

SUPPORTING INFORMATION

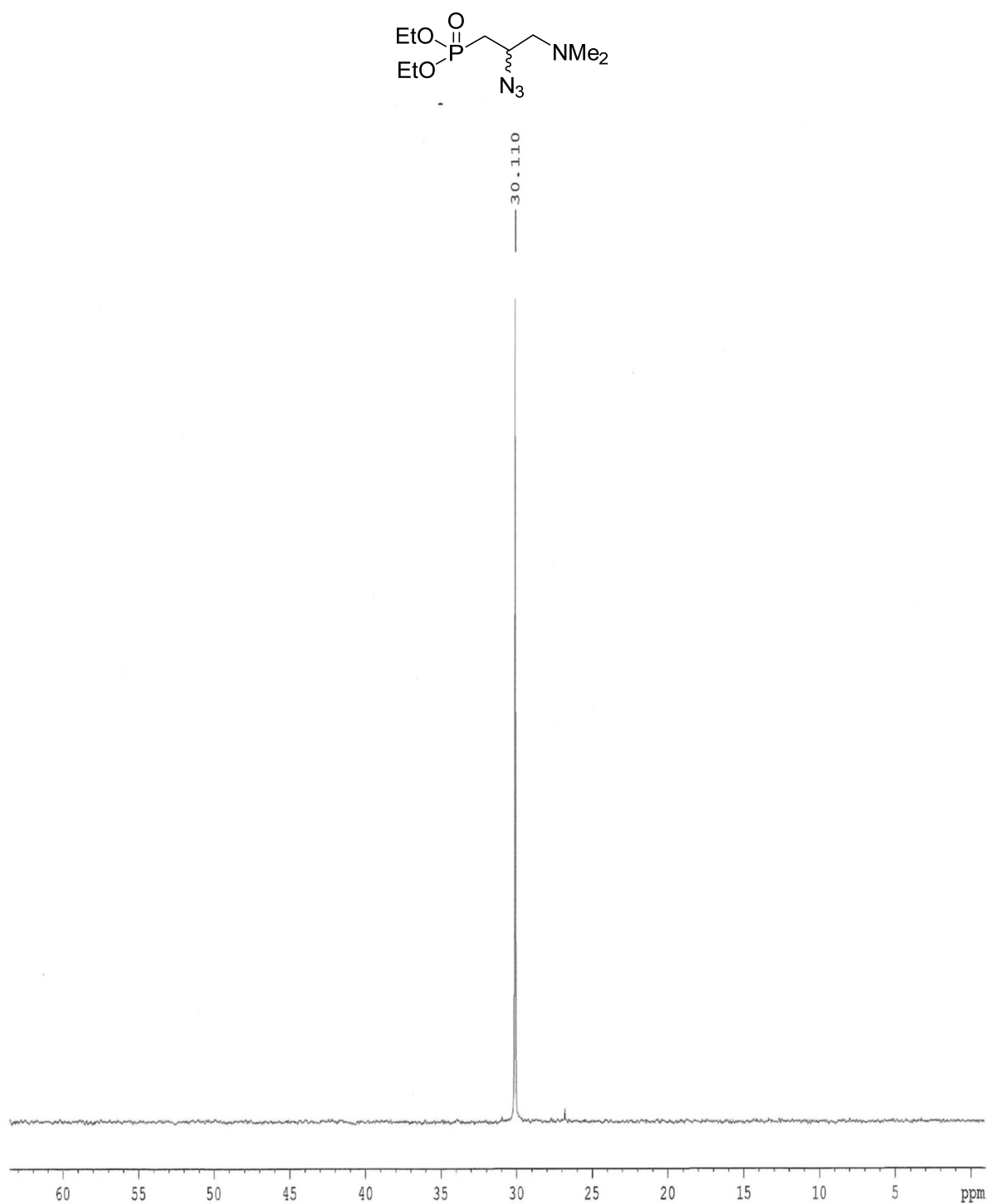
Towards Chemoenzymatic Syntheses of Both Enantiomers of Phosphoemeriamine

Piotr Kielbasiński *, Małgorzata Kwiatkowska, Piotr Łyzwa and Marian Mikołajczyk

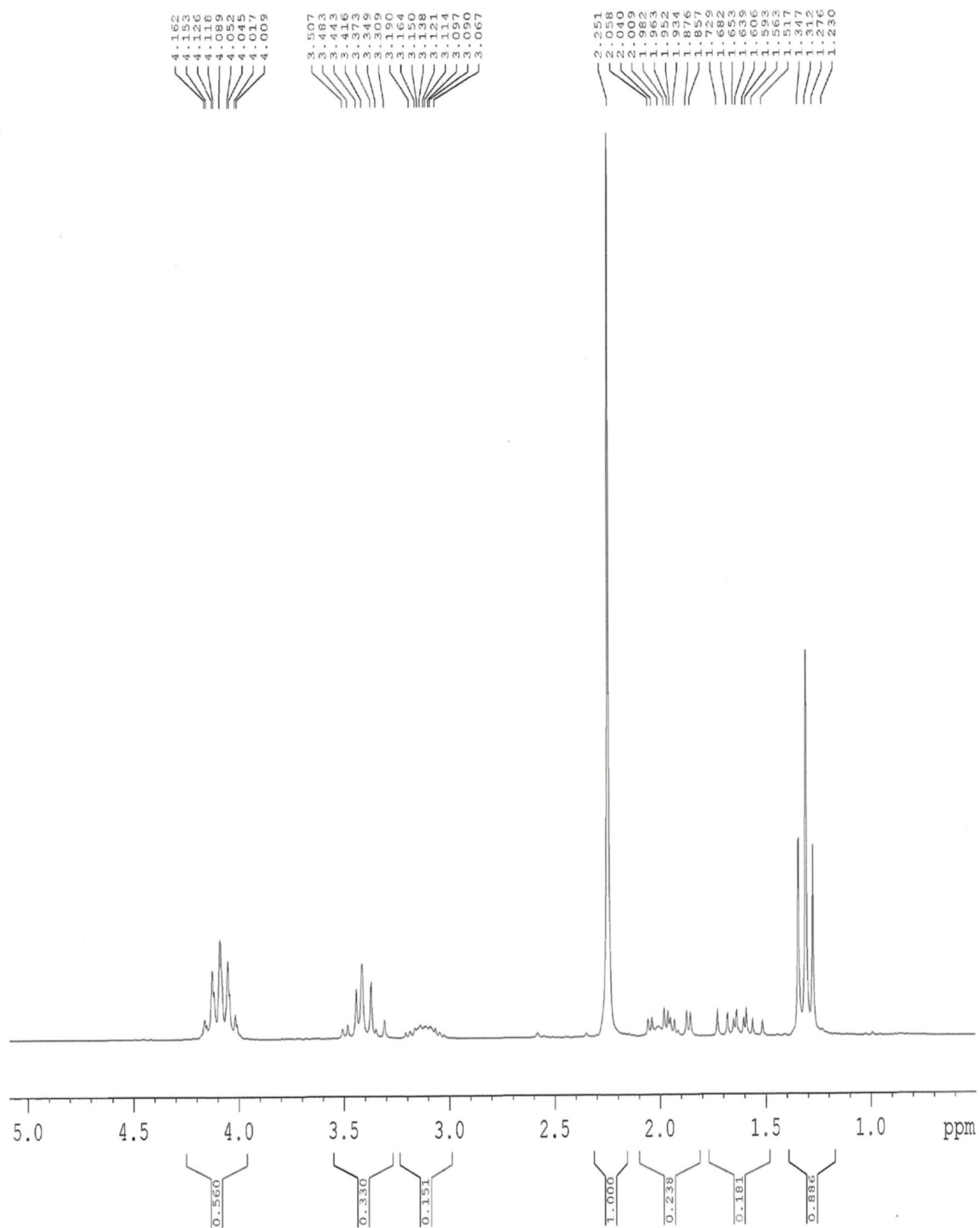
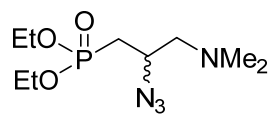
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malgorzata.kwiatkowska@cbmm.lodz.pl (M.K.); plyzwa@interia.pl (P.Ł.);
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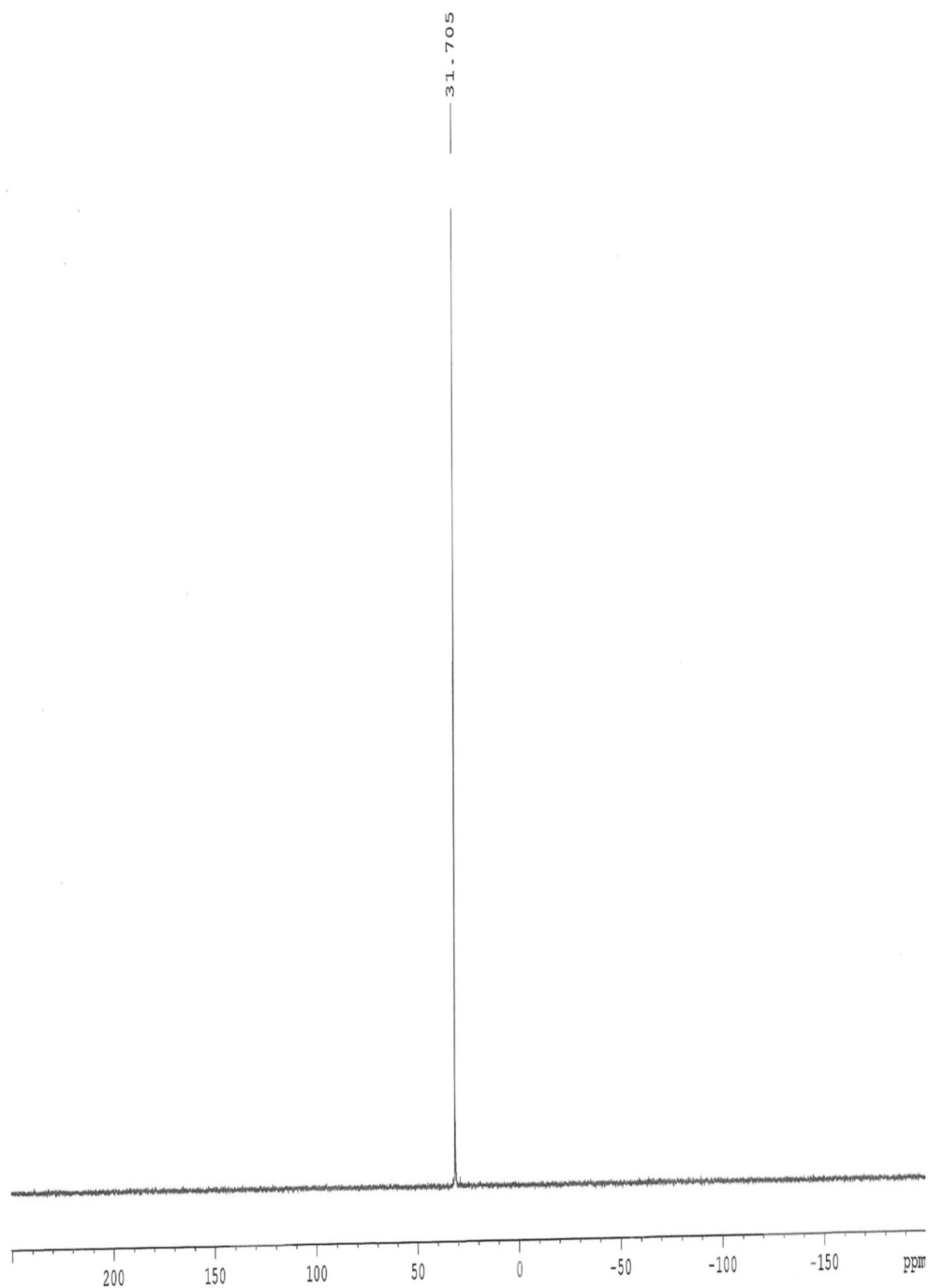
*Diethyl 2-azido-3-*N,N*-dimethylaminopropylphosphonate* **11**
³¹P NMR (CDCl₃)



