

Synthesis of aziridine *N*-methylenephosphonates: Reaction scope and mechanistic insights

Supporting Information

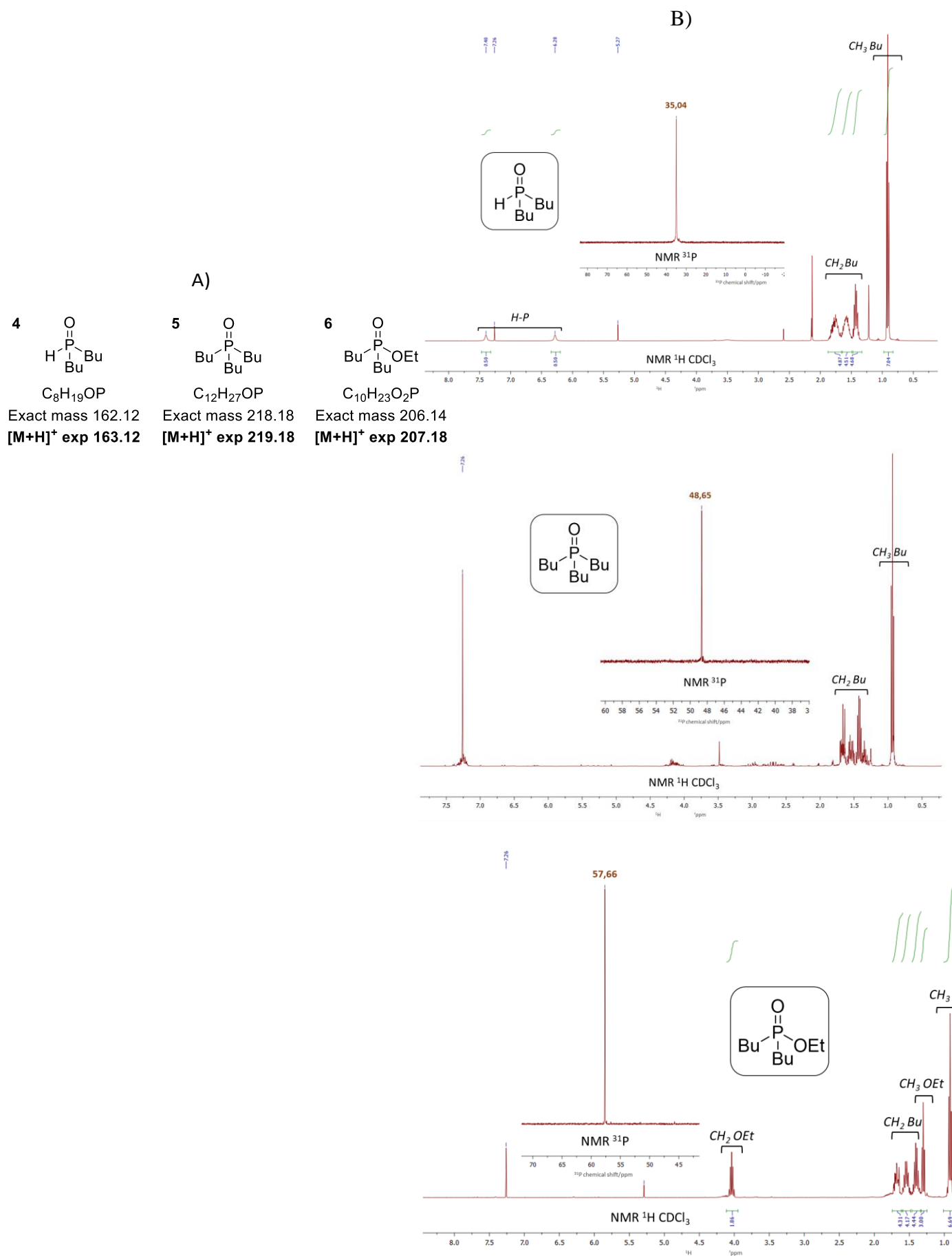
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Team Nucleosides & Phosphorylated Effectors, Institute for Biomolecules Max Mousseron (IBMM), Univ Montpellier, CNRS, ENSCM, Pole Chimie Balard Recherche, 1919, route de Mende, 34293 Montpellier, France

Table of Contents

Figure S1. A) Structures of the main identified by-products and MS data; B) their corresponding ^1H & $^{31}\text{P}\{^1\text{H}\}$ NMR spectra.

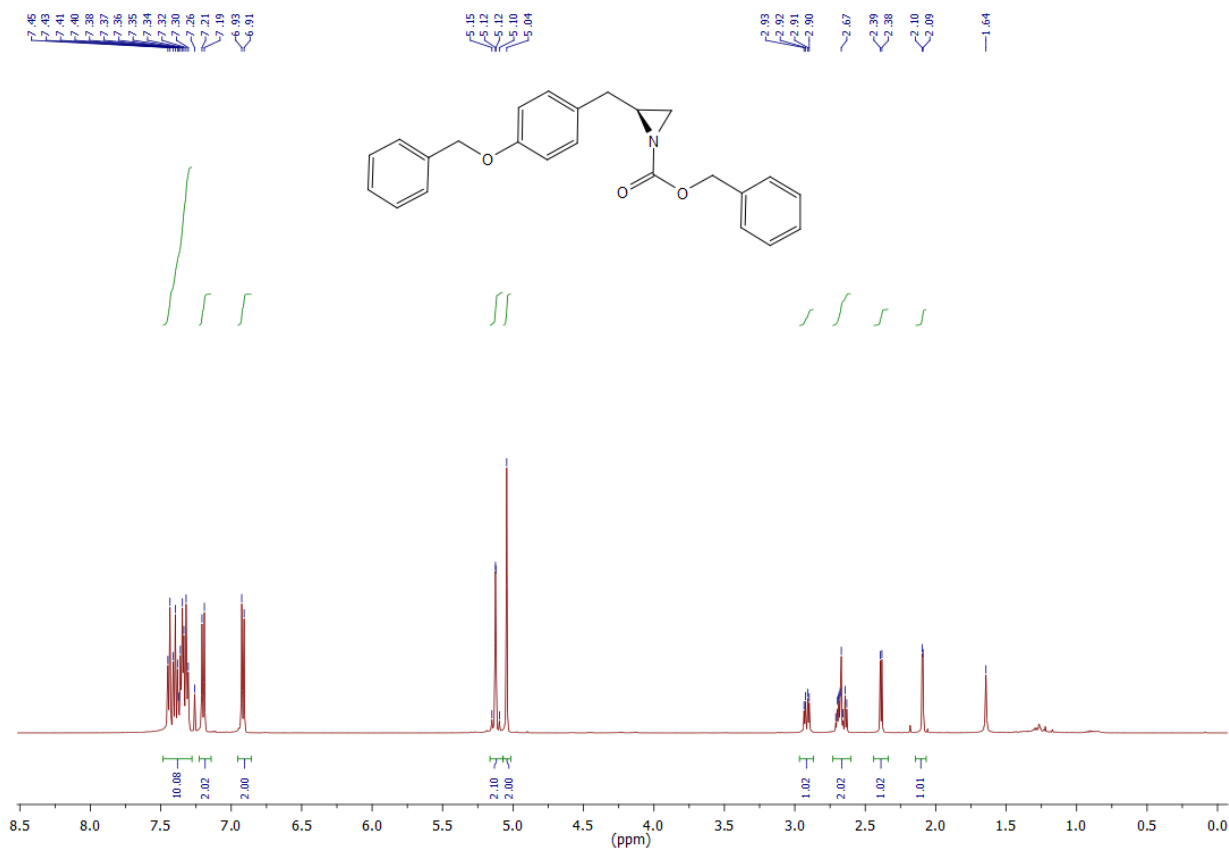
Copies of ^1H , ^{13}C and eventually ^{31}P NMR spectra of all new compounds



