

Electrophilic Trifluoromethylation of *S*-Hydrogen Phosphorothioates

Nico Santschi, Antonio Togni*

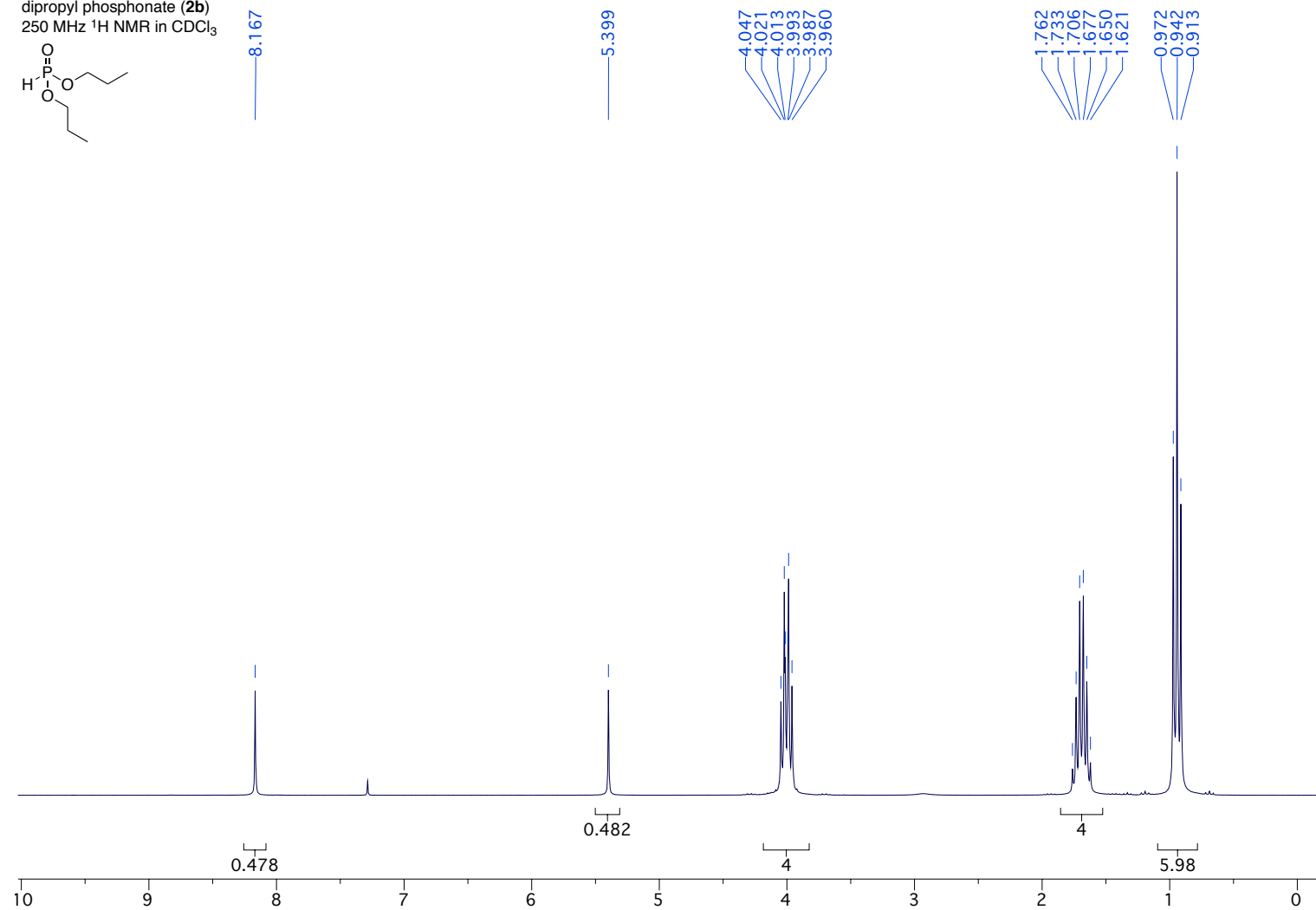
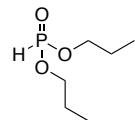
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SUPPORTING INFORMATION

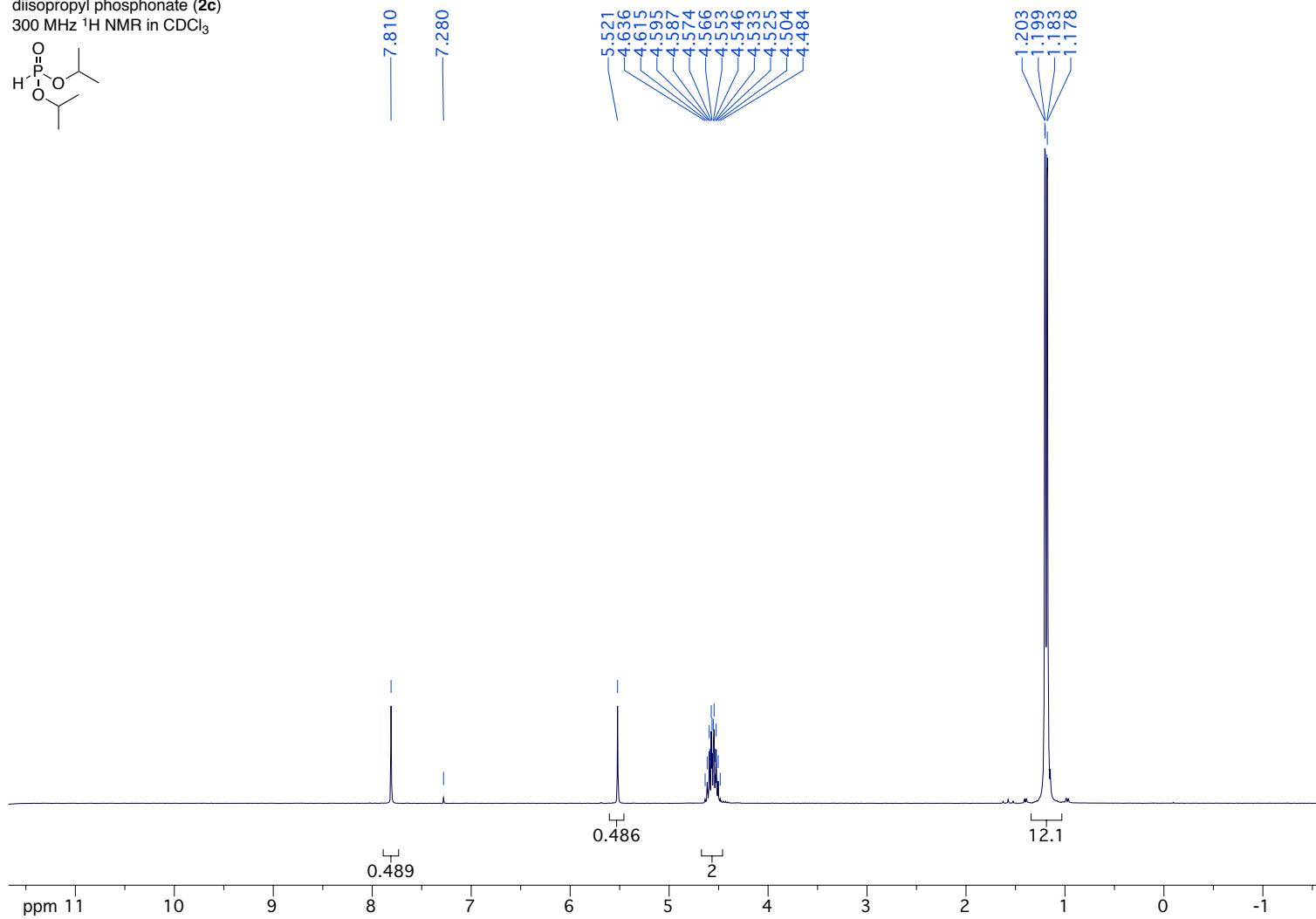
¹ H NMR of dipropyl phosphonate (2b).....	S2
¹ H NMR of diisopropyl phosphonate (2c).....	S3
¹ H NMR of diisobutyl phosphonate (2e).....	S4
¹ H NMR of dineopentyl phosphonate (2f).....	S5
¹ H NMR of dicyclohexyl phosphonate (2g).....	S6
¹ H NMR of bis(2-chloroethyl) phosphonate (2h).....	S7
¹ H NMR of bis(3-chloropropyl) phosphonate (2i).....	S8
¹ H, ¹³ C, ³¹ P NMR of bis(4-chlorobutyl) phosphonate (2j).....	S9
¹ H NMR of bis(2-methoxyethyl) phosphonate (2k).....	S12
¹ H NMR of <i>O,O</i> -diethyl <i>S</i> -hydrogen phosphorothioate (3a).....	S13
¹ H, ¹³ C, ³¹ P NMR of <i>O,O</i> -dipropyl <i>S</i> -hydrogen phosphorothioate (3b).....	S14
¹ H NMR of <i>O,O</i> -diisopropyl <i>S</i> -hydrogen phosphorothioate (3c).....	S17
¹ H NMR of <i>O,O</i> -dibutyl <i>S</i> -hydrogen phosphorothioate (3d).....	S18
¹ H NMR of <i>O,O</i> -diisobutyl <i>S</i> -hydrogen phosphorothioate (3e).....	S19
¹ H, ¹³ C, ³¹ P NMR of <i>O,O</i> -dineopentyl <i>S</i> -hydrogen phosphorothioate (3f).....	S20
¹ H, ¹³ C, ³¹ P NMR of <i>O,O</i> -dicyclohexyl <i>S</i> -hydrogen phosphorothioate (3g).....	S23
¹ H, ¹³ C, ³¹ P NMR of <i>O,O</i> -bis(2-chloroethyl) <i>S</i> -hydrogen phosphorothioate (3h).....	S26
¹ H, ¹³ C, ³¹ P NMR of <i>O,O</i> -bis(3-chloropropyl) <i>S</i> -hydrogen phosphorothioate (3i).....	S29
¹ H, ¹³ C, ³¹ P NMR of <i>O,O</i> -bis(4-chlorobutyl) <i>S</i> -hydrogen phosphorothioate (3j).....	S32

^1H , ^{13}C , ^{31}P NMR of <i>O,O</i> -bis(2-methoxyethyl) <i>S</i> -hydrogen phosphorothioate (3k).....	S35
^1H , ^{13}C NMR of <i>O,O</i> -diethyl <i>S</i> -trifluoromethyl phosphorothioate (4a).....	S38
^1H , ^{13}C NMR of <i>O,O</i> -diisopropyl <i>S</i> -trifluoromethyl phosphorothioate (4c).....	S40
^1H , ^{13}C , ^{31}P , ^{19}F NMR of <i>O,O</i> -dicyclohexyl <i>S</i> -trifluoromethyl phosphorothioate (4g).....	S42

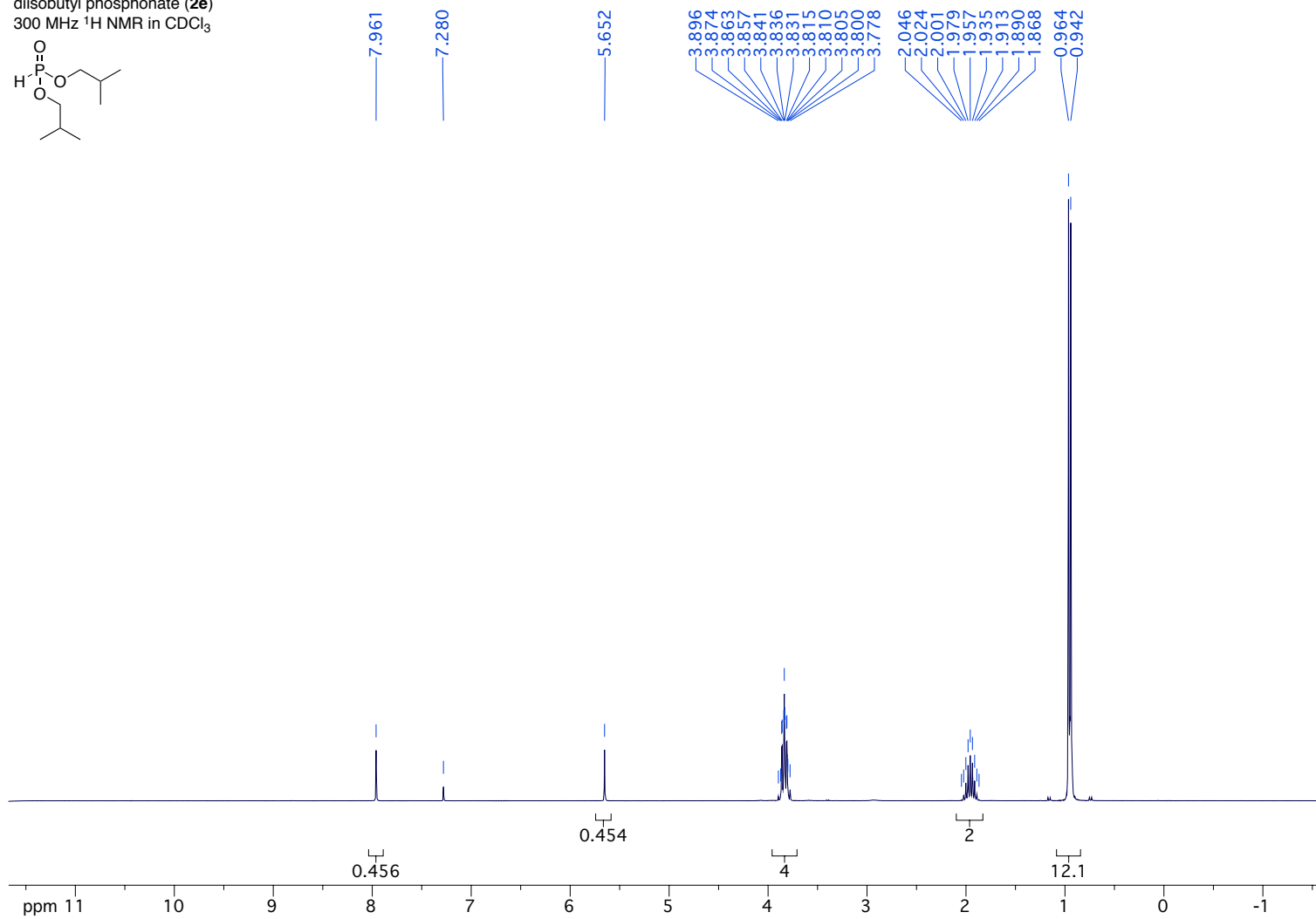
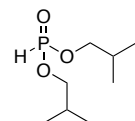
dipropyl phosphonate (**2b**)
250 MHz ^1H NMR in CDCl_3



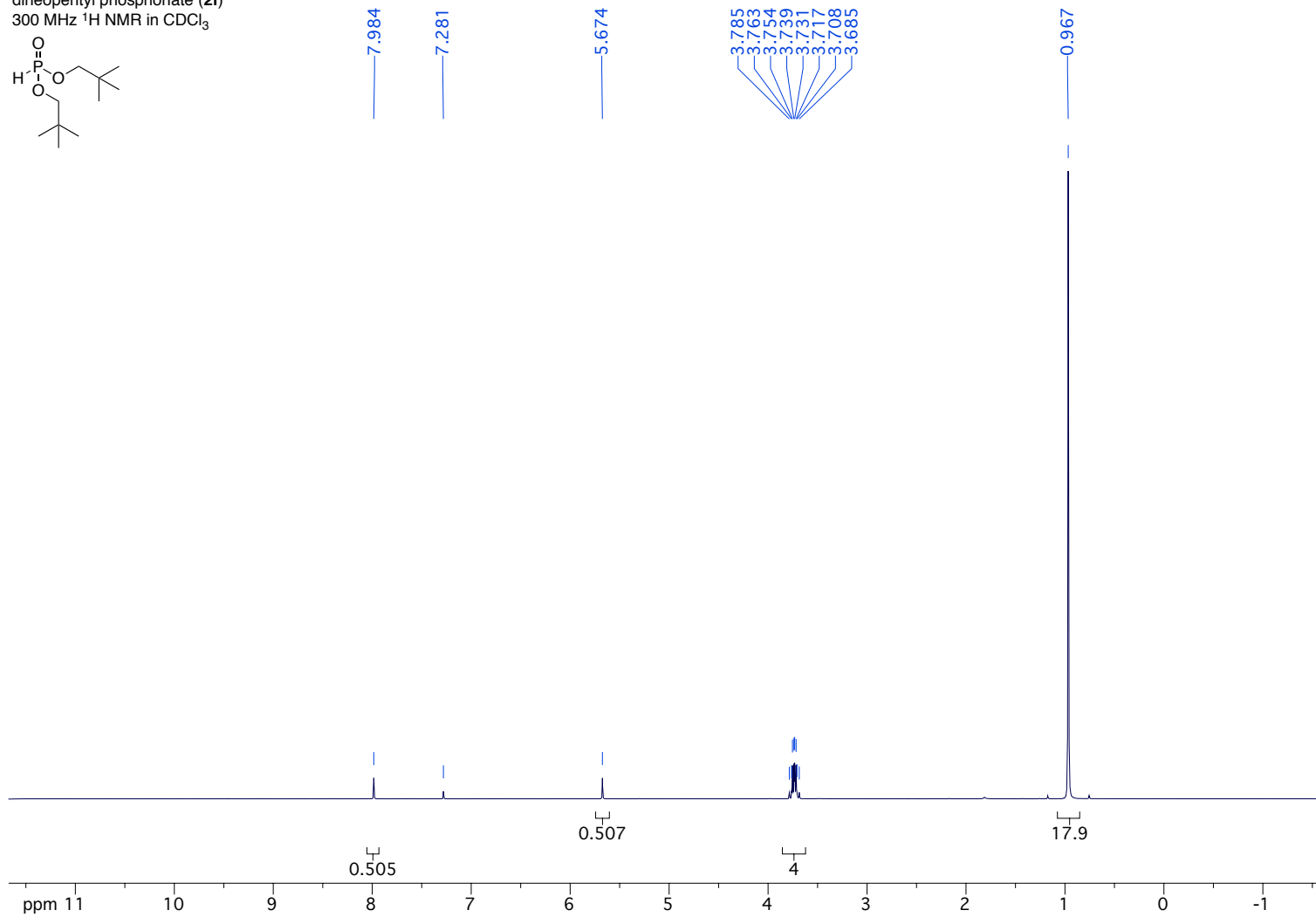
diisopropyl phosphonate (**2c**)
300 MHz ^1H NMR in CDCl_3