Diethyl 2-azido-3-*N,N*-dimethyloaminopropylphosphonate **11**
¹H NMR (CDCl₃)

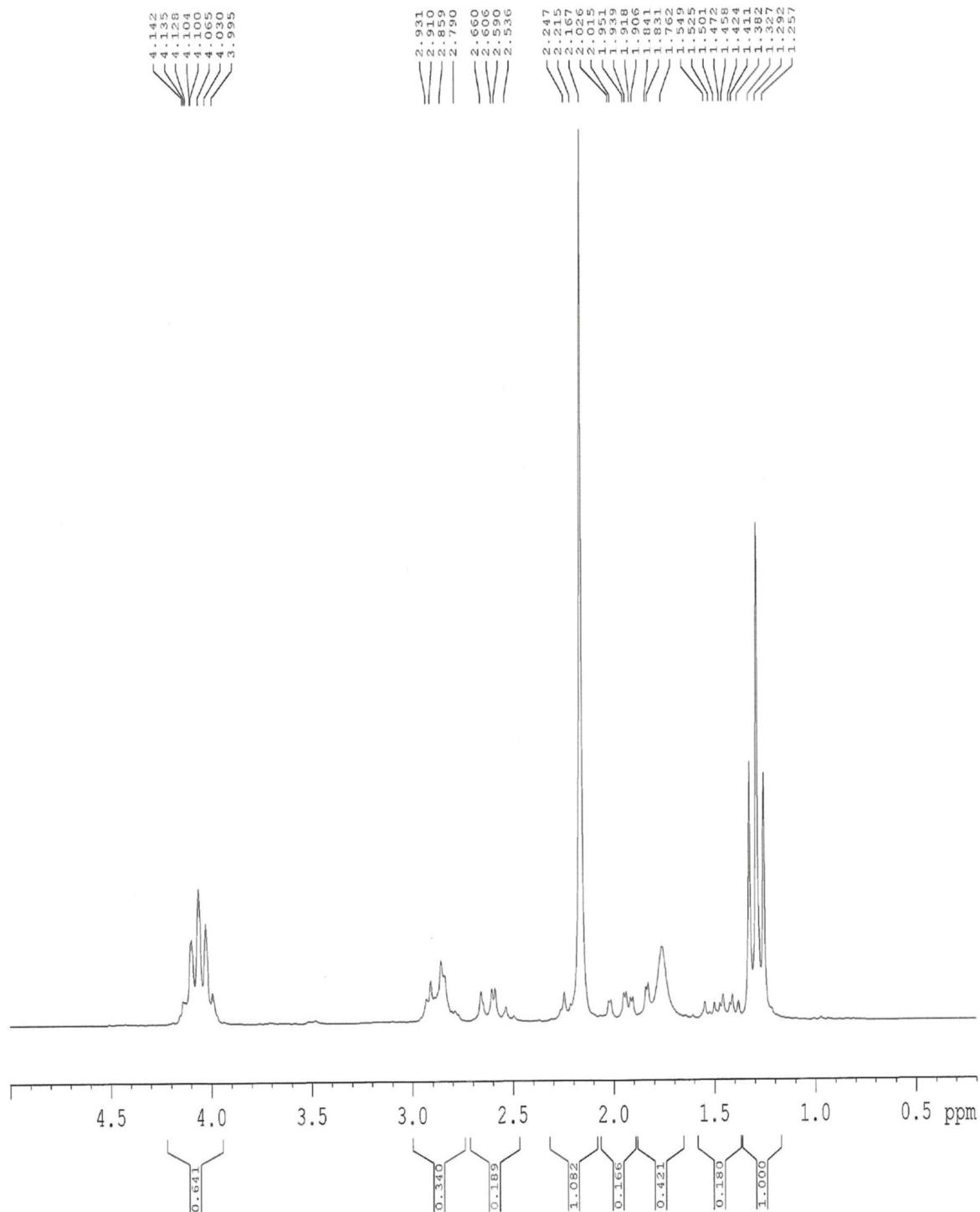
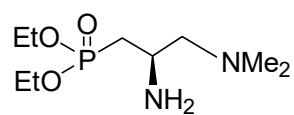