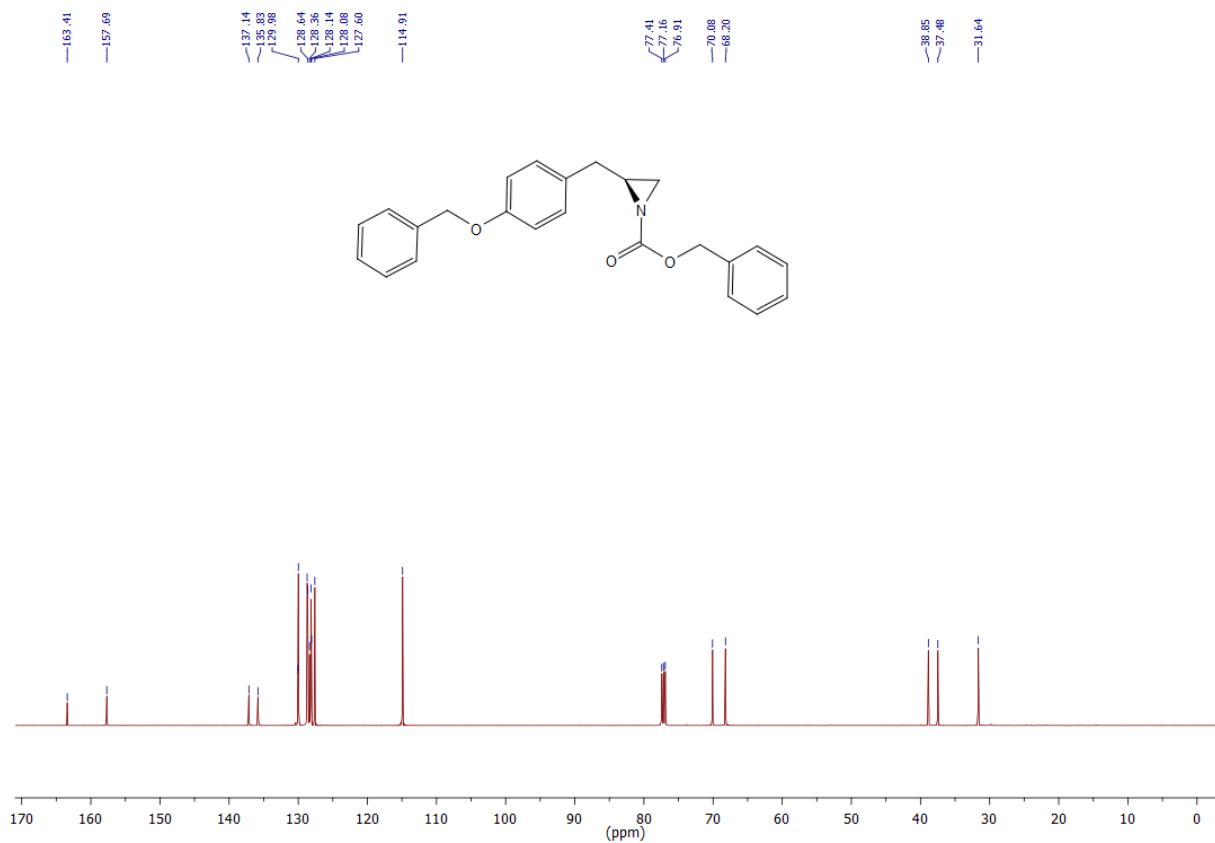
Copies of ^1H , ^{13}C and eventually ^{31}P NMR spectra of all new compounds

