

Electronic Supplementary Information

Synthesis of 2-aryl-3-(2-cyanoethyl)aziridines and their chemical and enzymatic hydrolysis towards γ -lactams and γ -lactones

Karen Mollet,¹ Lena Decuyper,¹ Saskia Vander Meeren,¹ Nicola Piens,¹ Karel De Winter,²
Tom Desmet² and Matthias D'hooghe^{1,*}

¹*SynBioC Research Group, Department of Sustainable Organic Chemistry and Technology, Faculty of Bioscience Engineering, Ghent University, Coupure links 653, B-9000 Ghent, Belgium
matthias.dhooghe@UGent.be*

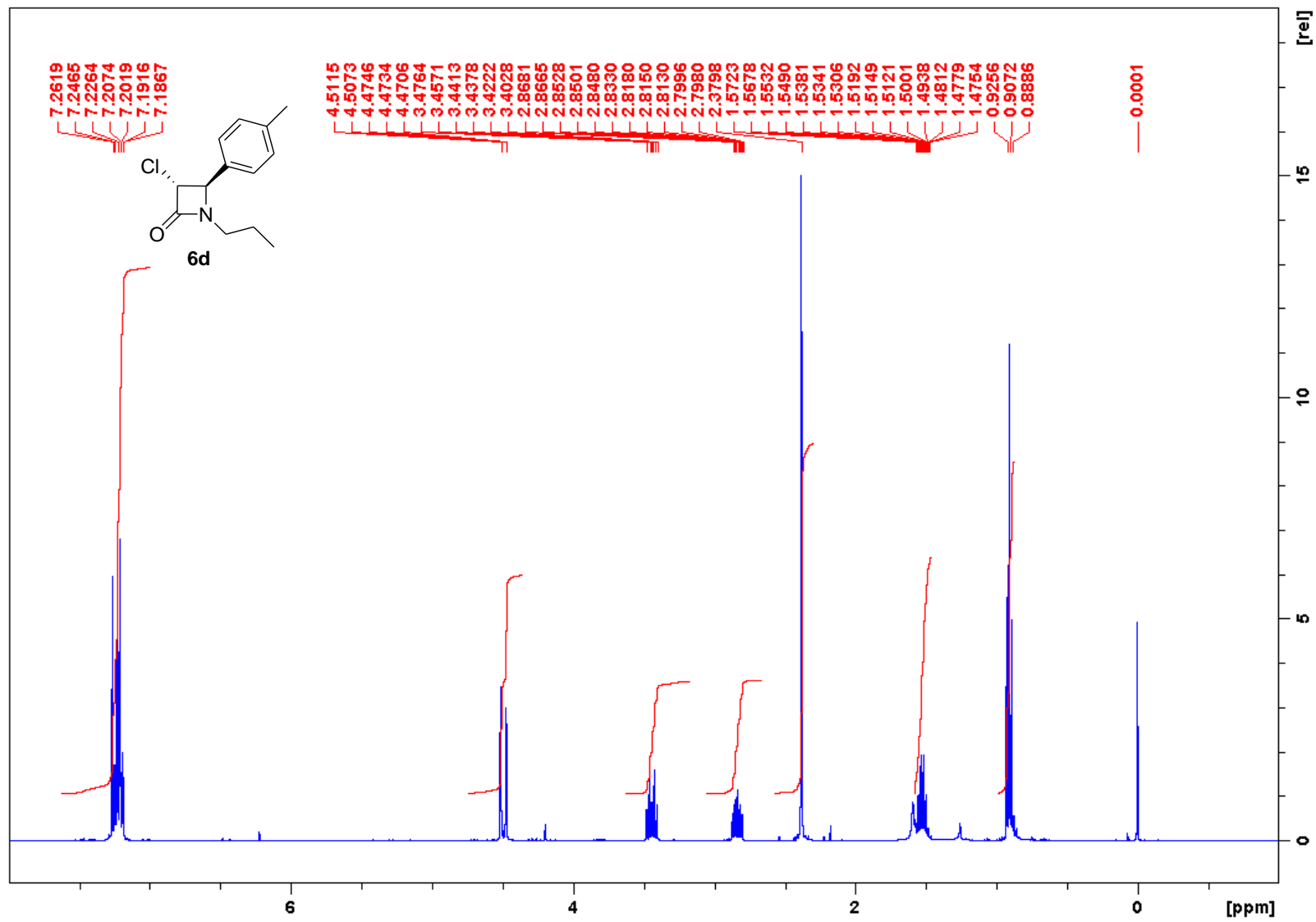
²*Department of Biochemical and Microbial Technology, Faculty of Bioscience Engineering, Ghent University, Coupure links 653, B-9000 Ghent, Belgium*

Contents

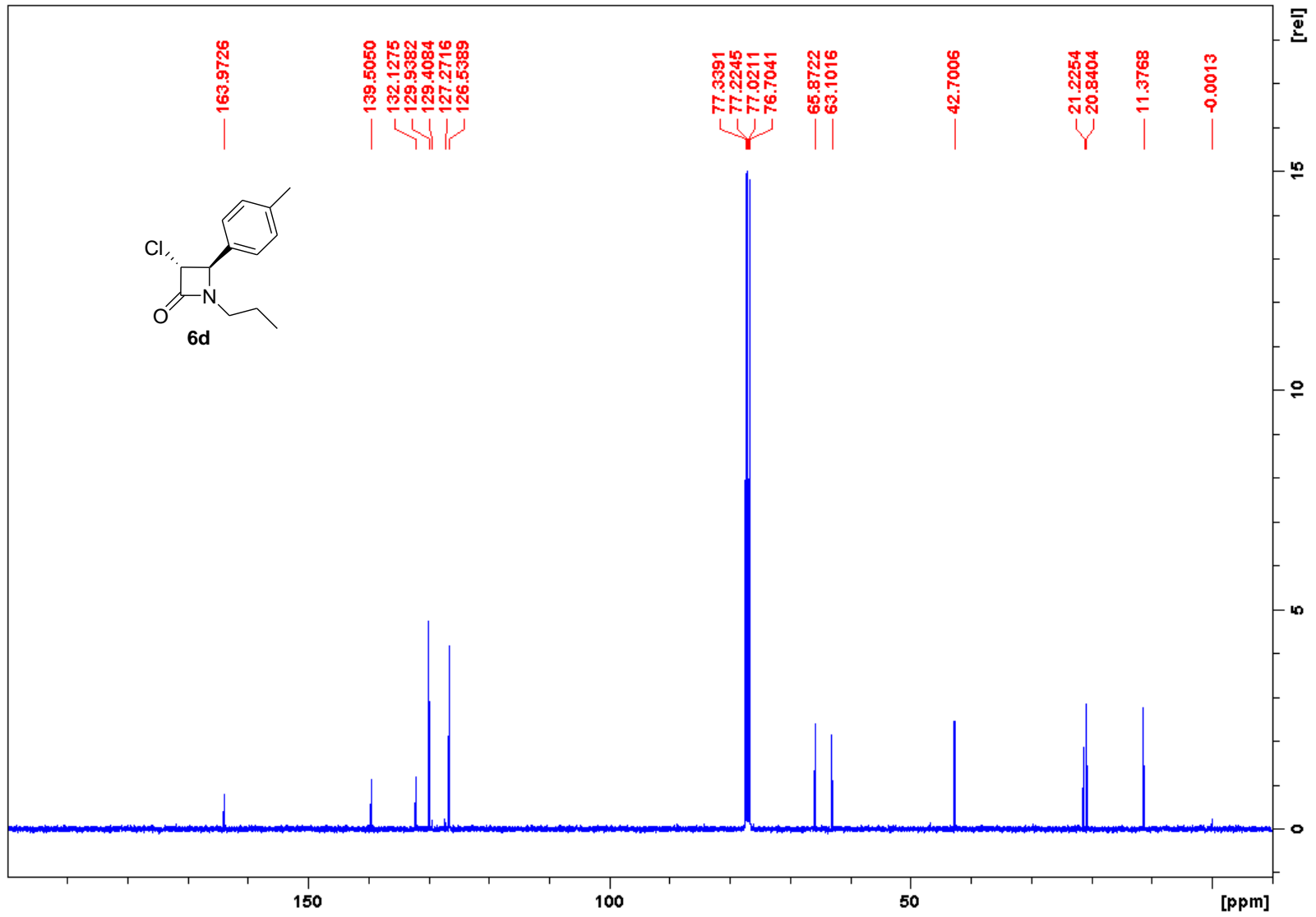
¹H NMR and ¹³C NMR spectra of compounds **6d**, **7a-e**, **9a-c,e**, **10a-c,e**, **11b,c**

S2 – S34

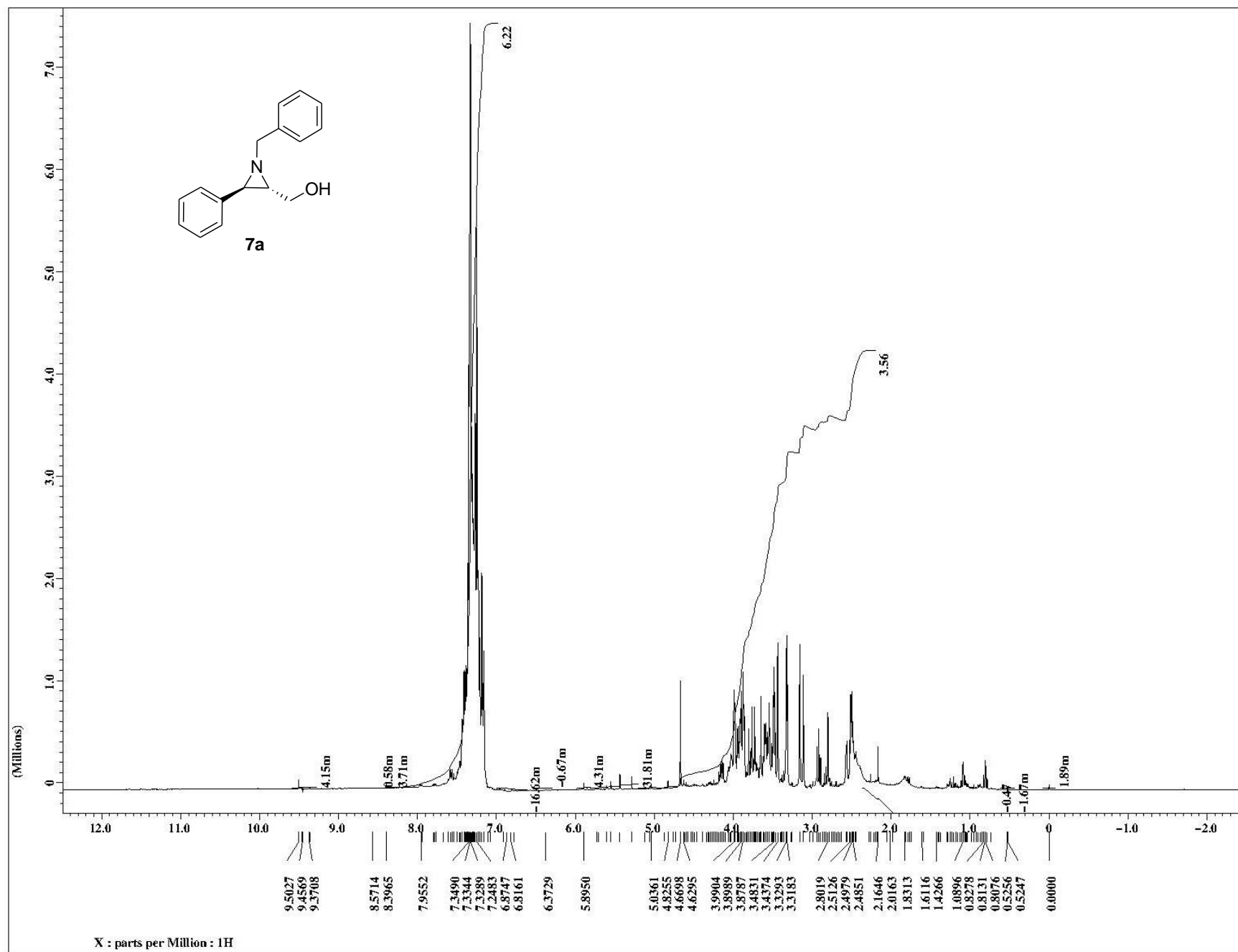
Trans-3-chloro-4-(4-methylphenyl)-1-propylazetidin-2-one **6d**: ¹H NMR



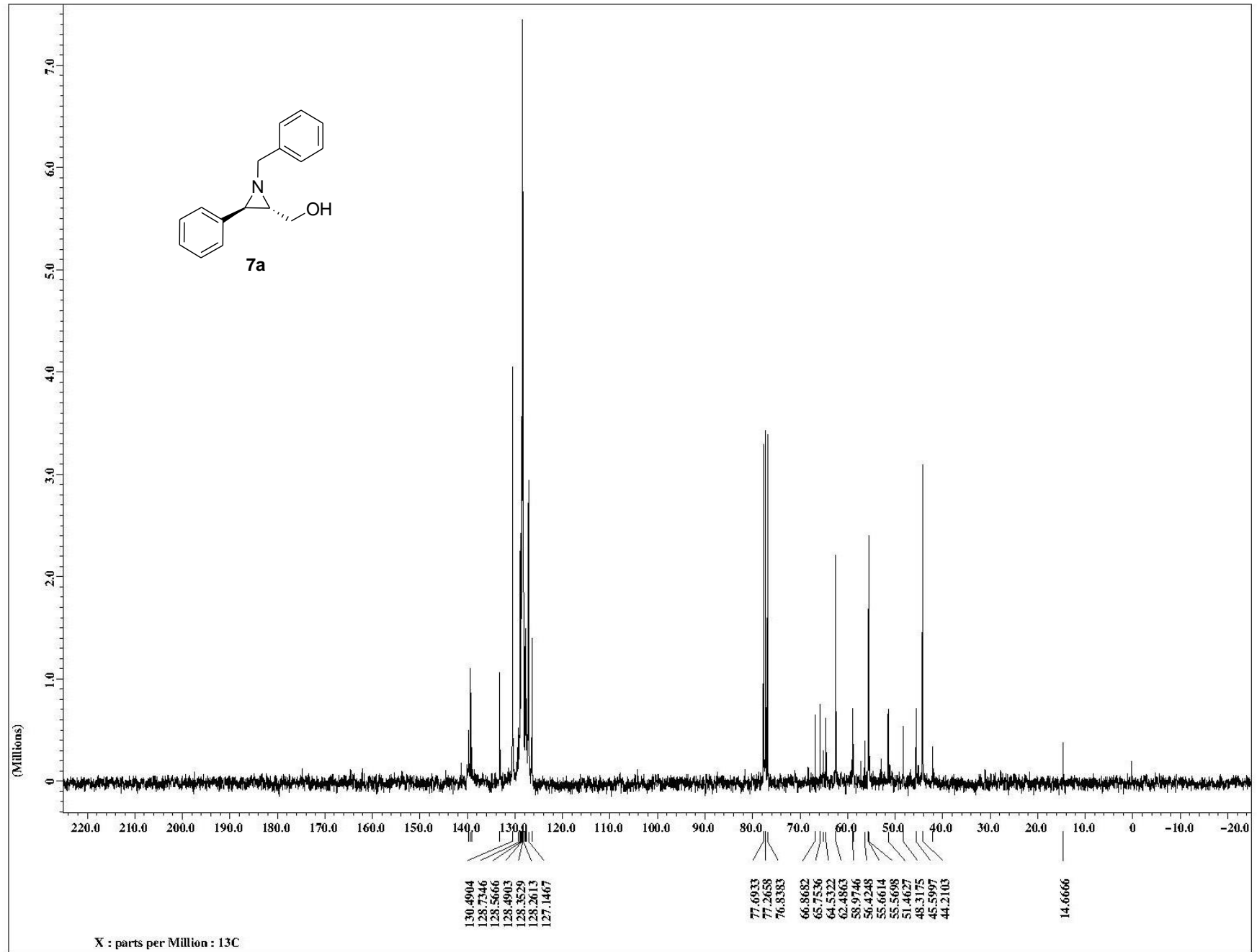
Trans-3-chloro-4-(4-methylphenyl)-1-propylazetidin-2-one **6d**: ^{13}C NMR