*Diethyl 2-amino-3-*N,N*-dimethyloaminopropylphosphonate* **12**
³¹P NMR



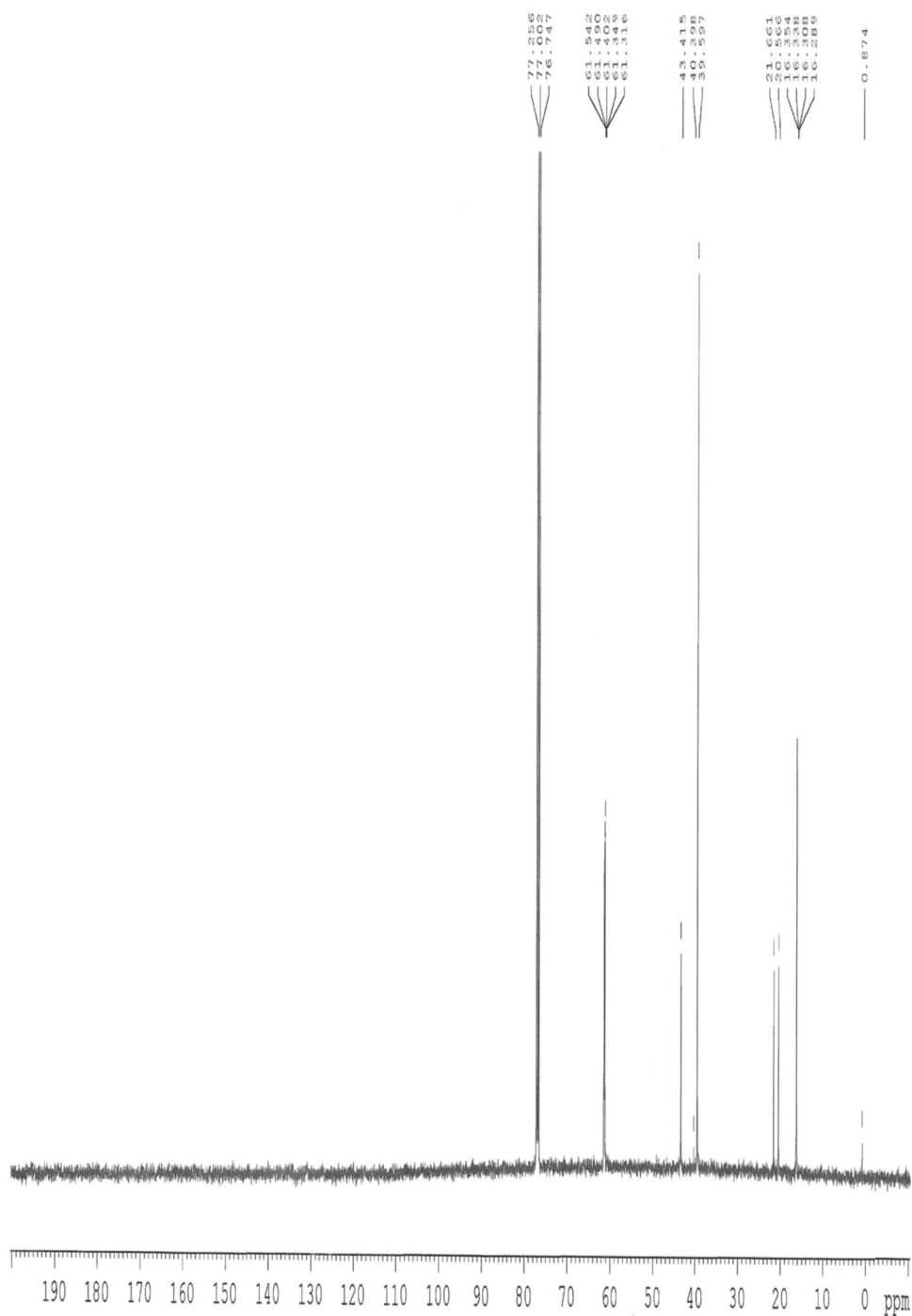
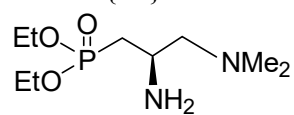
Diethyl 2-amino-3-*N,N*-dimethyloaminopropylphosphonate **12**