Benzyl (S)-2-(4-(benzyloxy)benzyl)aziridine-1-carbamate - **1e**

RMN ^1H

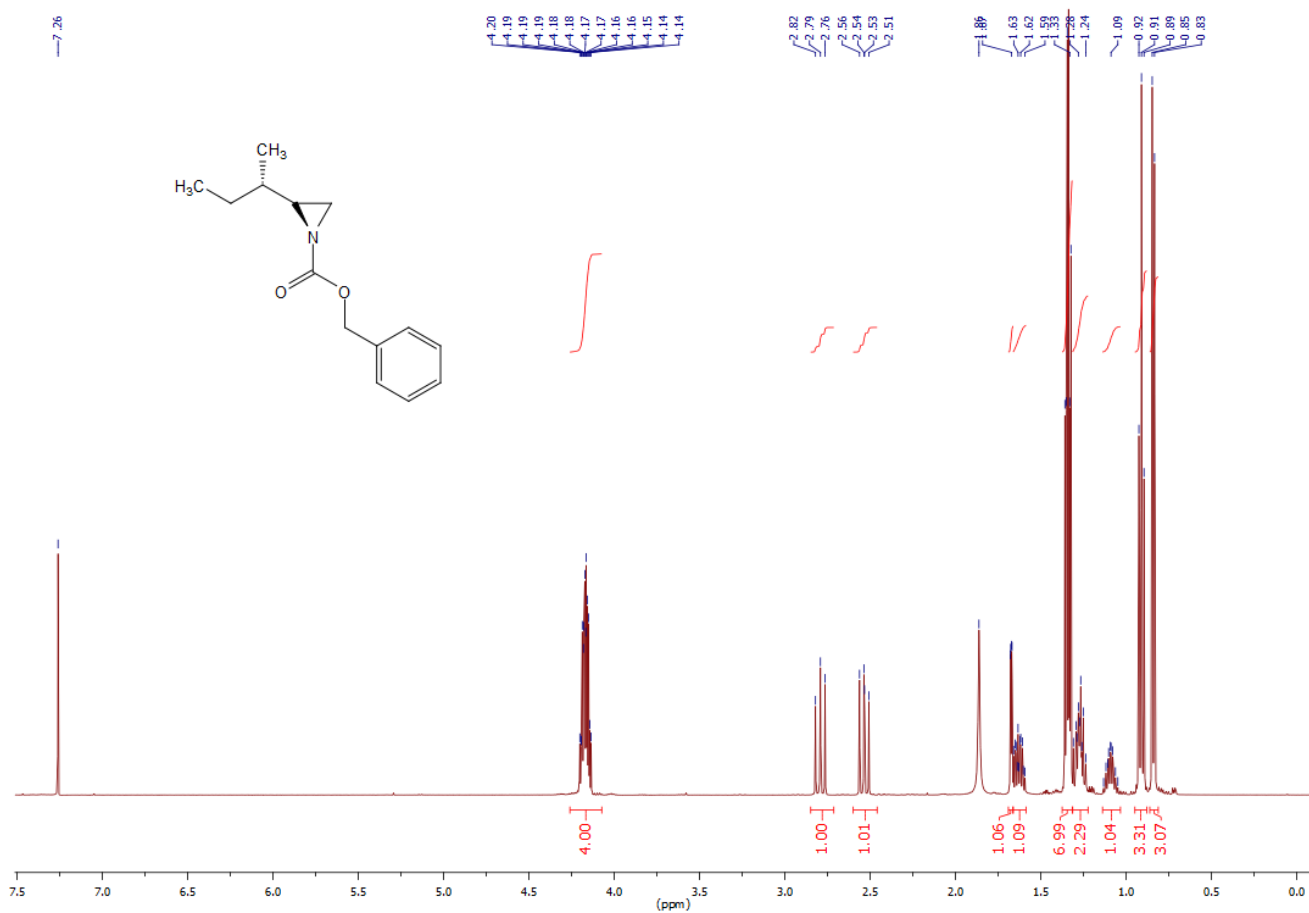


RMN $^{13}\text{C}\{^1\text{H}\}$

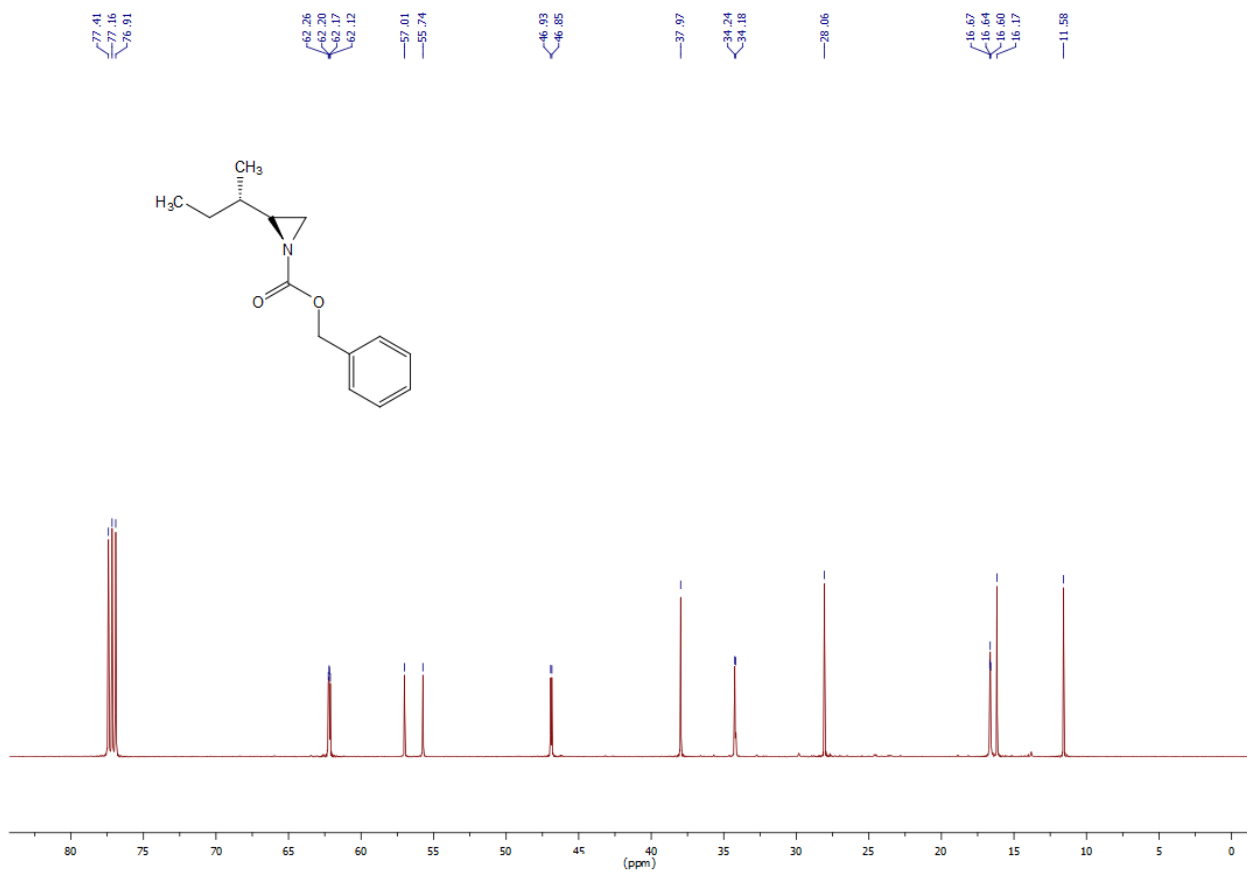


Benzyl (S)-2-((S)-sec-butyl)aziridine-1-carboxylate - **1i**