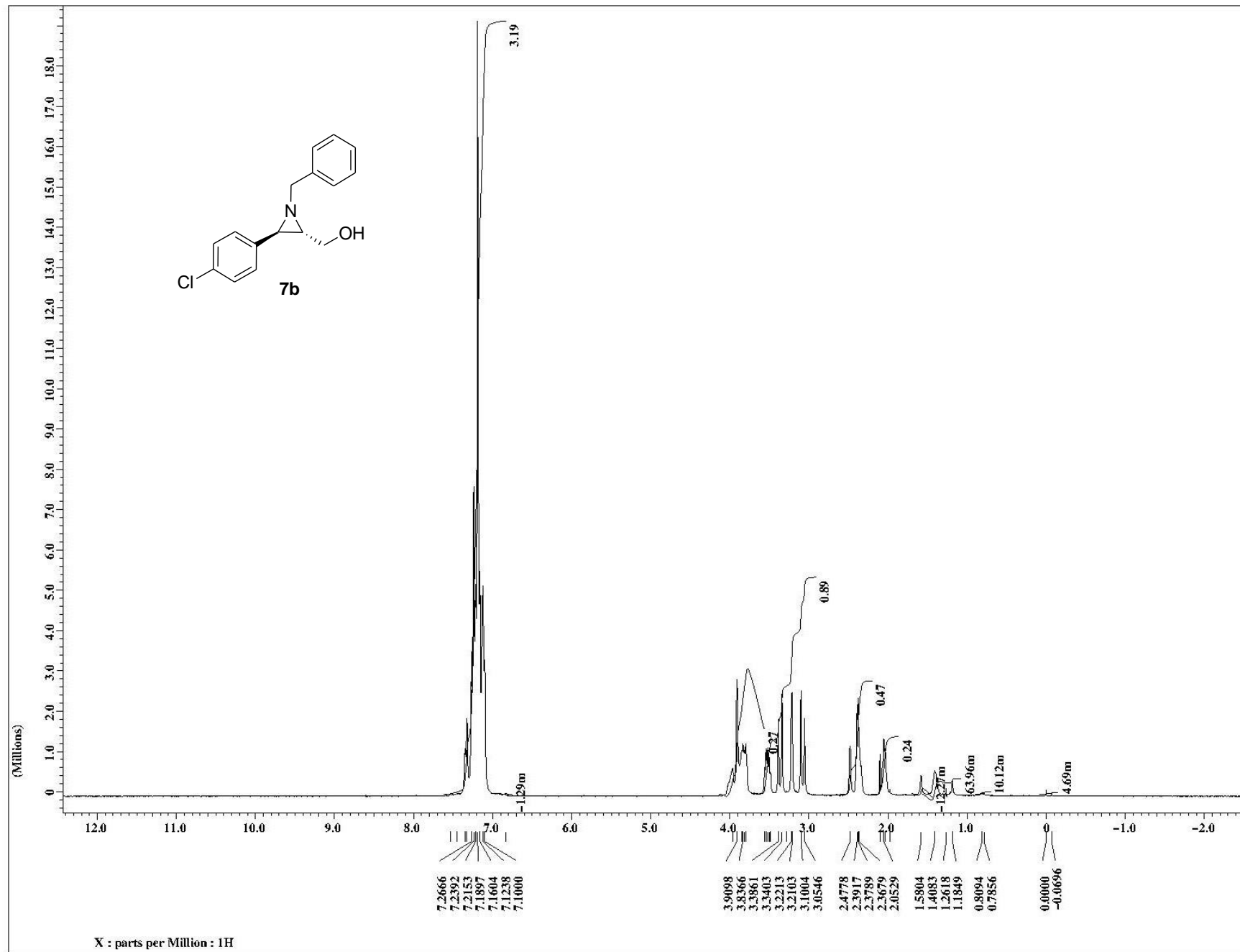
Trans-1-benzyl-3-hydroxymethyl-2-phenylaziridine **7a**: ^1H NMR



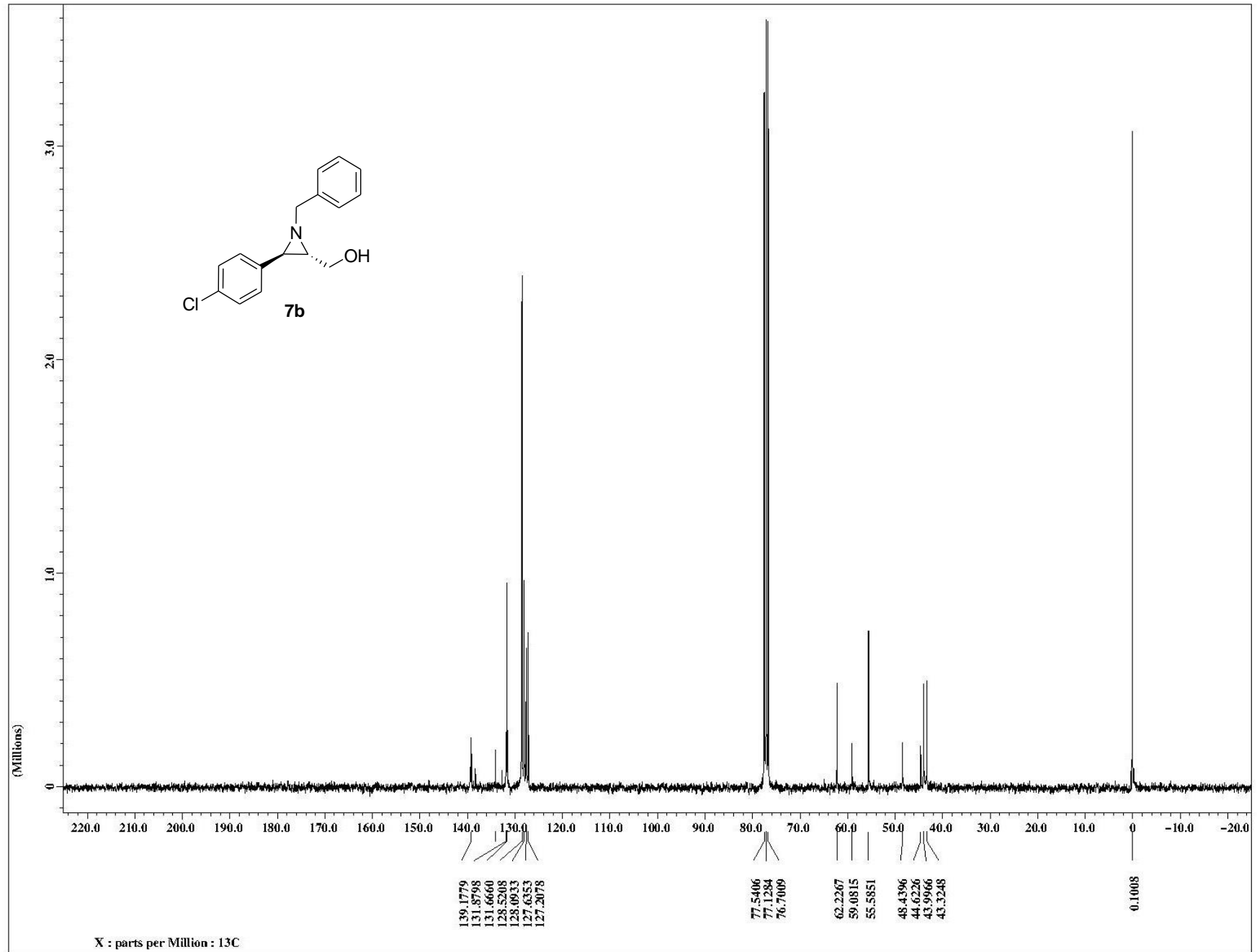
Trans-1-benzyl-3-hydroxymethyl-2-phenylaziridine **7a**: ^{13}C NMR



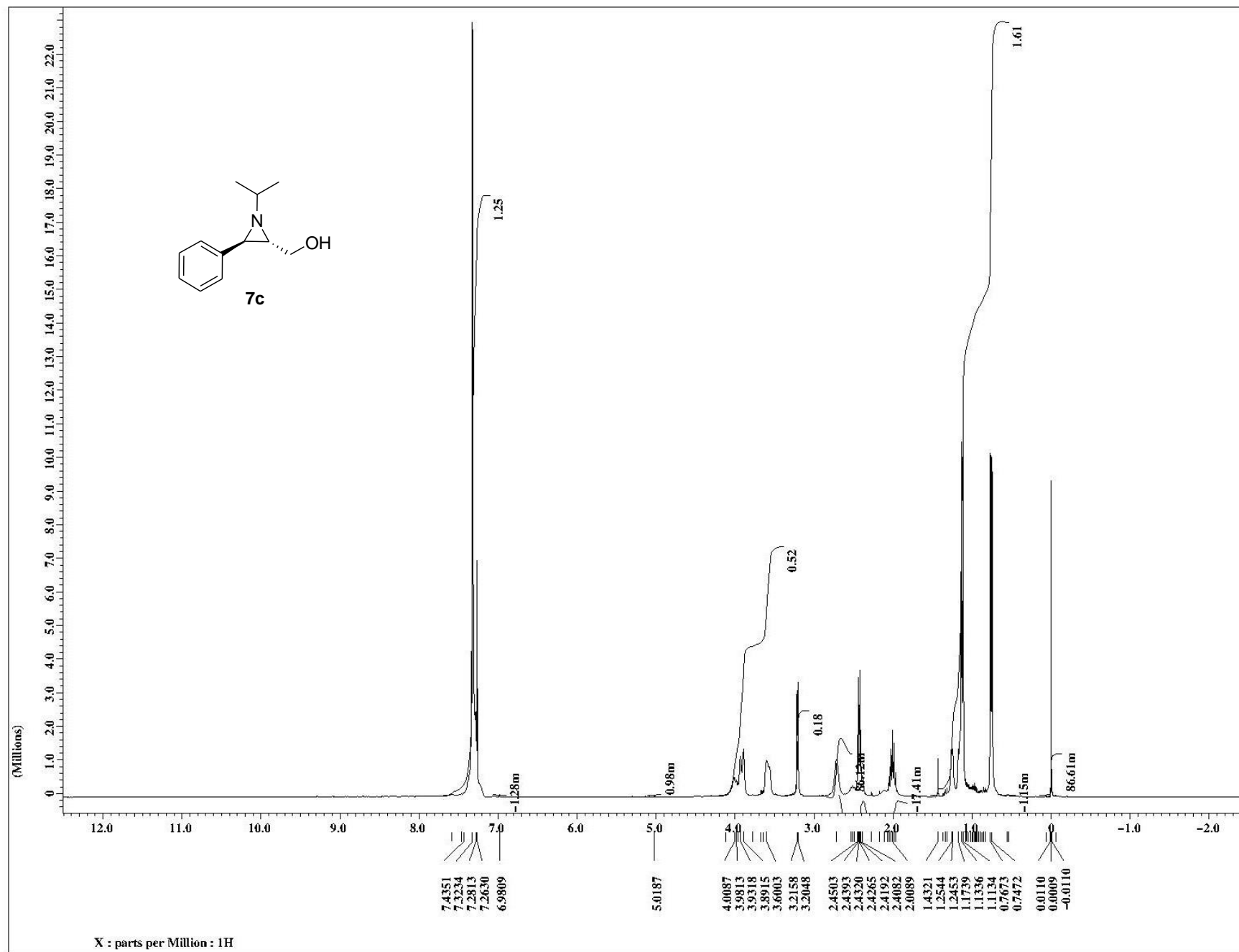
Trans-1-benzyl-2-(4-chlorophenyl)-3-(hydroxymethyl)aziridine **7b**: ^1H NMR



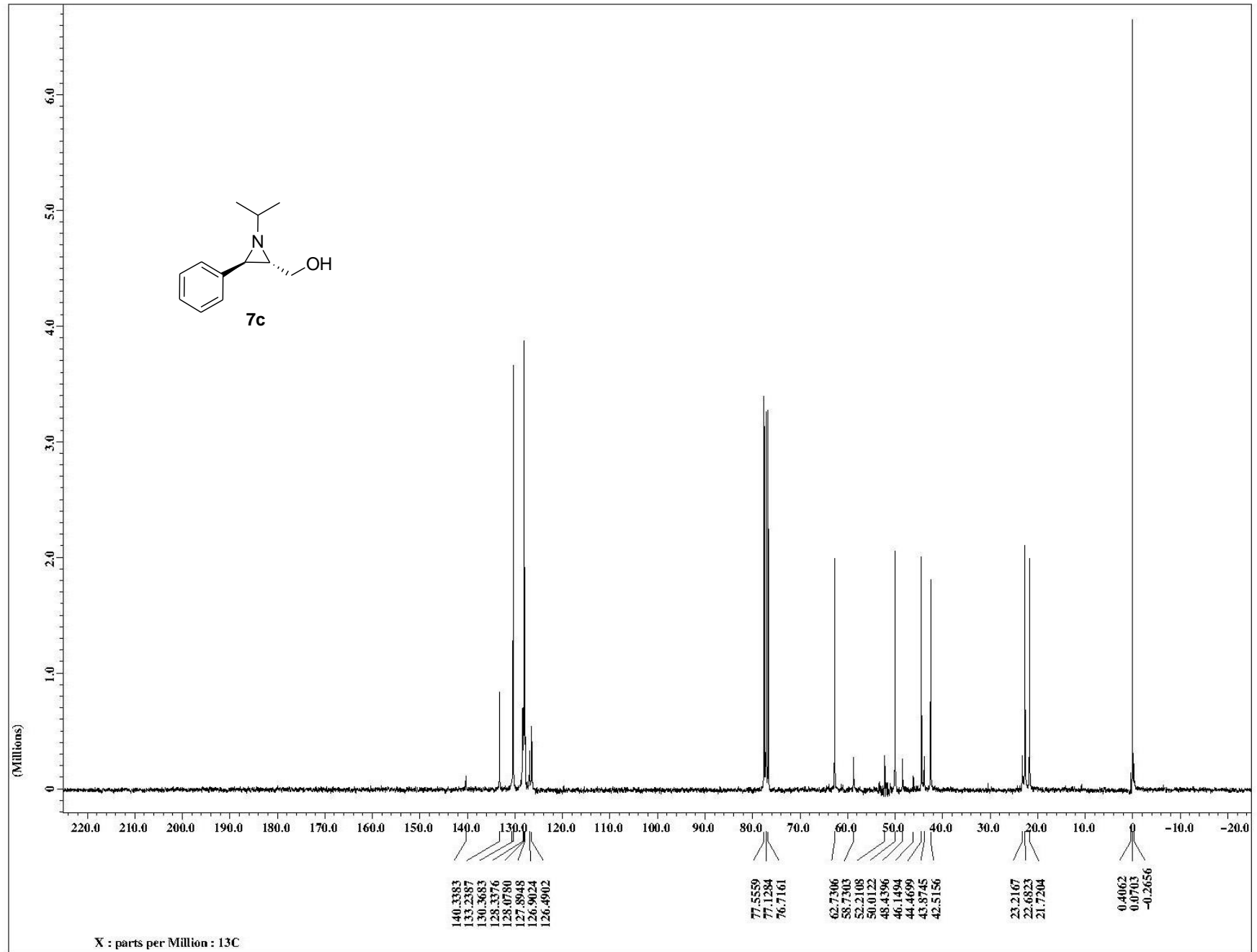
Trans-1-benzyl-2-(4-chlorophenyl)-3-(hydroxymethyl)aziridine **7b**: ^{13}C NMR