¹H NMR



*Diethyl 2-amino-3-*N,N*-dimethylaminopropylphosphonate* **12**

$^{13}\text{C}\{^1\text{H}\}$ NMR

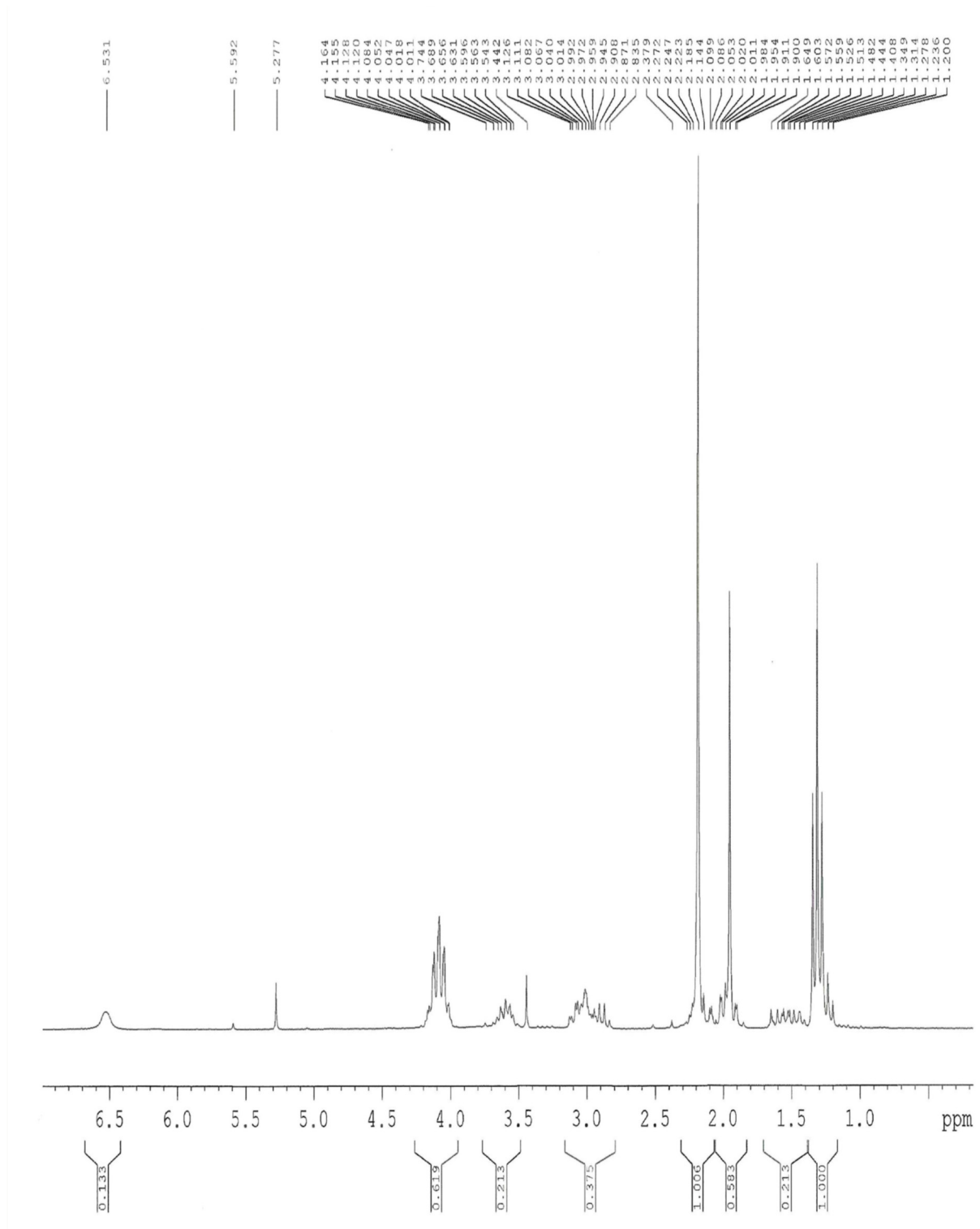


N-(Diethoxyphosphoryl)methyl(*N*',*N*'-dimethylaminomethyl)acetamide **13**

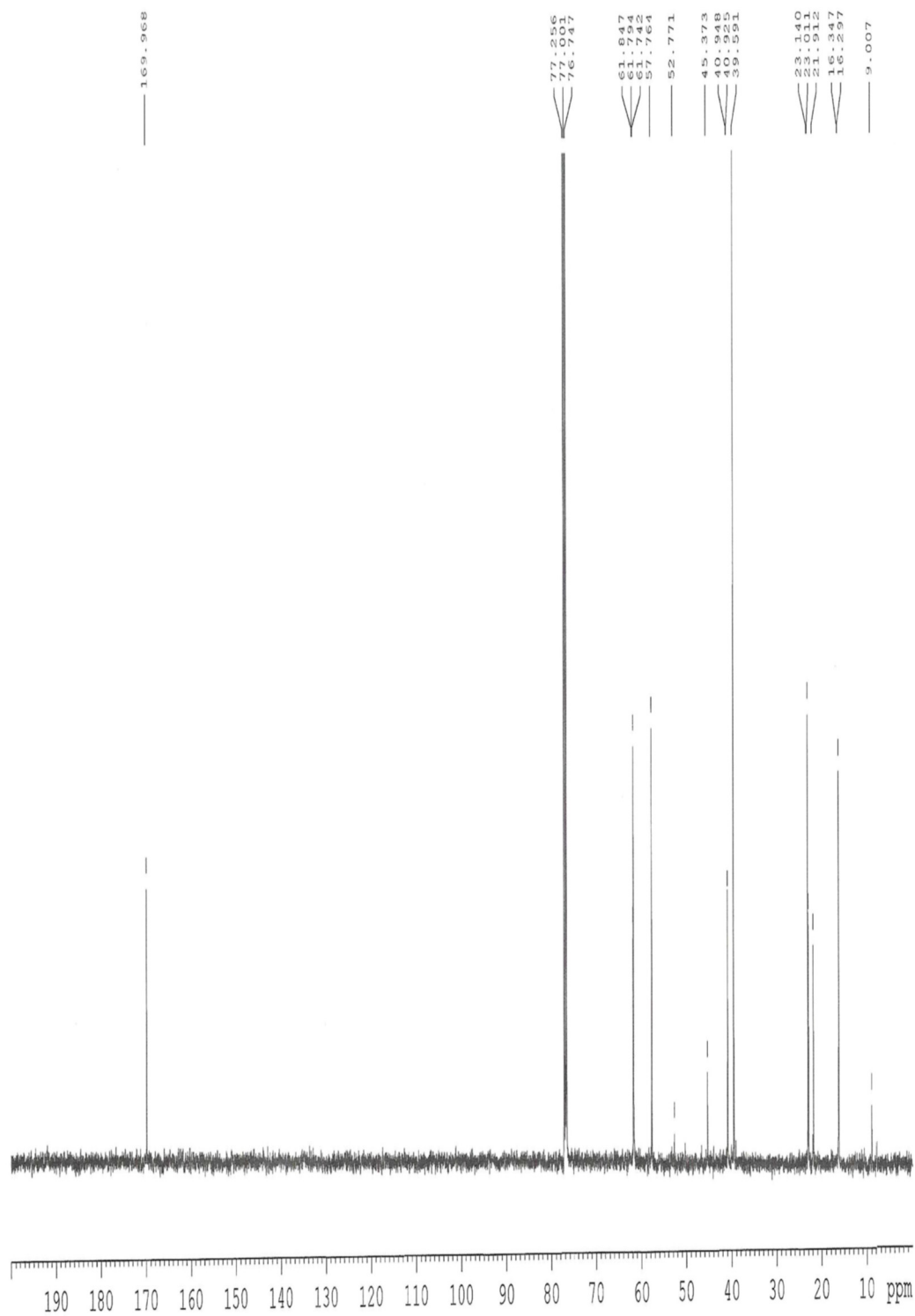
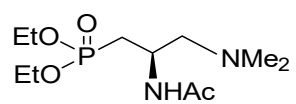


N-(Diethoxyphosphoryl)methyl(*N*',*N*'-dimethylaminomethyl)acetamide **13**

^1H NMR

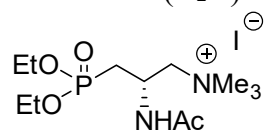


N-(Diethoxyphosphoryl)methyl(*N*',*N*'-dimethylaminomethyl)acetamide **13**
 $^{13}\text{C}\{^1\text{H}\}$ NMR



Trimethyl (2-acetamido)-(3-diethoxyphosphoryl)propylammonium iodide **14**

^{31}P NMR (D_2O)

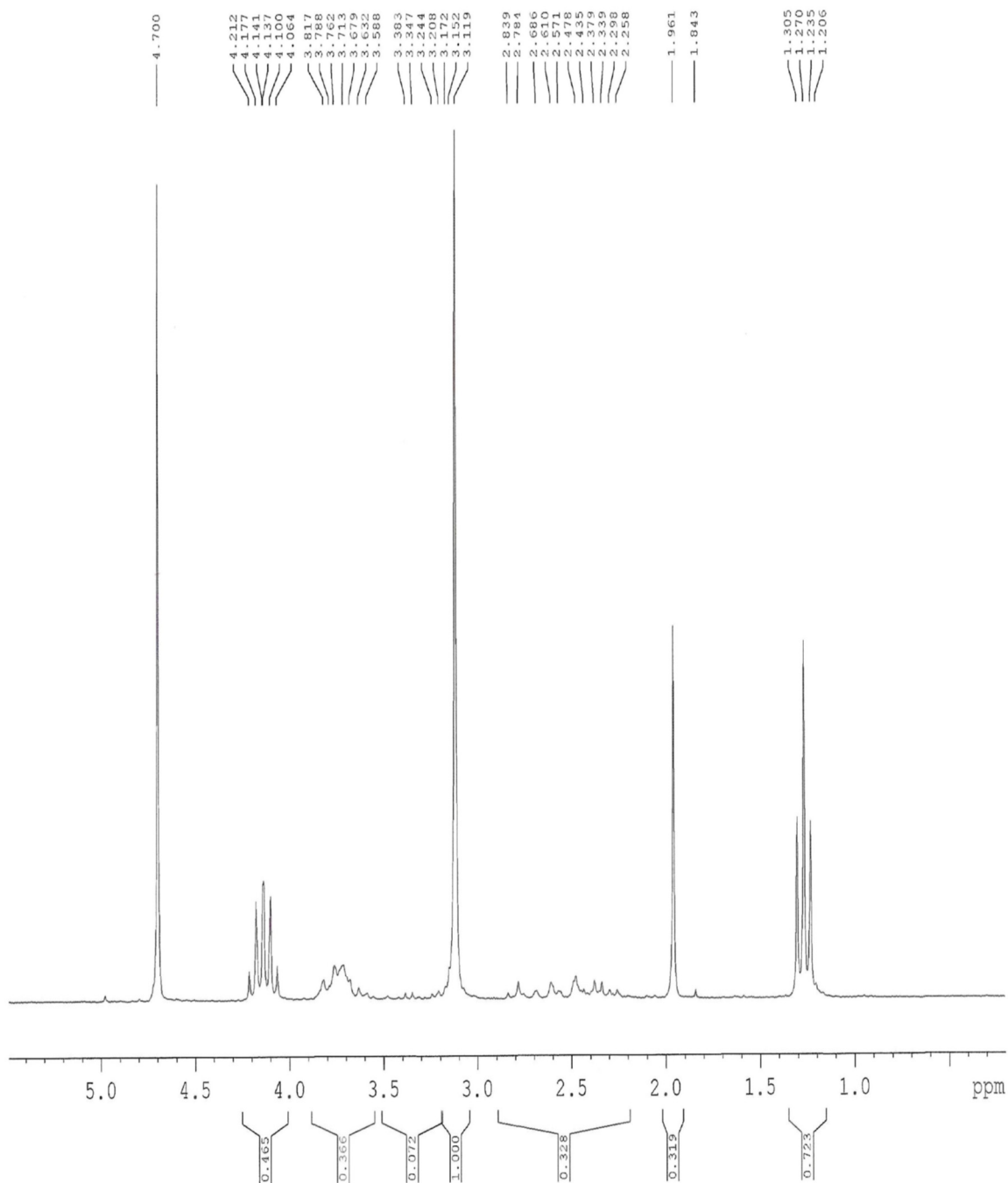
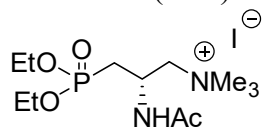