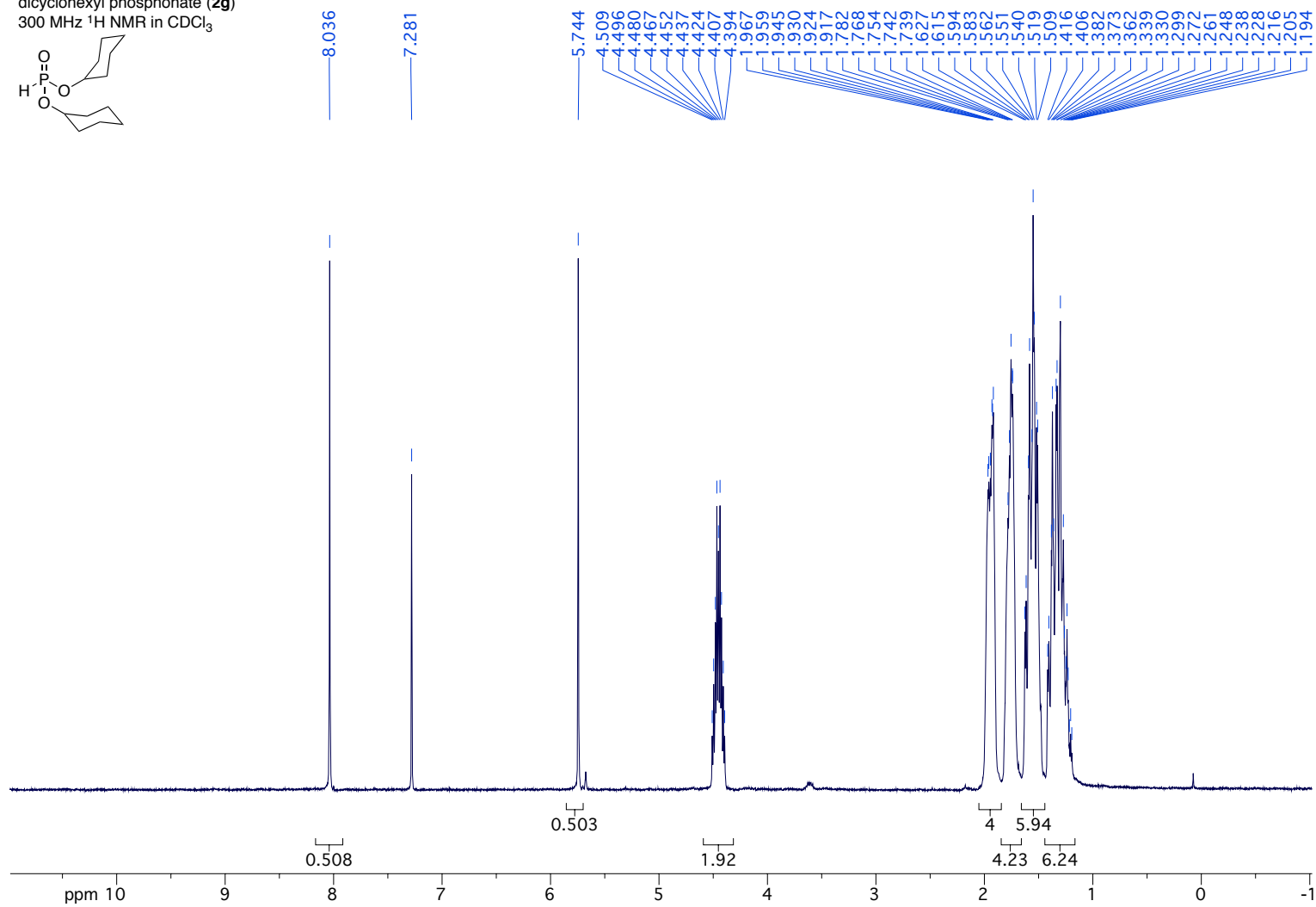
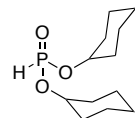
diisobutyl phosphonate (**2e**)
300 MHz ^1H NMR in CDCl_3



dineopentyl phosphonate (**2f**)
300 MHz ^1H NMR in CDCl_3

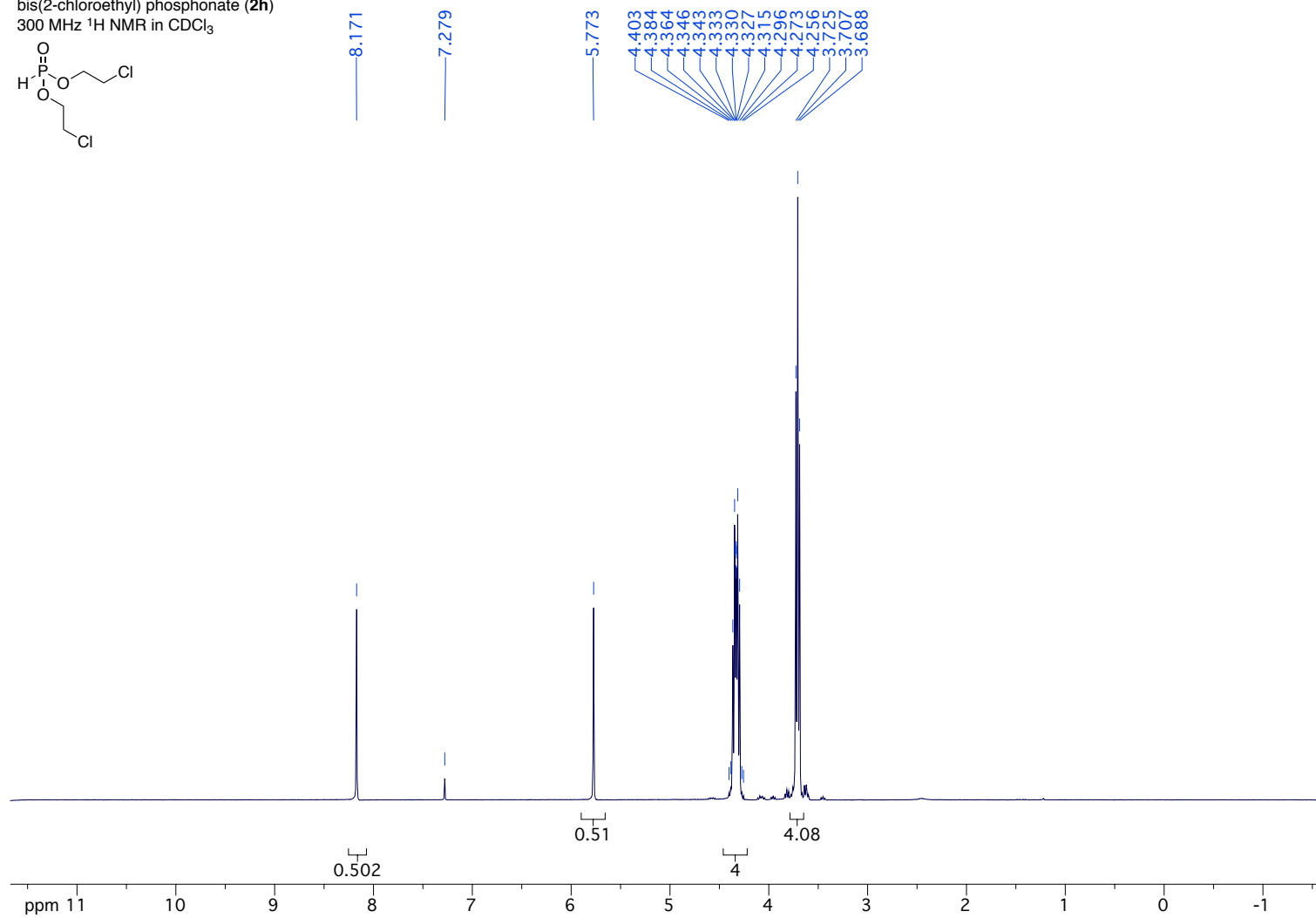
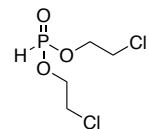


dicyclohexyl phosphonate (**2g**)
300 MHz ^1H NMR in CDCl_3

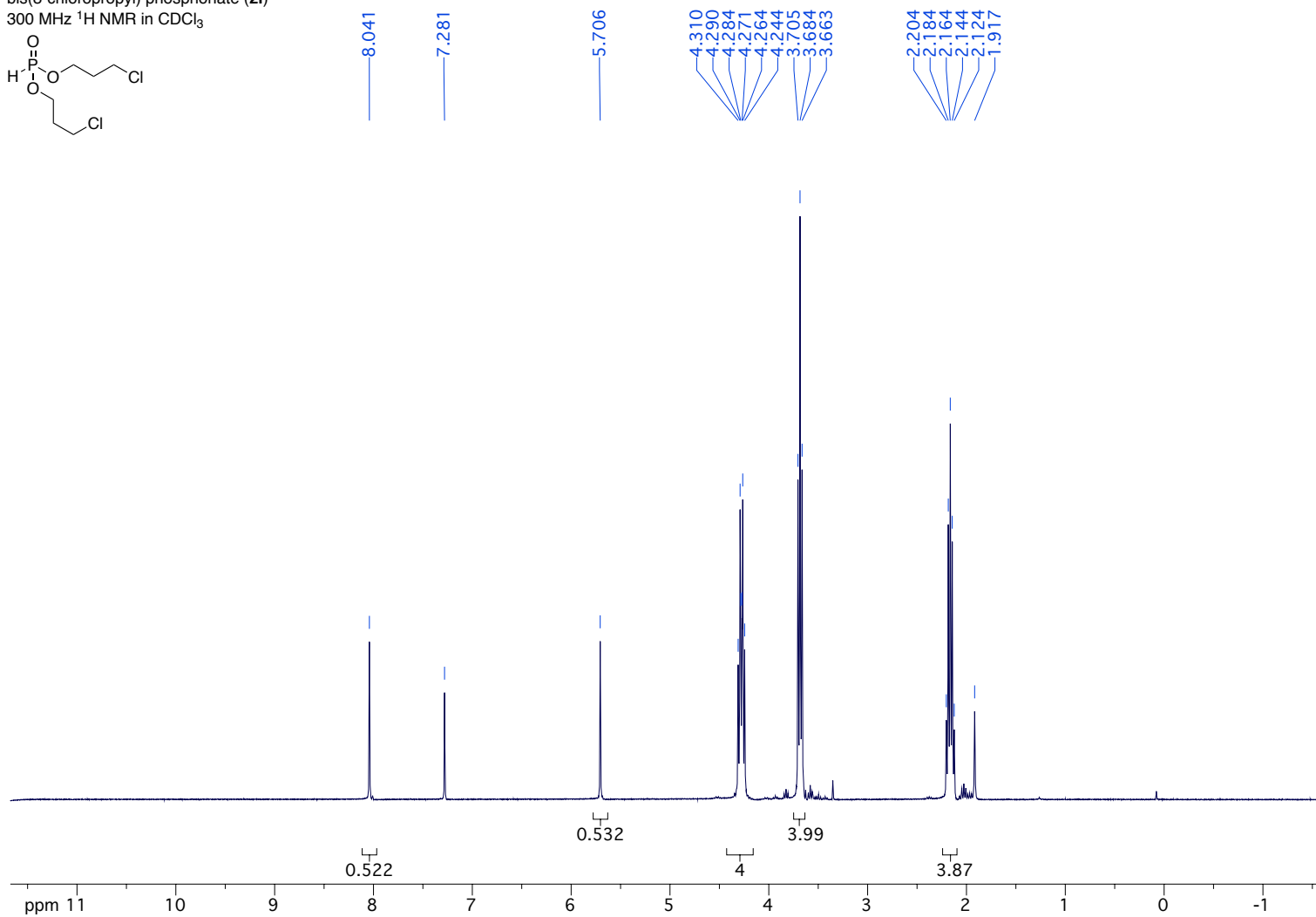
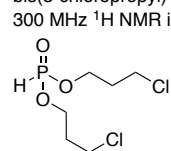


bis(2-chloroethyl) phosphonate (**2h**)

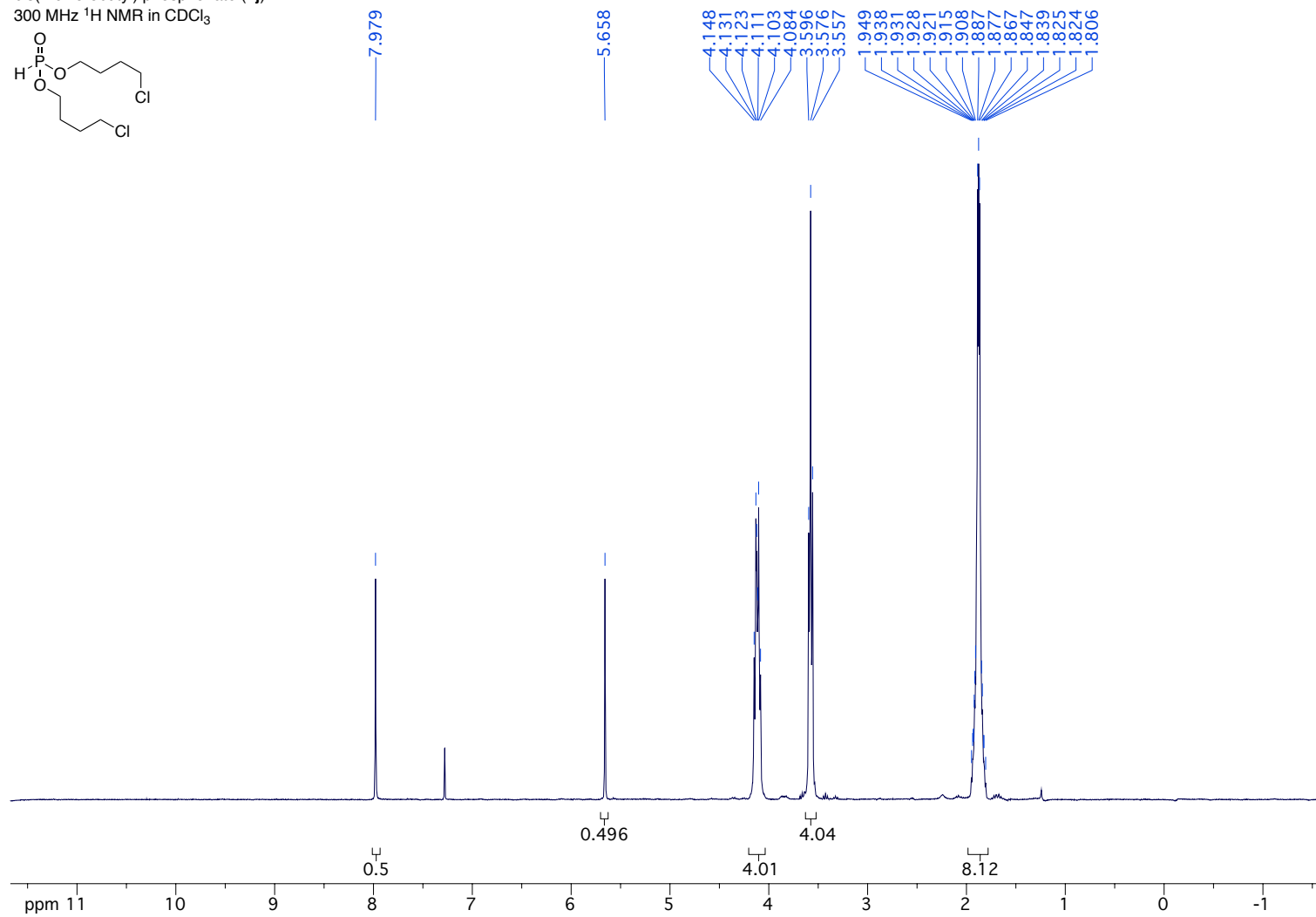
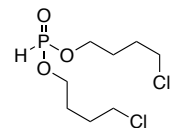
300 MHz ^1H NMR in CDCl_3



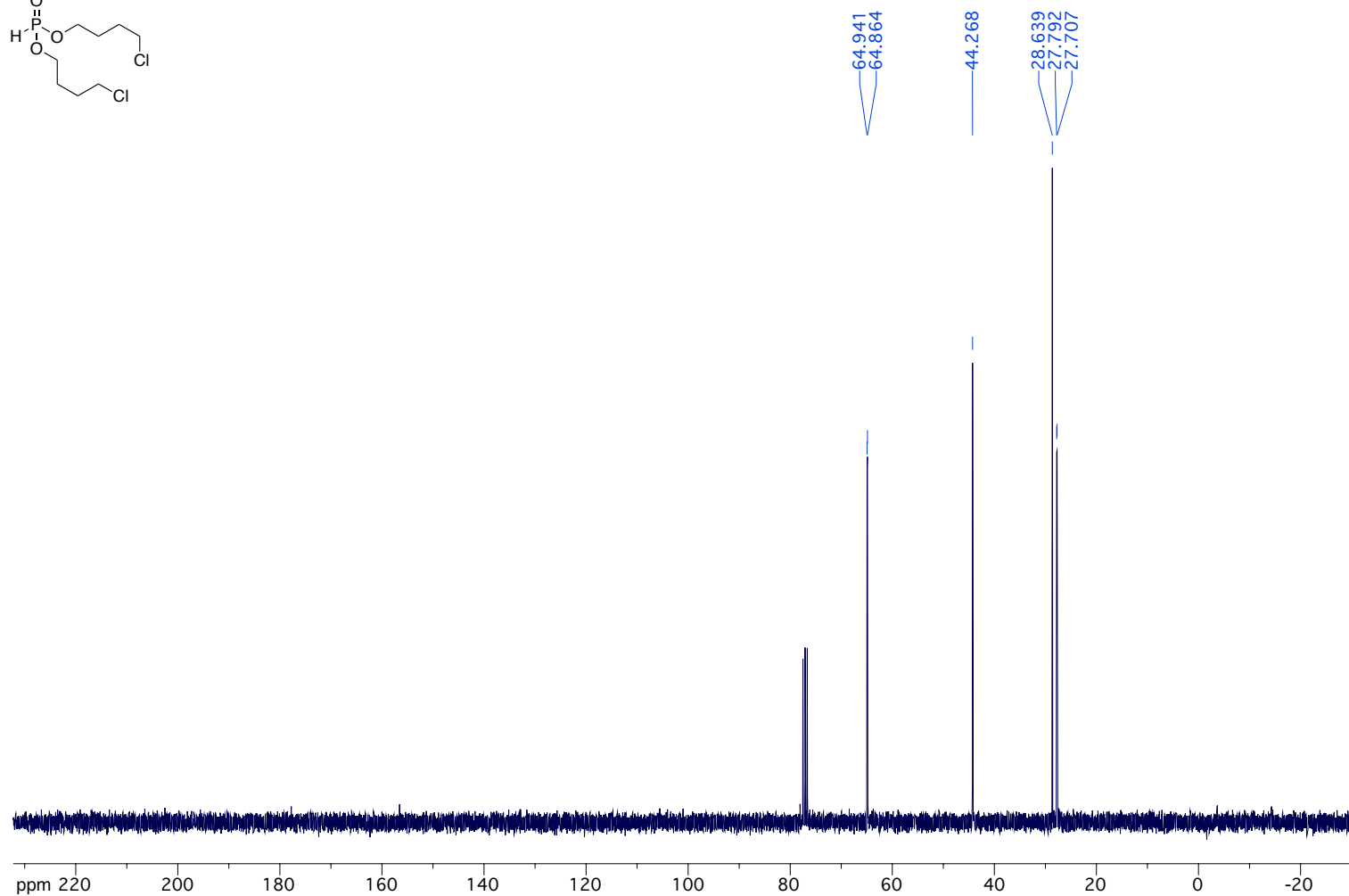
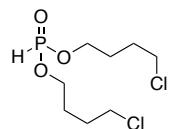
bis(3-chloropropyl) phosphonate (**2i**)
 300 MHz ^1H NMR in CDCl_3



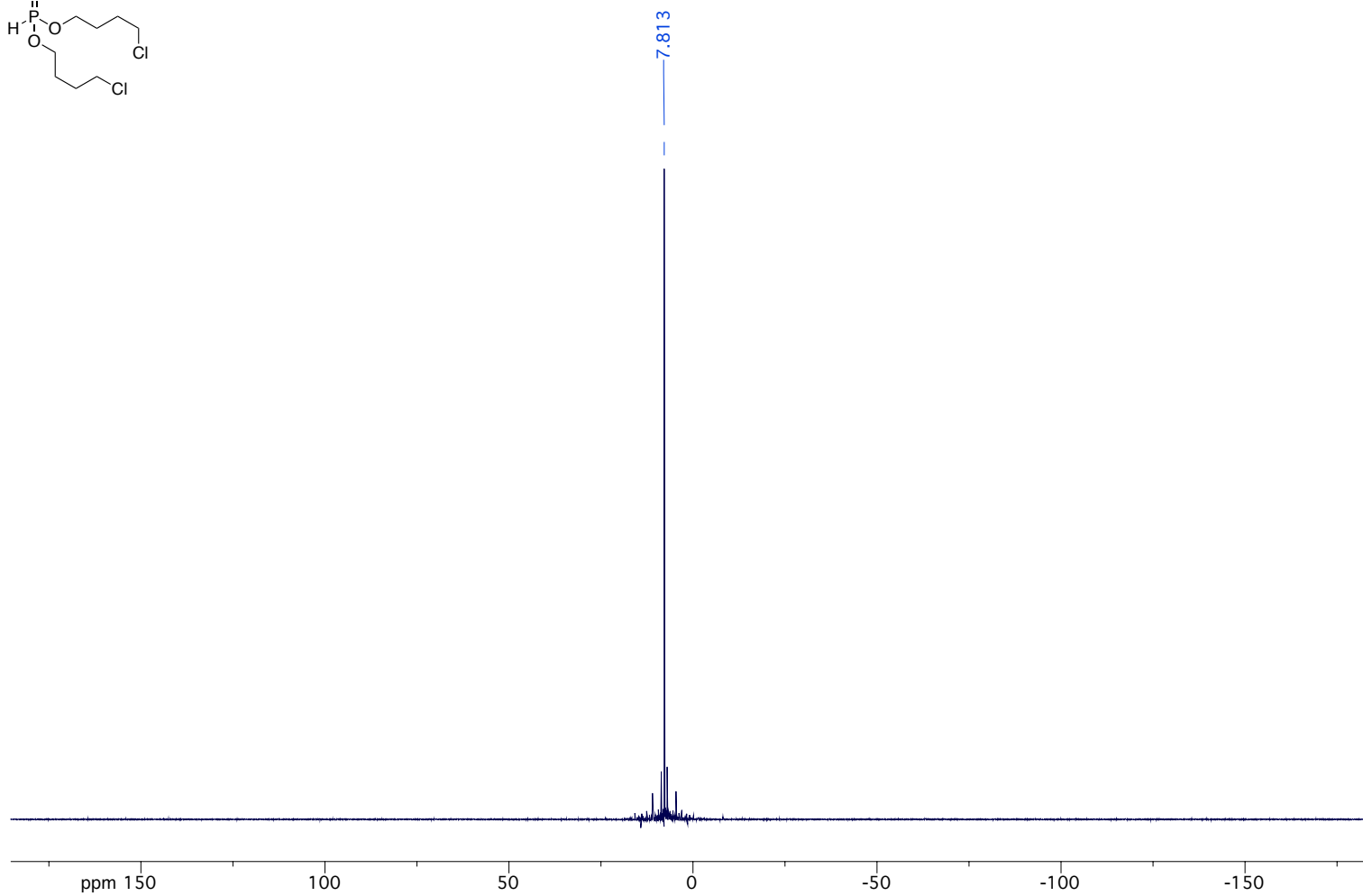
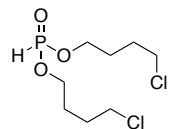
bis(4-chlorobutyl) phosphonate (**2j**)
300 MHz ^1H NMR in CDCl_3