RMN ^1H

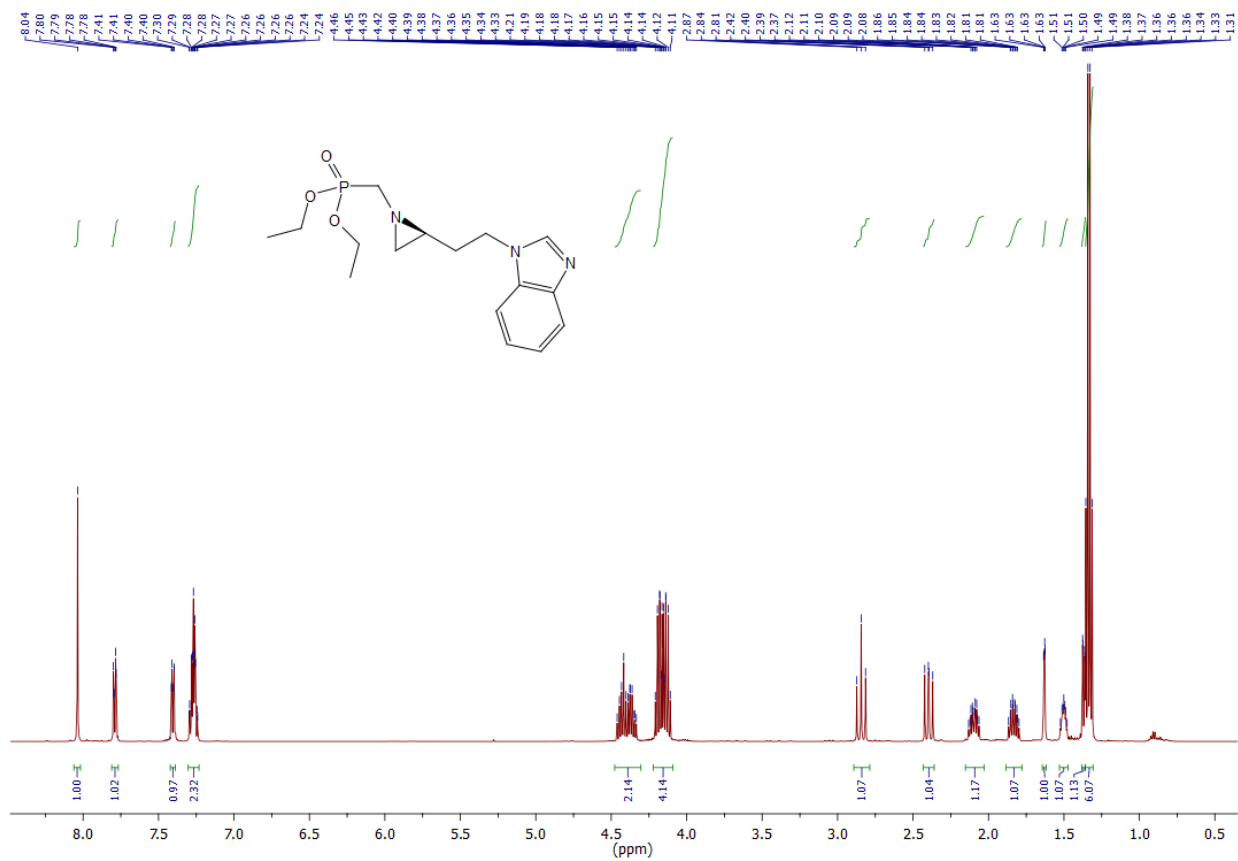


RMN $^{13}\text{C}\{^1\text{H}\}$

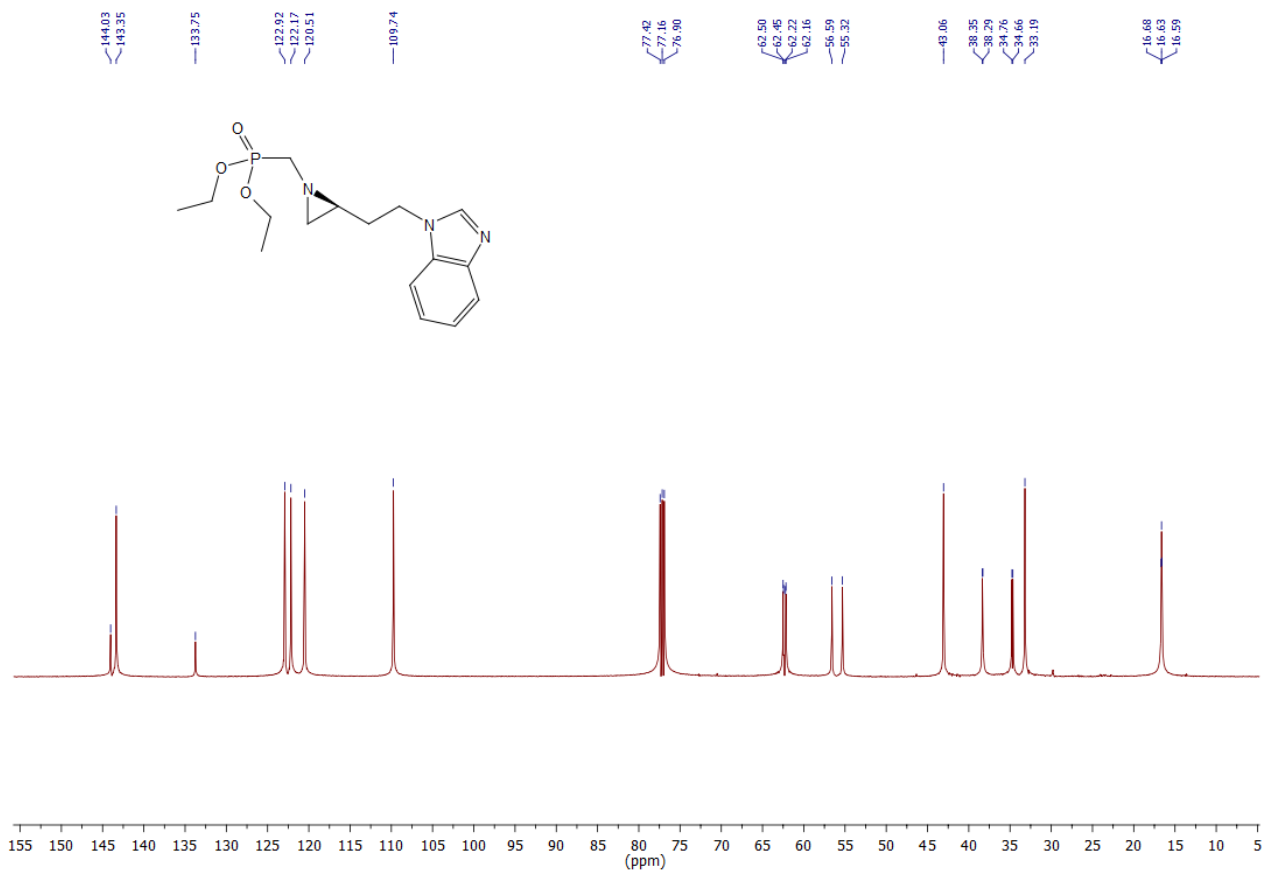


Diethyl (S)-((2-(2-(1H-benzo[d]imidazol-1-yl)ethyl)aziridin-1-yl)methyl)phosphonate – **2a**

