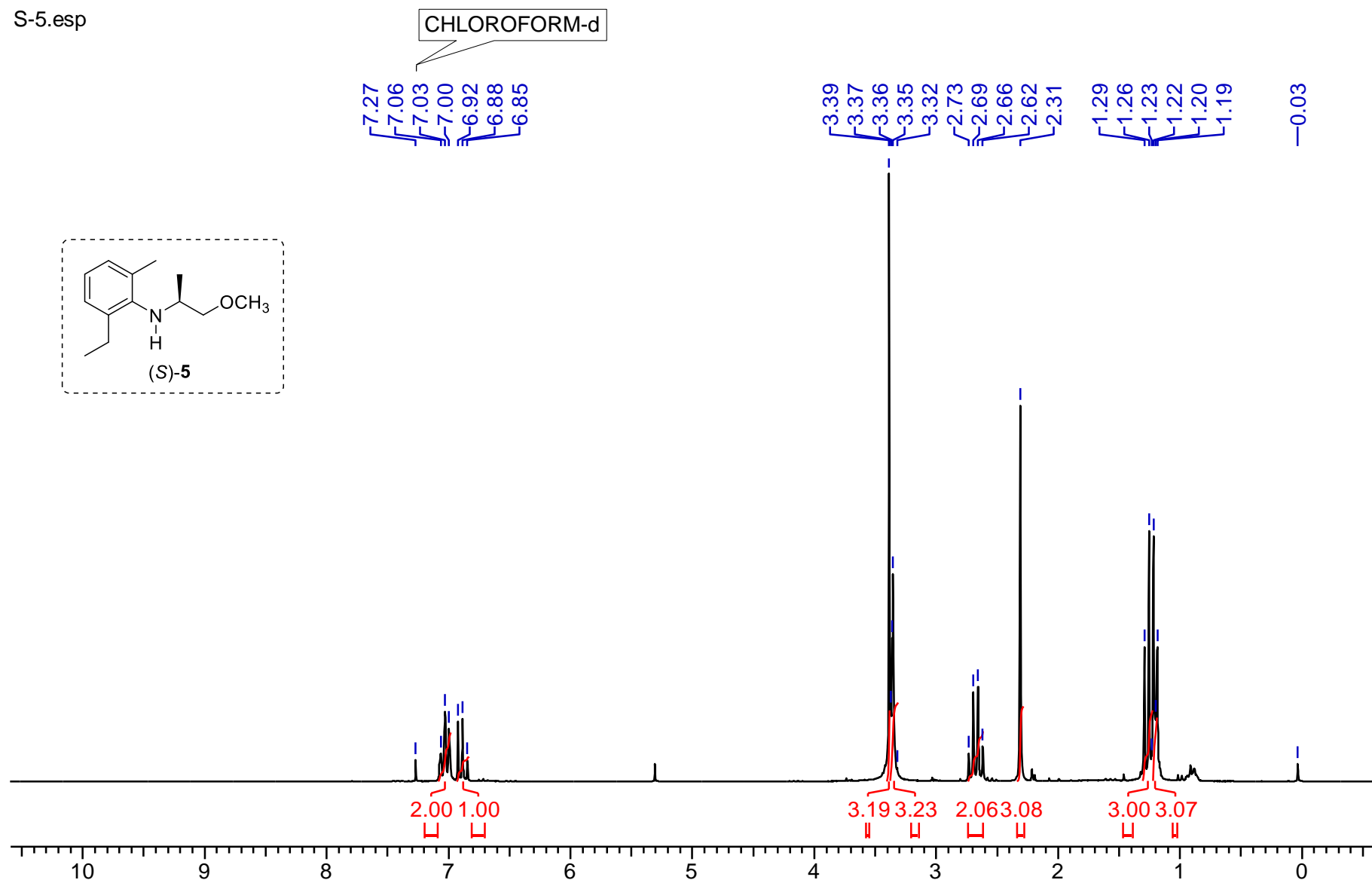
^{13}C NMR (50 MHz, CDCl_3) of compound (S)-4:

S-4.ESP



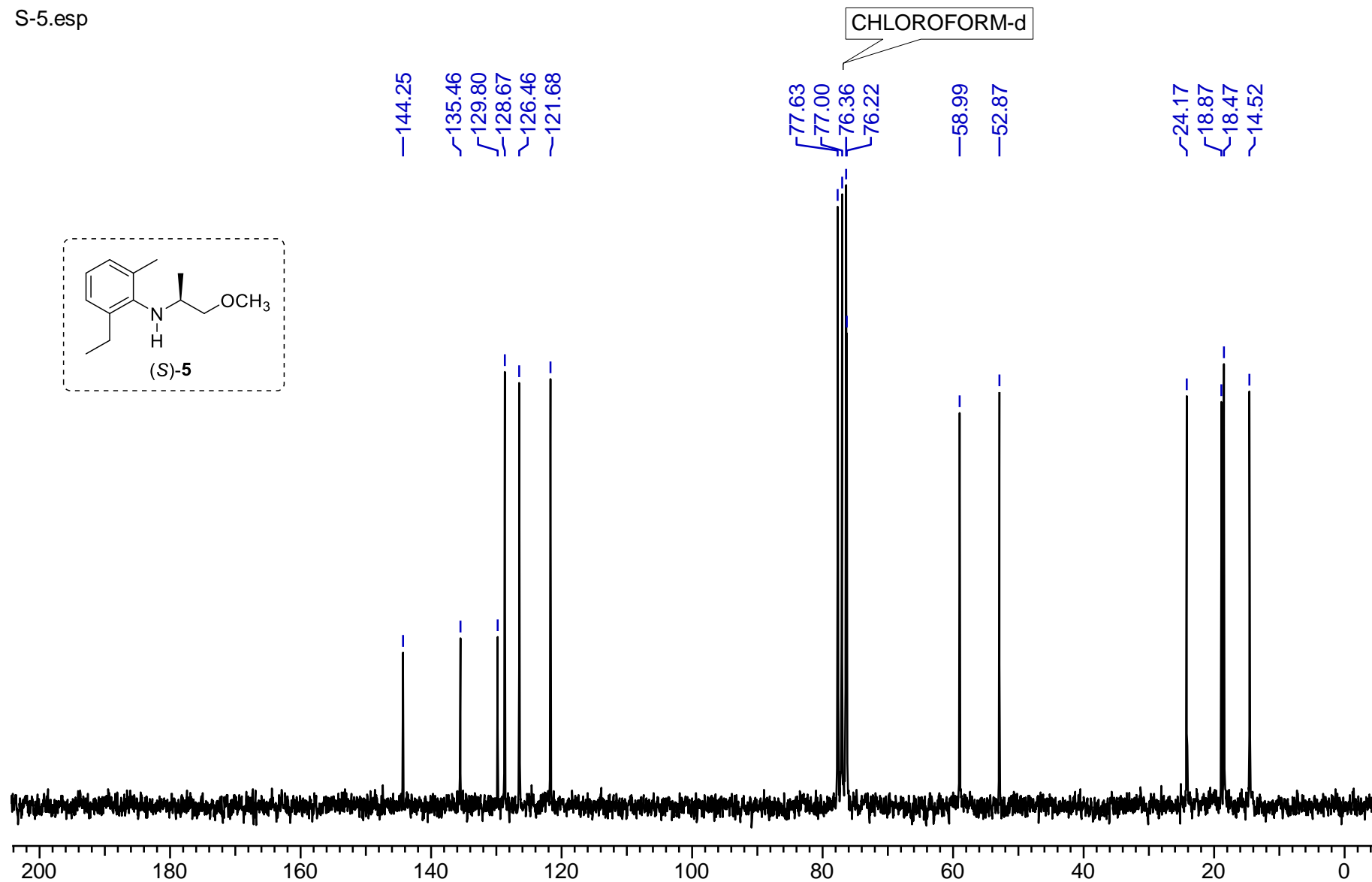
^1H NMR (200 MHz, CDCl_3) of compound (S)-5:

S-5.esp



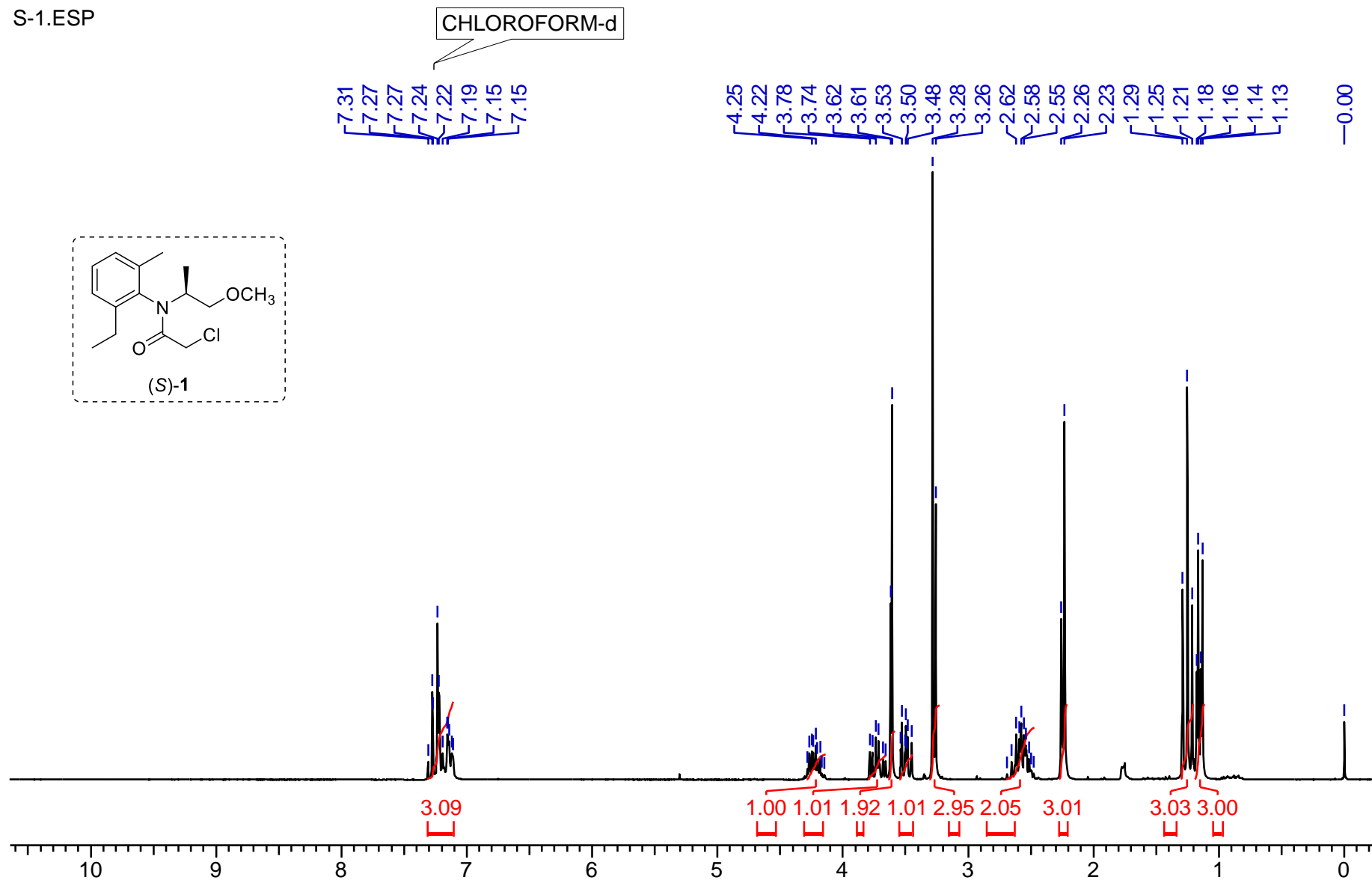
^{13}C NMR (50 MHz, CDCl_3) of compound (S)-5:

S-5.esp



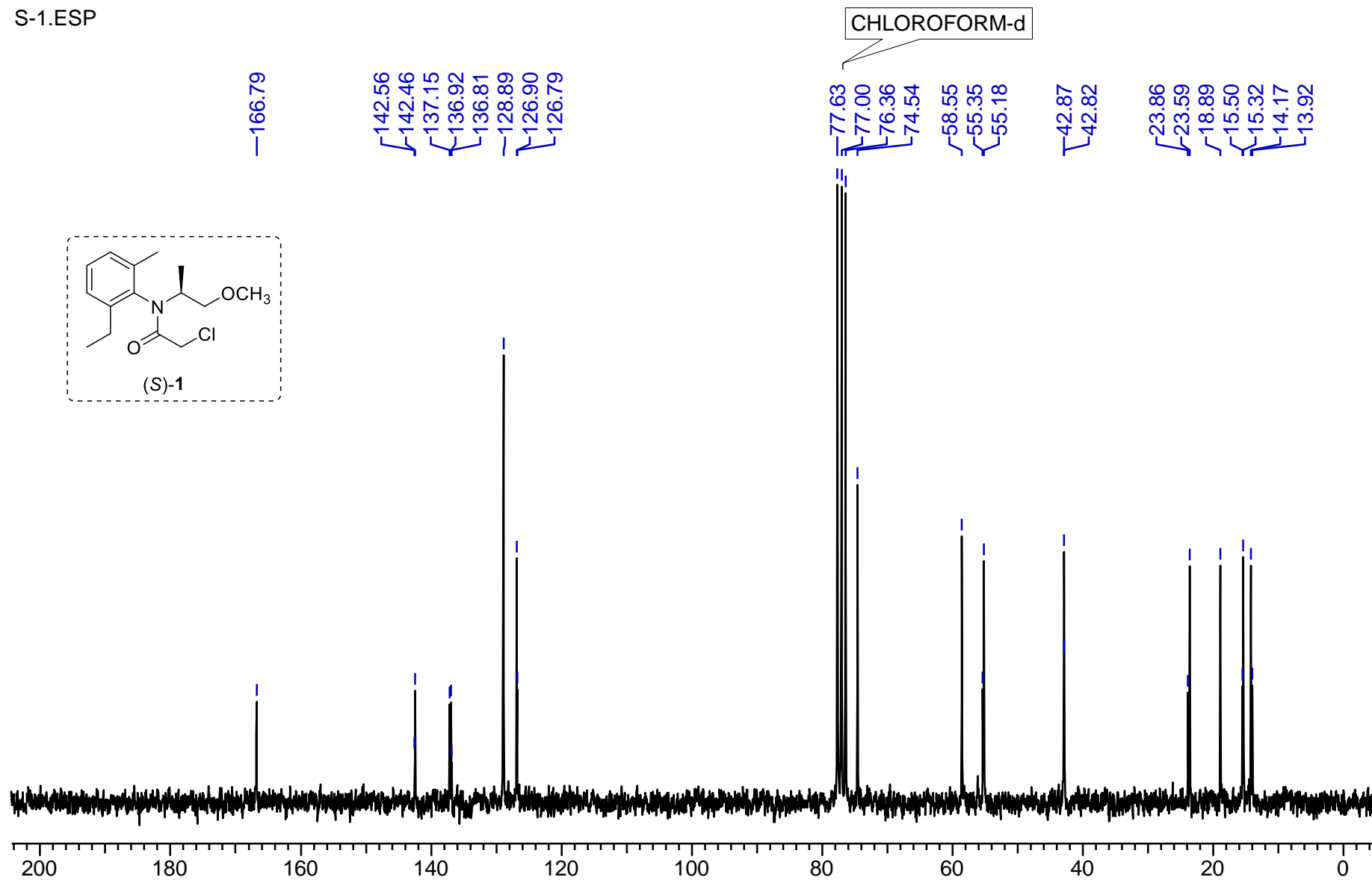
^1H NMR (200 MHz, CDCl_3) of compound (S)-1:

S-1.ESP



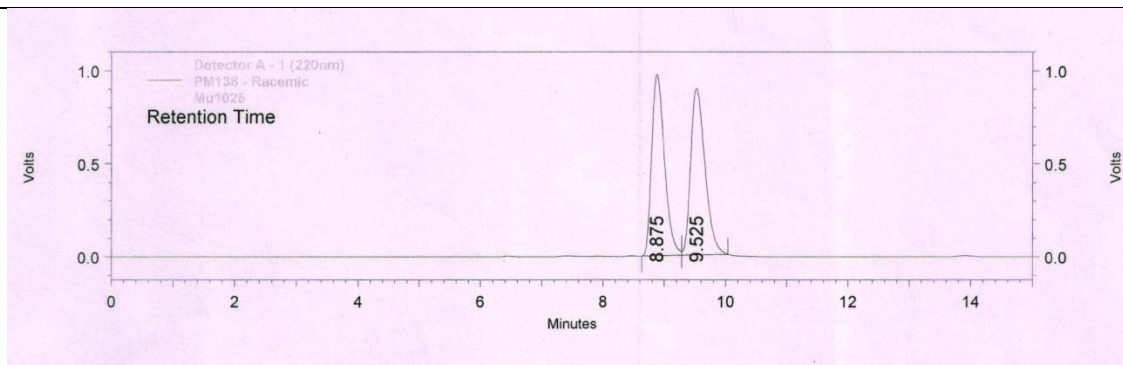
^{13}C NMR (50 MHz, CDCl_3) of compound (S)-1:

S-1.ESP

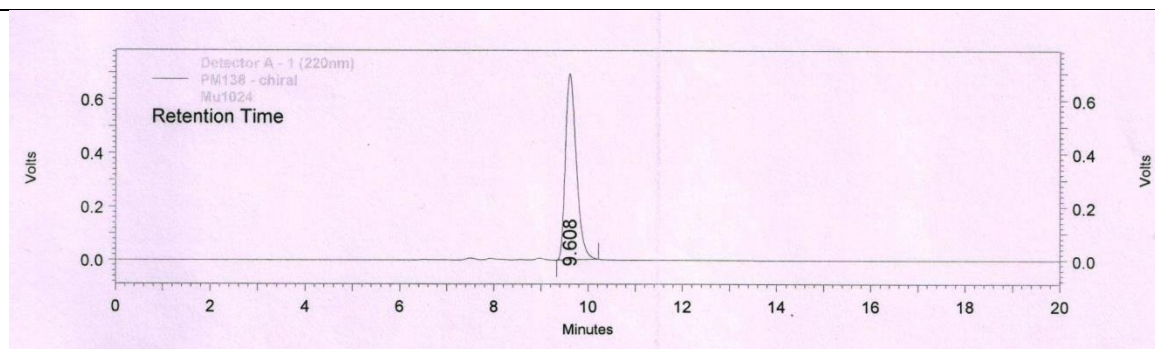


Chiral HPLC analysis of Compound (S)-5:

Conditions: Chiralcel OD-H (250 X 4.6 mm) column; eluent: n-Hexane/isopropanol (99.75:0.25); flow rate: 0.5mL/min; detector 220 nm.

**Racemic Sample Chromatograph**

Pk #	Retention Time (mins)	Area	Area %
1	8.875	14342294	49.725
2	9.525	14500801	50.275
Totals			

**Chiral Sample Chromatograph**

Pk #	Retention Time (mins)	Area	Area %
1	9.608	11219758	100.000
Totals		11219758	100.000