— 26.780



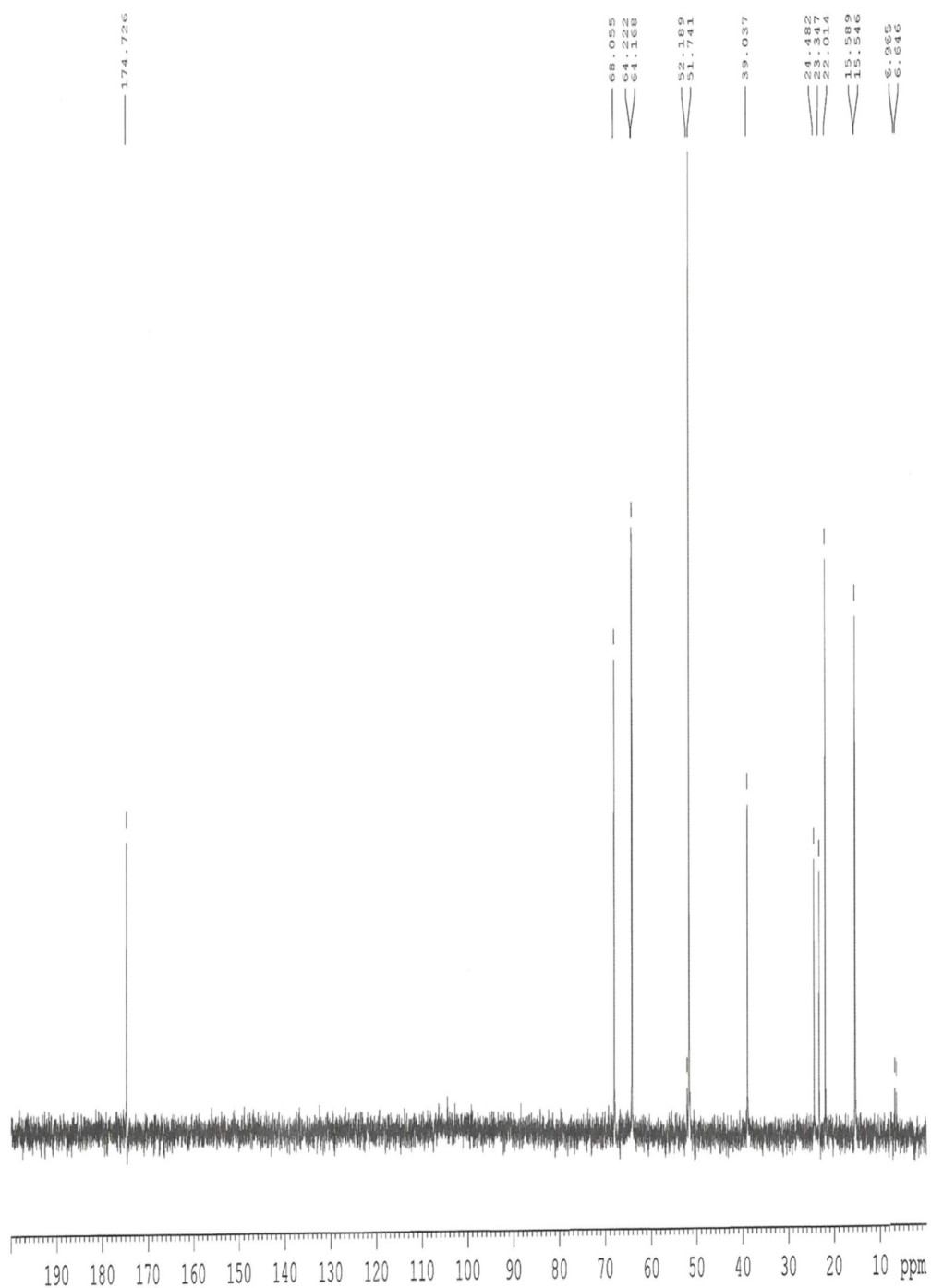
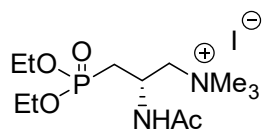
Trimethyl (2-acetamido)-(3-diethoxyphosphoryl)propylammonium iodide **14**

^1H NMR (D_2O)

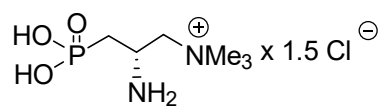


Trimethyl (2-acetamido)-(3-diethoxyphosphoryl)propylammonium iodide **14**

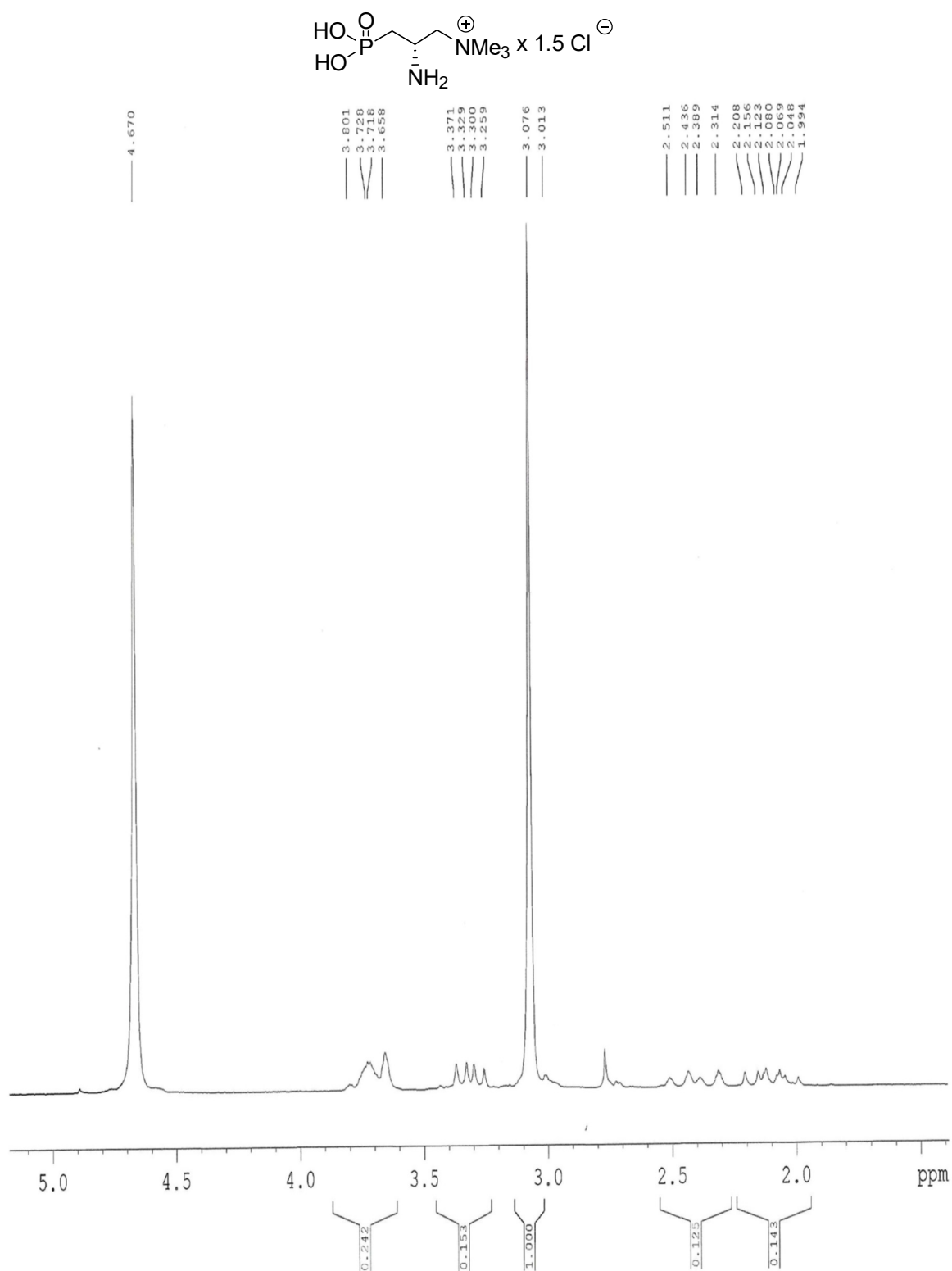
$^{13}\text{C}\{^1\text{H}\}$ NMR (D_2O)



2-Amino-3-phosphoryl-1-trimethylammonium (emeriamine) sesquichloride **8a**
³¹P NMR (D₂O)