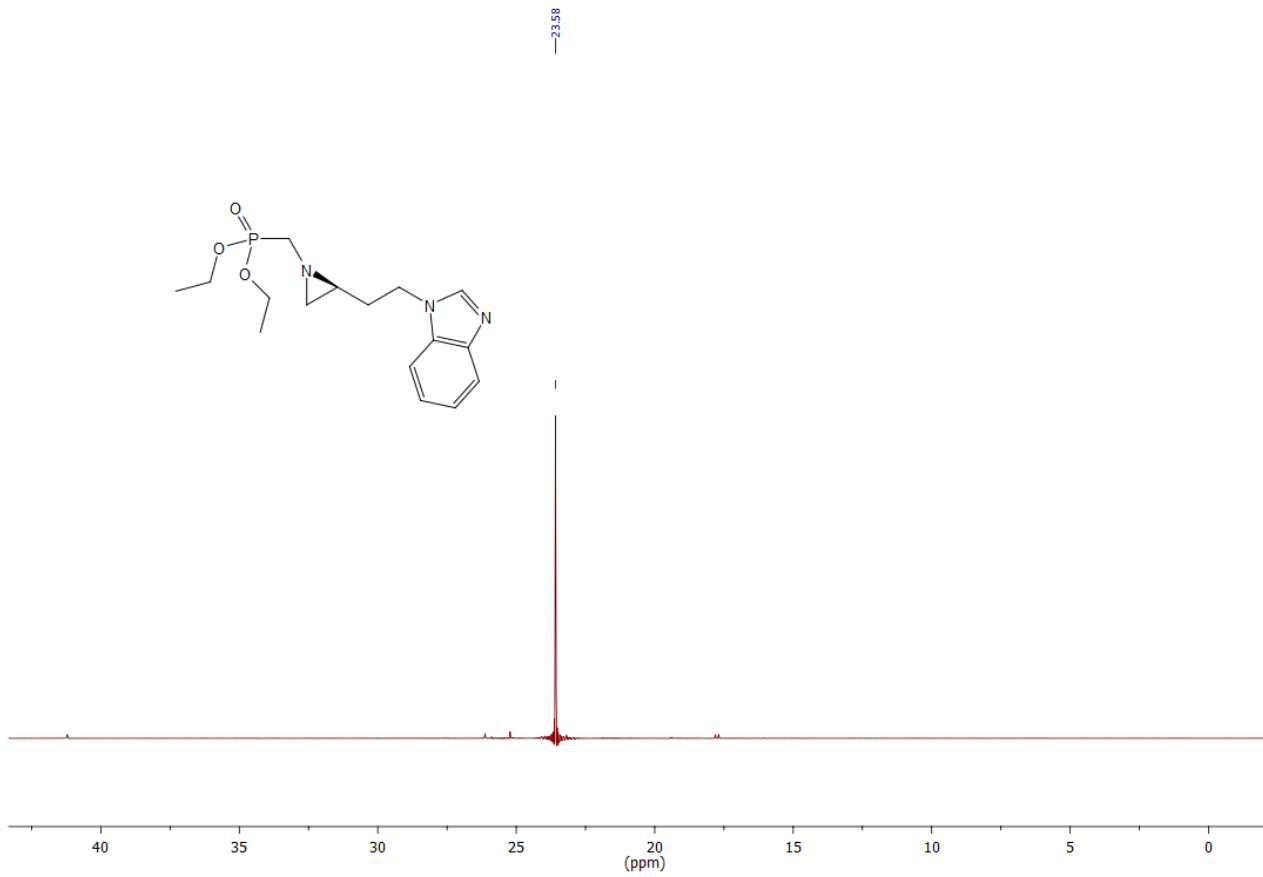
RMN ^1H



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

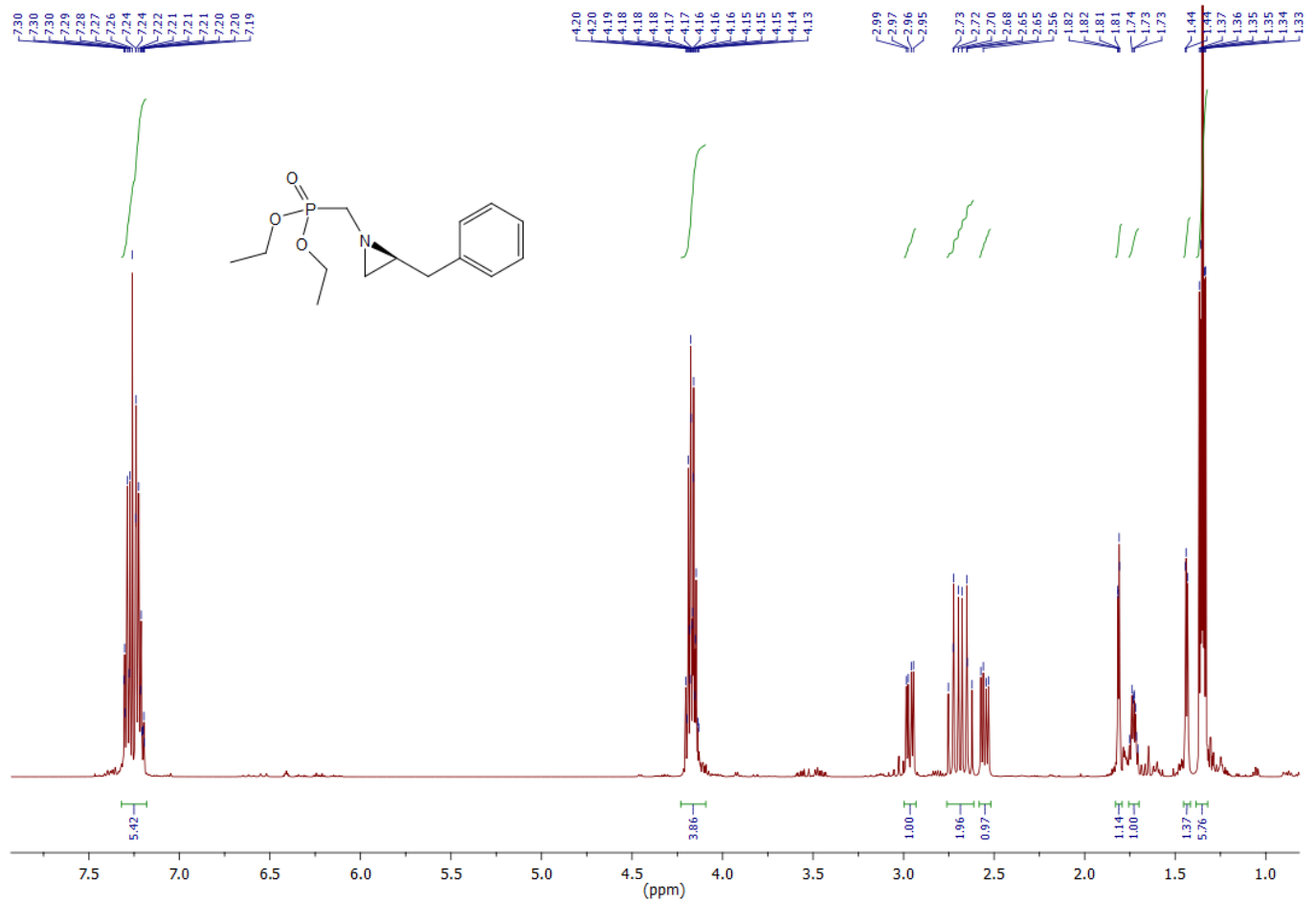