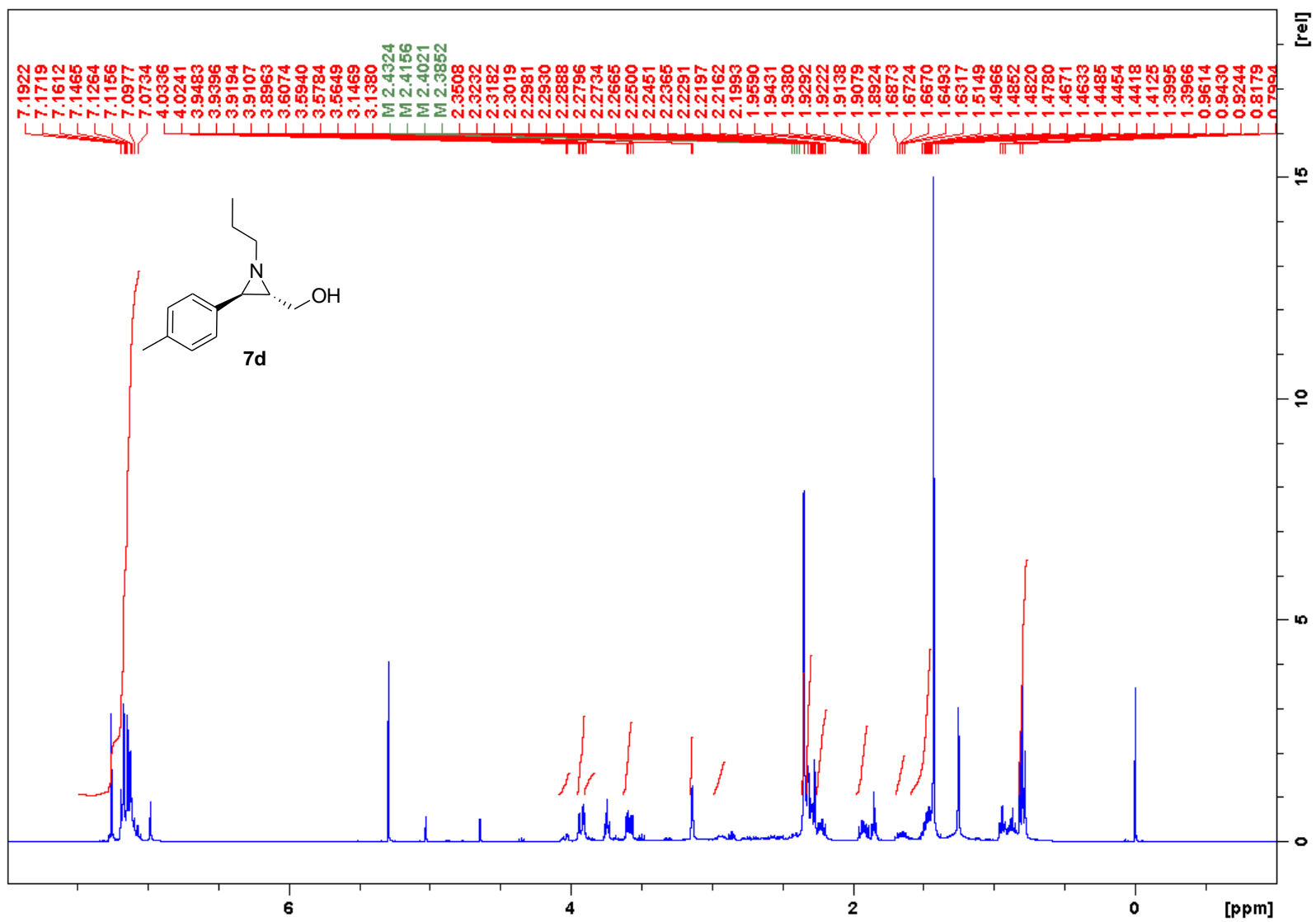
Trans-3-hydroxymethyl-1-isopropyl-2-phenylaziridine **7c**: ^1H NMR



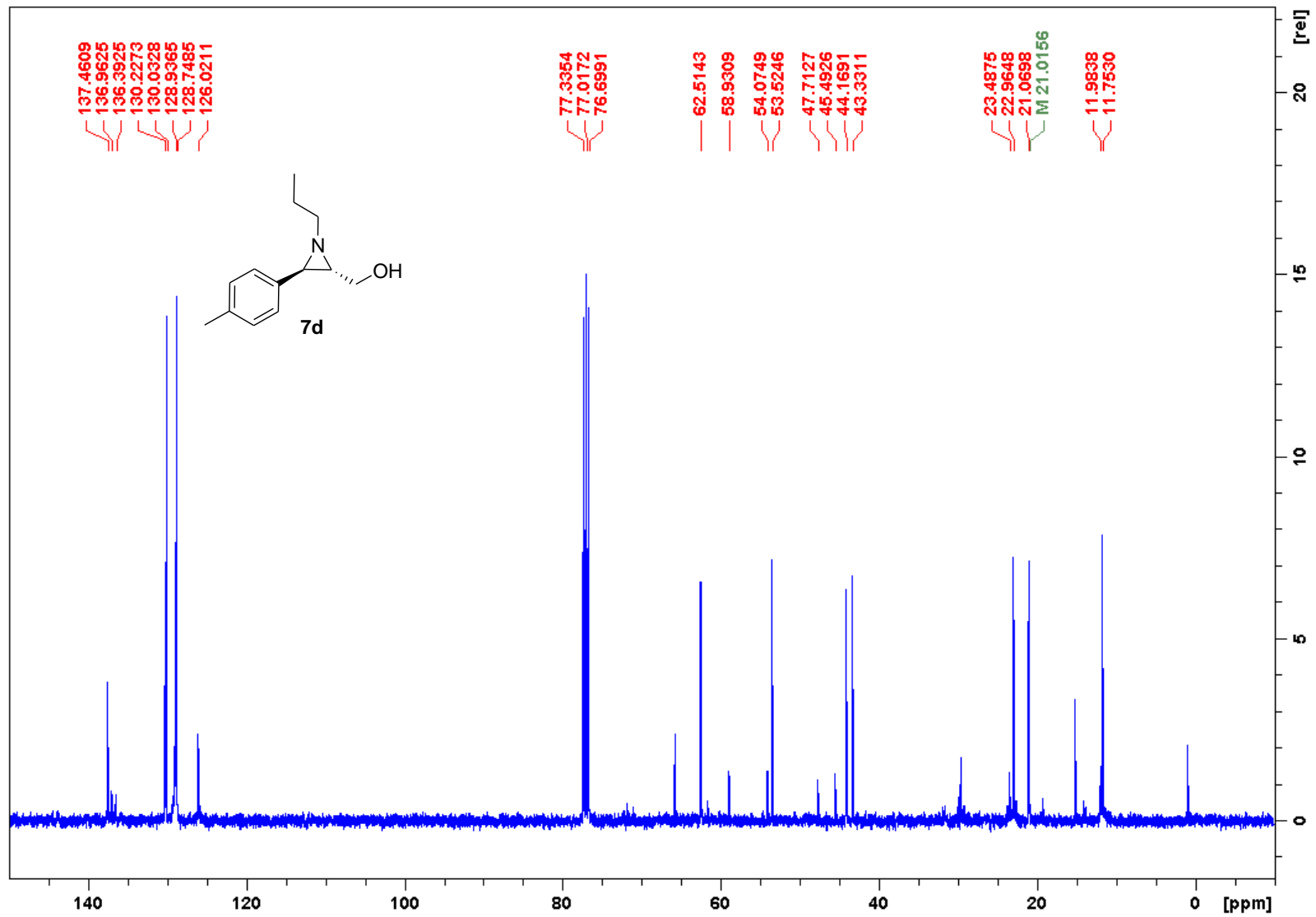
Trans-3-hydroxymethyl-1-isopropyl-2-phenylaziridine **7c**: ^{13}C NMR



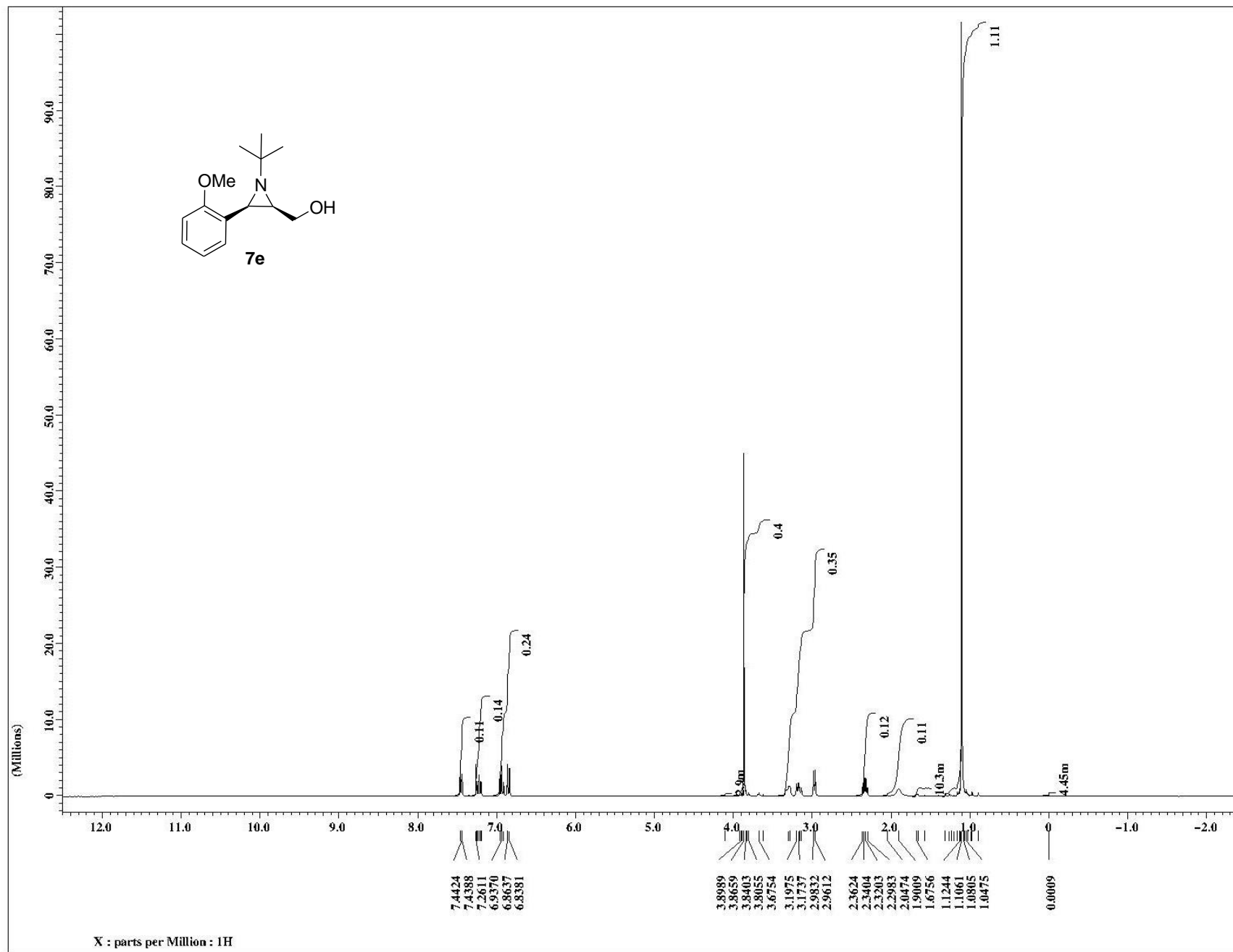
Trans-3-hydroxymethyl-2-(4-methylphenyl)-1-propylaziridine **7d**: ¹H NMR



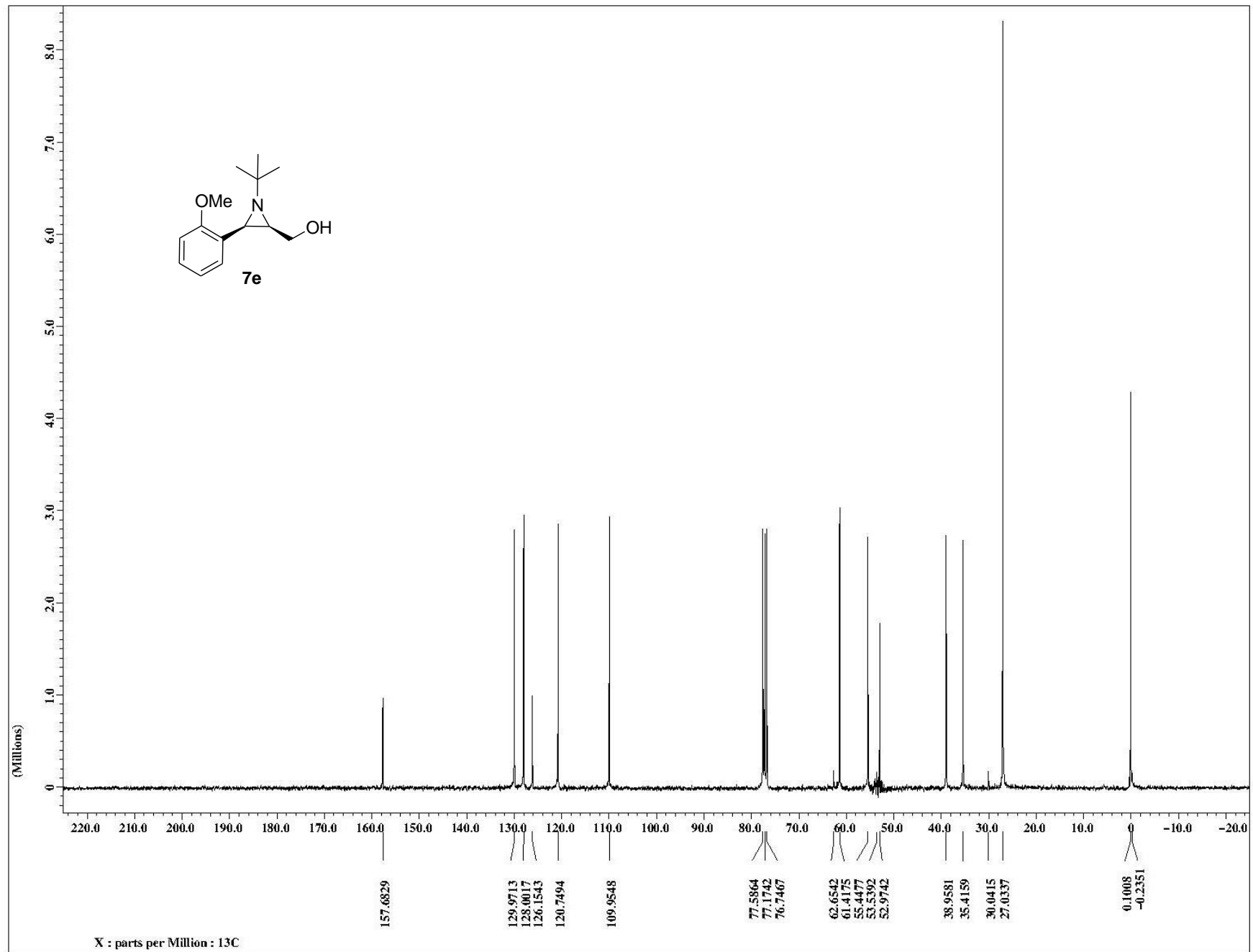
Trans-3-hydroxymethyl-2-(4-methylphenyl)-1-propylaziridine **7d**: ^{13}C NMR