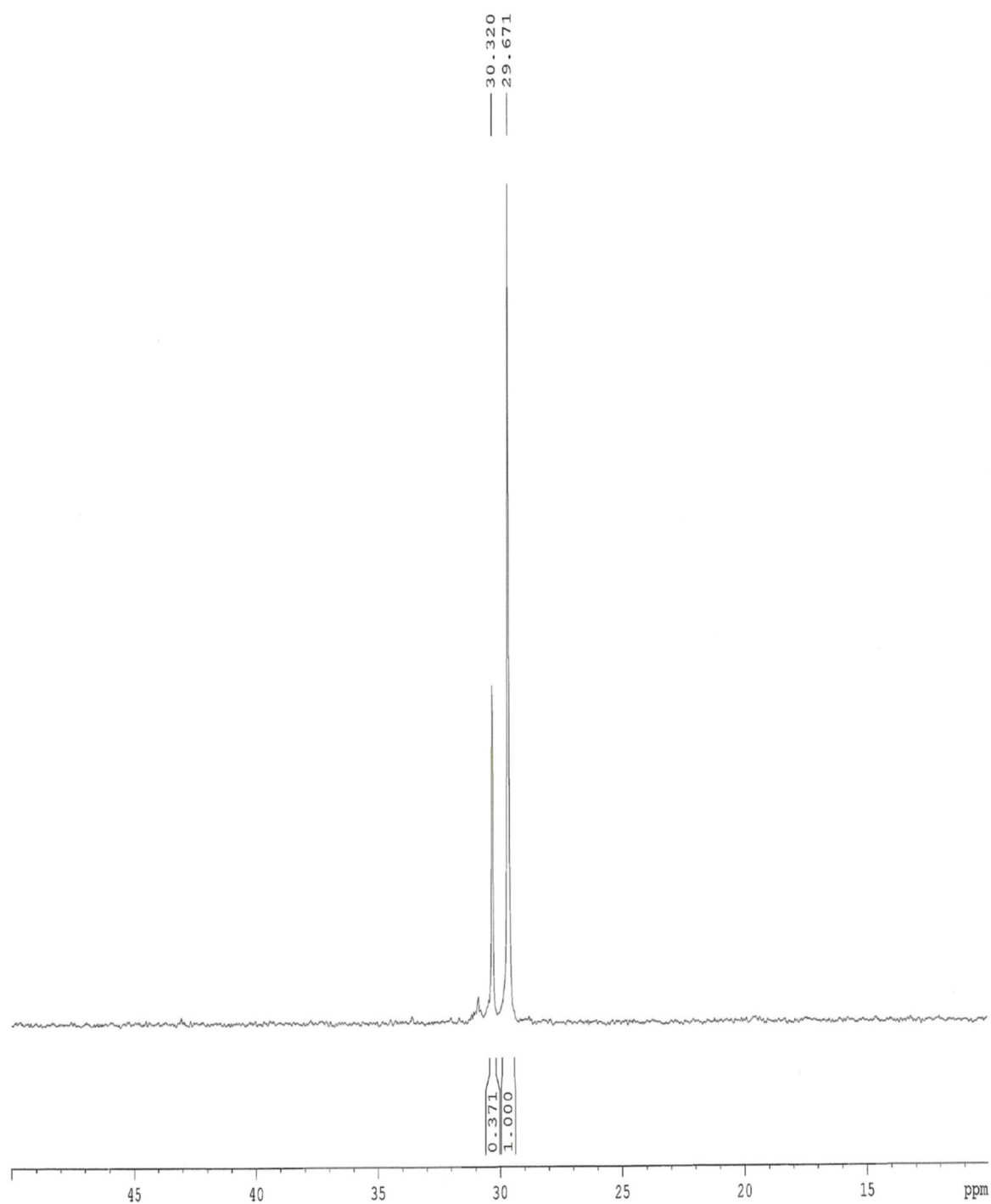


2-Amino-3-phosphoryl-1-trimethylammonium (emeriamine) sesquichloride **8a**
 ^1H NMR (D_2O)

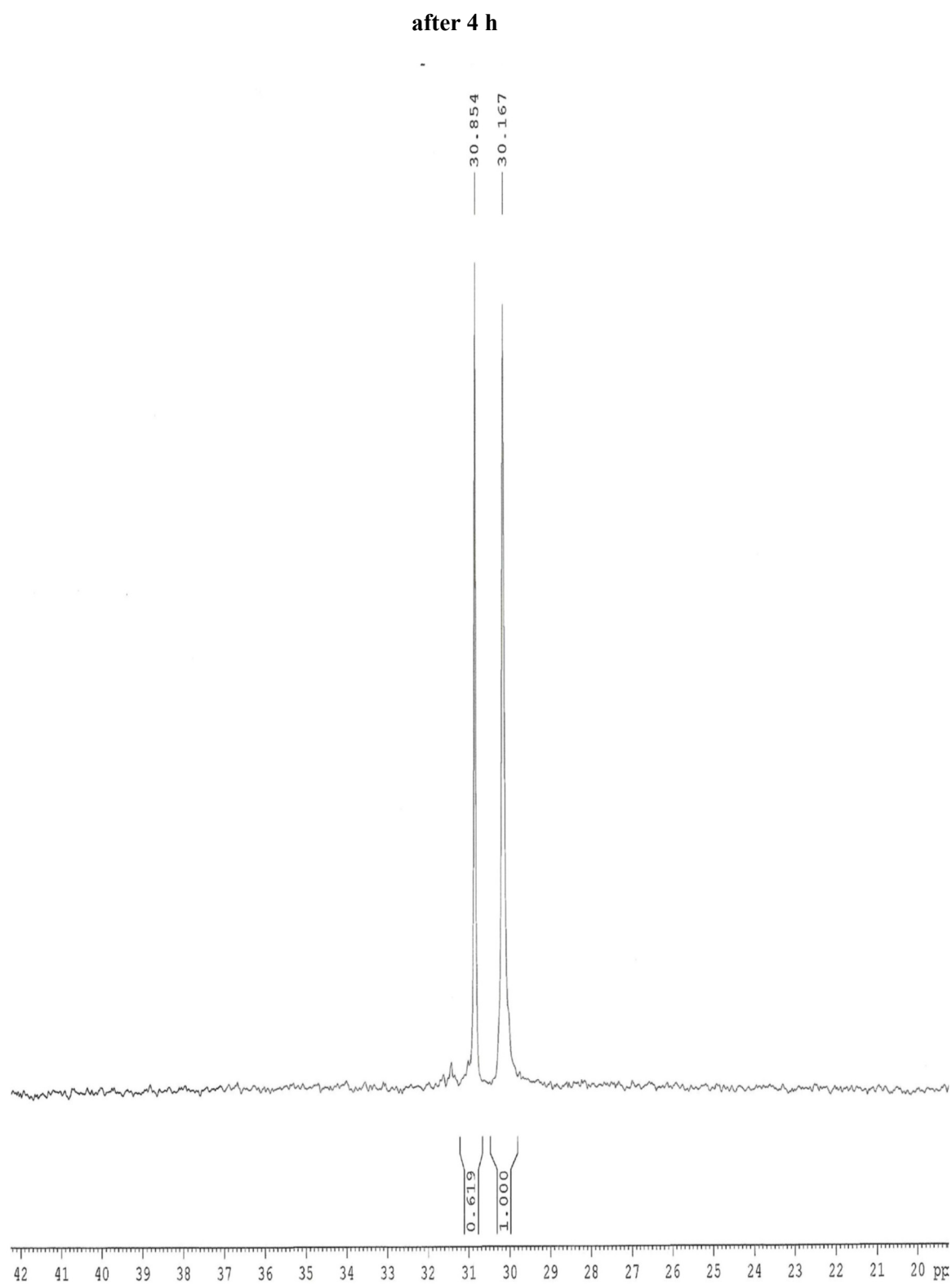


^{31}P NMR control of the progress of the enzymatic kinetic resolution of *diethyl 2-amino-3-N,N*-dimethyloaminopropylphosphonate **12**

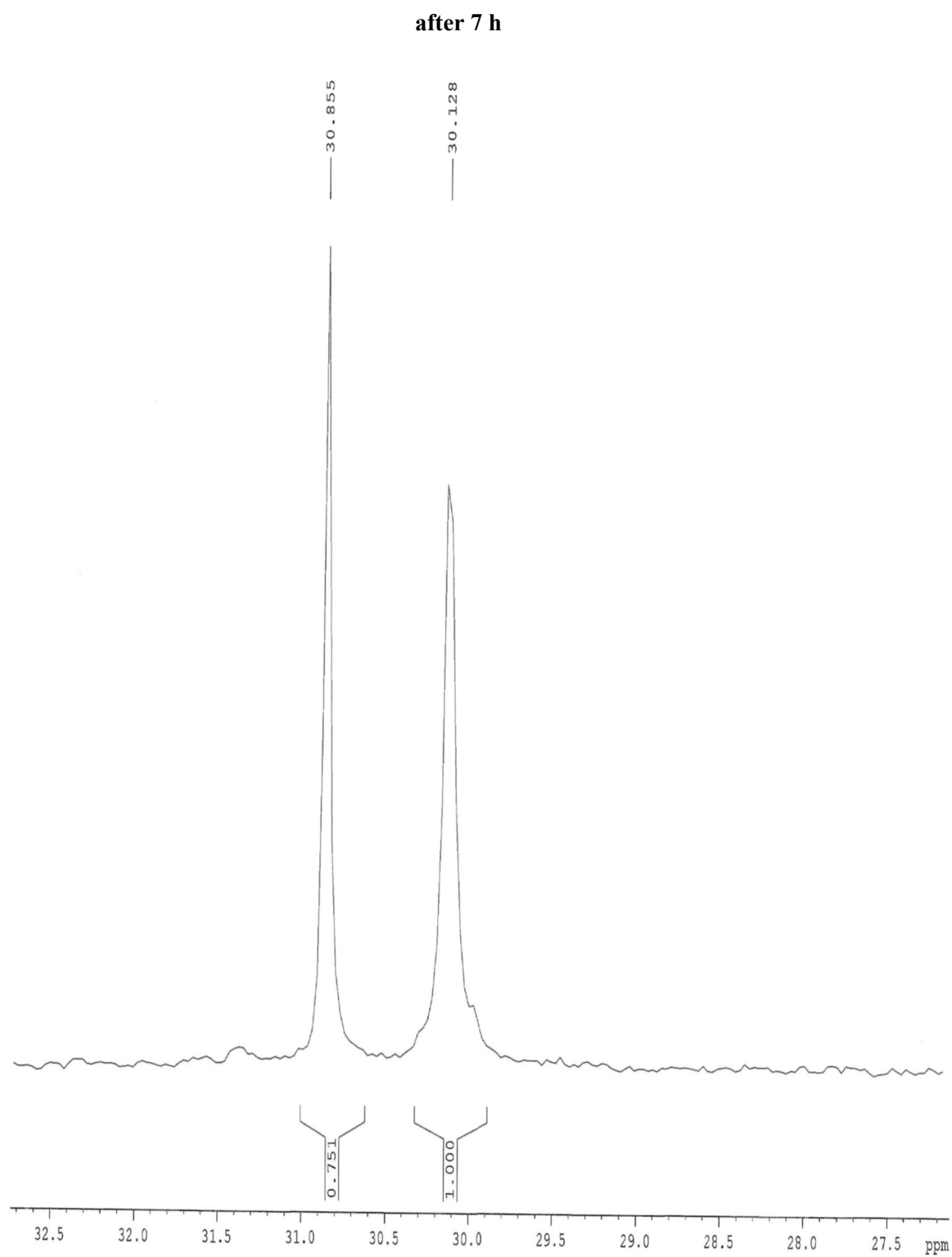
after 2 h



^{31}P NMR control of the progress of the enzymatic kinetic resolution of *diethyl 2-amino-3- N,N -dimethyloaminopropylphosphonate* **12**