RMN $^{31}\text{P}\{^1\text{H}\}$

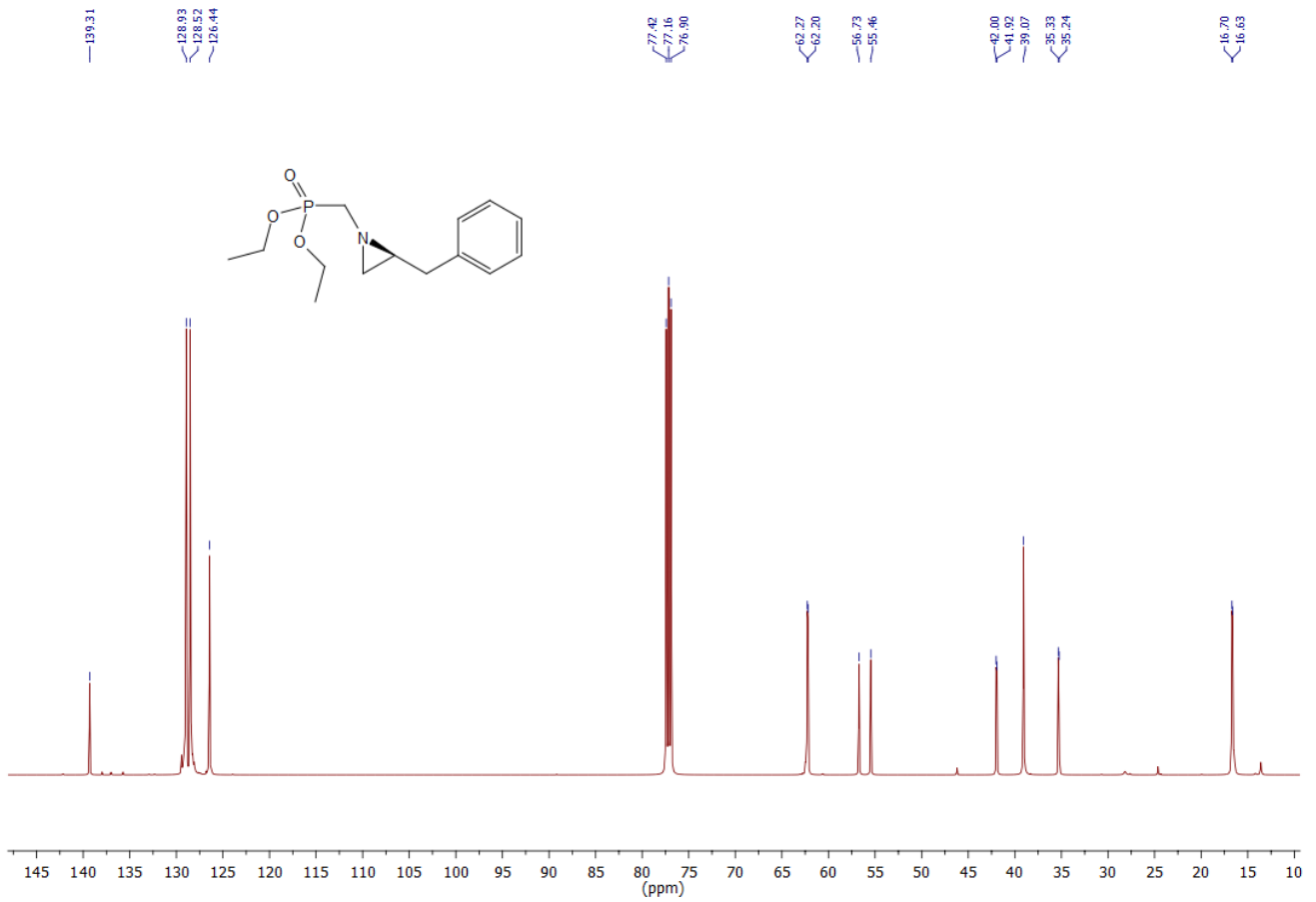


Diethyl (*S*)-((2-benzylaziridin-1-yl)methyl)phosphonate – **2b**