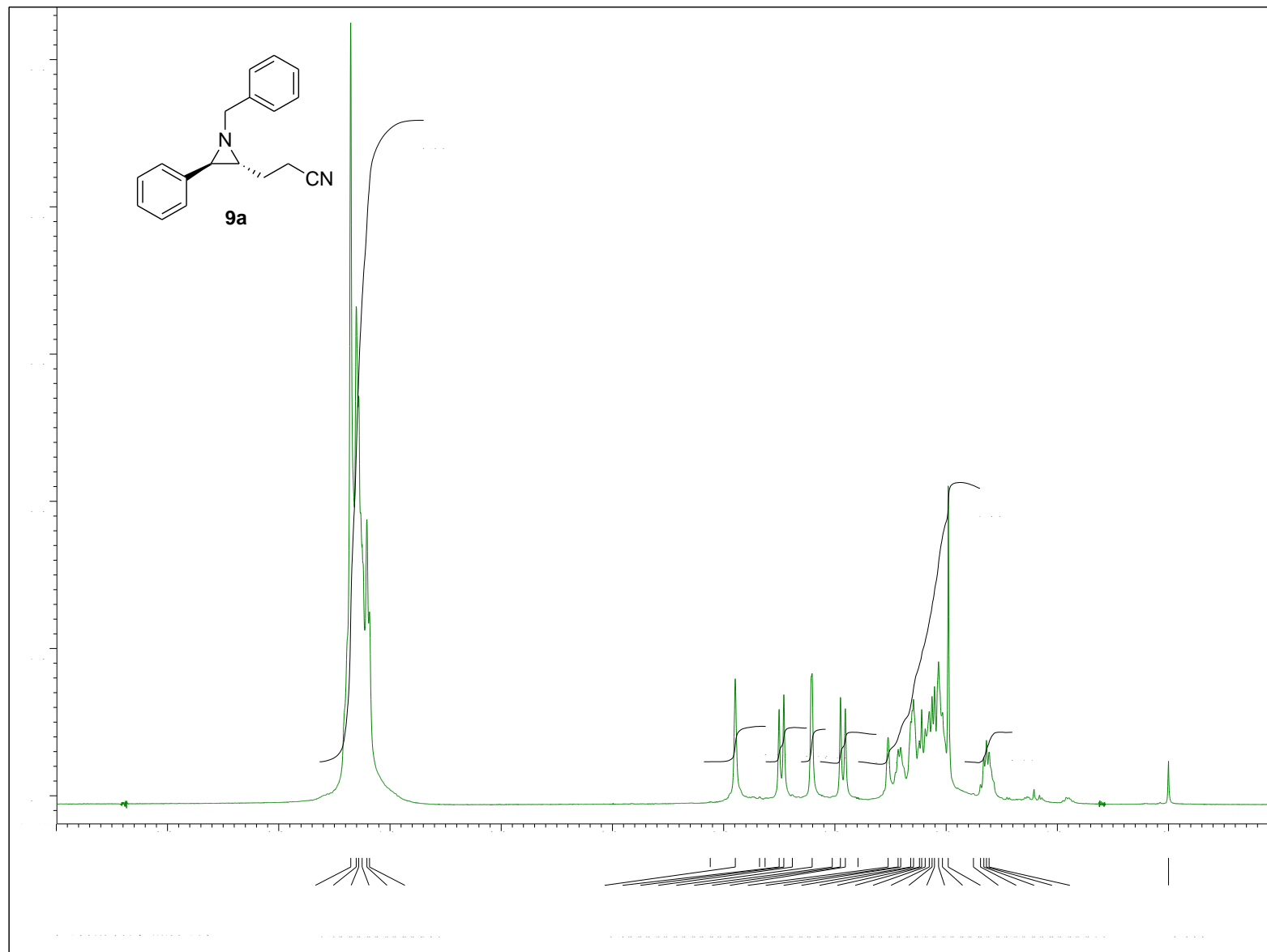
Cis-1-*tert*-butyl-3-hydroxymethyl-2-(2-methoxyphenyl)aziridine **7e**: ^1H NMR



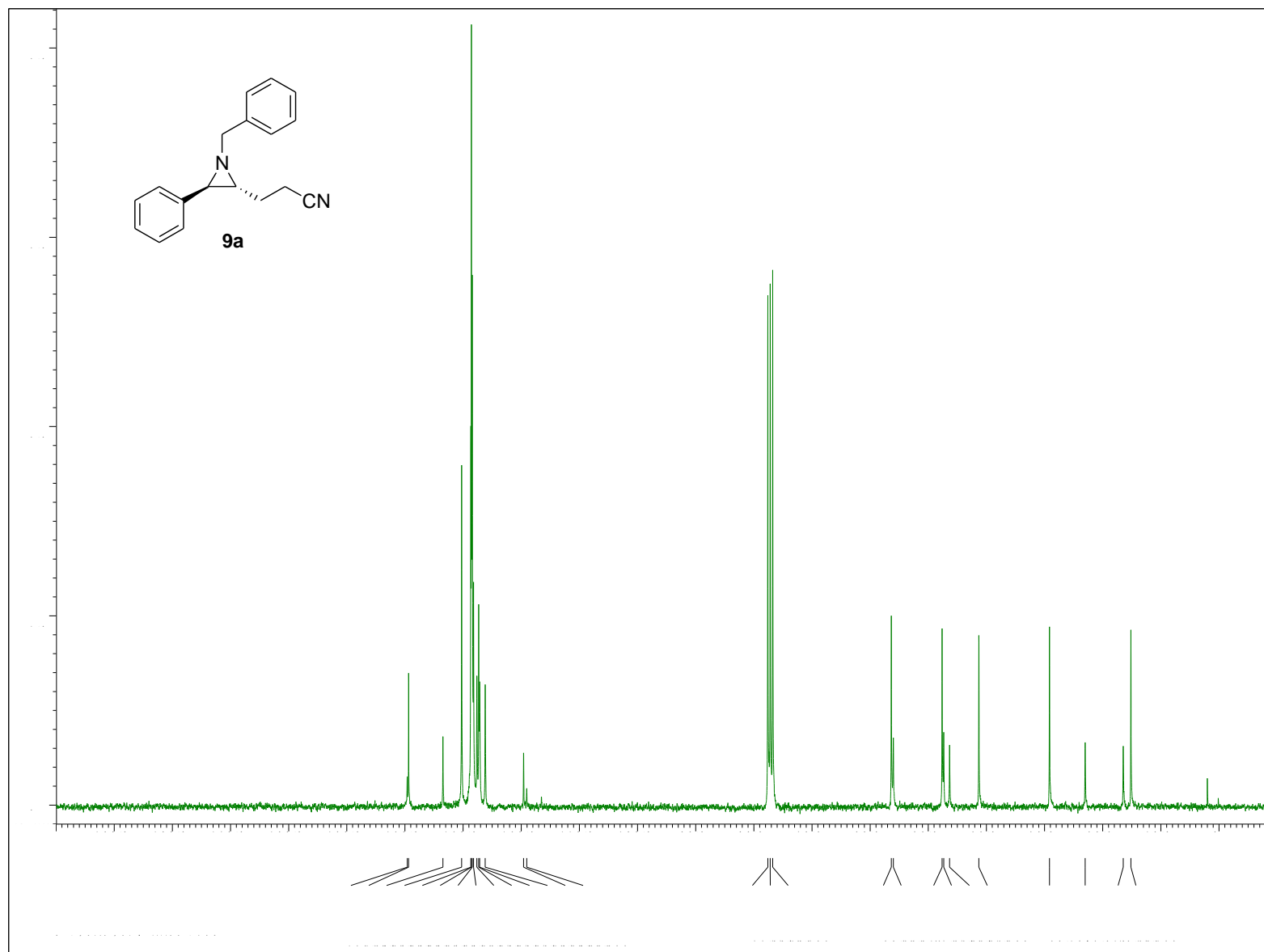
Cis-1-*tert*-butyl-3-hydroxymethyl-2-(2-methoxyphenyl)aziridine **7e**: ^{13}C NMR



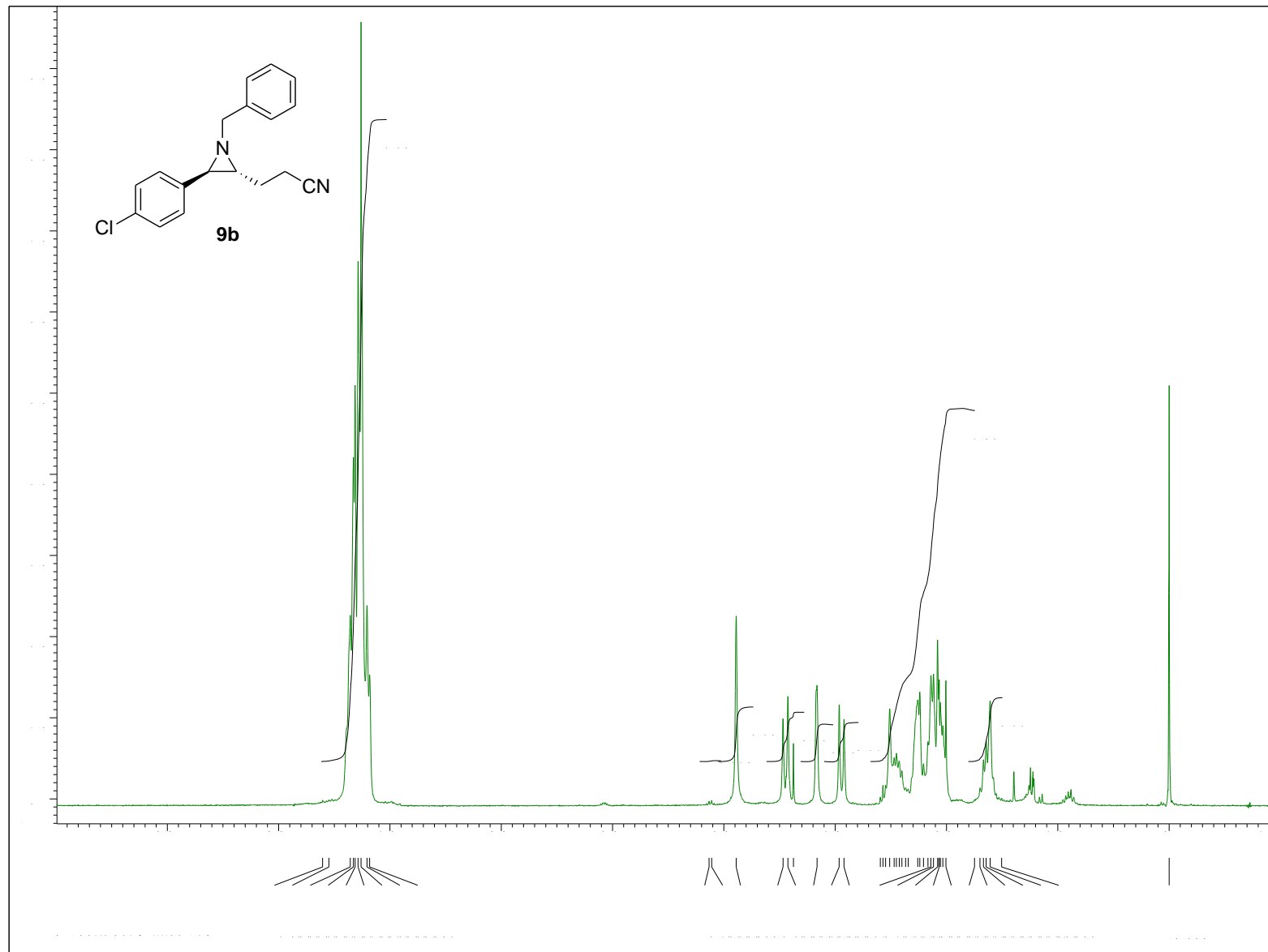
Trans-1-benzyl-3-(2-cyanoethyl)-2-phenylaziridine **9a**: ^1H NMR



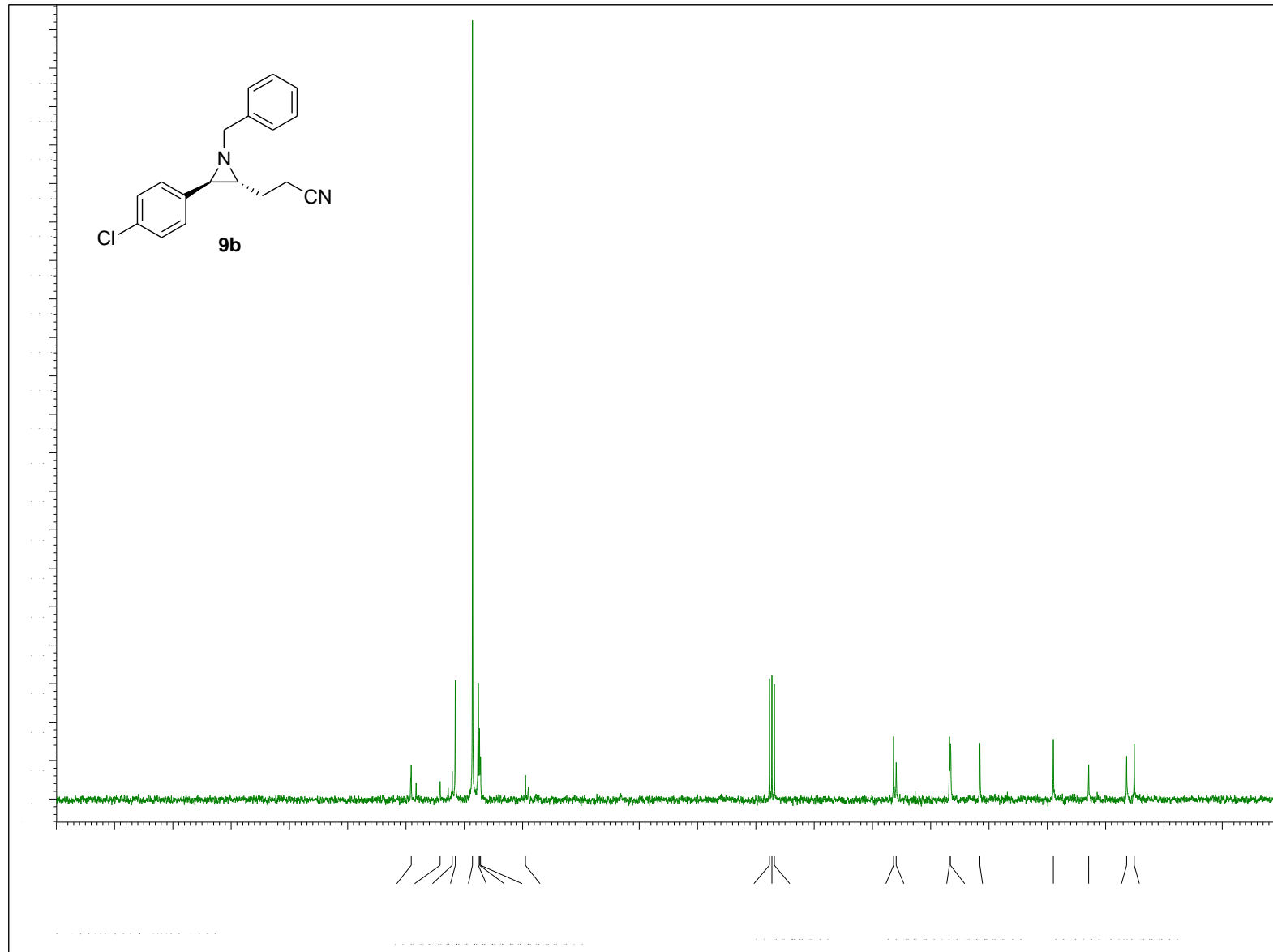
Trans-1-benzyl-3-(2-cyanoethyl)-2-phenylaziridine **9a**: ^{13}C NMR