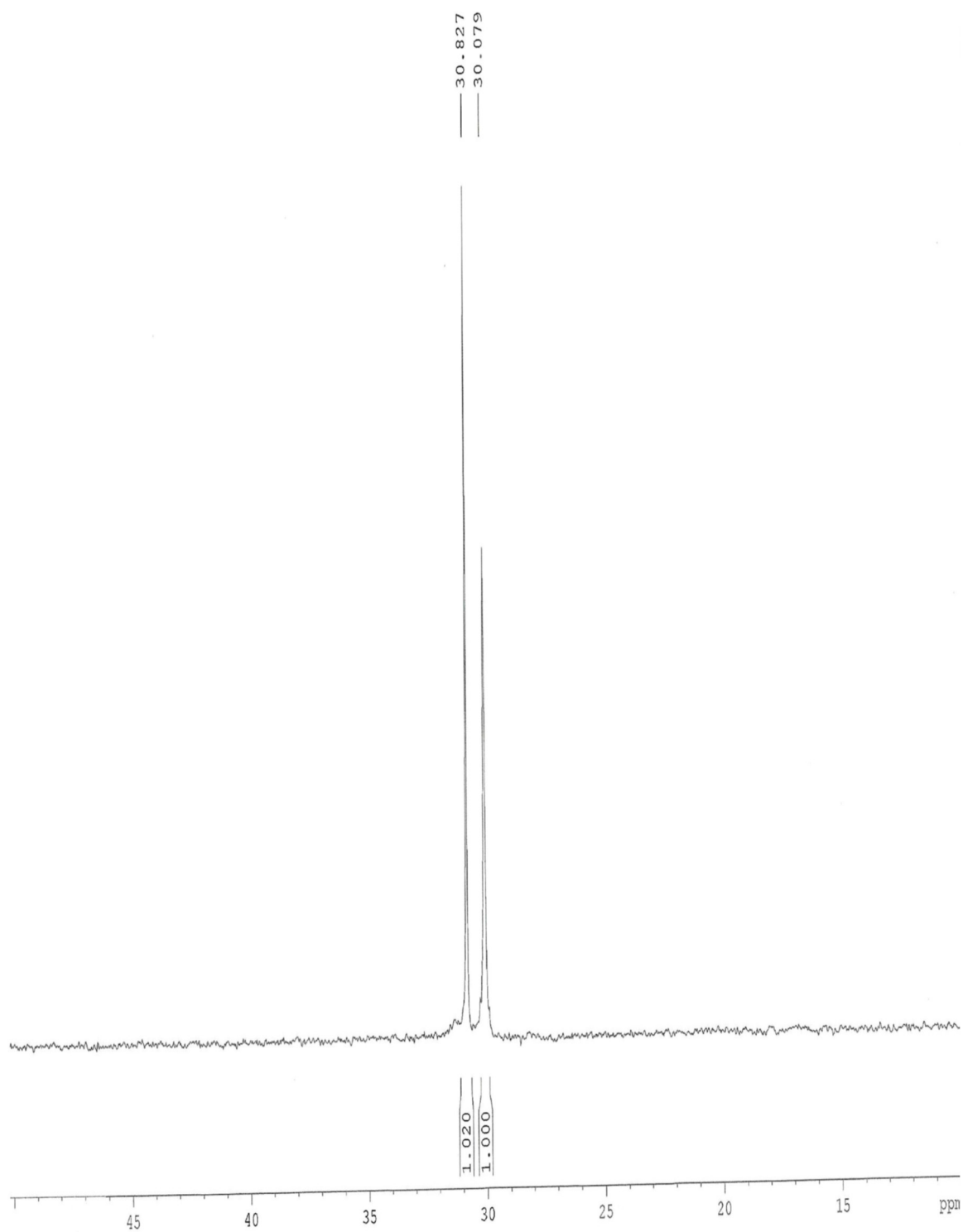


^{31}P NMR control of the progress of the enzymatic kinetic resolution of *diethyl 2-amino-3- N,N -dimethyloaminopropylphosphonate* **12**



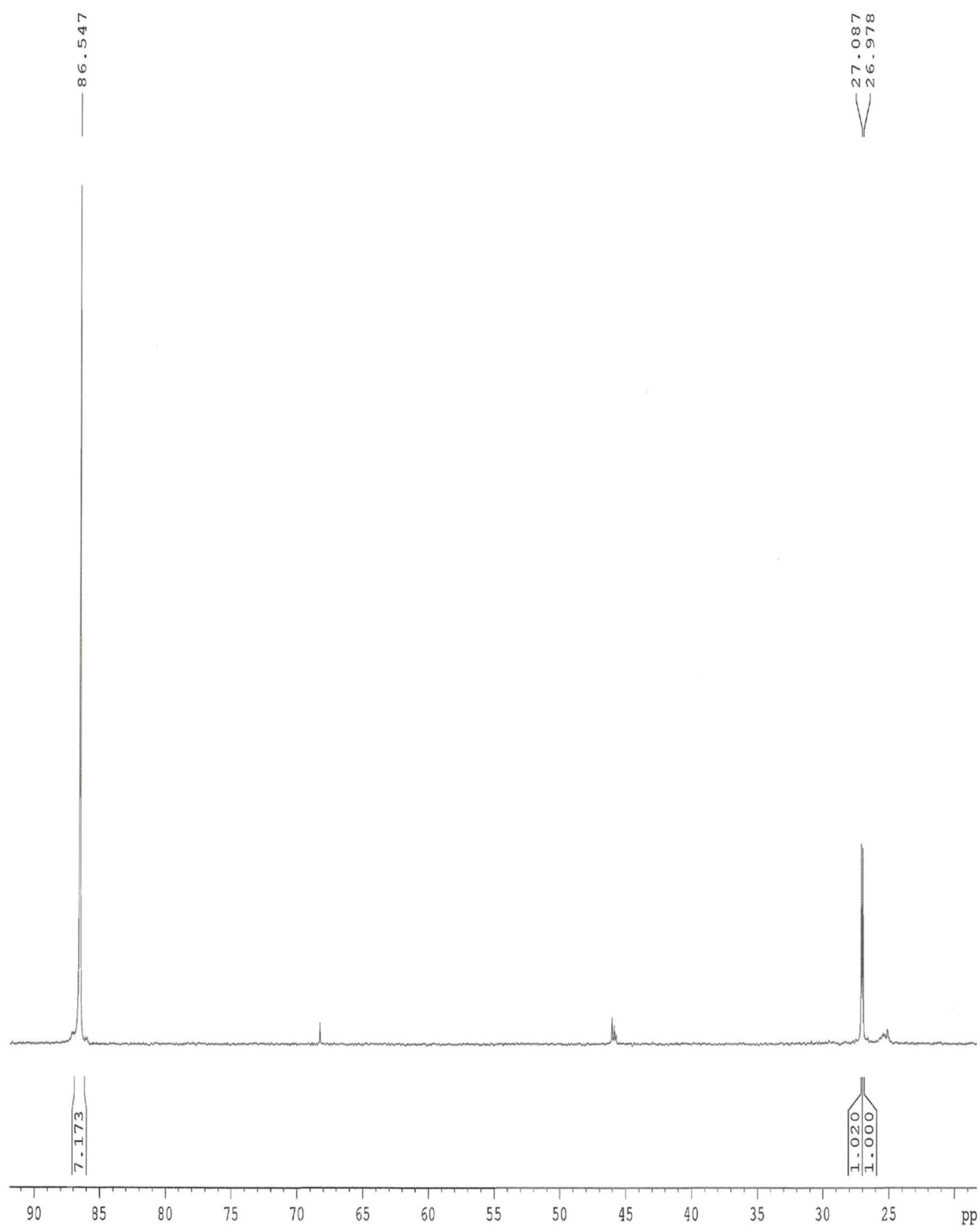
^{31}P NMR control of the progress of the enzymatic kinetic resolution of *diethyl 2-amino-3-*N,N*-dimethyloaminopropylphosphonate* **12**