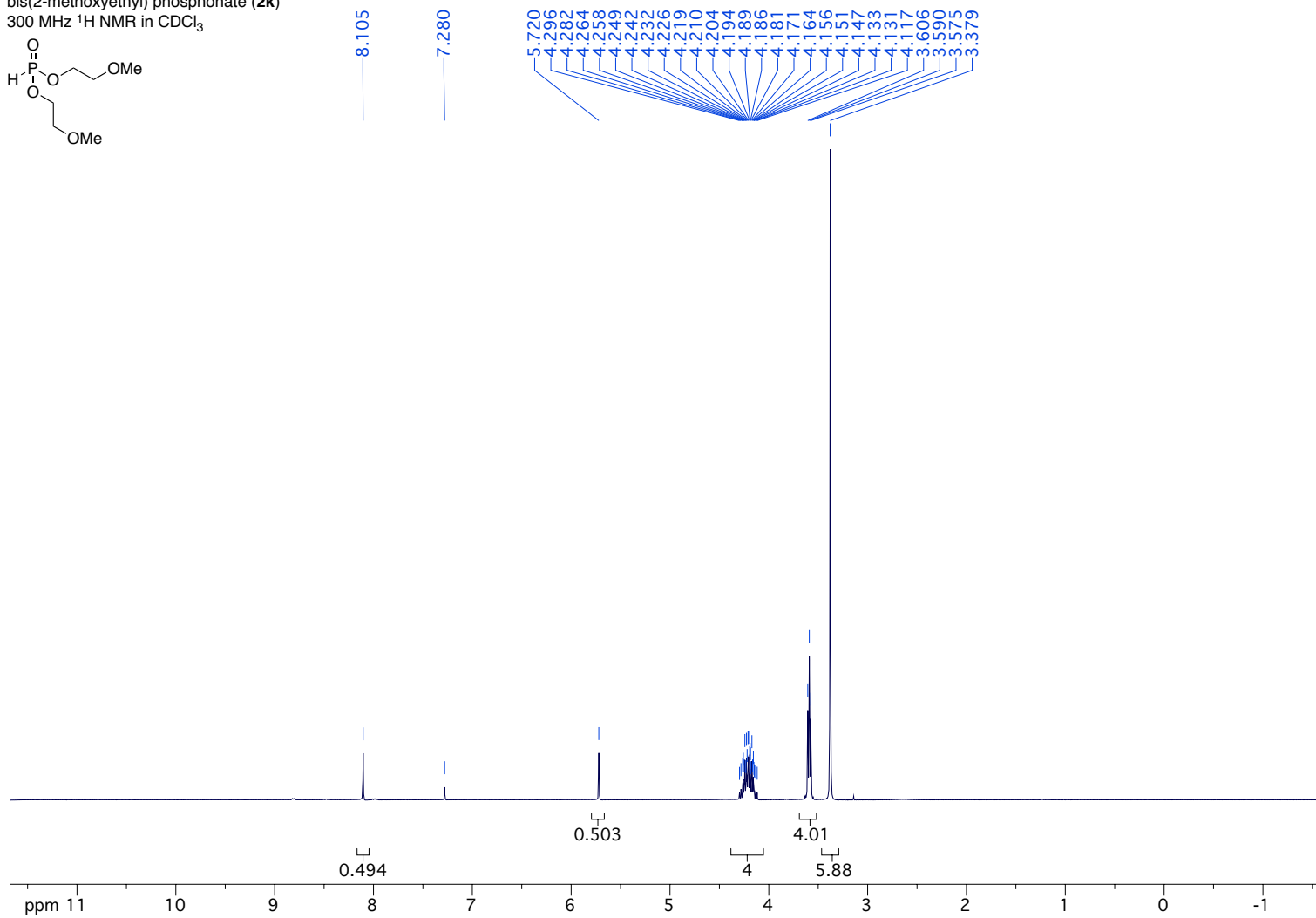
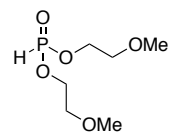
bis(4-chlorobutyl) phosphonate (**2j**)
75.5 MHz ^{13}C NMR in CDCl_3



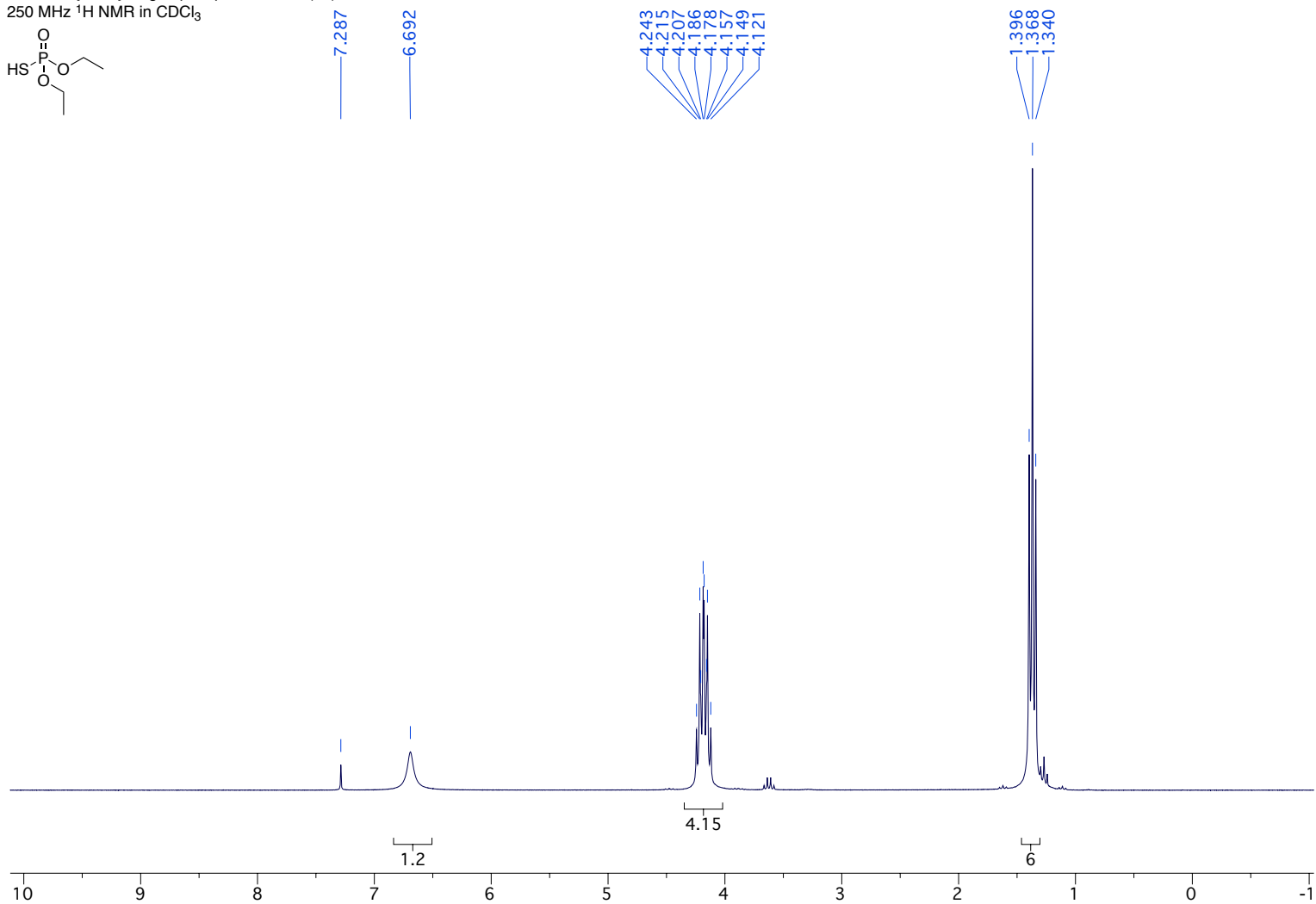
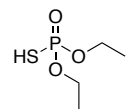
bis(4-chlorobutyl) phosphonate (**2j**)
121.5 MHz ^{31}P NMR in CDCl_3



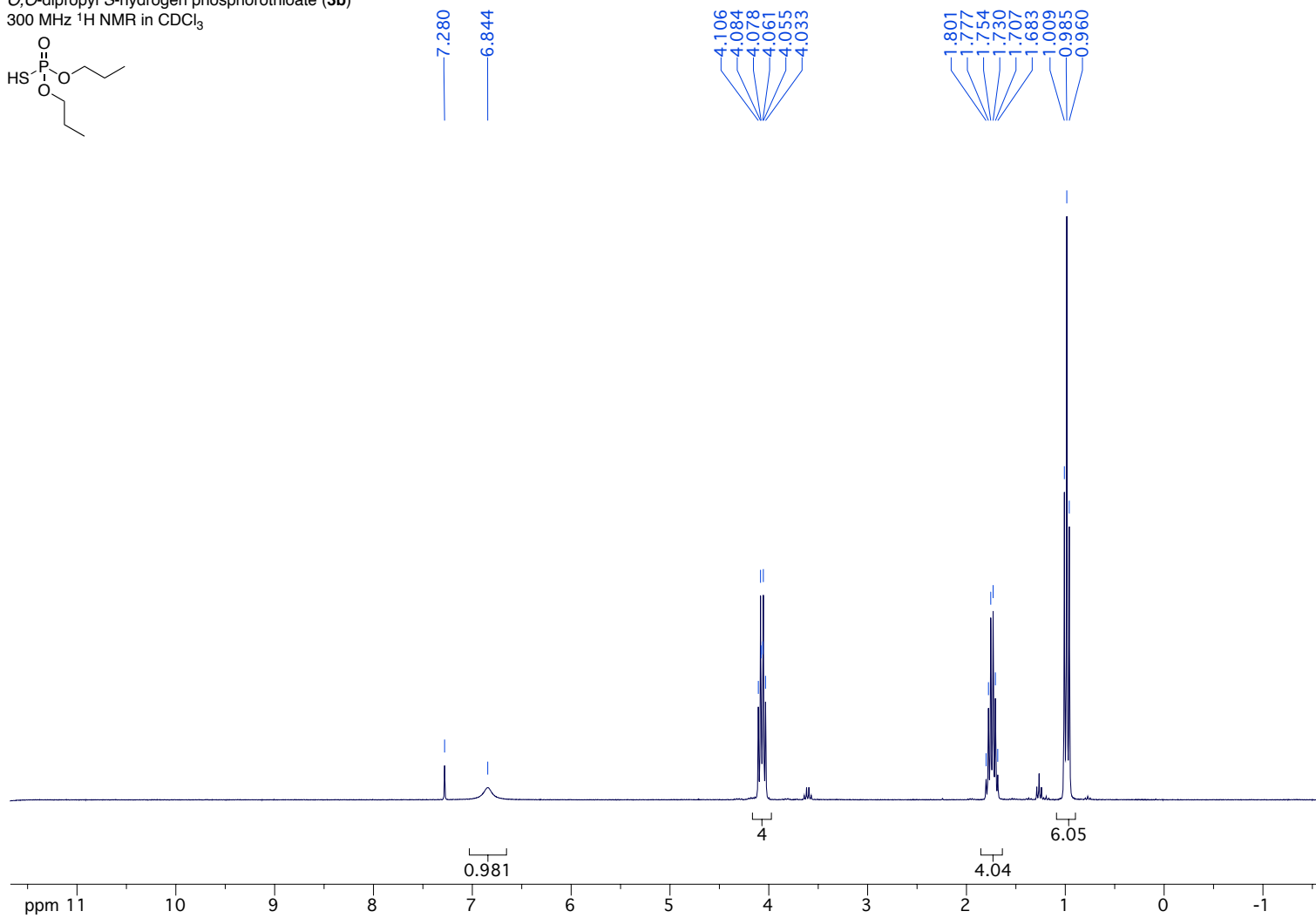
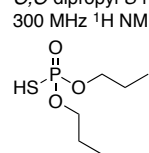
bis(2-methoxyethyl) phosphonate (**2k**)
 300 MHz ^1H NMR in CDCl_3



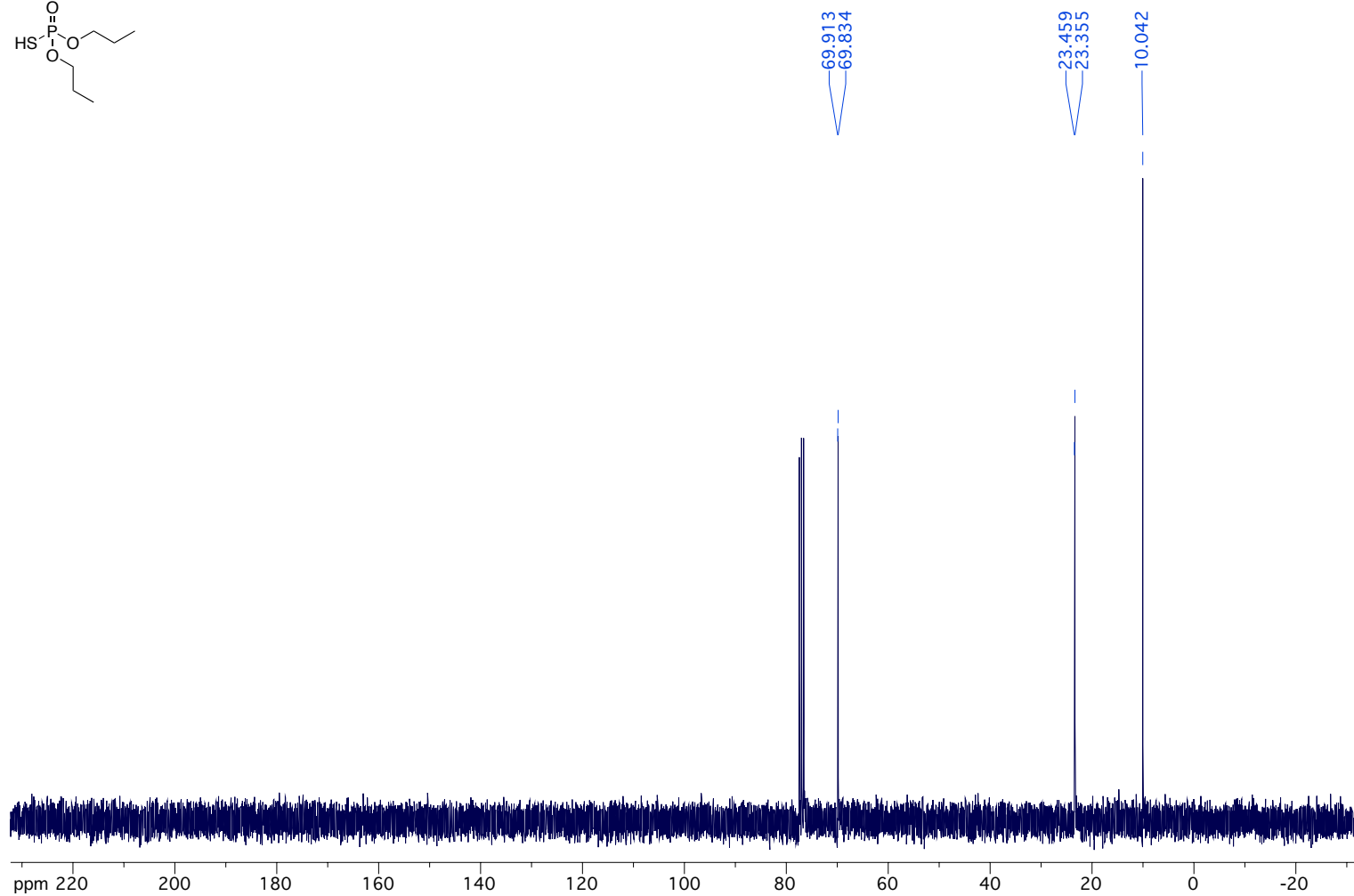
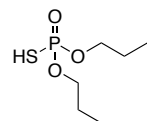
O,O-diethyl *S*-hydrogen phosphorothioate (**3a**)
 250 MHz ^1H NMR in CDCl_3



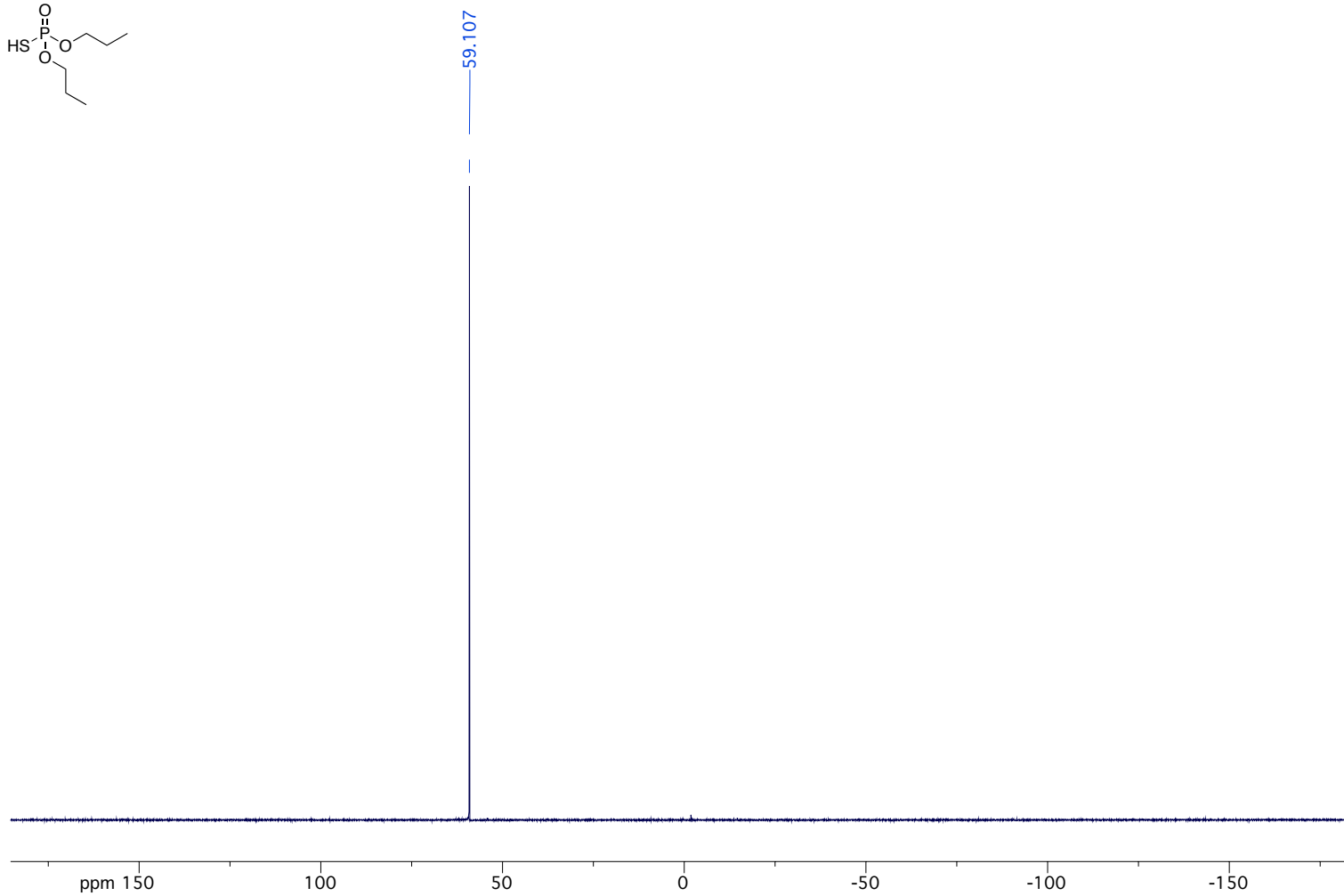
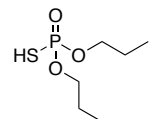
O,O-dipropyl *S*-hydrogen phosphorothioate (**3b**)
 300 MHz ^1H NMR in CDCl_3



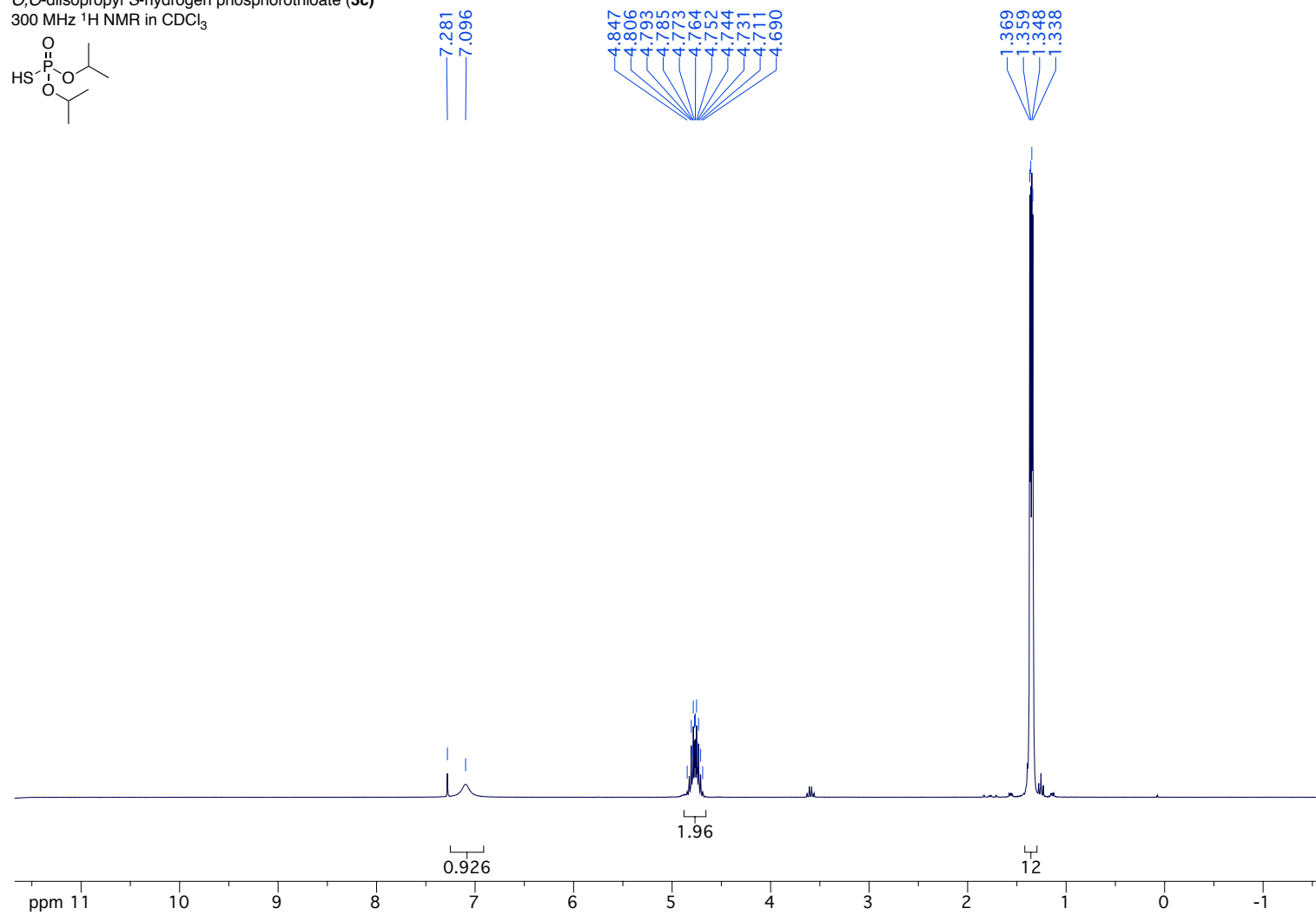
O,O-dipropyl *S*-hydrogen phosphorothioate (**3b**)
75.5 MHz ^{13}C NMR in CDCl_3