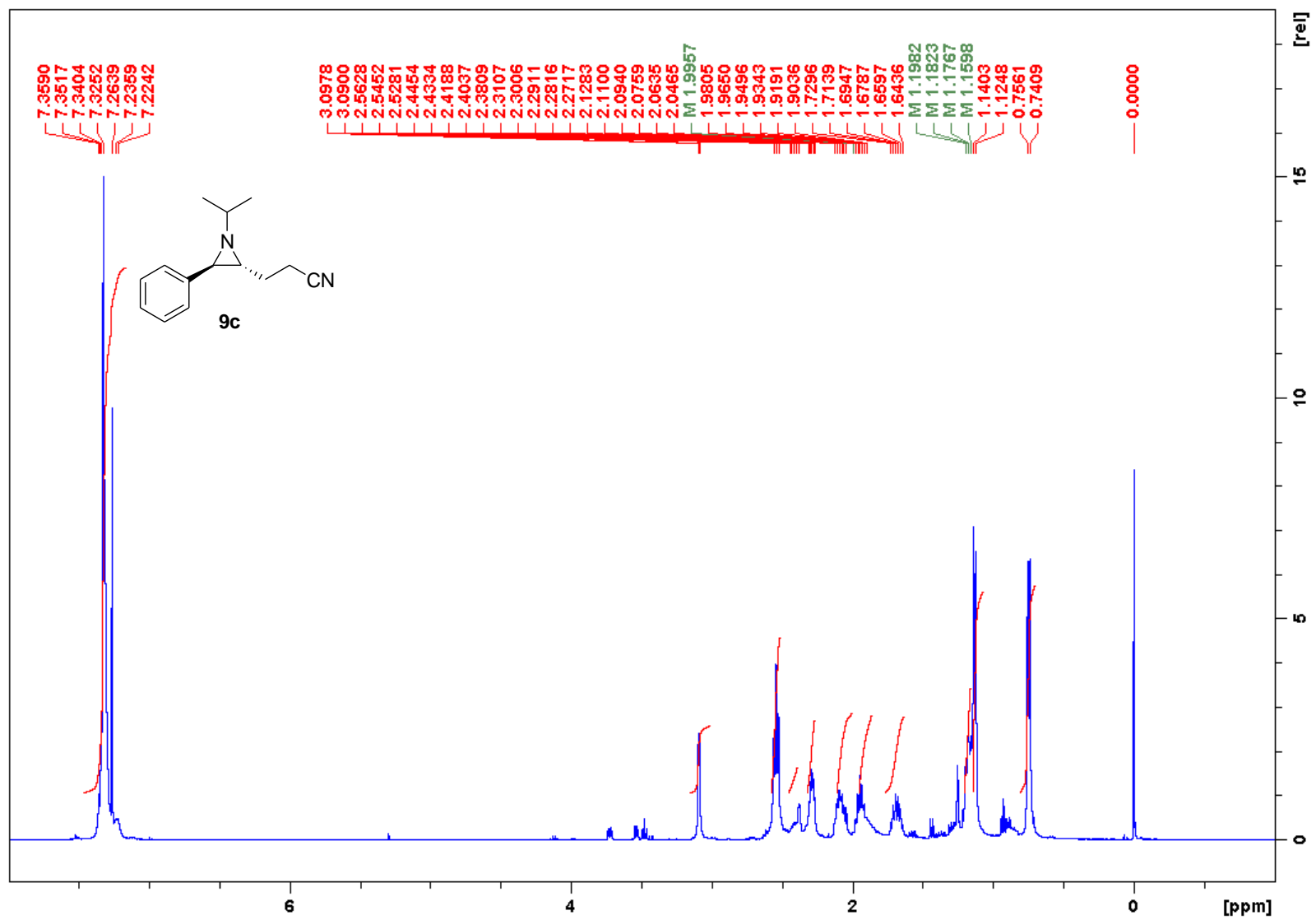
Trans-1-benzyl-2-(4-chlorophenyl)-3-(2-cyanoethyl)aziridine **9b**: ^1H NMR



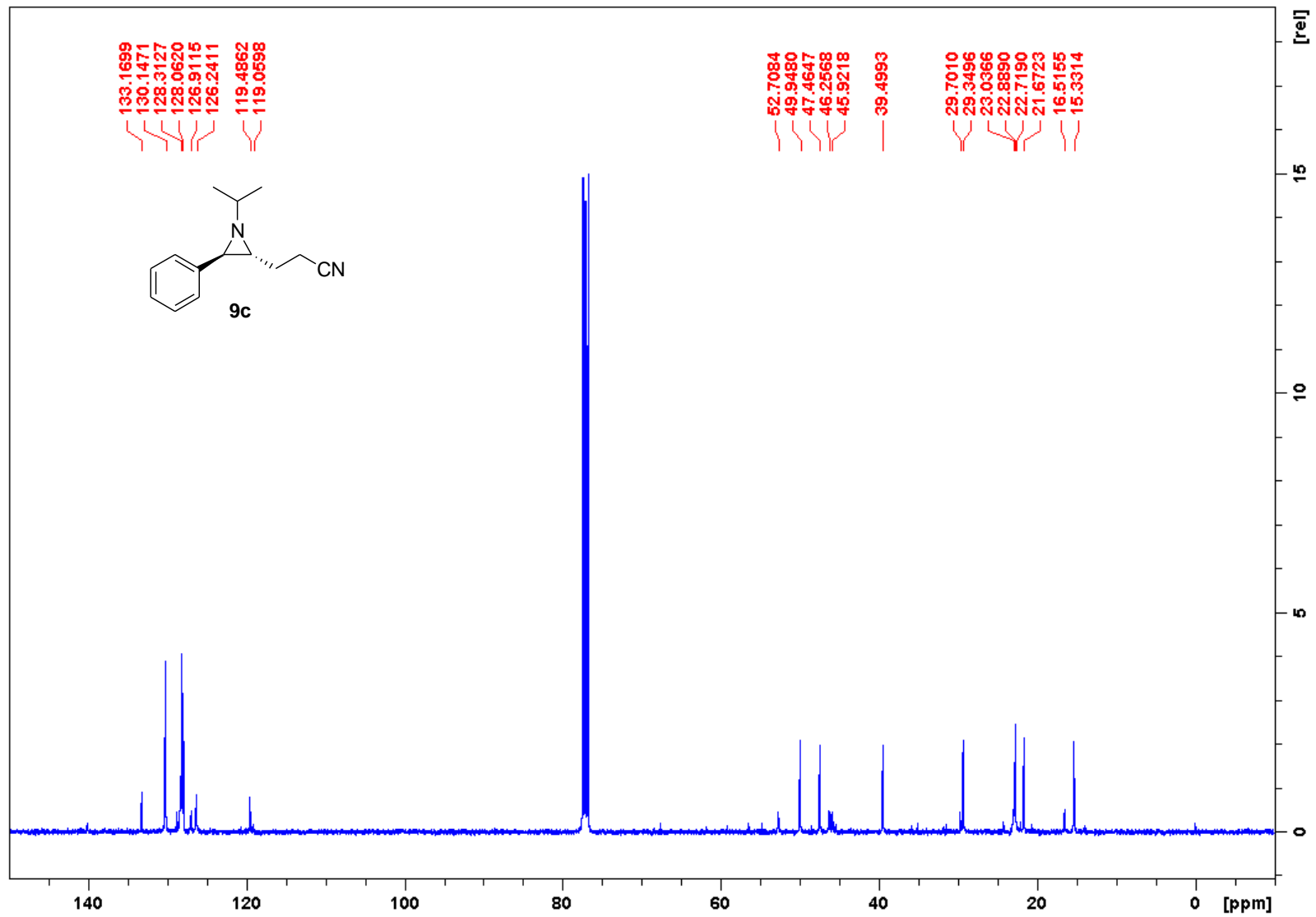
Trans-1-benzyl-2-(4-chlorophenyl)-3-(2-cyanoethyl)aziridine **9b**: ^{13}C NMR



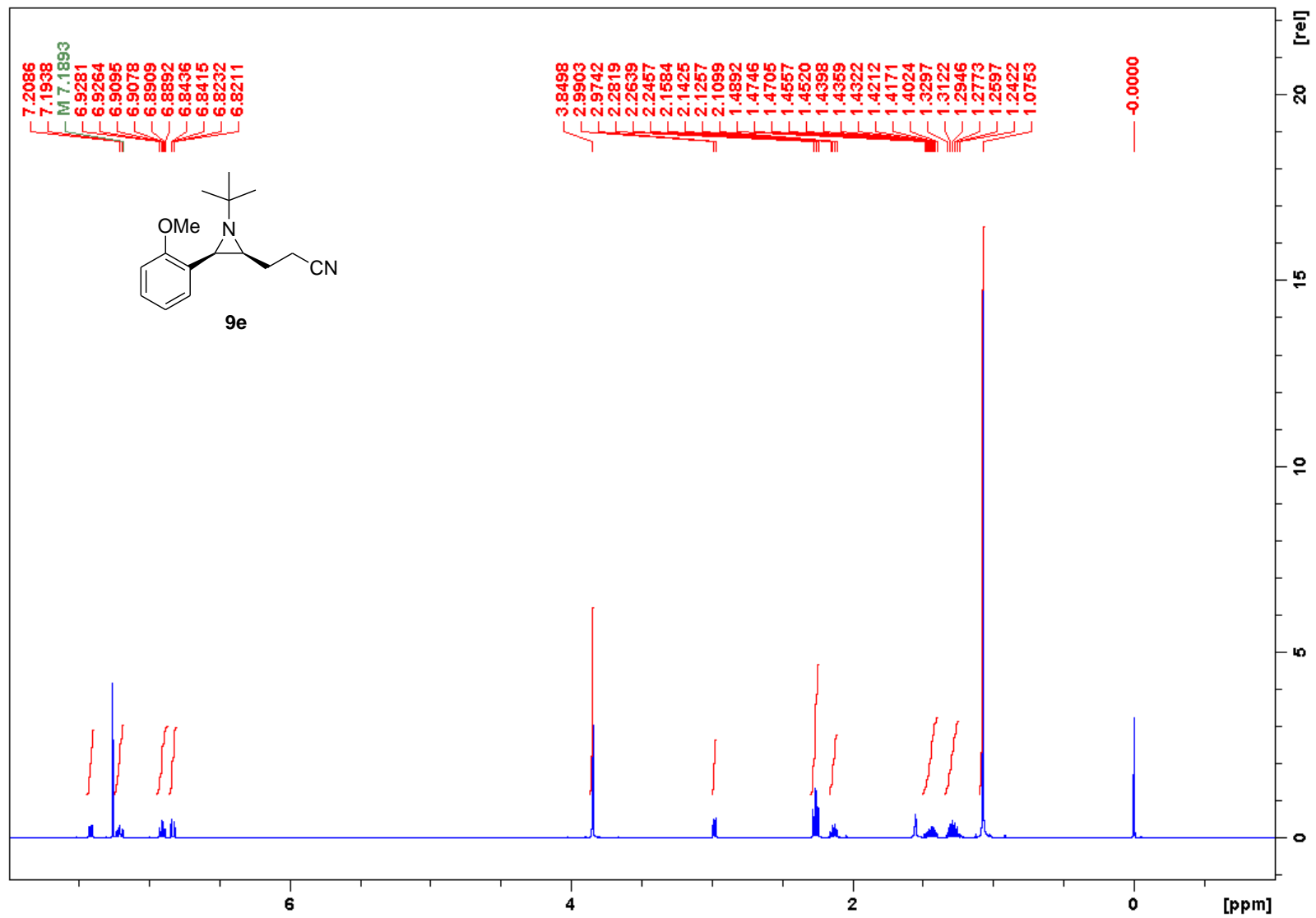
Trans-3-(2-cyanoethyl)-1-isopropyl-2-phenylaziridine **9c**: ^1H NMR



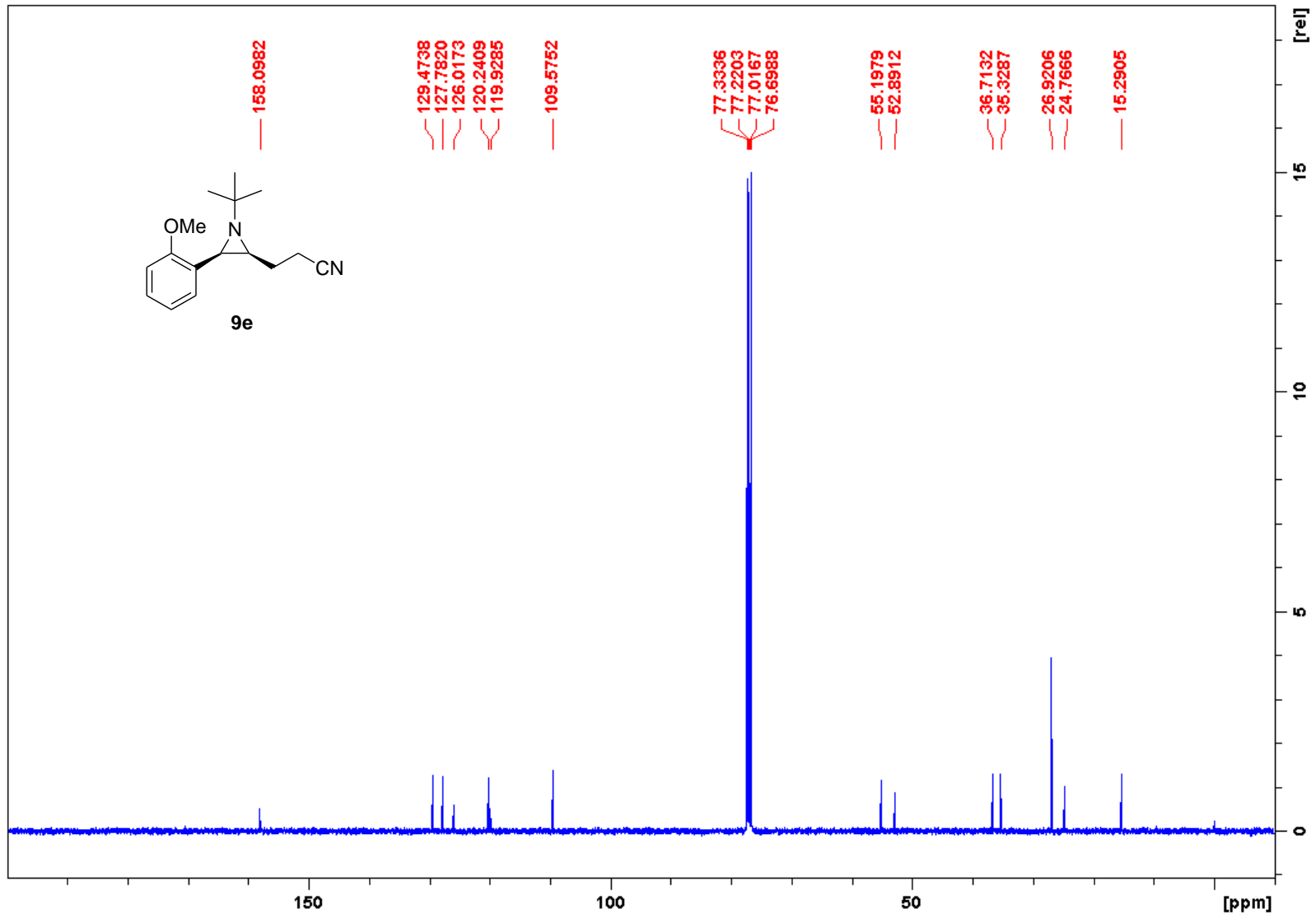
Trans-3-(2-cyanoethyl)-1-isopropyl-2-phenylaziridine **9c**: ^{13}C NMR