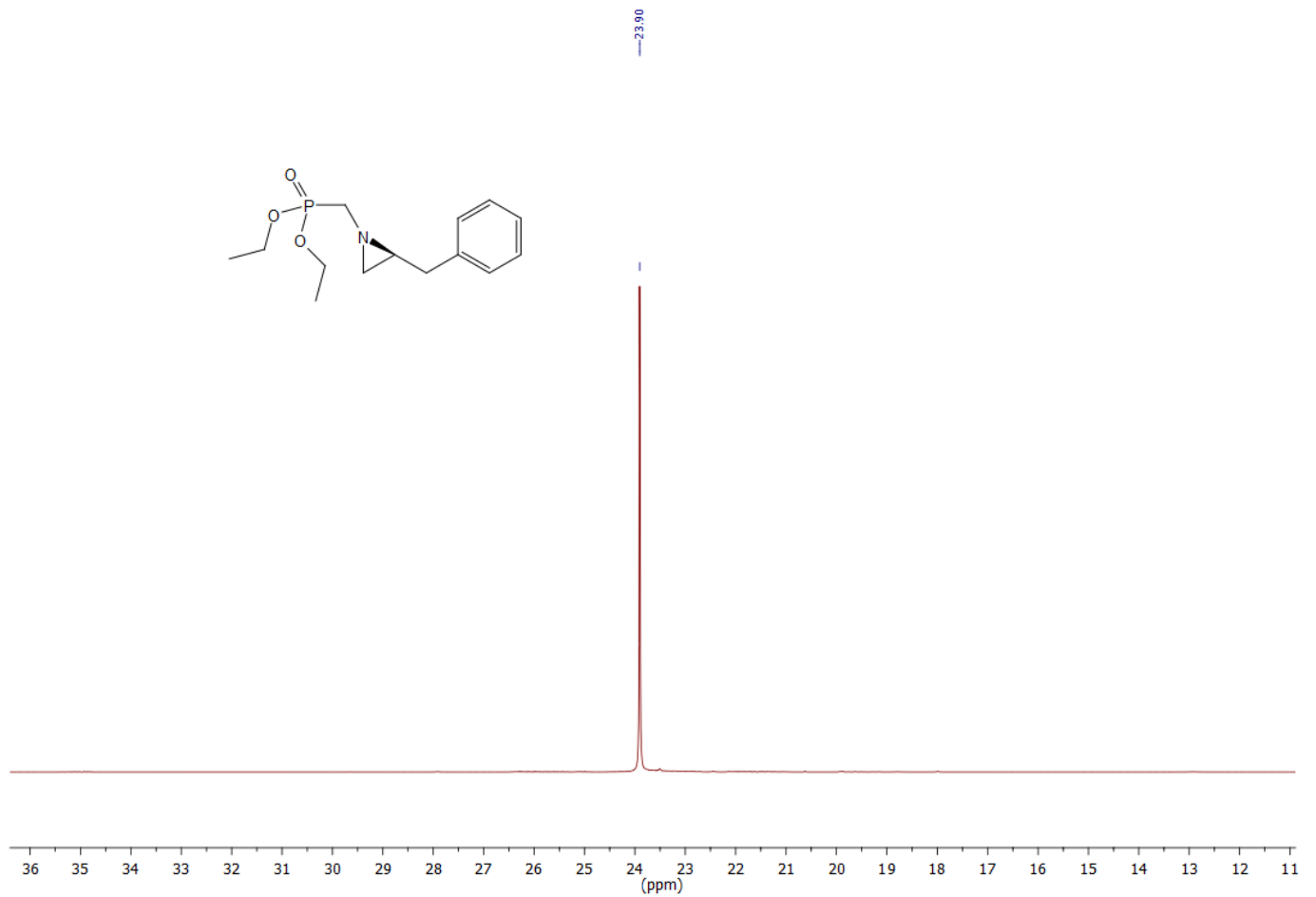
RMN ^1H

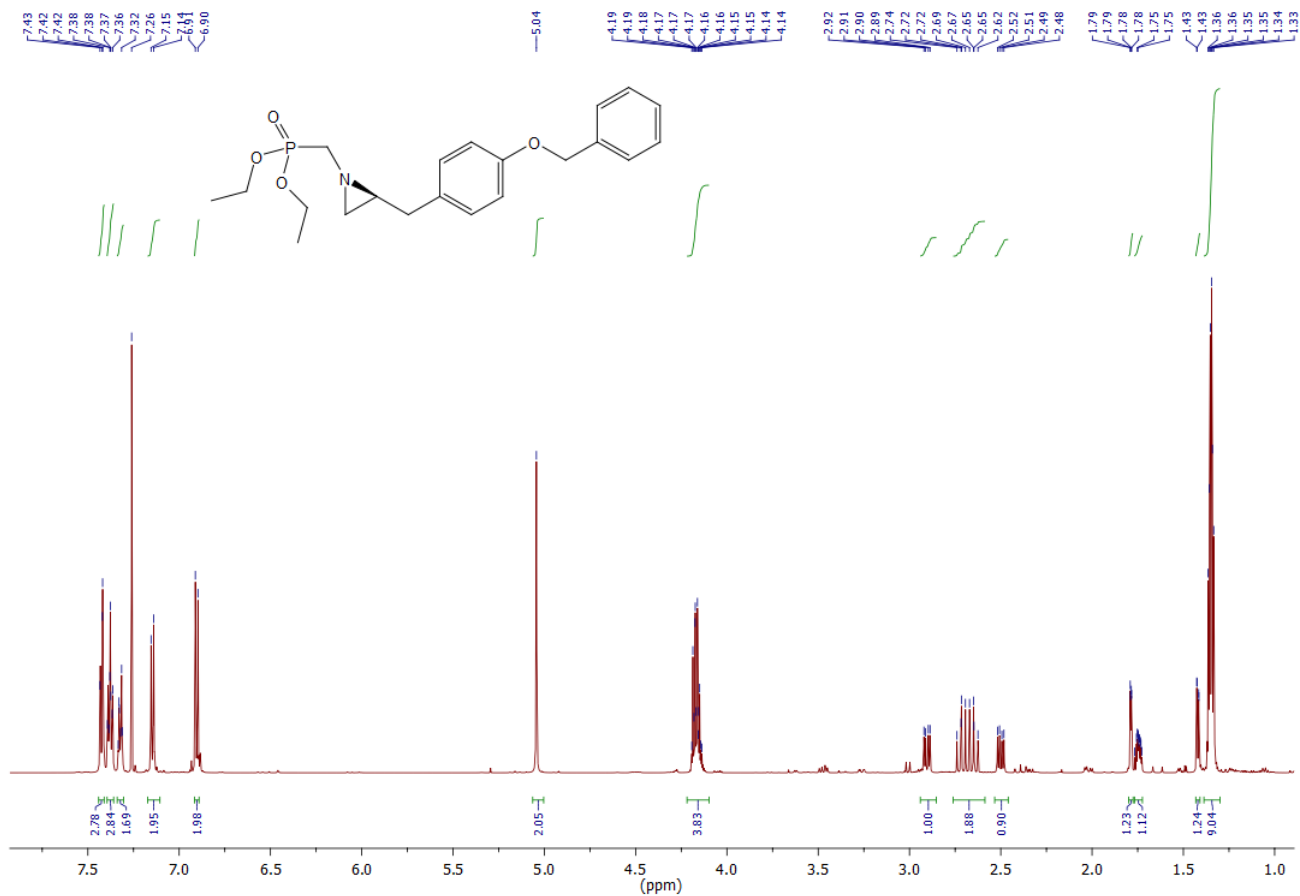


RMN $^{13}\text{C}\{^1\text{H}\}$

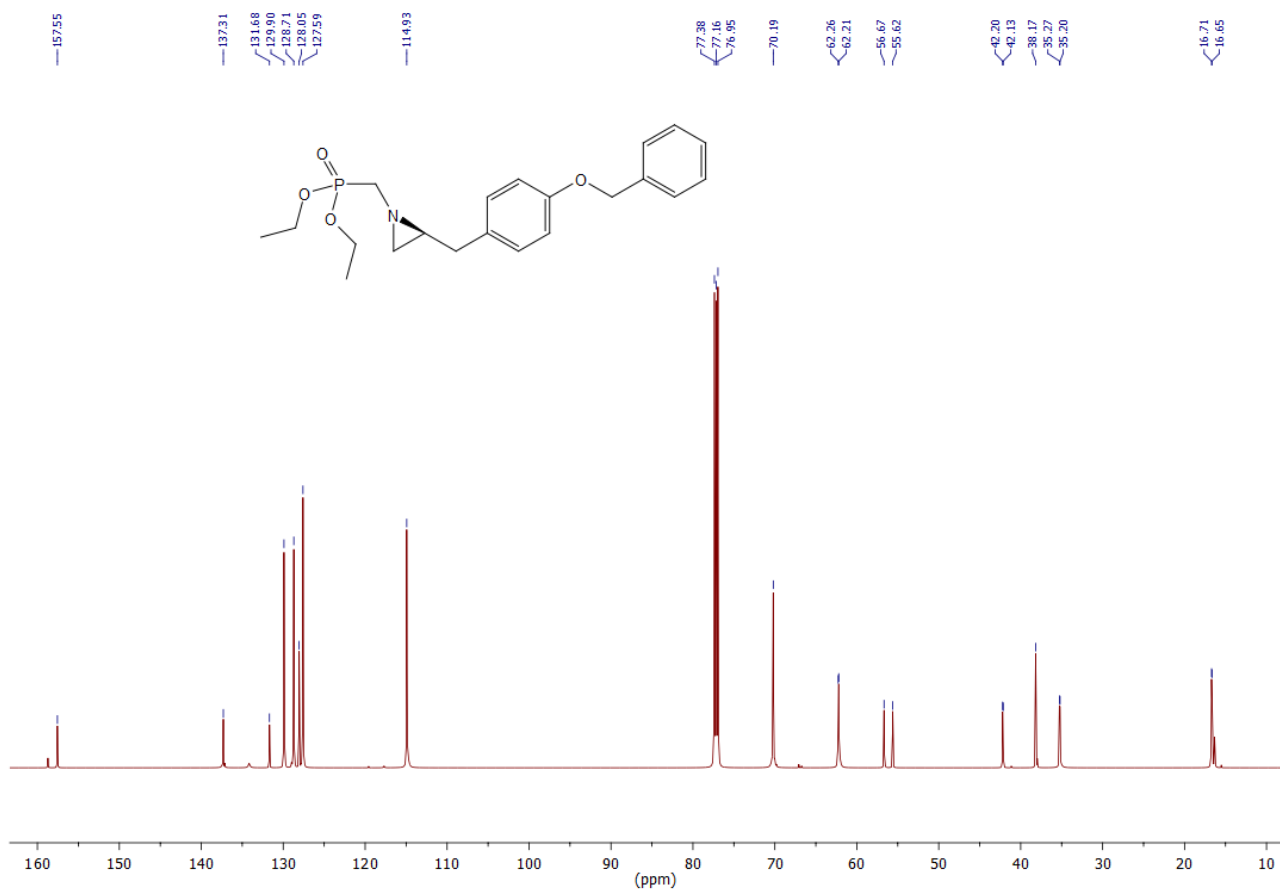