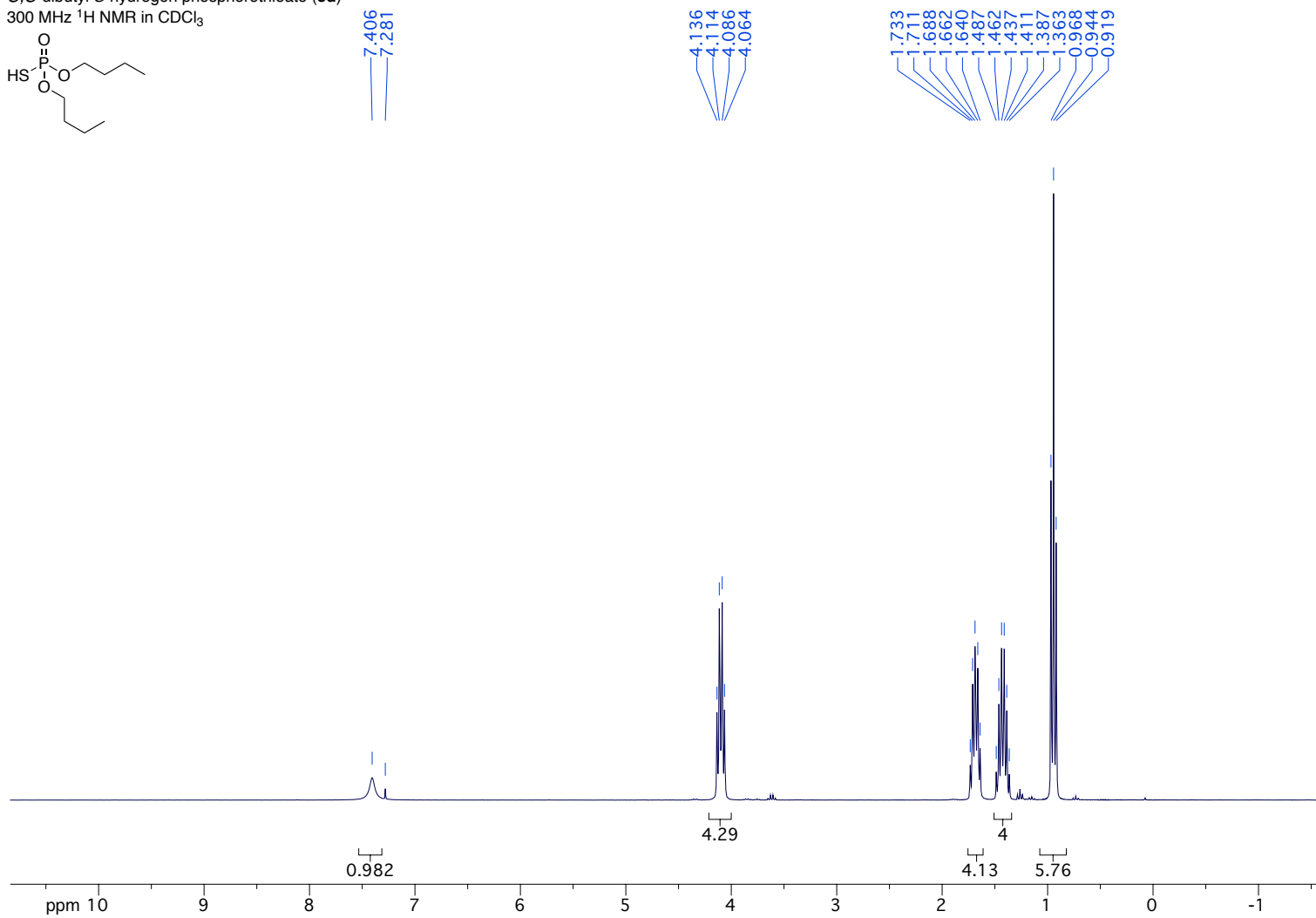
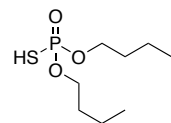
O,O-dipropyl *S*-hydrogen phosphorothioate (**3b**)
121.5 MHz ^{31}P NMR in CDCl_3



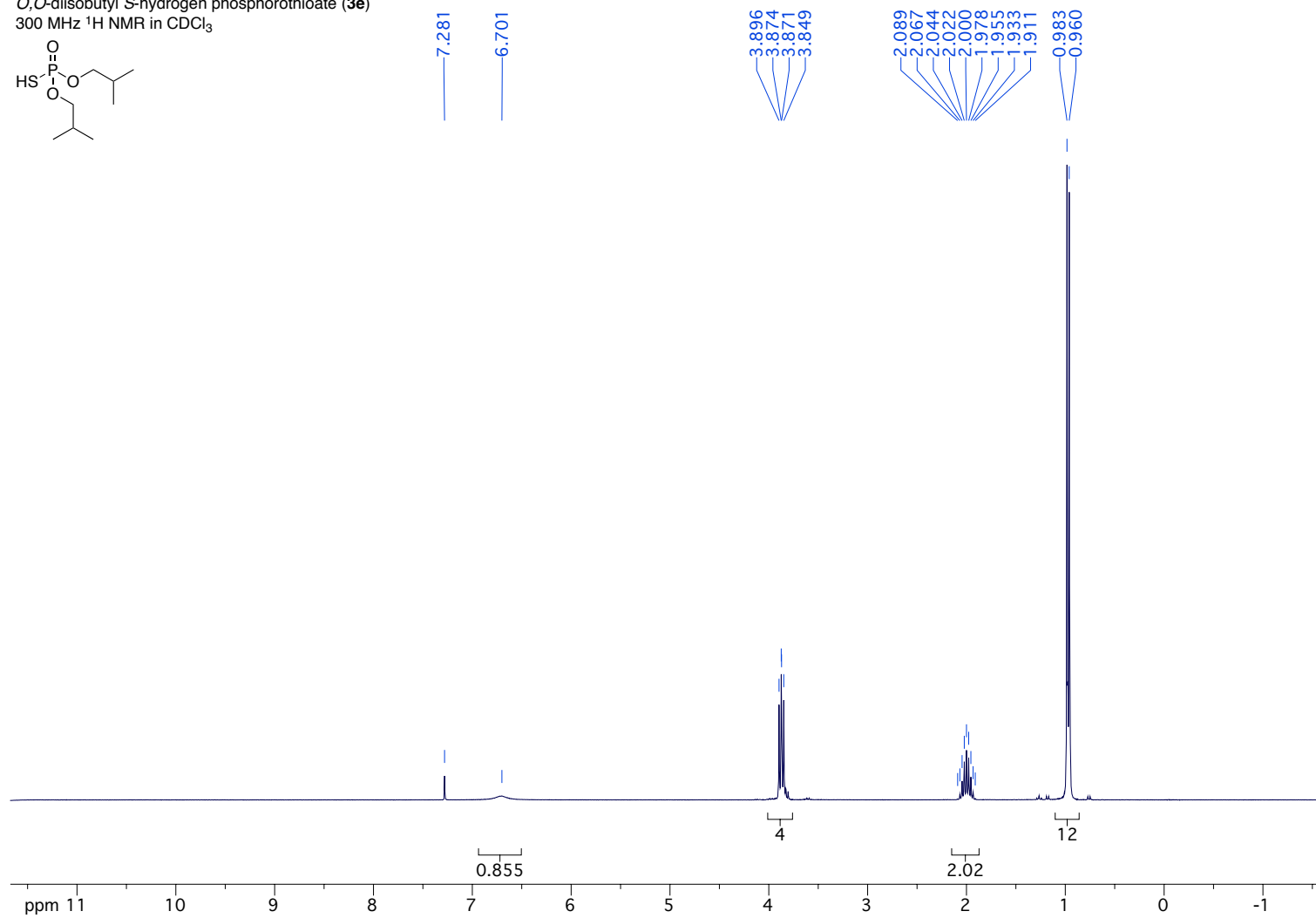
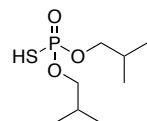
O,O-diisopropyl *S*-hydrogen phosphorothioate (**3c**)
300 MHz ^1H NMR in CDCl_3



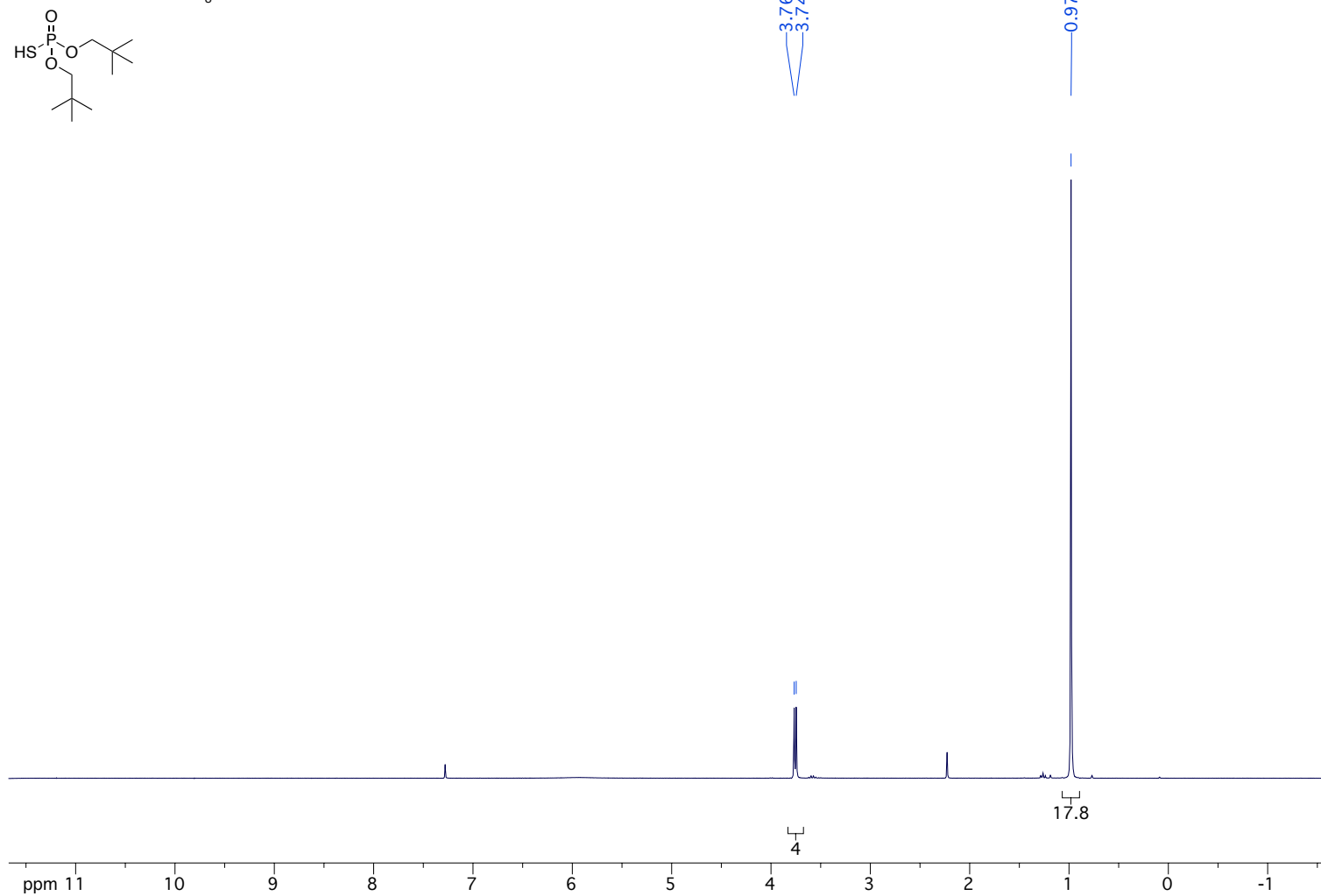
O,O-dibutyl *S*-hydrogen phosphorothioate (**3d**)
 300 MHz ^1H NMR in CDCl_3



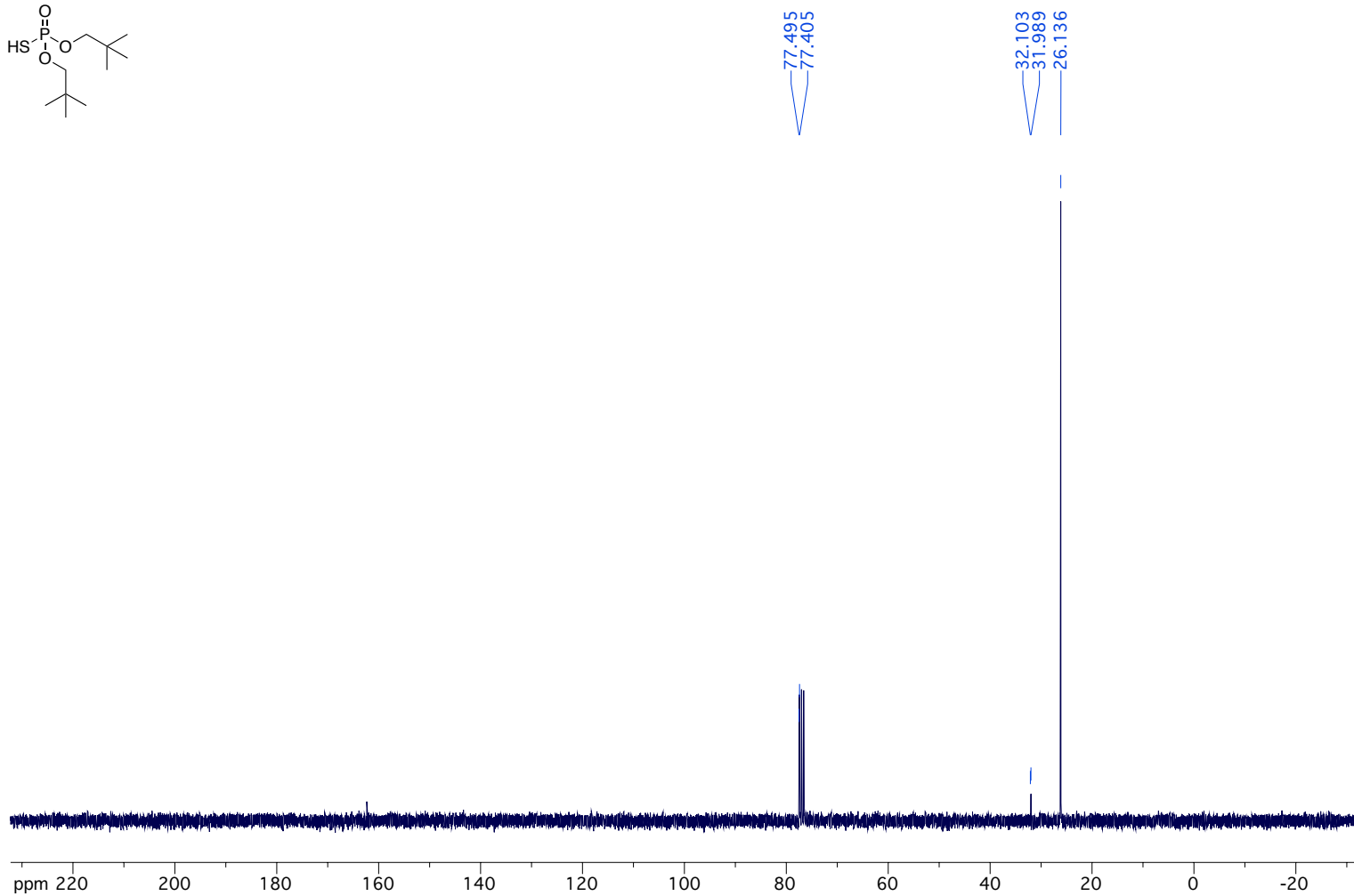
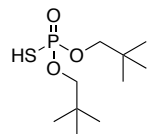
O,O-diisobutyl *S*-hydrogen phosphorothioate (**3e**)
300 MHz ^1H NMR in CDCl_3



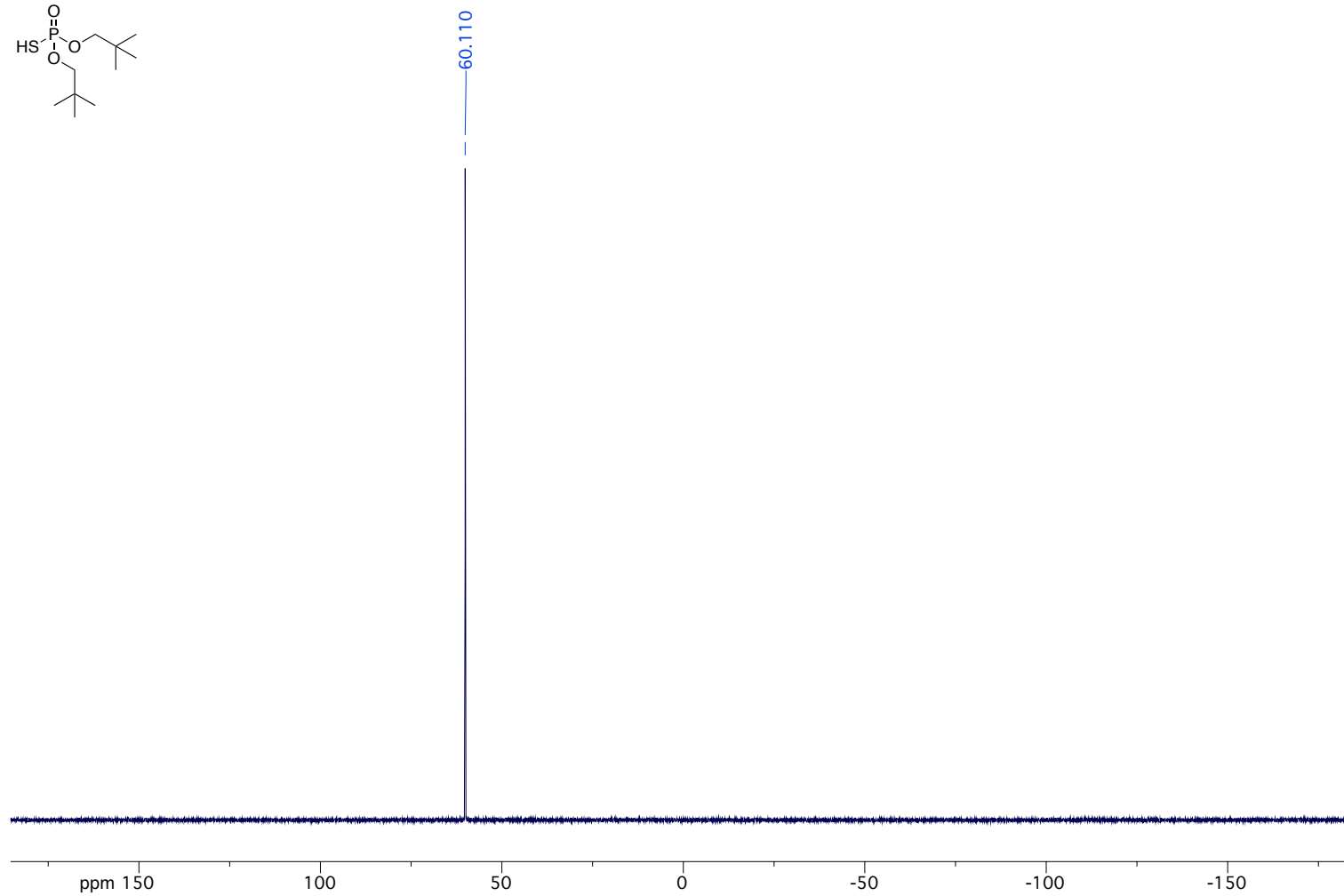
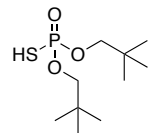
O,O-dineopentyl *S*-hydrogen phosphorothioate (**3f**)
300 MHz ^1H NMR in CDCl_3