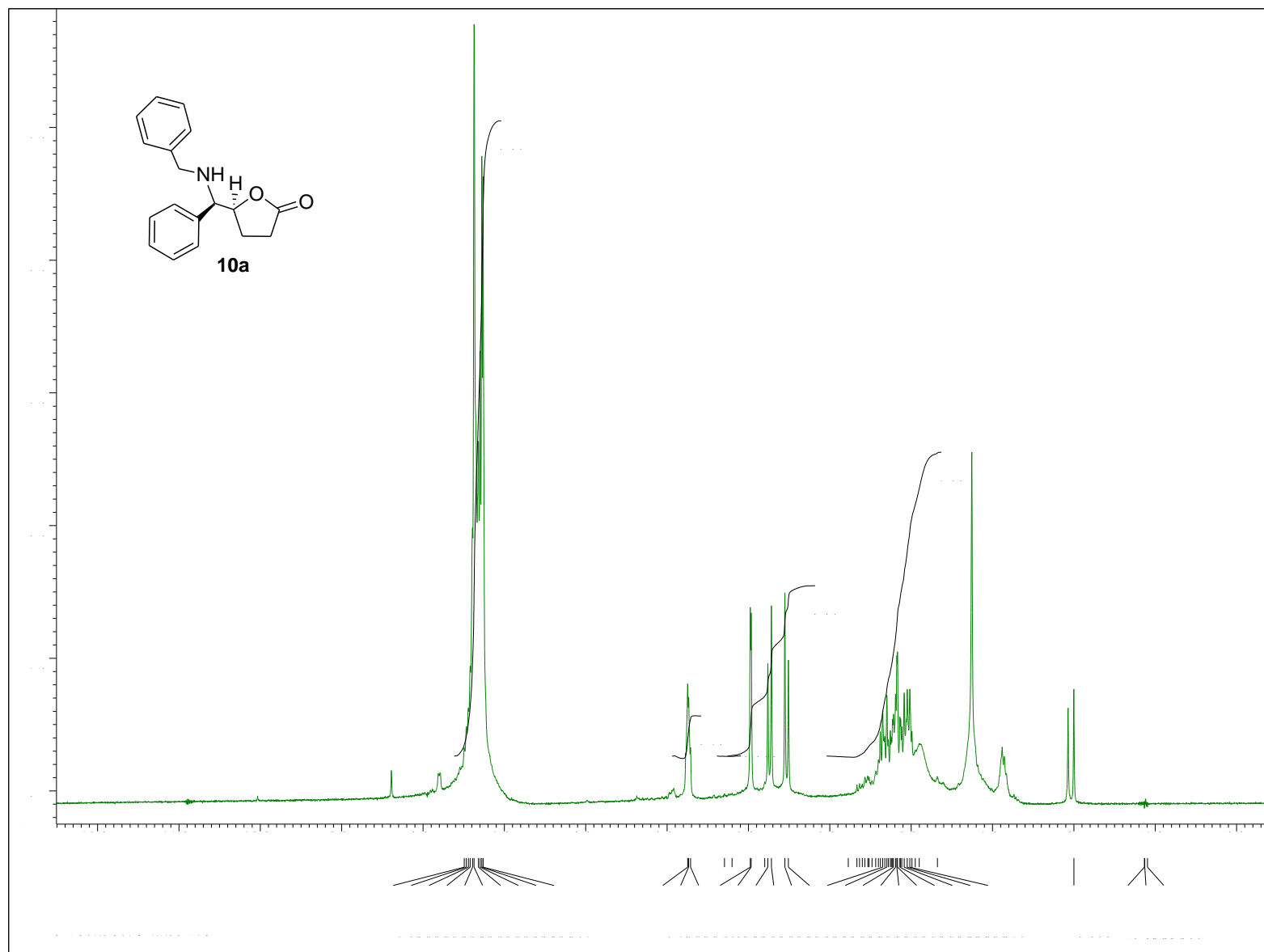
Cis-1-tert-butyl-3-(2-cyanoethyl)-2-(2-methoxyphenyl)aziridine **9e**: ^1H NMR



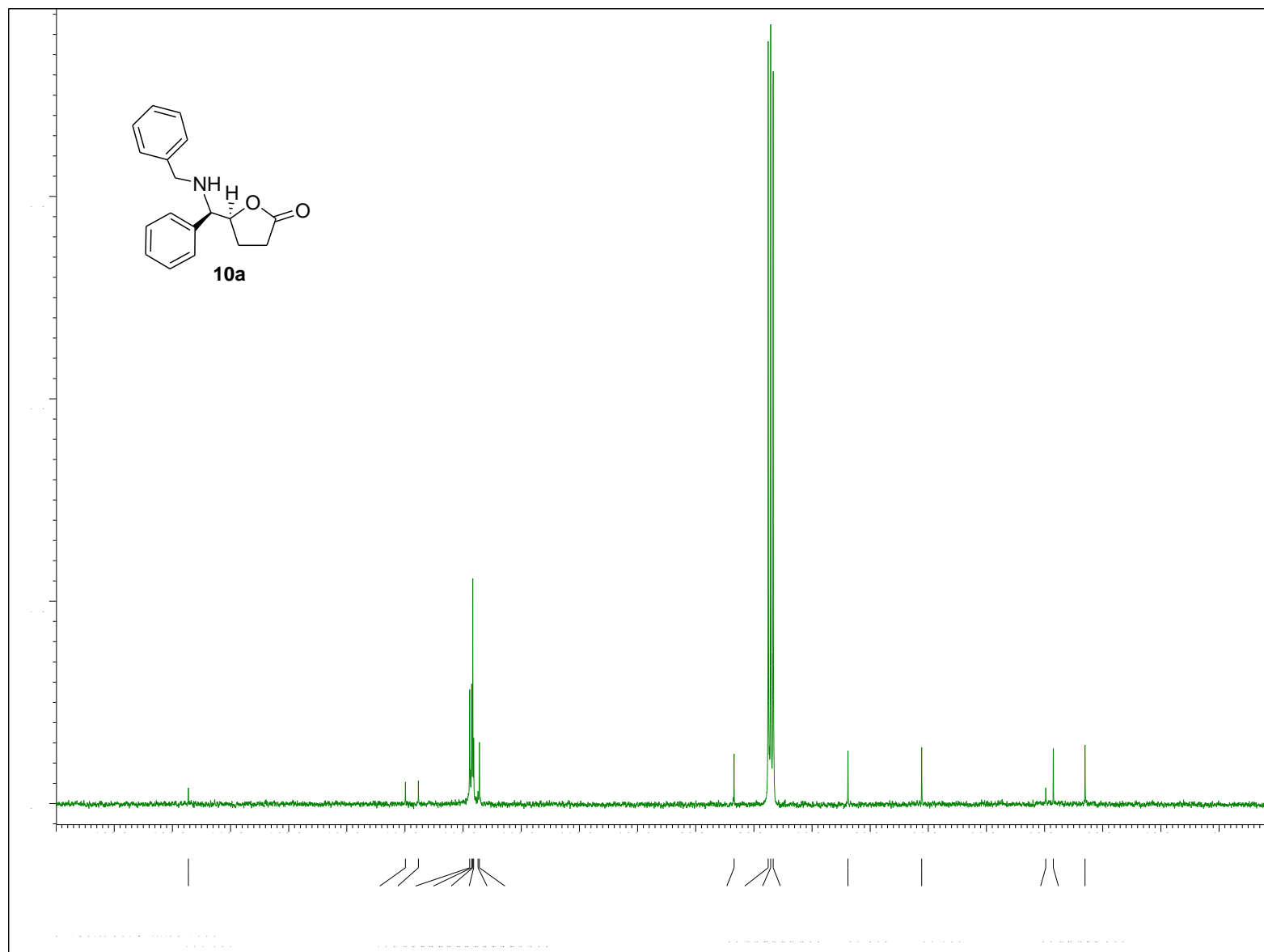
Cis-1-*tert*-butyl-3-(2-cyanoethyl)-2-(2-methoxyphenyl)aziridine **9e**: ^{13}C NMR



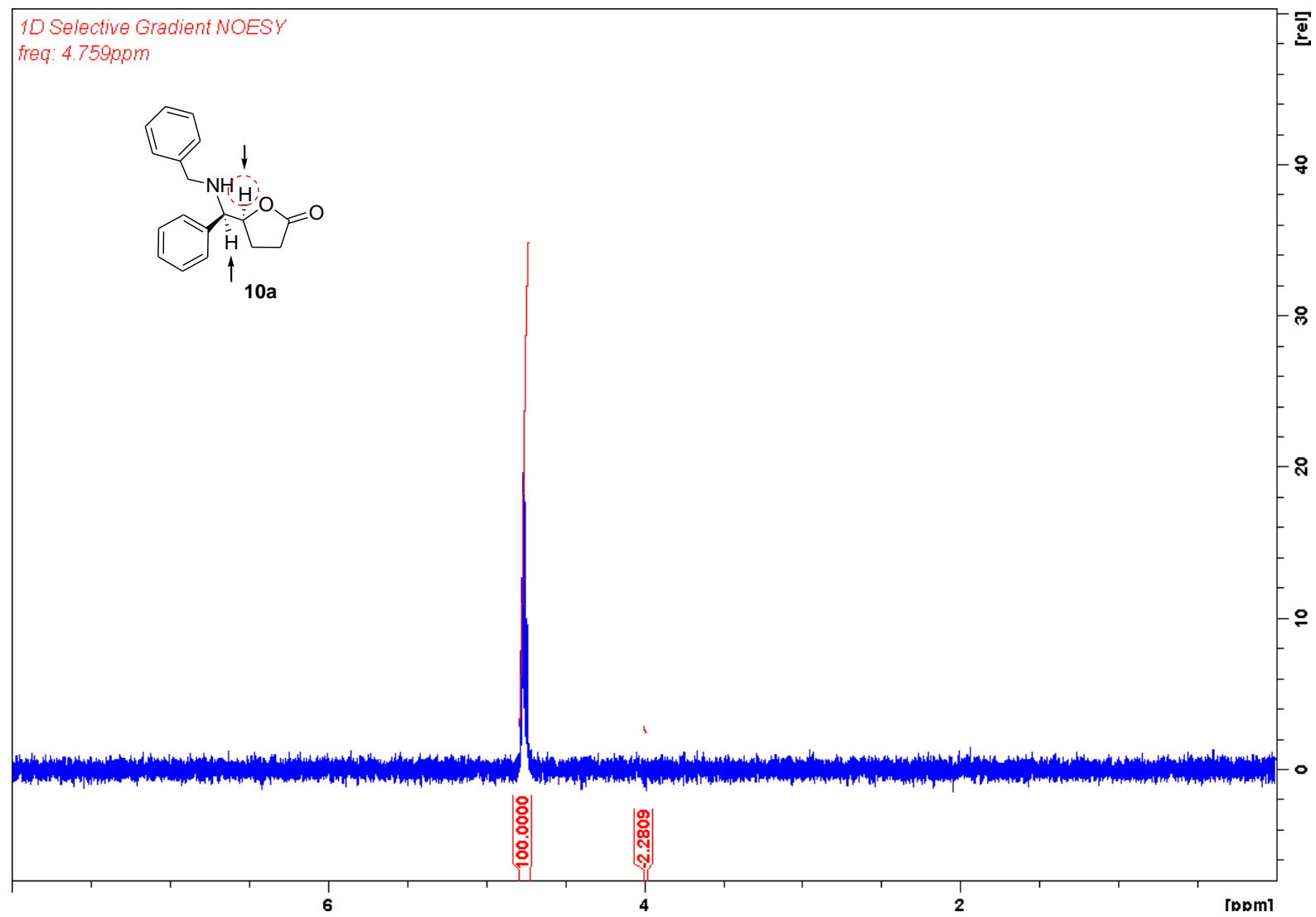
(4*S**,1'*R*'*)-4-(Benzylaminophenylmethyl)butyrolactone **10a**: ^1H NMR



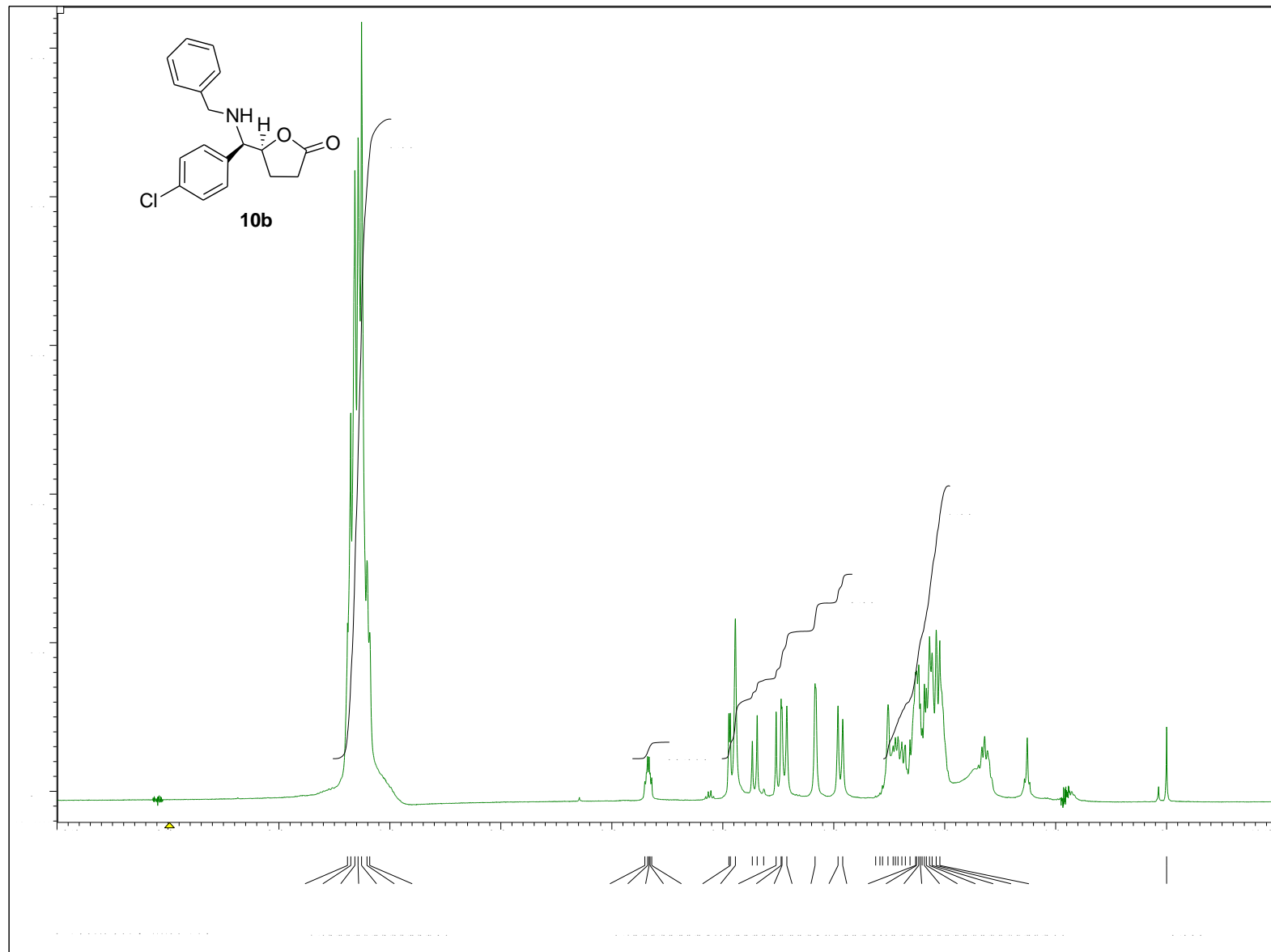
(4*S**,1'*R*'*)-4-(Benzylaminophenylmethyl)butyrolactone **10a**: ^{13}C NMR