after 24 h



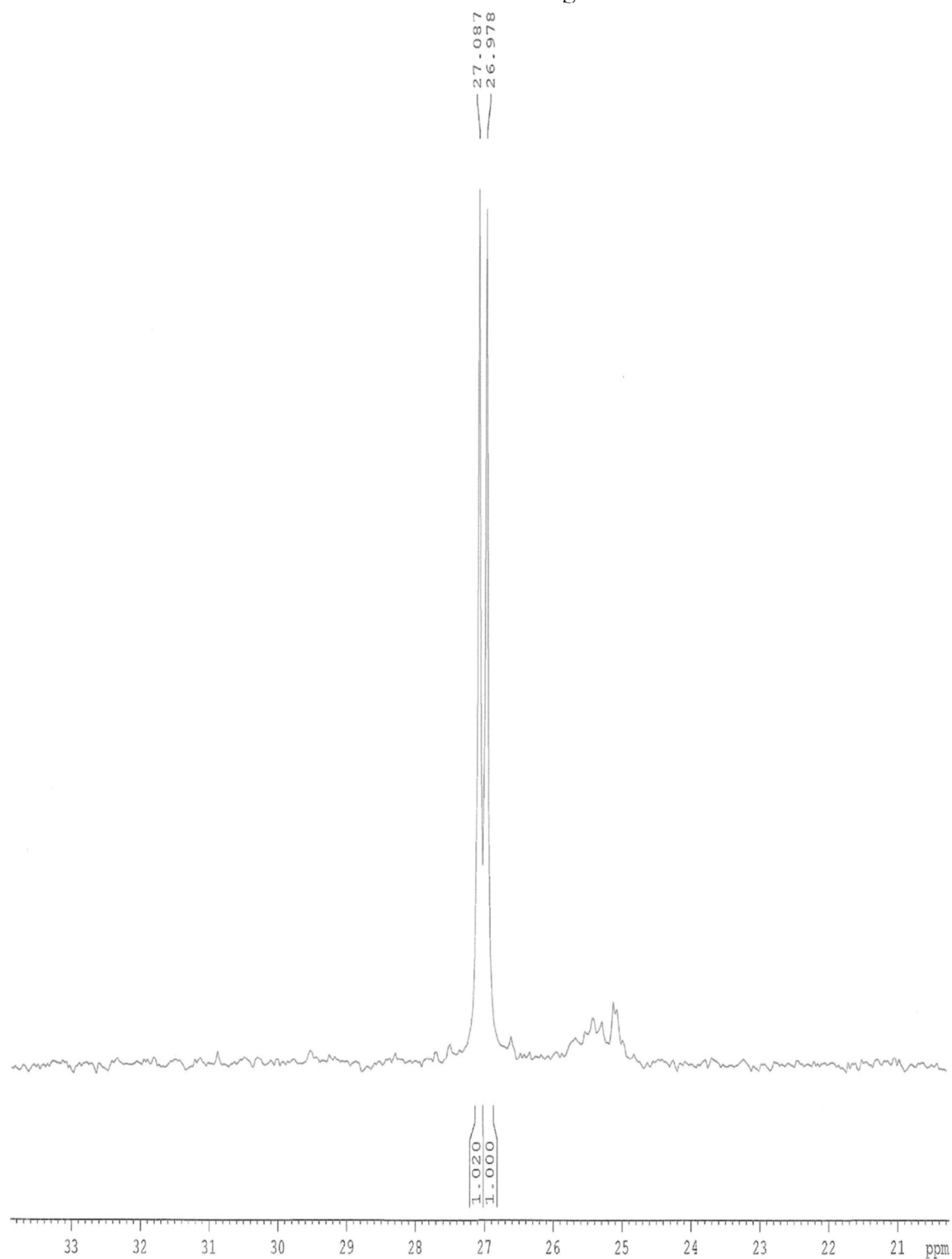
Determination of enantiomeric excess of *diethyl 2-amino-3-N,N-dimethyloaminopropylphosphonate* **12**

^{31}P NMR (CDCl_3) of racemic **12** with (+)-(*R*)-*t*-butylphenylphosphinothioic acid



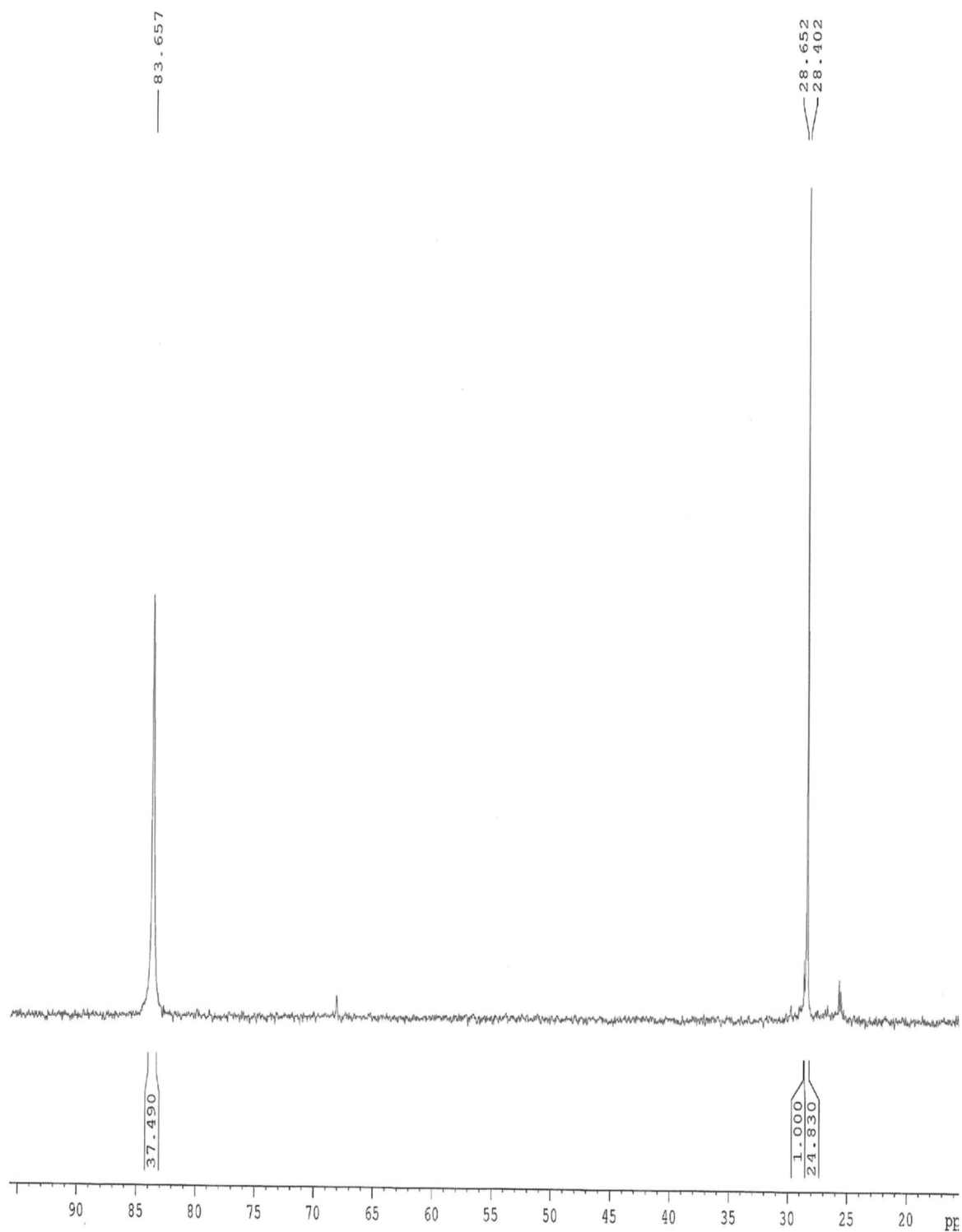
Determination of enantiomeric excess of *diethyl 2-amino-3-N,N*-

dimethyloaminopropylphosphonate **12**
 ^{31}P NMR (CDCl_3) of racemic **12** with (+)-(*R*)-*t*-butylphenylphosphinothioic acid;
extension of the amine signals



Determination of enantiomeric excess of *diethyl 2-amino-3-N,N*-

dimethyloaminopropylphosphonate 12
 ^{31}P NMR (CDCl_3) of enantiomerically enriched (+)-(*R*)-**12**
 with (+)-(*R*)-*t*-butylphenylphosphinothioic acid



Determination of enantiomeric excess of *diethyl 2-amino-3-N,N*-*dimethyloaminopropylphosphonate 12*
 ^{31}P NMR (CDCl_3) of enantiomerically enriched (+)-(*R*)-**12**
 with (+)-(*R*)-*t*-butylphenylphosphinothioic acid

extension of the amine signals