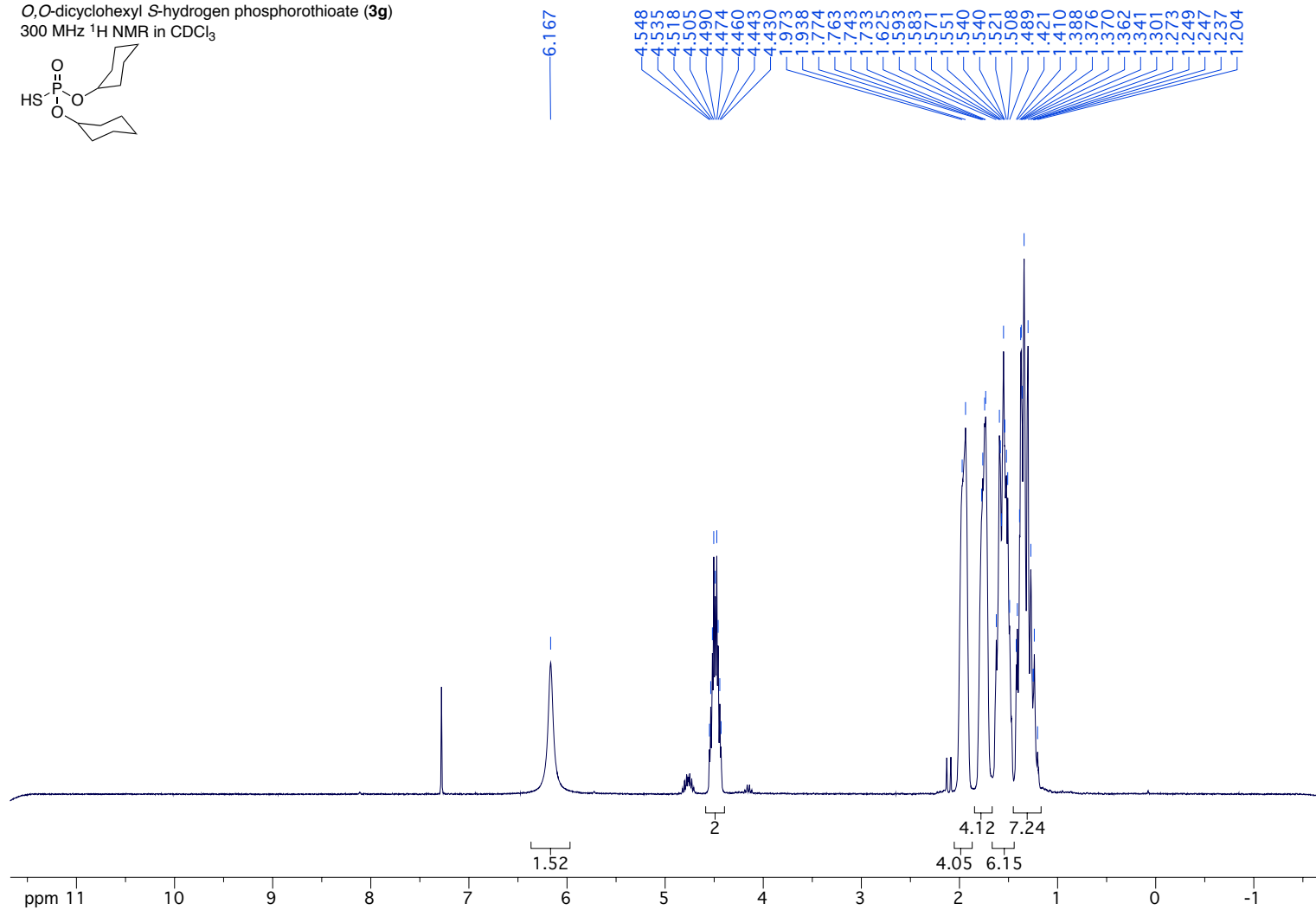
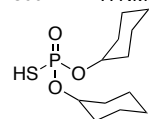
O,O-dineopentyl *S*-hydrogen phosphorothioate (**3f**)
75.5 MHz ^{13}C NMR in CDCl_3



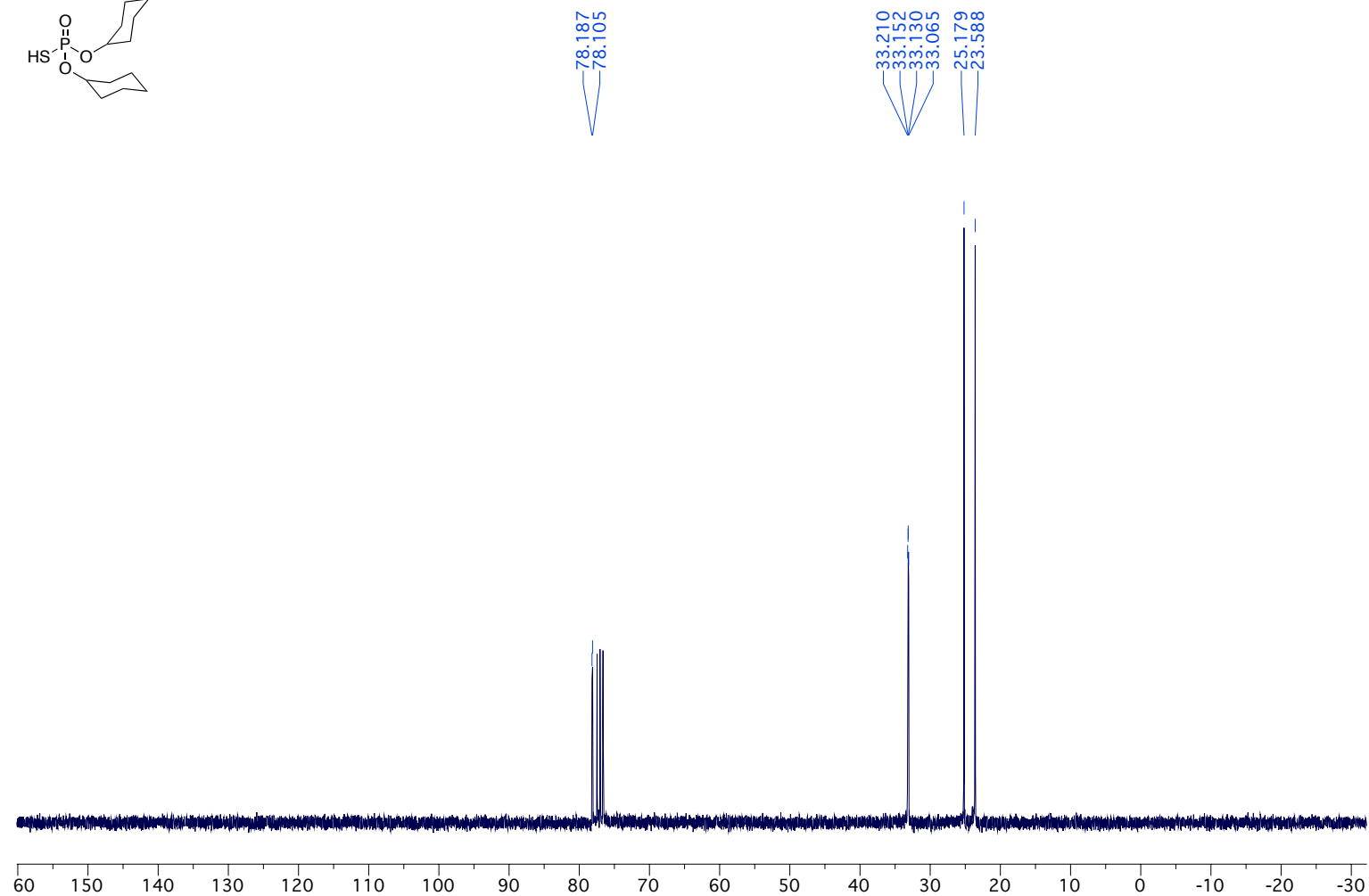
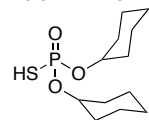
O,O-dineopentyl *S*-hydrogen phosphorothioate (**3f**)
121.5 MHz ^{31}P NMR in CDCl_3



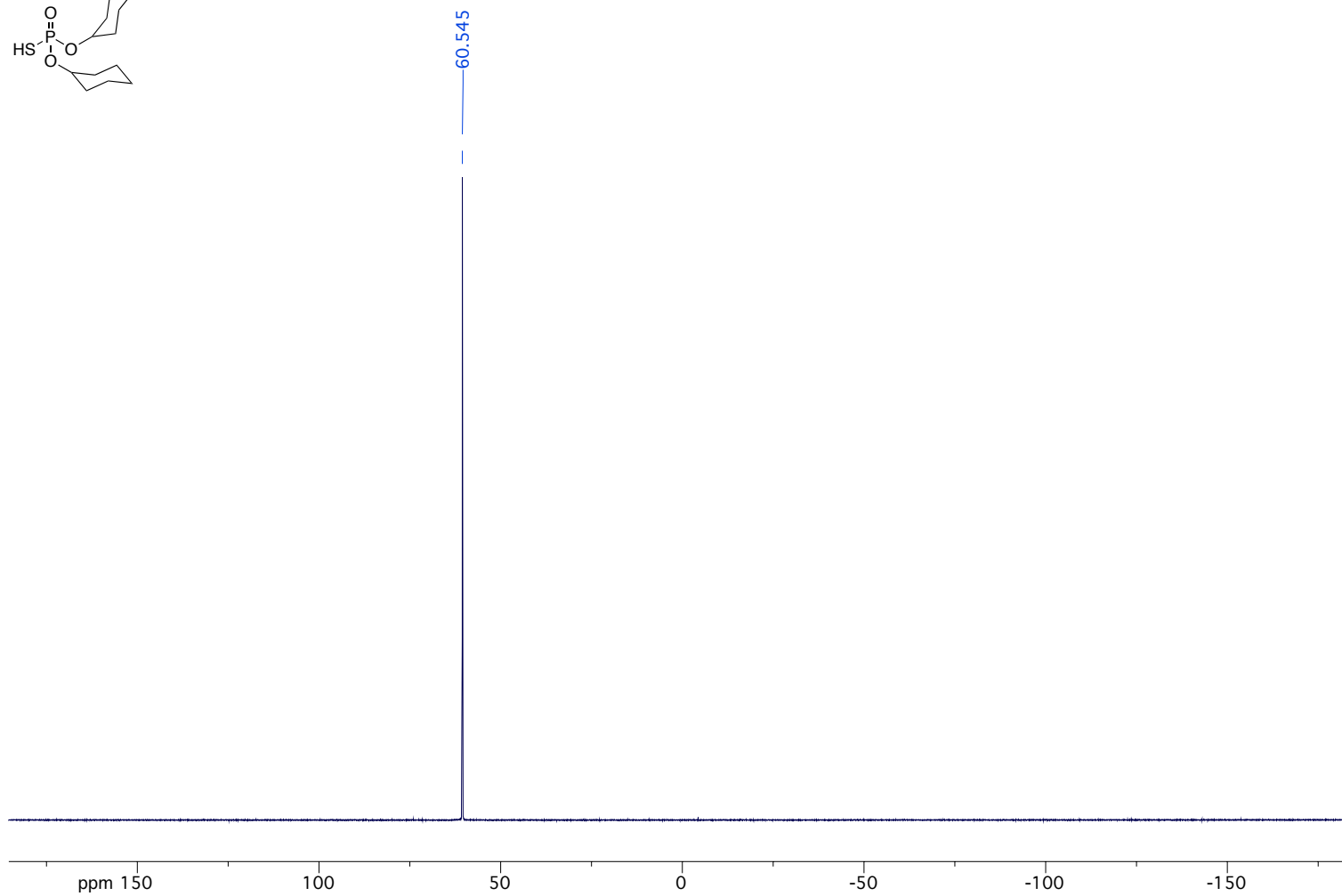
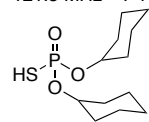
O,O-dicyclohexyl *S*-hydrogen phosphorothioate (**3g**)
300 MHz ^1H NMR in CDCl_3



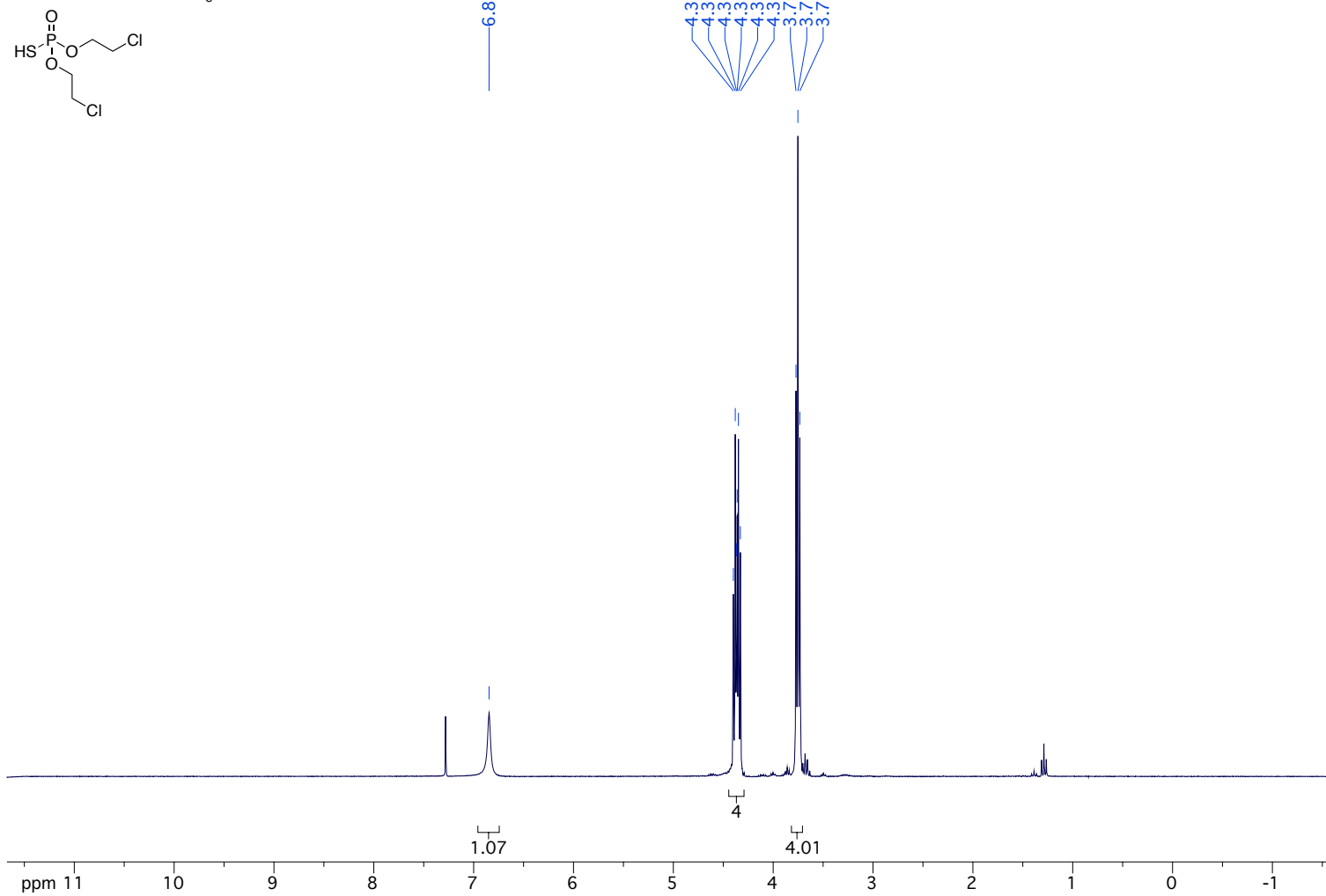
O,O-dicyclohexyl *S*-hydrogen phosphorothioate (**3g**)
75.5 MHz ^{13}C NMR in CDCl_3



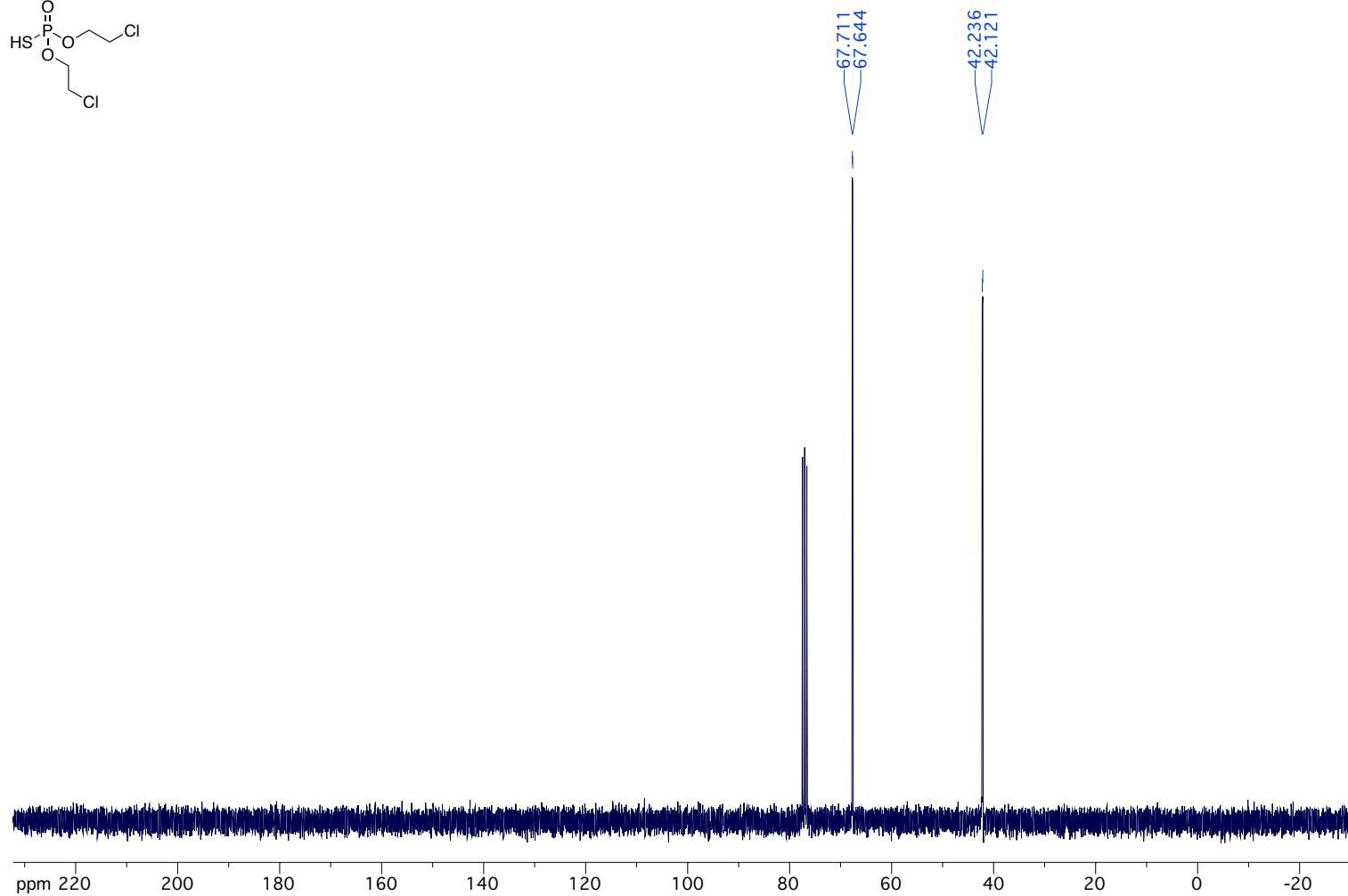
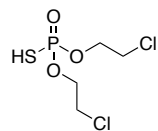
O,O-dicyclohexyl *S*-hydrogen phosphorothioate (**3g**)
121.5 MHz ^{31}P NMR in CDCl_3



O,O-bis(2-chloroethyl) *S*-hydrogen phosphorothioate (**3h**)
300 MHz ^1H NMR in CDCl_3

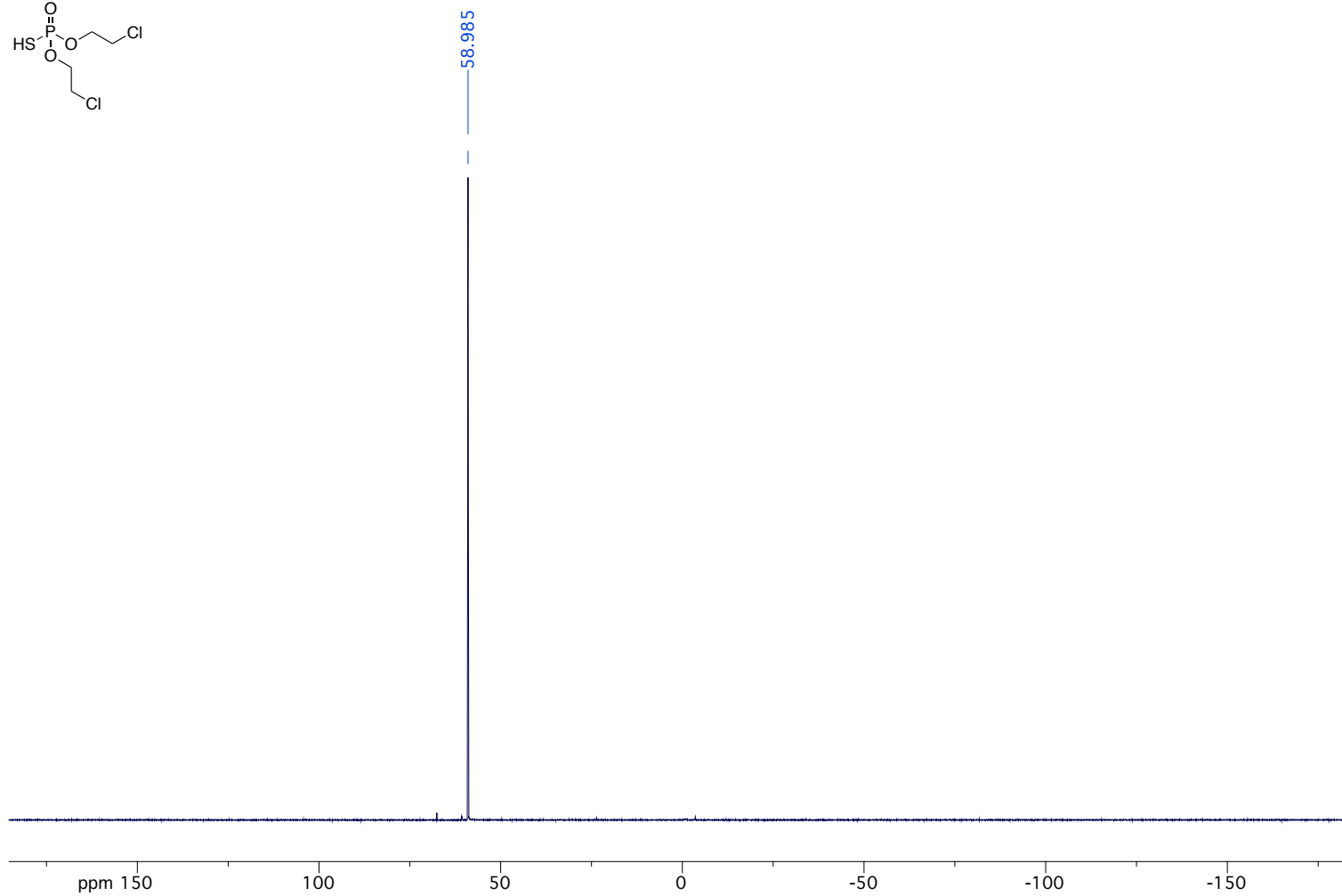
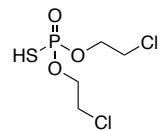