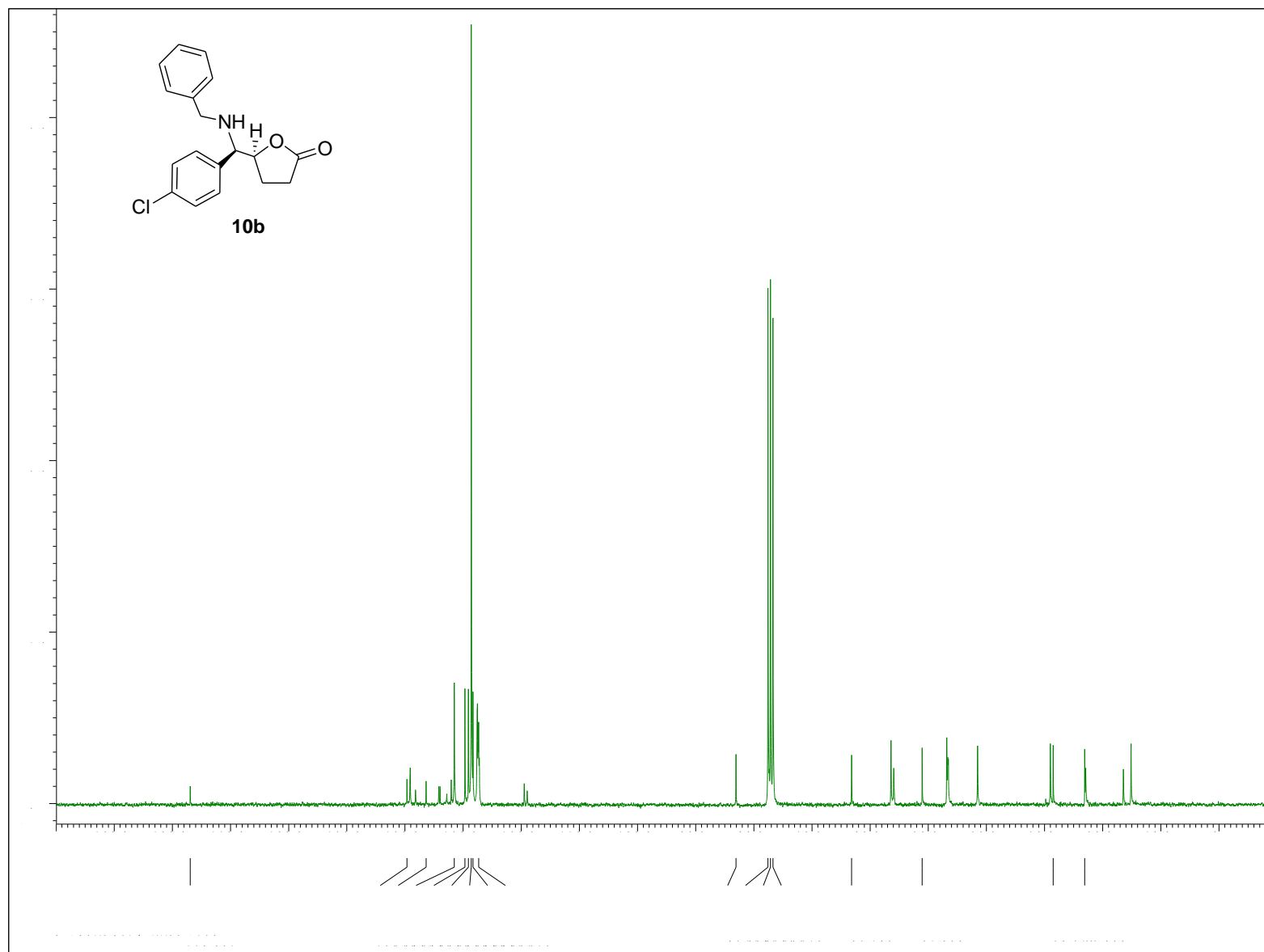
(4*S**,1'*R*'*)-4-(Benzylaminophenylmethyl)butyrolactone **10a**: 1D NOESY



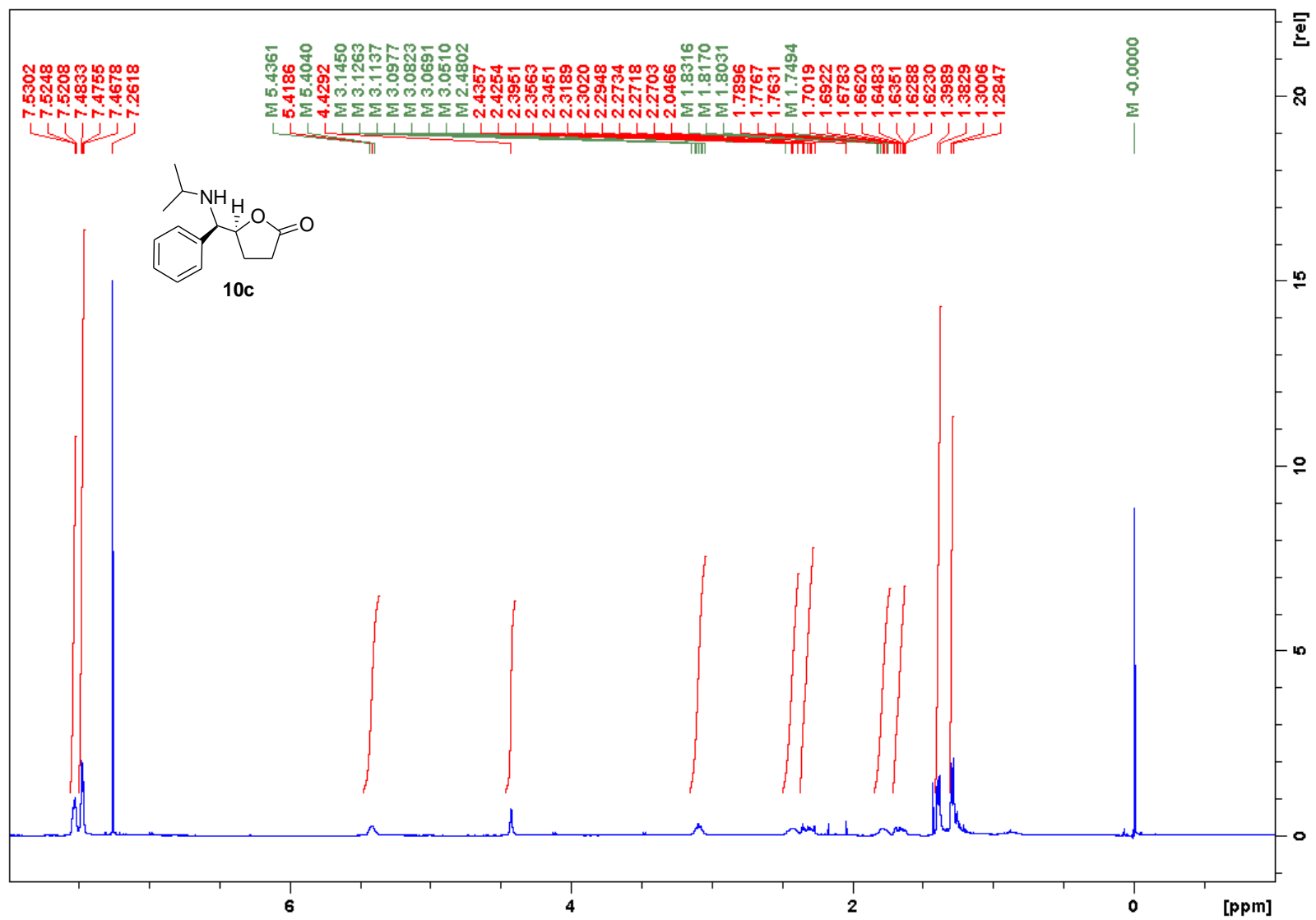
(4*S**,1'*R*'*)-4-[Benzylamino(4-chlorophenyl)methyl]butyrolactone **10b**: ¹H NMR



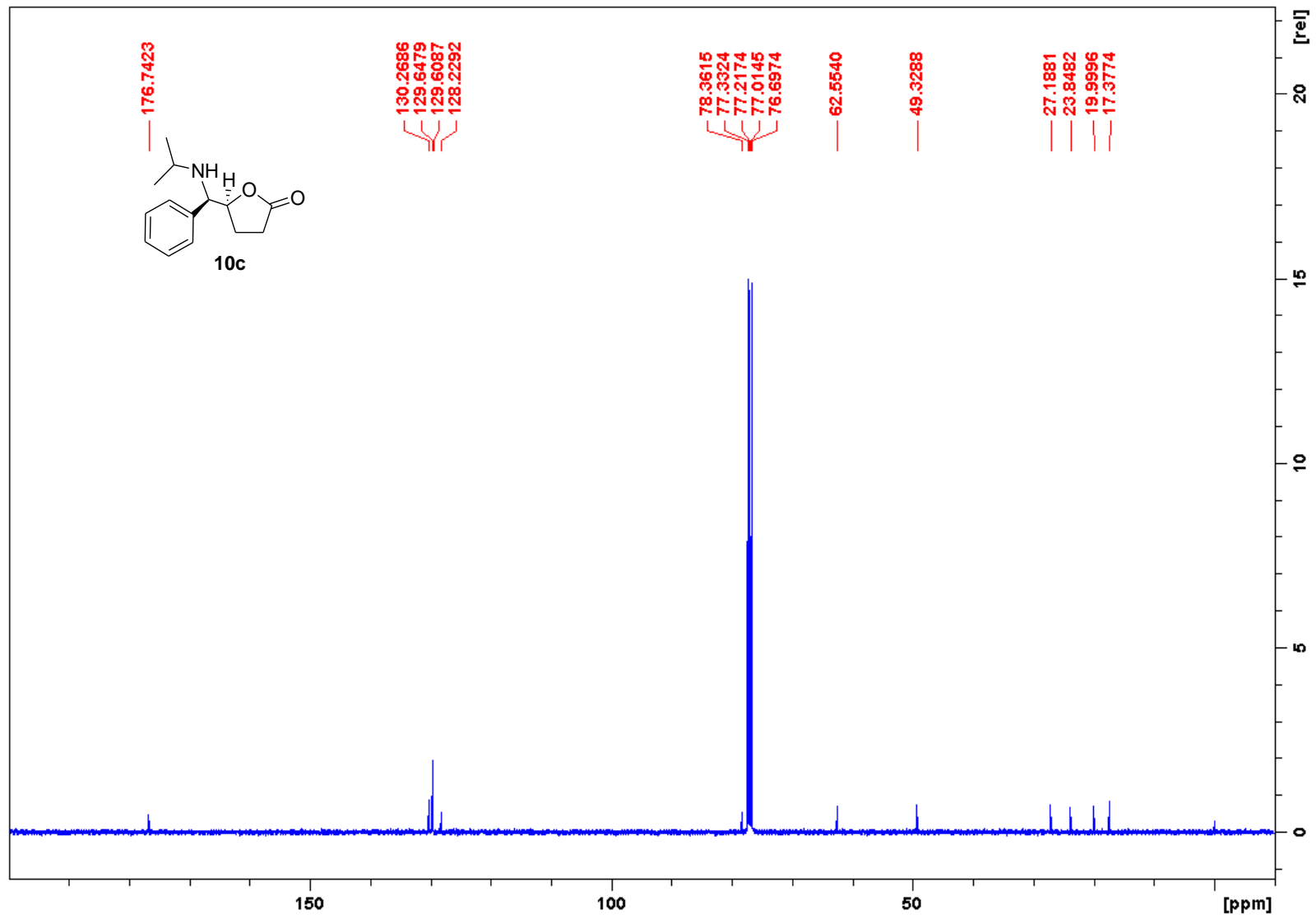
(4*S**,1'*R*'*)-4-[Benzylamino(4-chlorophenyl)methyl]butyrolactone **10b**: ^{13}C NMR



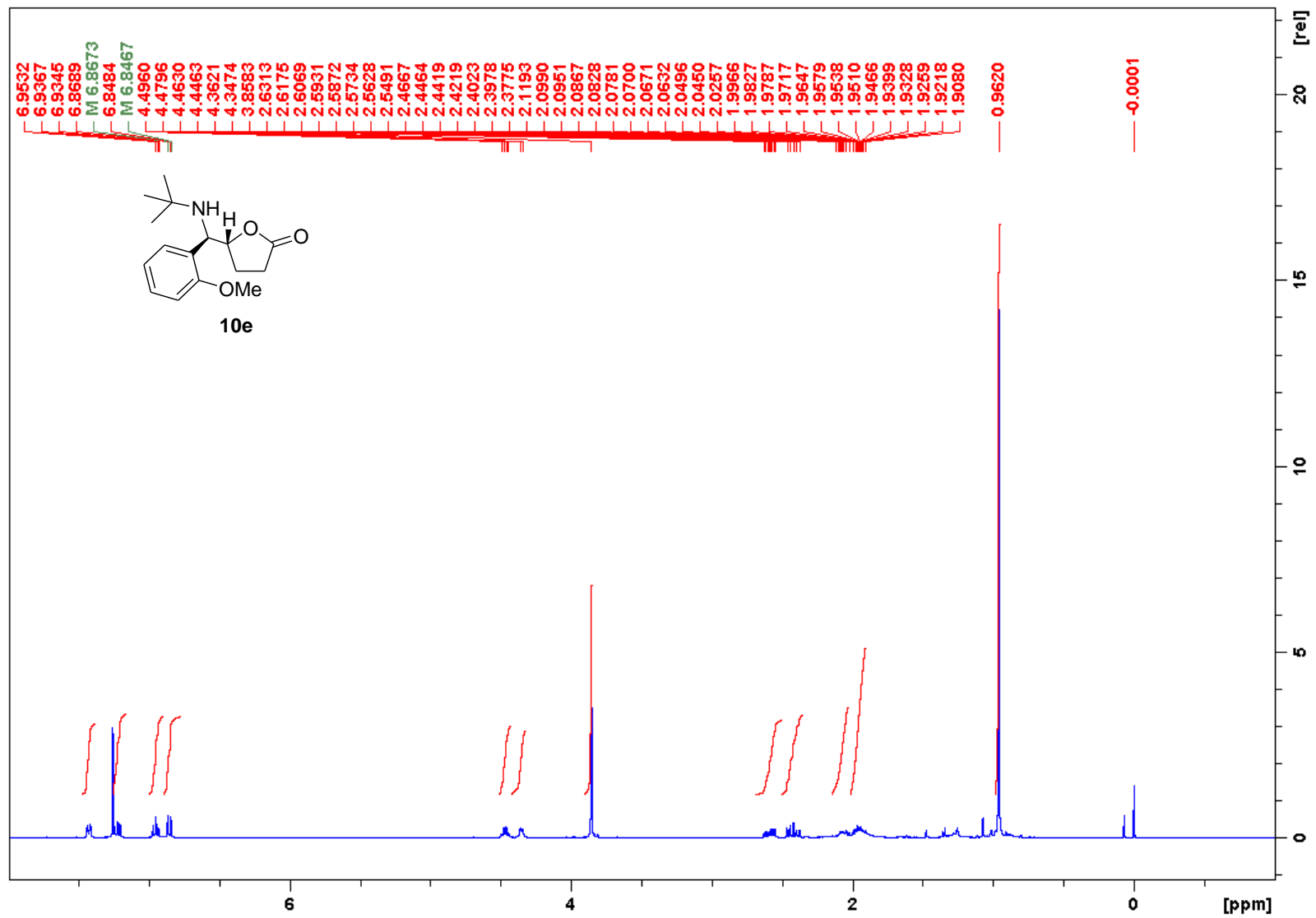
(4*S**,1'*R*'*)-4-[(Isopropylamino)phenylmethyl]butyrolactone **10c**: ¹H NMR