O,O-bis(2-chloroethyl) *S*-hydrogen phosphorothioate (**3h**)
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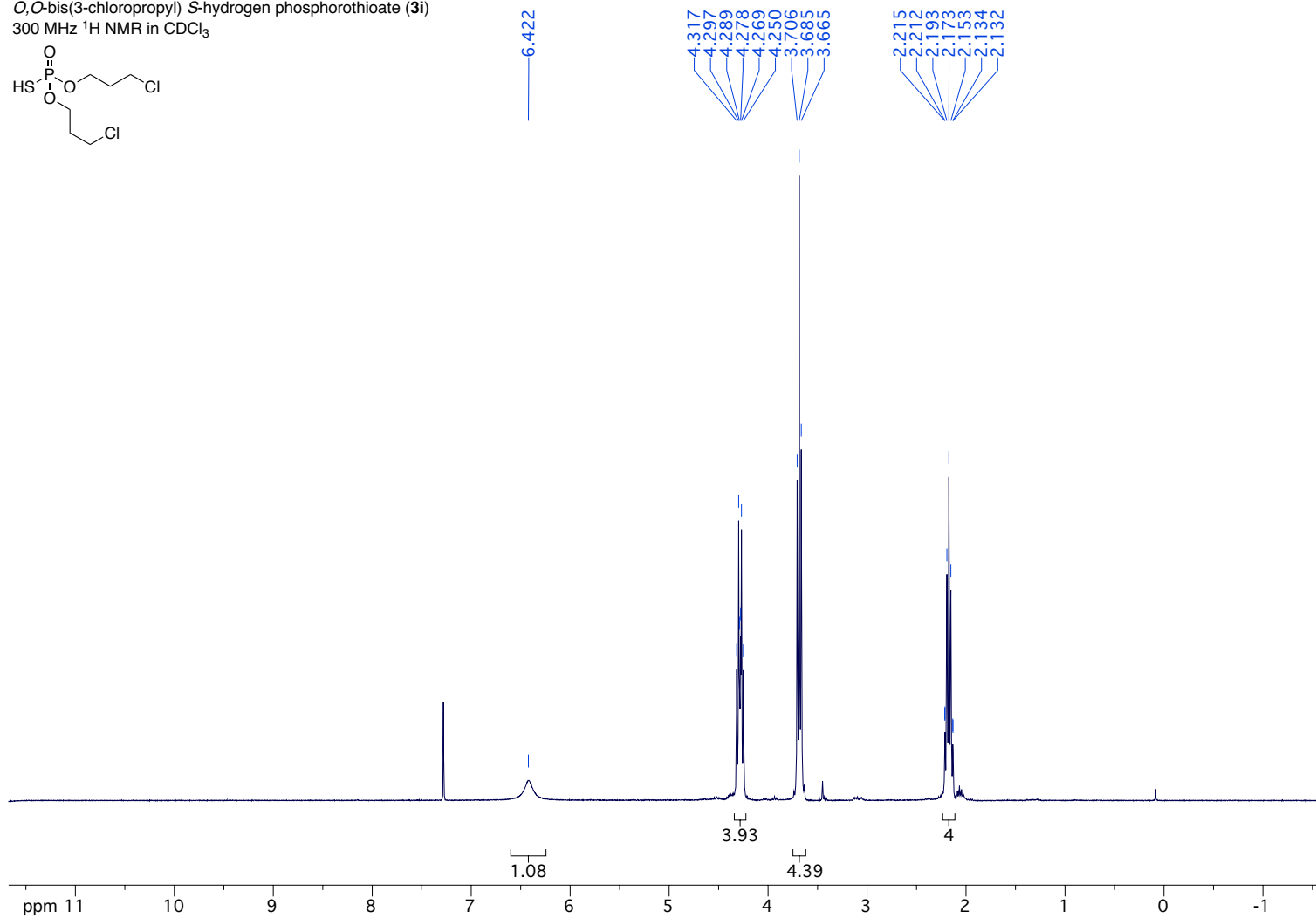


O,O-bis(2-chloroethyl) *S*-hydrogen phosphorothioate (**3h**)

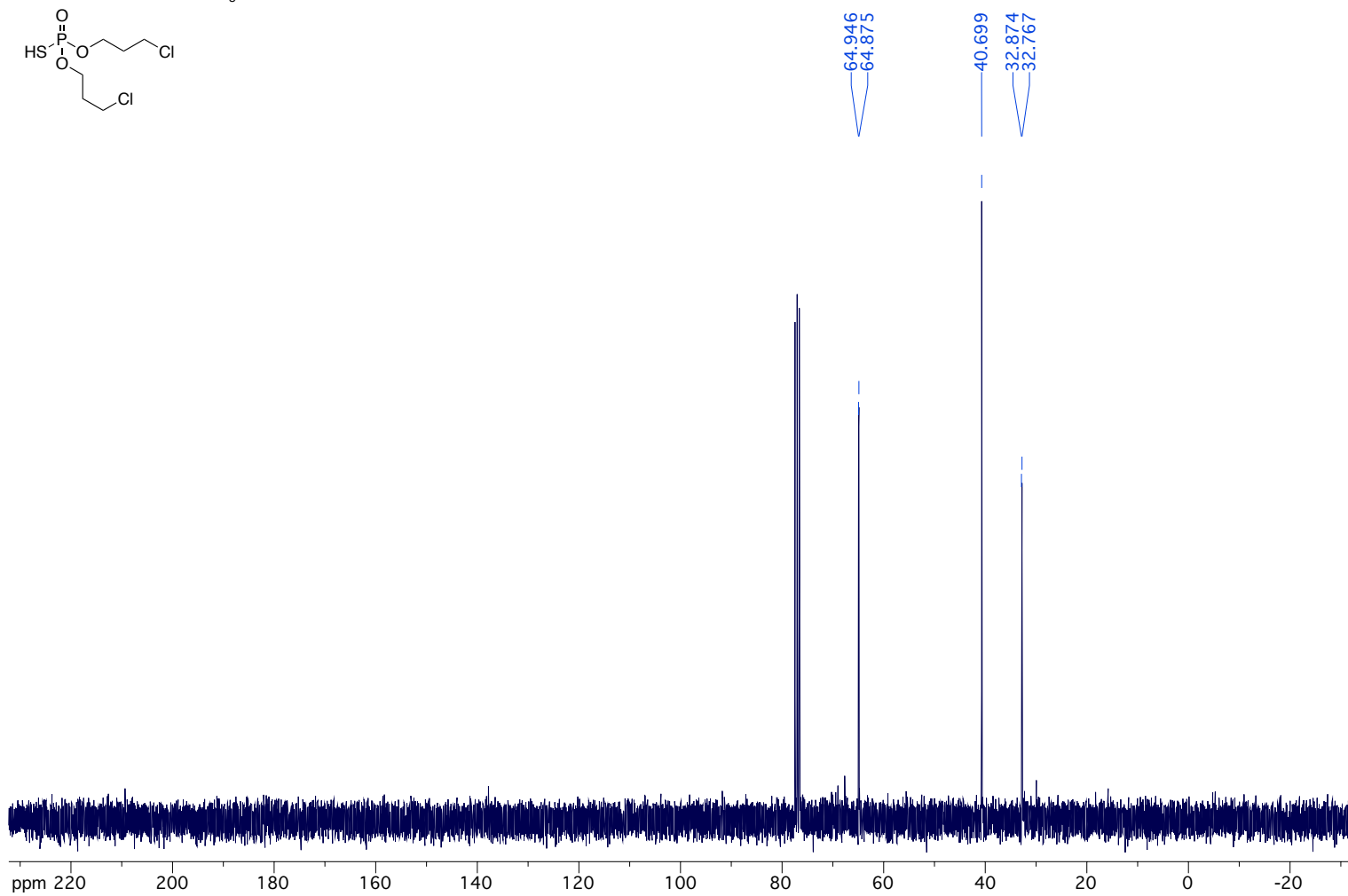
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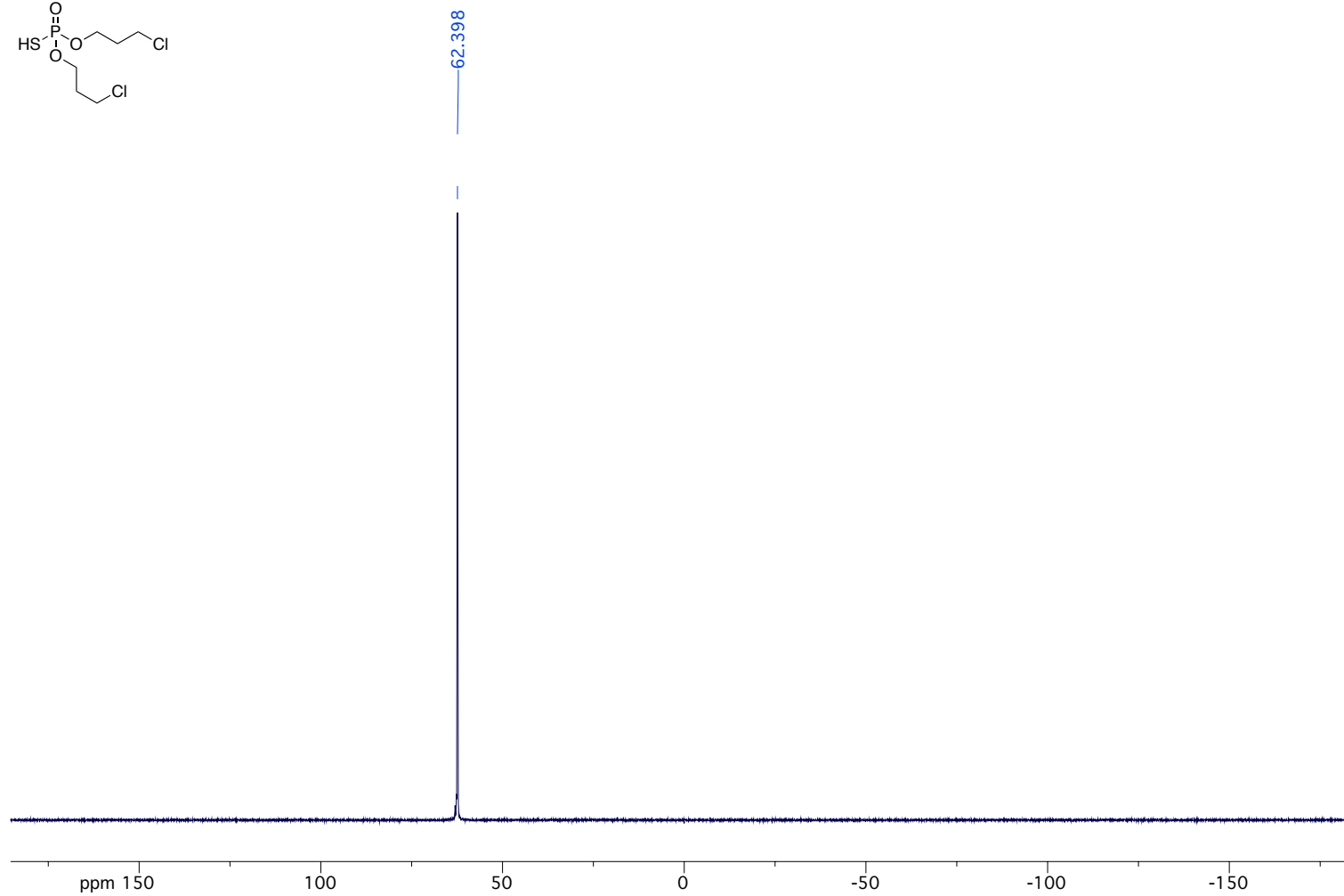
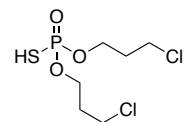
O,O-bis(3-chloropropyl) *S*-hydrogen phosphorothioate (**3i**)
300 MHz ^1H NMR in CDCl_3



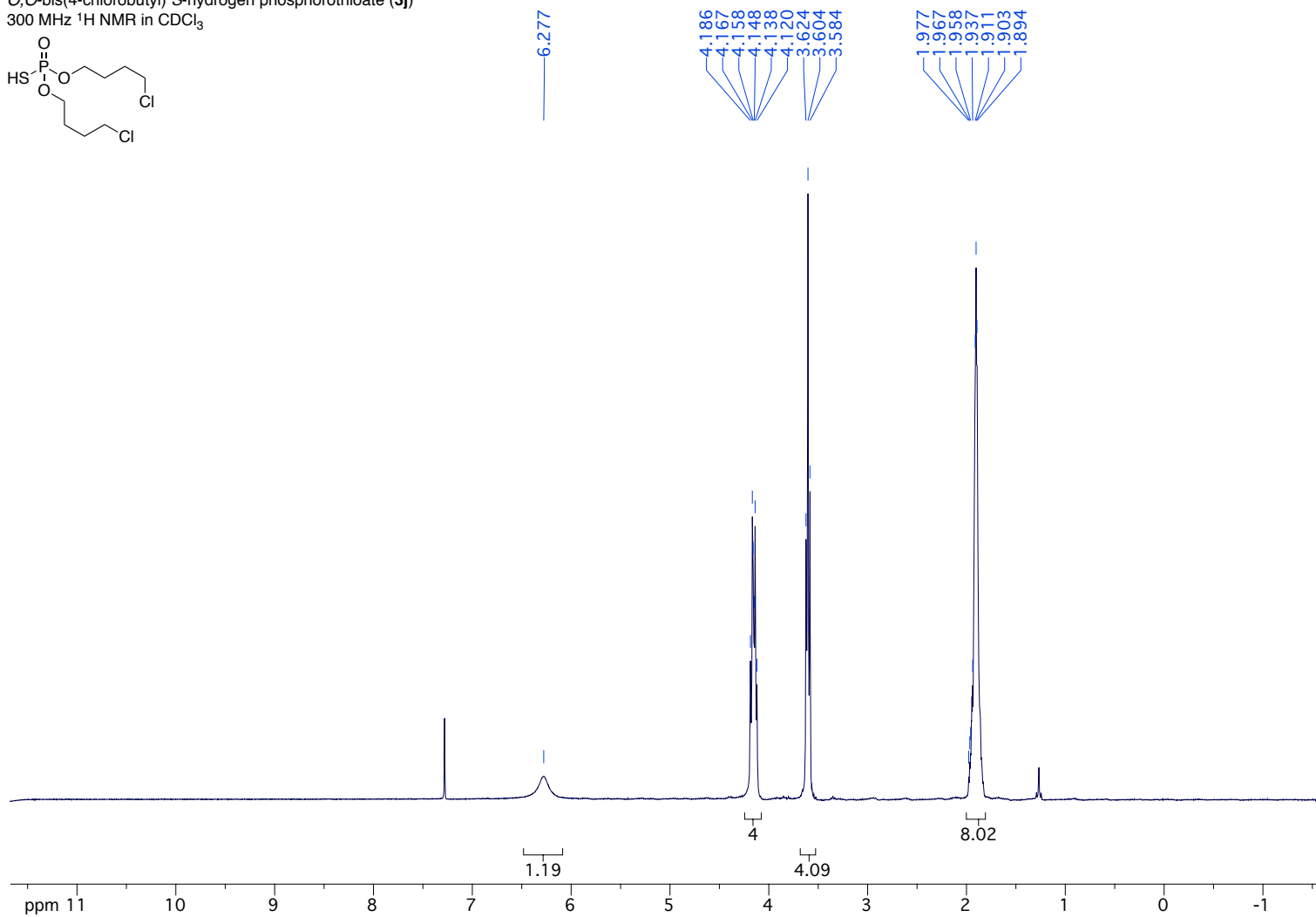
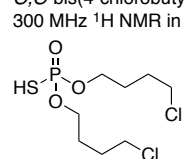
O,O-bis(3-chloropropyl) *S*-hydrogen phosphorothioate (**3i**)
75.5 MHz ^{13}C NMR in CDCl_3



O,O-bis(3-chloropropyl) *S*-hydrogen phosphorothioate (**3i**)
121.5 MHz ^{31}P NMR in CDCl_3

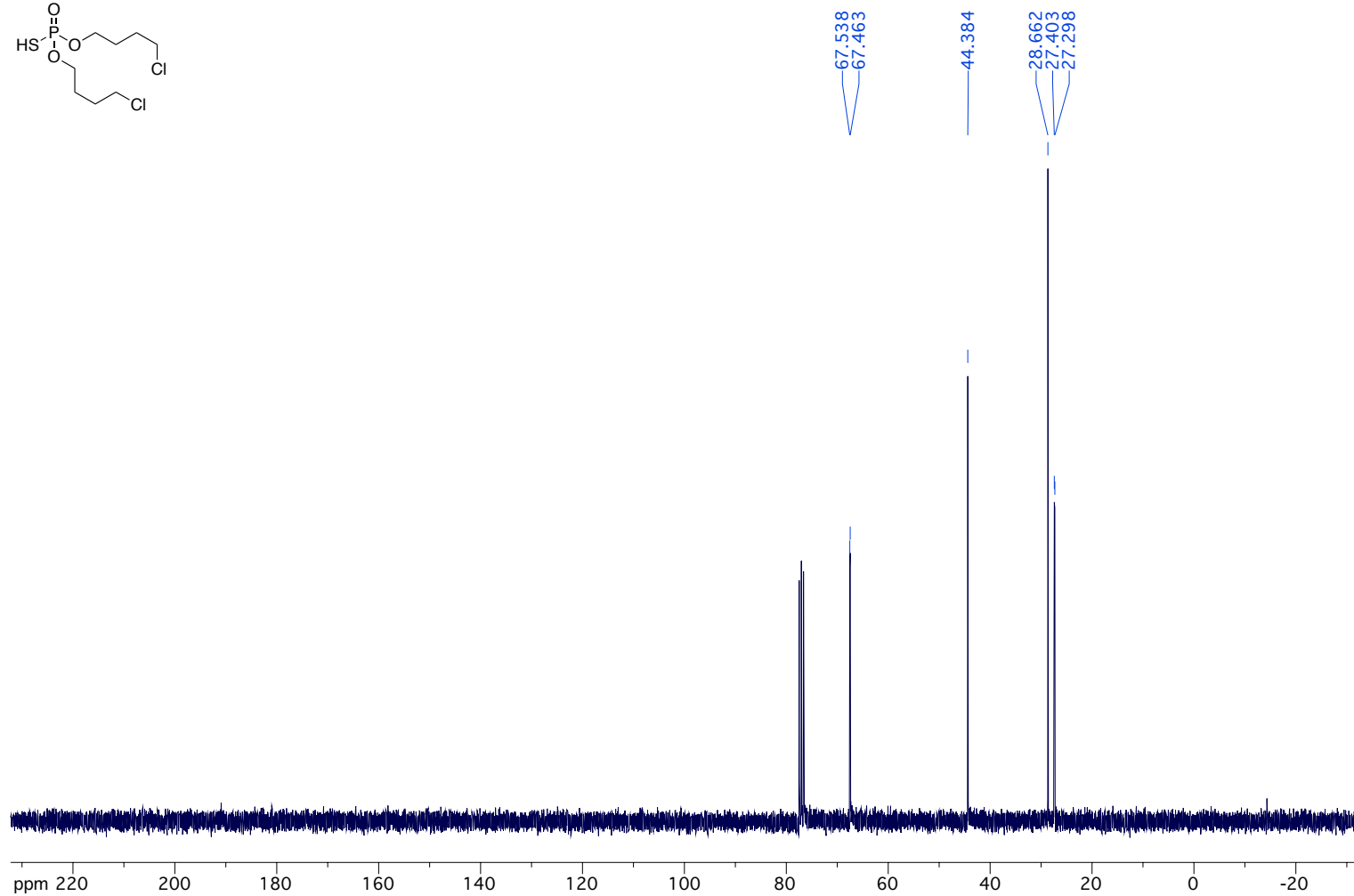
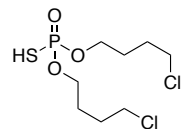


O,O-bis(4-chlorobutyl) *S*-hydrogen phosphorothioate (**3j**)
300 MHz ^1H NMR in CDCl_3

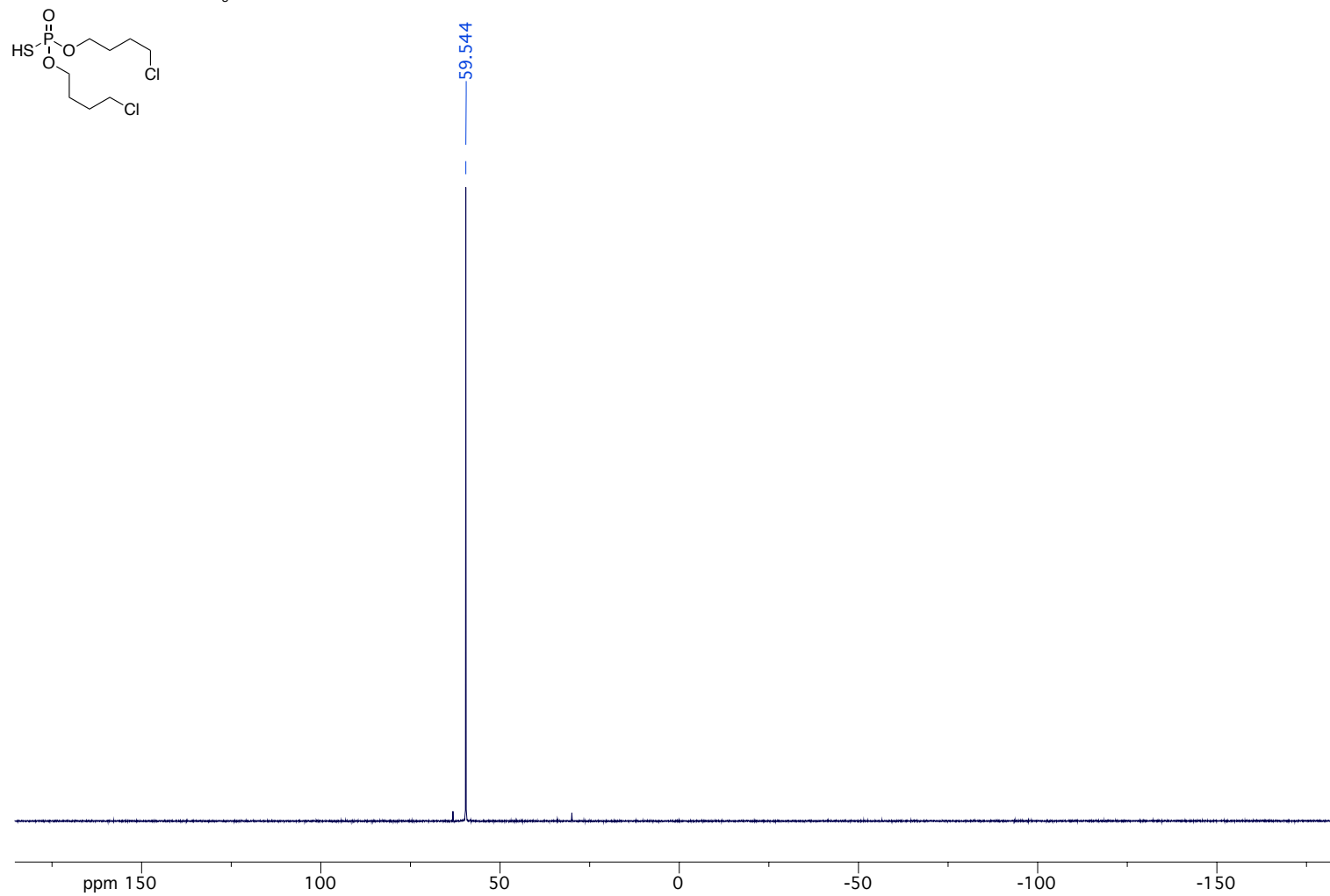


O,O-bis(4-chlorobutyl) *S*-hydrogen phosphorothioate (**3j**)

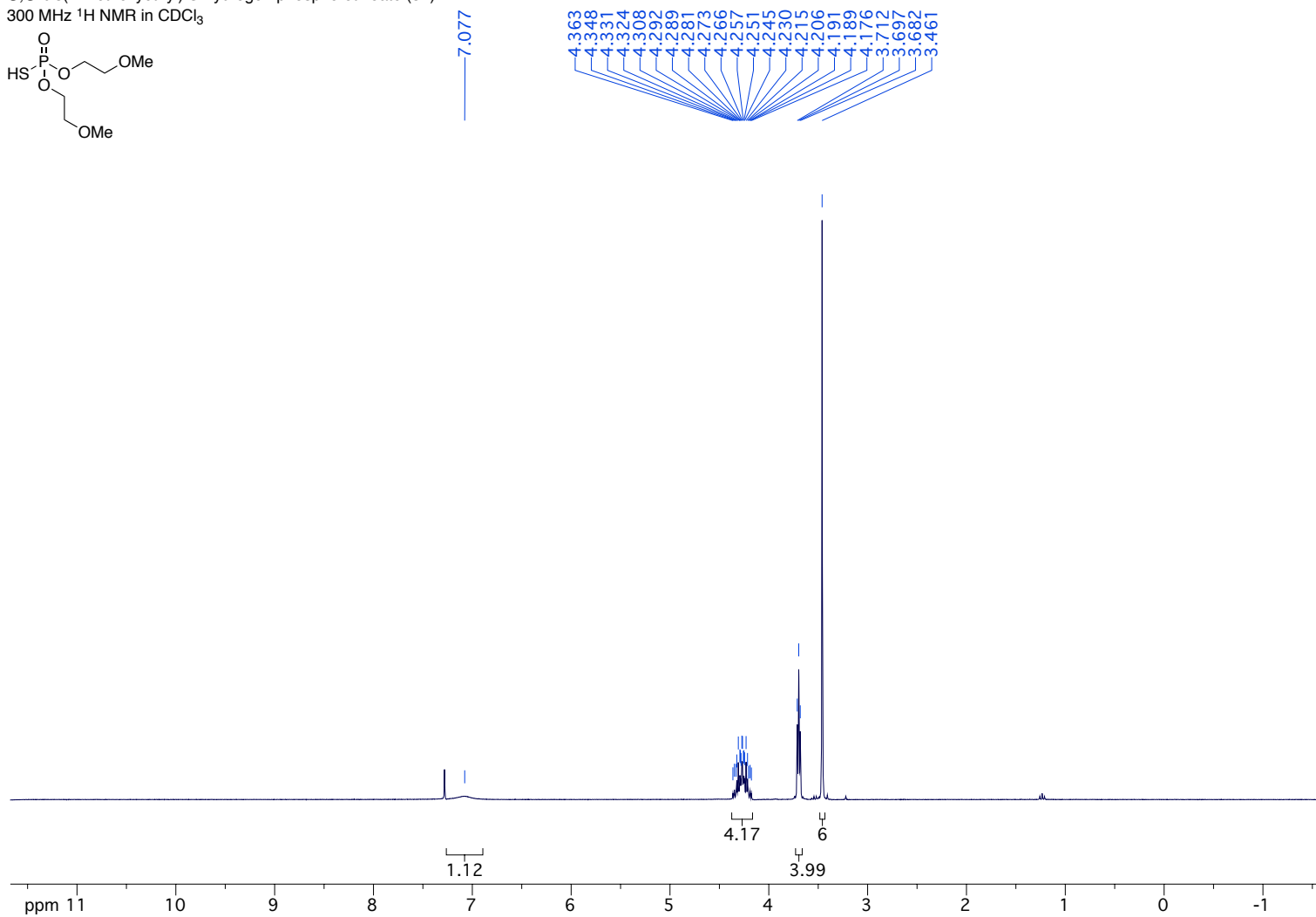
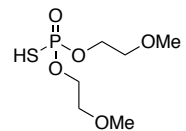
75.5 MHz ^{13}C NMR in CDCl_3



O,O-bis(4-chlorobutyl) *S*-hydrogen phosphorothioate (**3j**)
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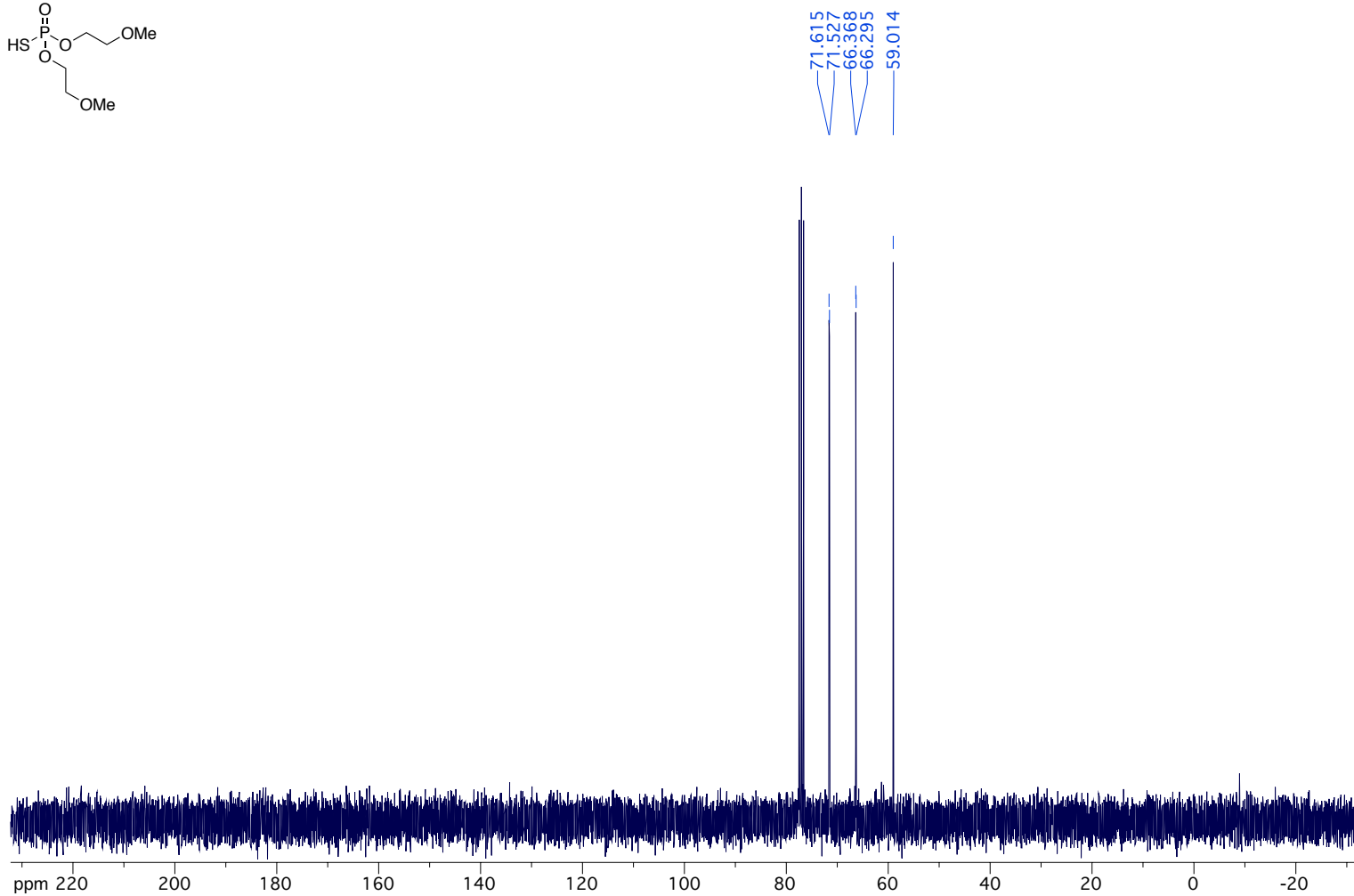
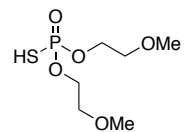


O,O-bis(2-methoxyethyl) *S*-hydrogen phosphorothioate (**3k**)
300 MHz ^1H NMR in CDCl_3

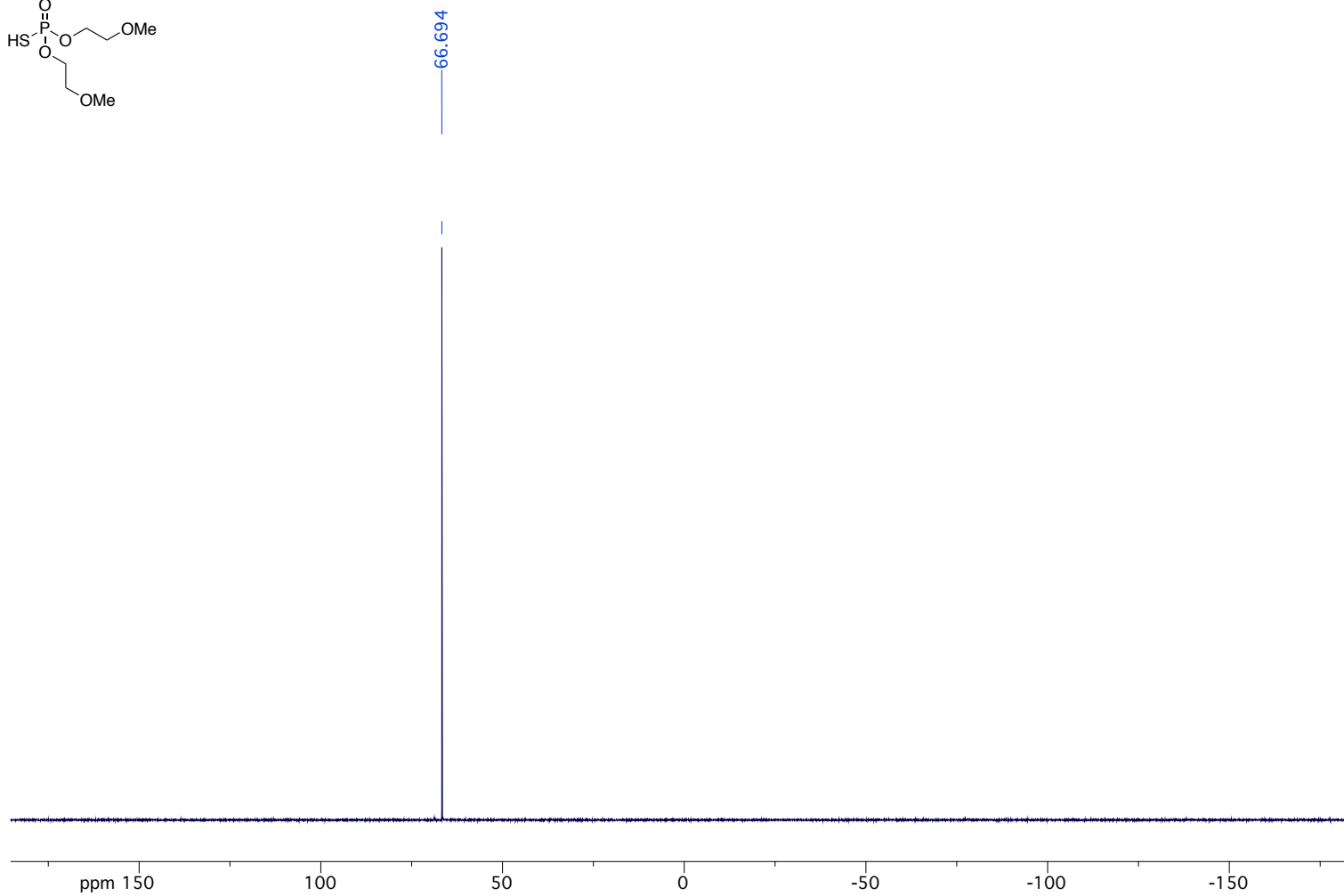
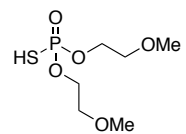


O,O-bis(2-methoxyethyl) *S*-hydrogen phosphorothioate (**3k**)

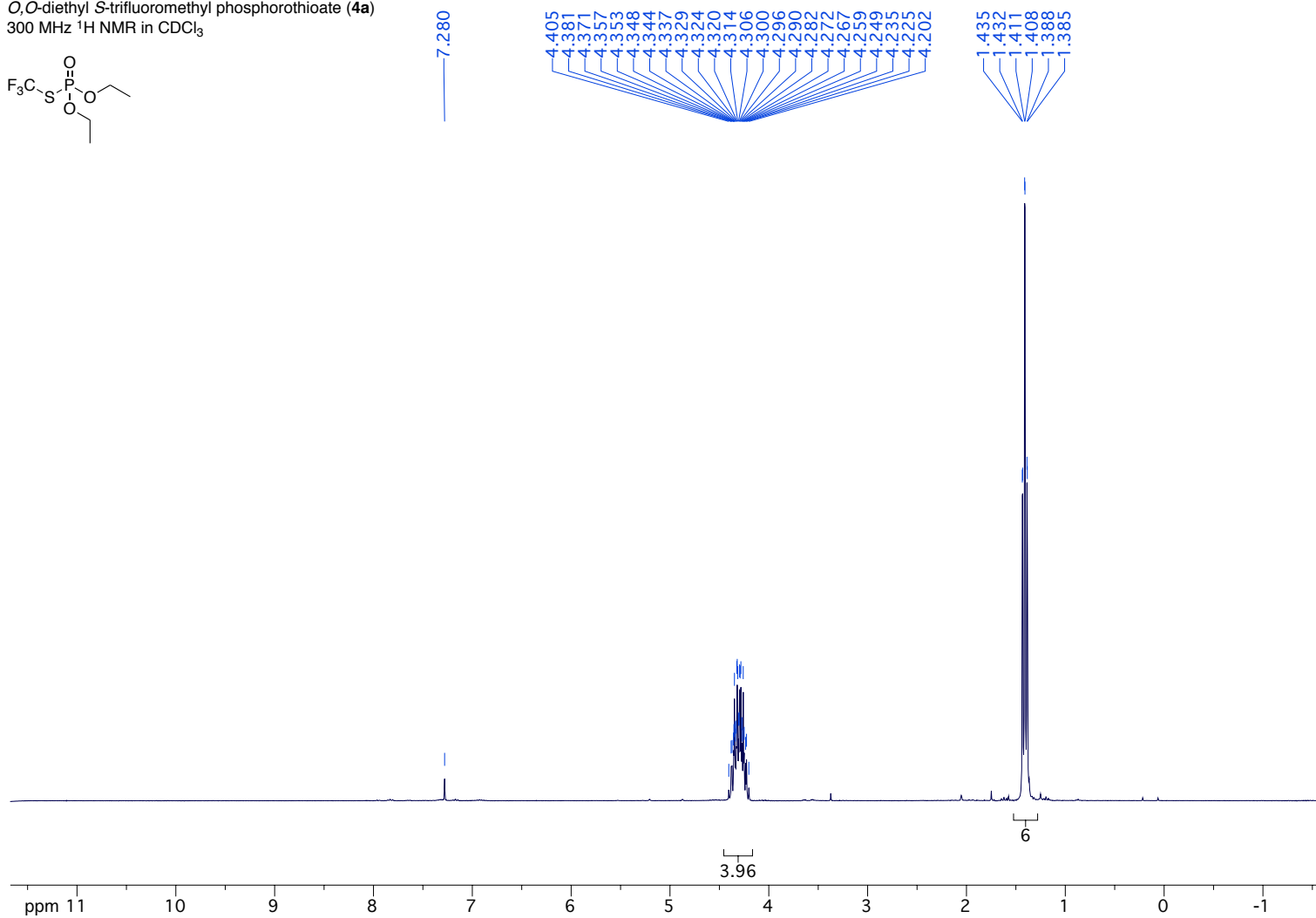
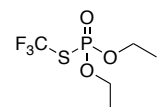
75.5 MHz ^{13}C NMR in CDCl_3



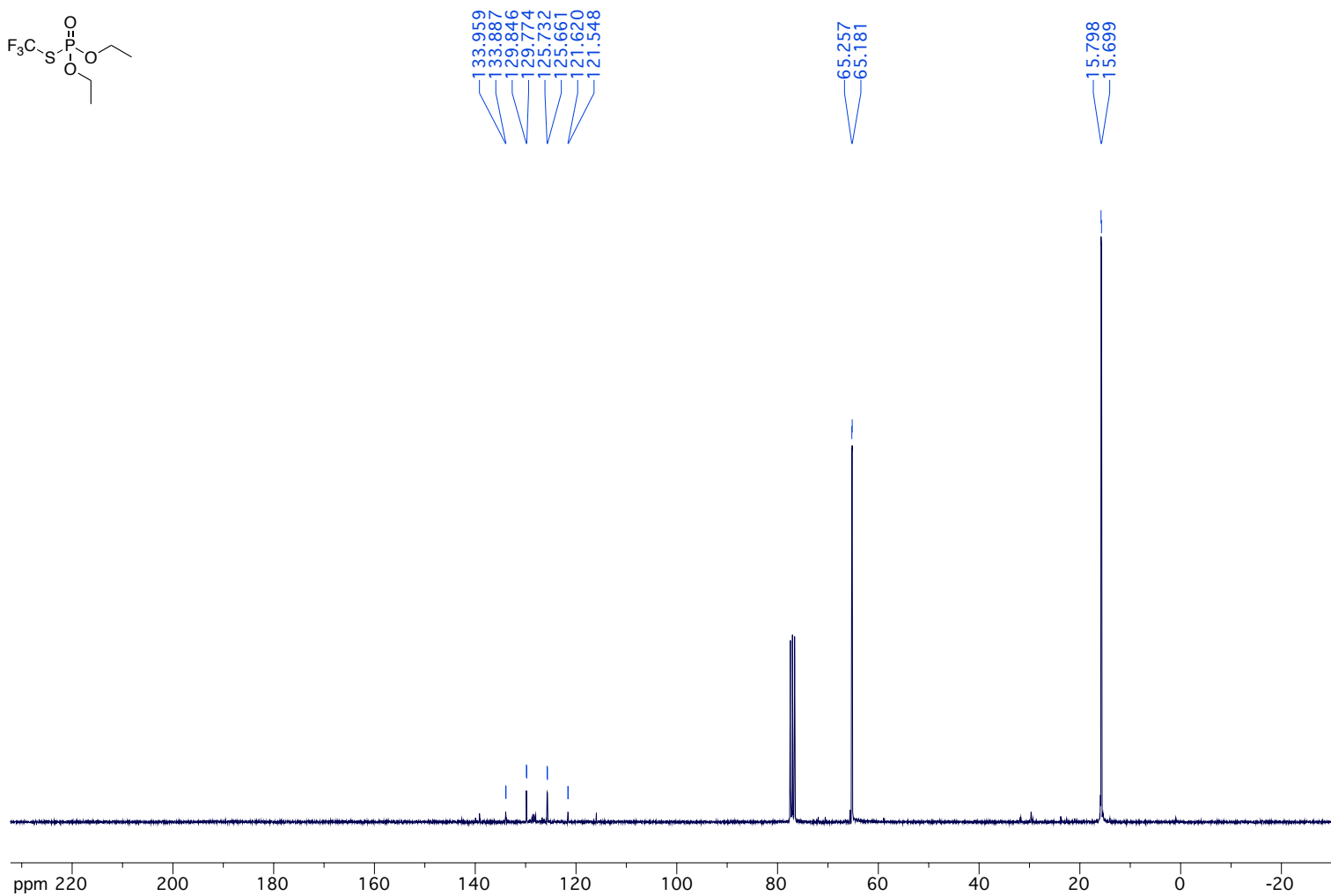
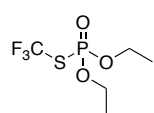
O,O-bis(2-methoxyethyl) *S*-hydrogen phosphorothioate (**3k**)
121.5 MHz ^{31}P NMR in CDCl_3