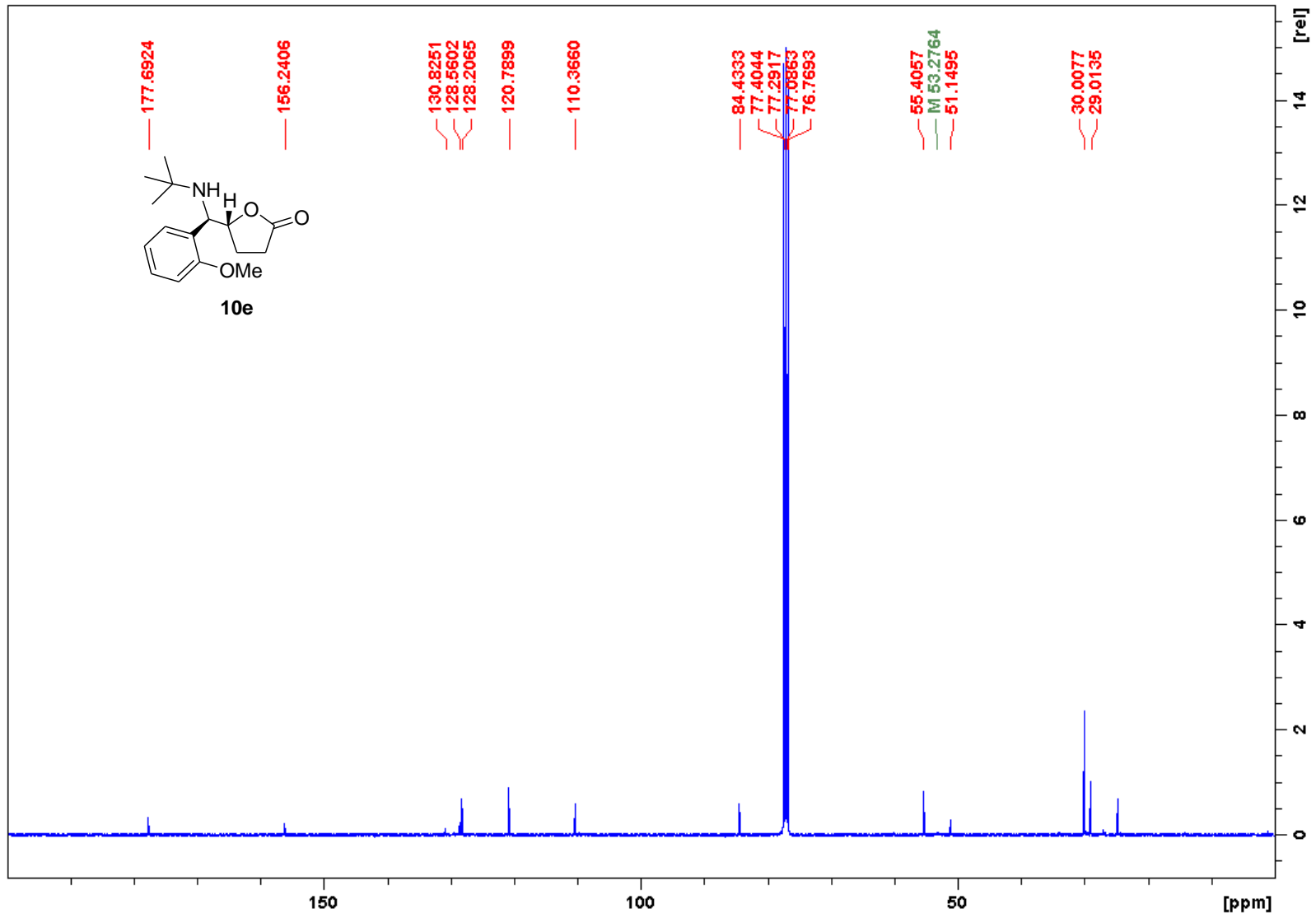
(4*S**,1'*R*'*)-4-[(Isopropylamino)phenylmethyl]butyrolactone **10c**: ¹³C NMR



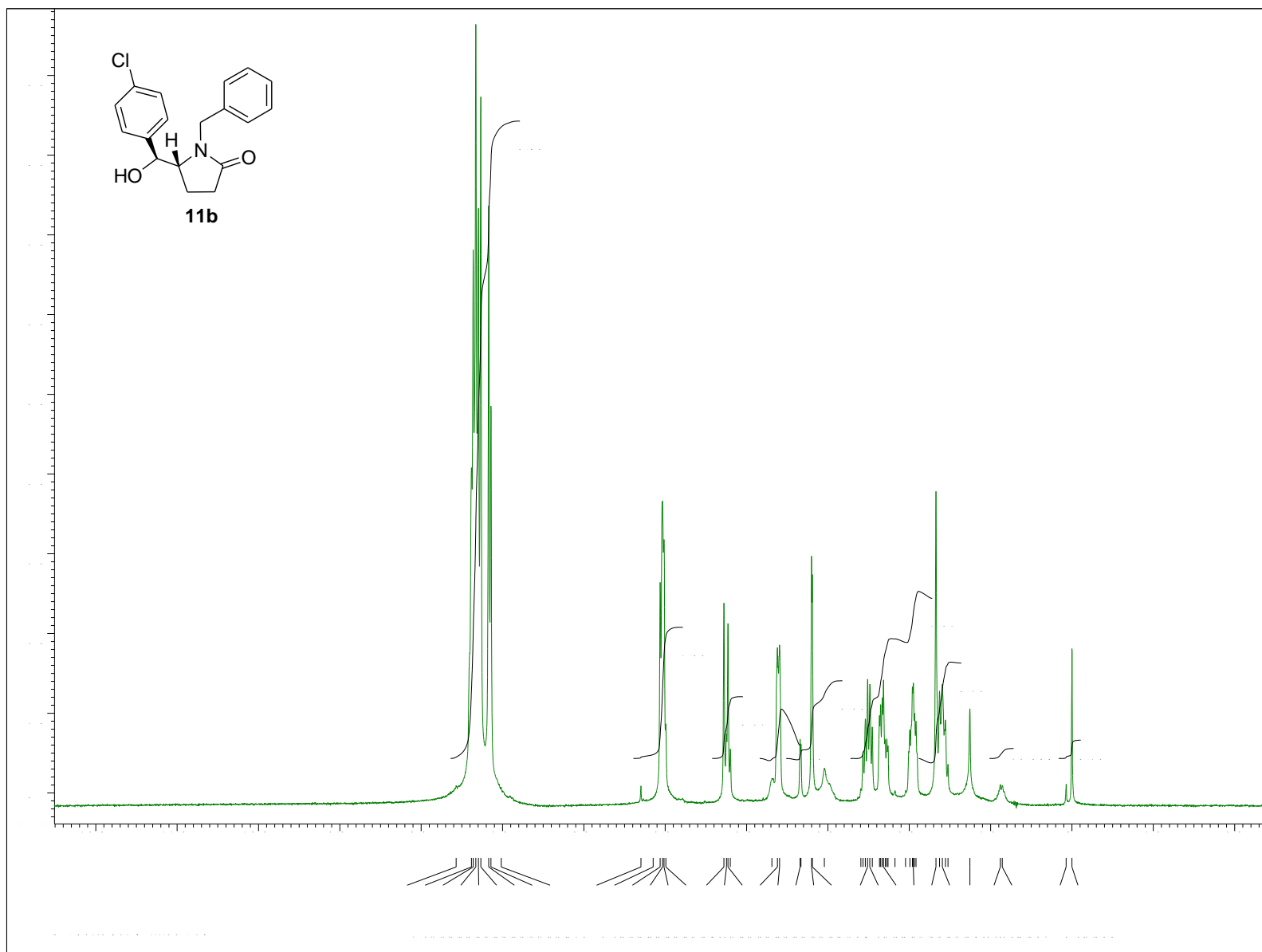
(4*R**,1'*R*'*)-4-[(*tert*-Butylamino)(2-methoxyphenyl)methyl]butyrolactone **10e**: ¹H NMR



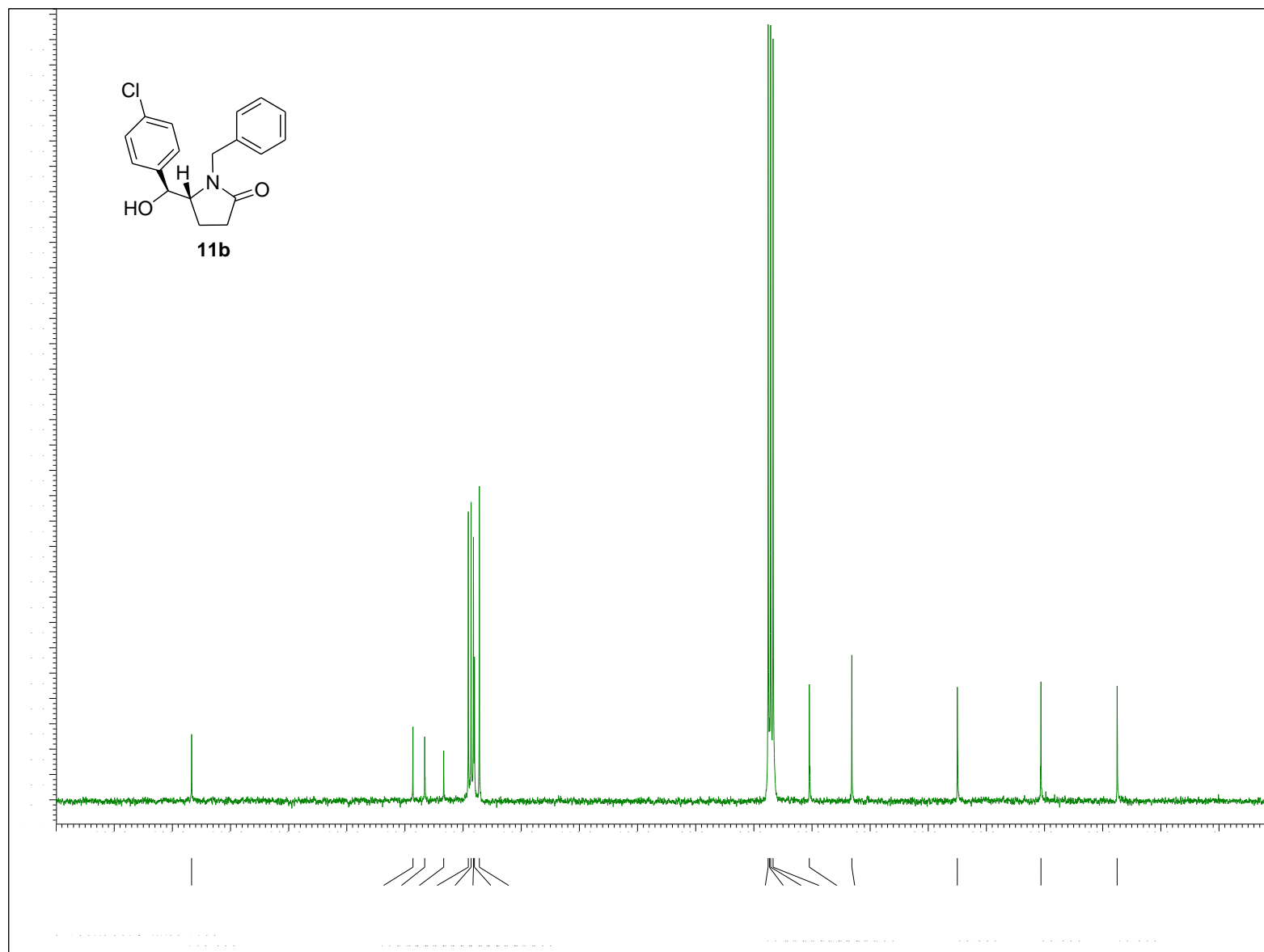
(4*R**,1'*R*'*)-4-[(*tert*-Butylamino)(2-methoxyphenyl)methyl]butyrolactone **10e**: ¹³C NMR



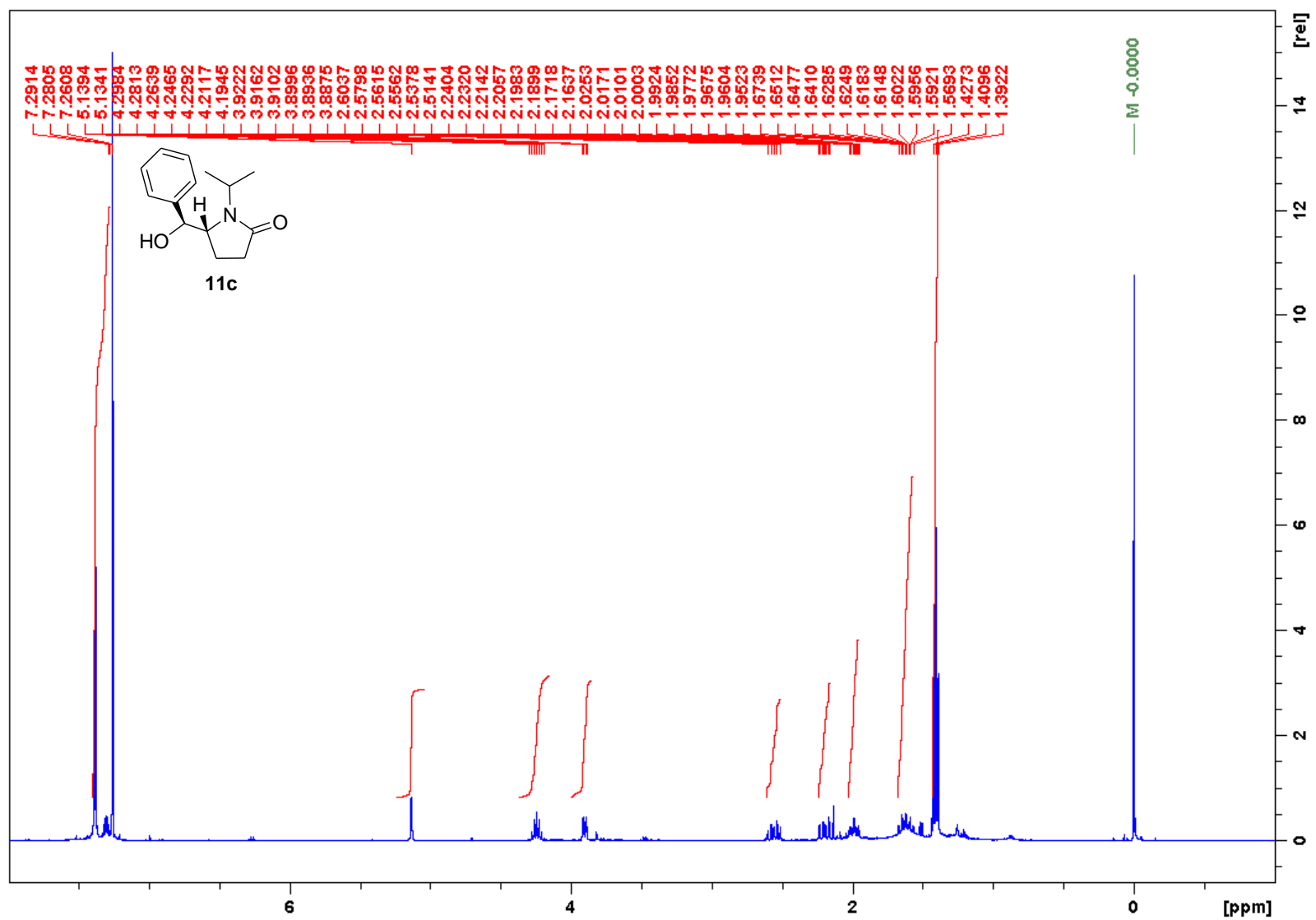
(5*R**,1'*S*'*)-1-Benzyl-5-[(4-chlorophenyl)hydroxymethyl]pyrrolidin-2-one **11b**: ^1H NMR



(5*R**,1'*S*')-1-Benzyl-5-[(4-chlorophenyl)hydroxymethyl]pyrrolidin-2-one **11b**: ^{13}C NMR



(5*R**,1'*S*'*)-1-Isopropyl-5-[hydroxyl(phenyl)methyl]pyrrolidin-2-one **11c**: ¹H NMR



(5*R**,1'*S*'*)-1-Isopropyl-5-[hydroxyl(phenyl)methyl]pyrrolidin-2-one **11c**: ¹³C NMR