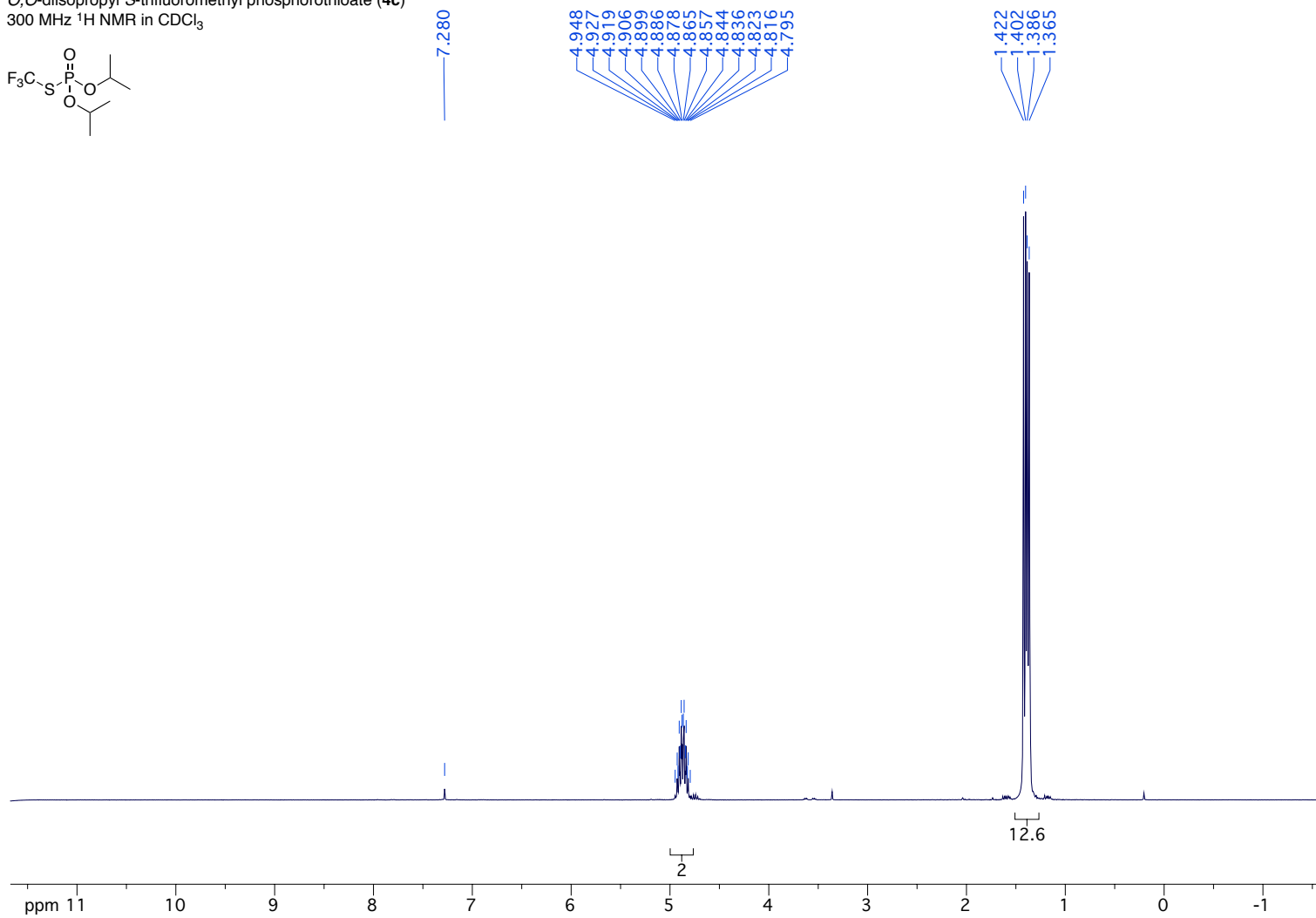
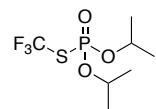
O,O-diethyl *S*-trifluoromethyl phosphorothioate (**4a**)
300 MHz ^1H NMR in CDCl_3



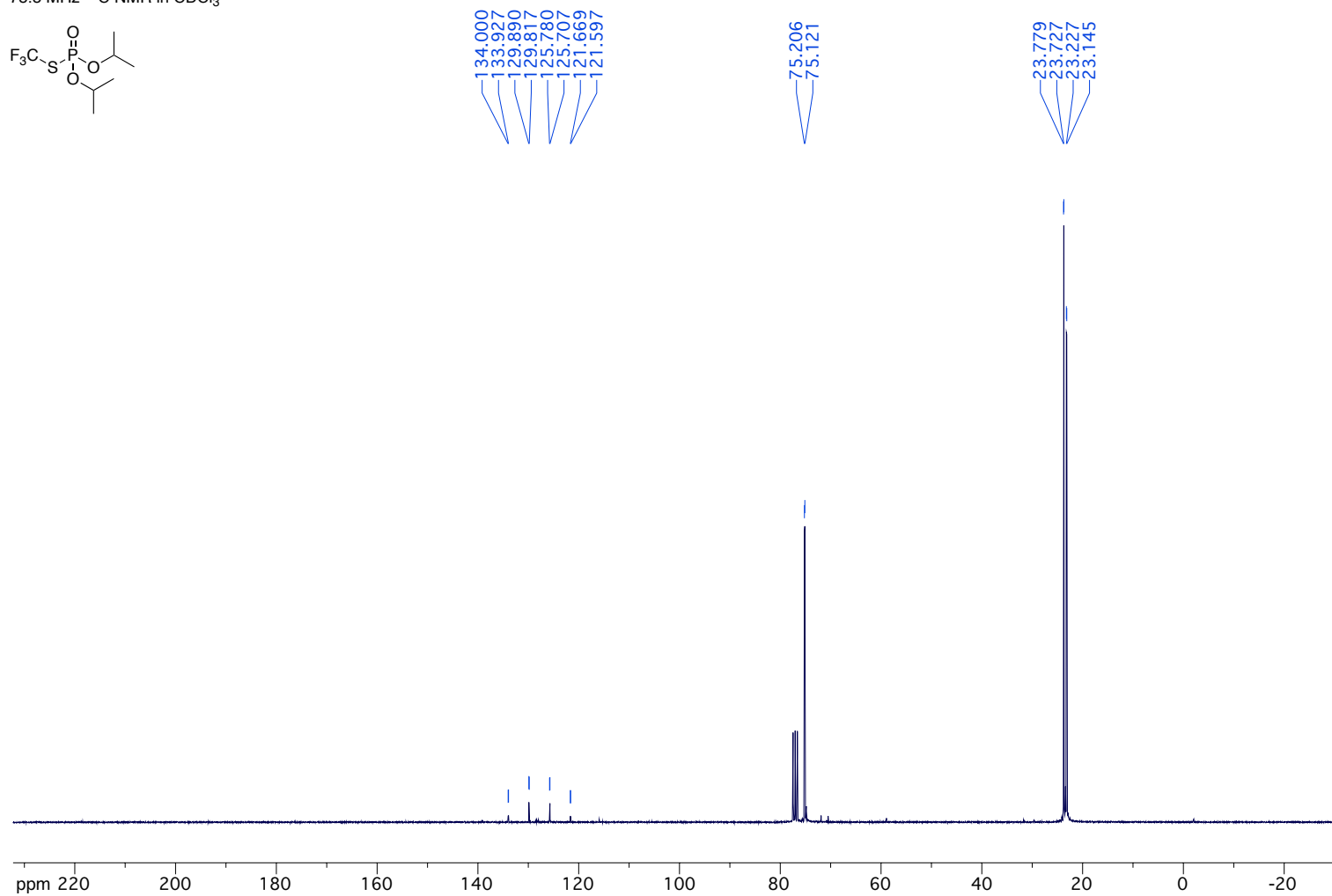
O,O-diethyl *S*-trifluoromethyl phosphorothioate (**4a**)
75.5 MHz ^{13}C NMR in CDCl_3



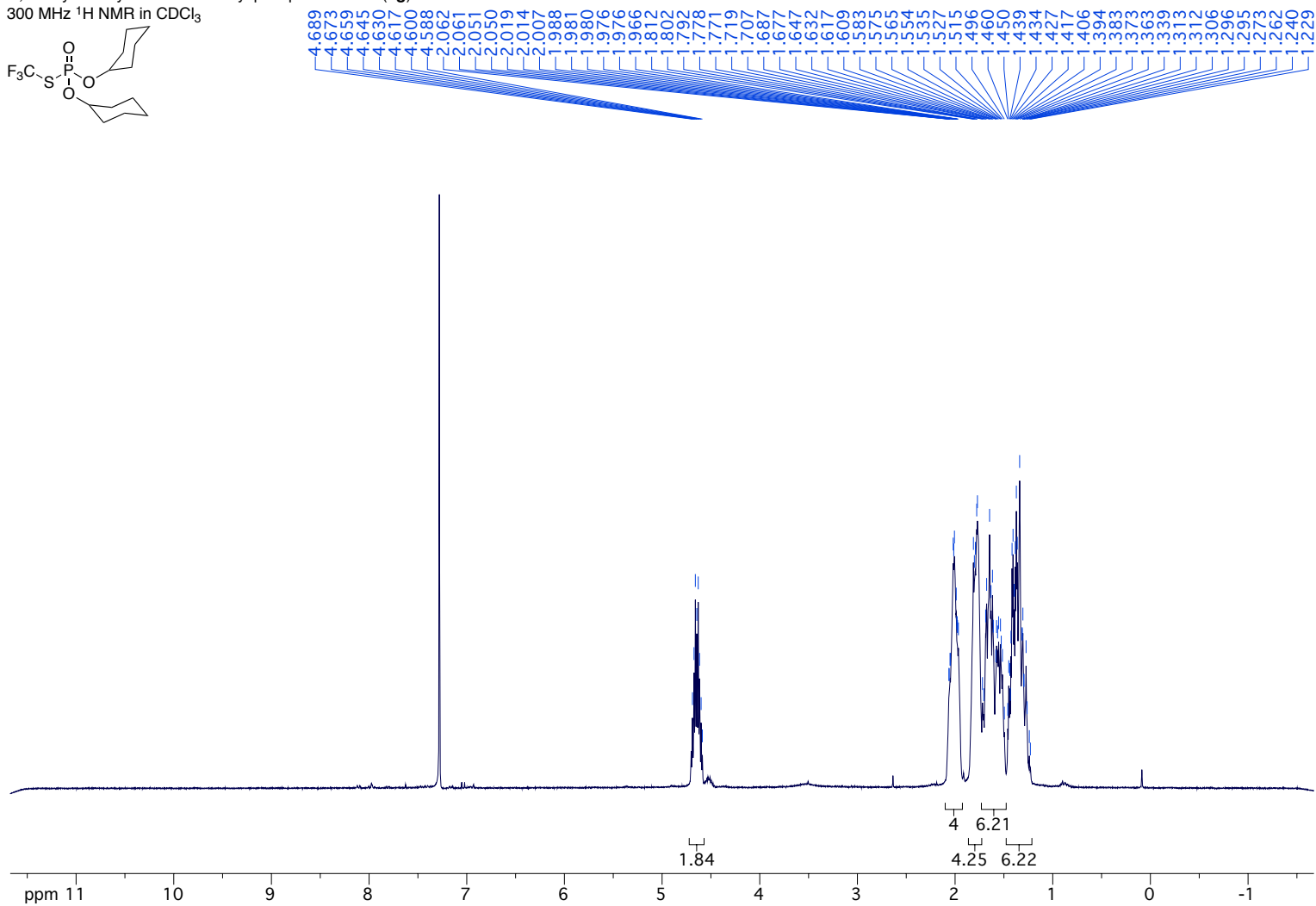
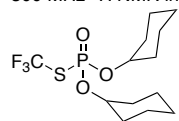
O,O-diisopropyl *S*-trifluoromethyl phosphorothioate (**4c**)
300 MHz ^1H NMR in CDCl_3



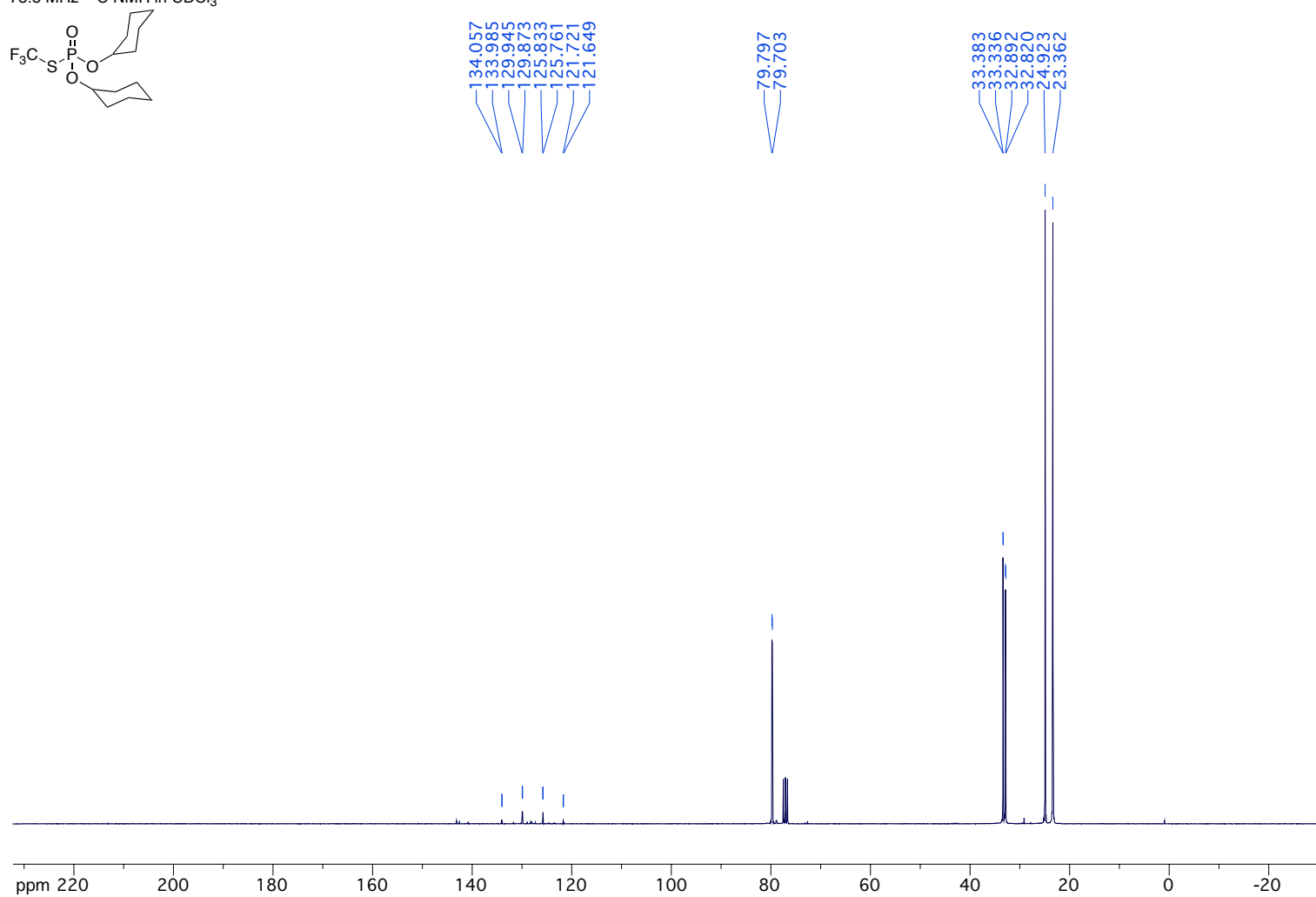
O,O-diisopropyl *S*-trifluoromethyl phosphorothioate (**4c**)
75.5 MHz ^{13}C NMR in CDCl_3



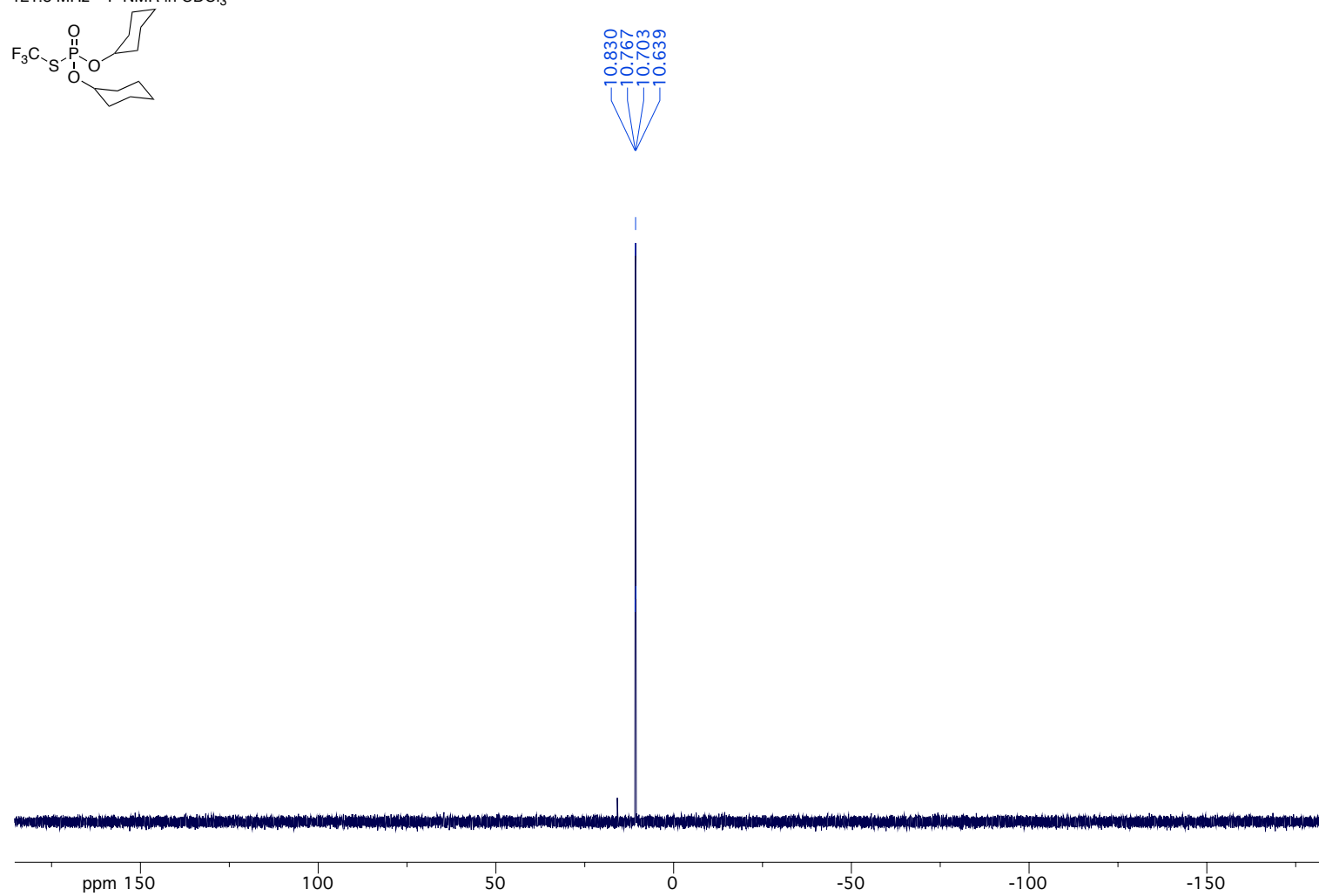
O,O-dicyclohexyl *S*-trifluoromethyl phosphorothioate (**4g**)
 300 MHz ^1H NMR in CDCl_3



O,O-dicyclohexyl *S*-trifluoromethyl phosphorothioate (**4g**)
75.5 MHz ^{13}C NMR in CDCl_3



O,O-dicyclohexyl *S*-trifluoromethyl phosphorothioate (**4g**)
121.5 MHz ^{31}P NMR in CDCl_3



O,O-dicyclohexyl *S*-trifluoromethyl phosphorothioate (**4g**)
188.3 MHz ^{19}F NMR in CDCl_3