RMN $^{31}\text{P}\{^1\text{H}\}$



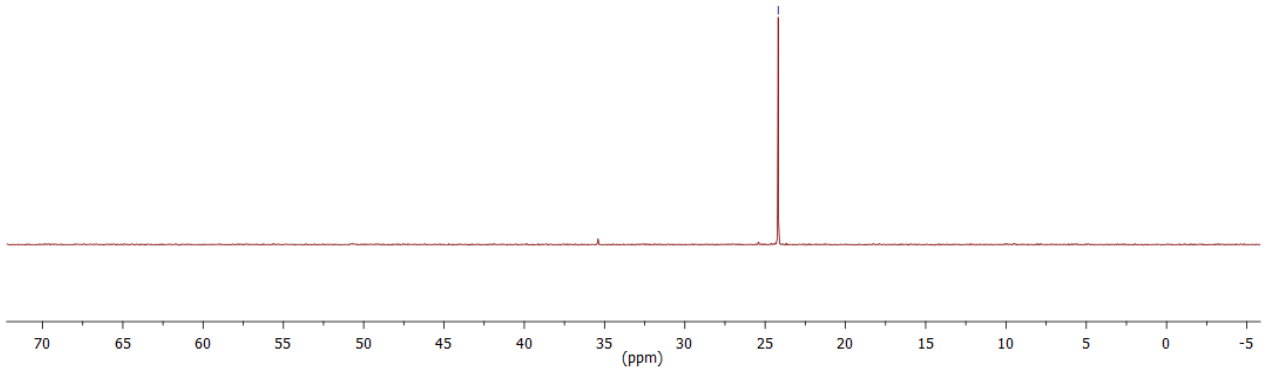
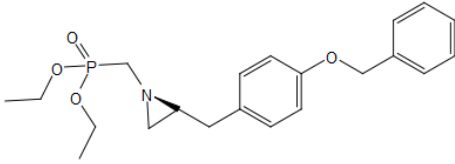


RMN ¹³C{¹H}



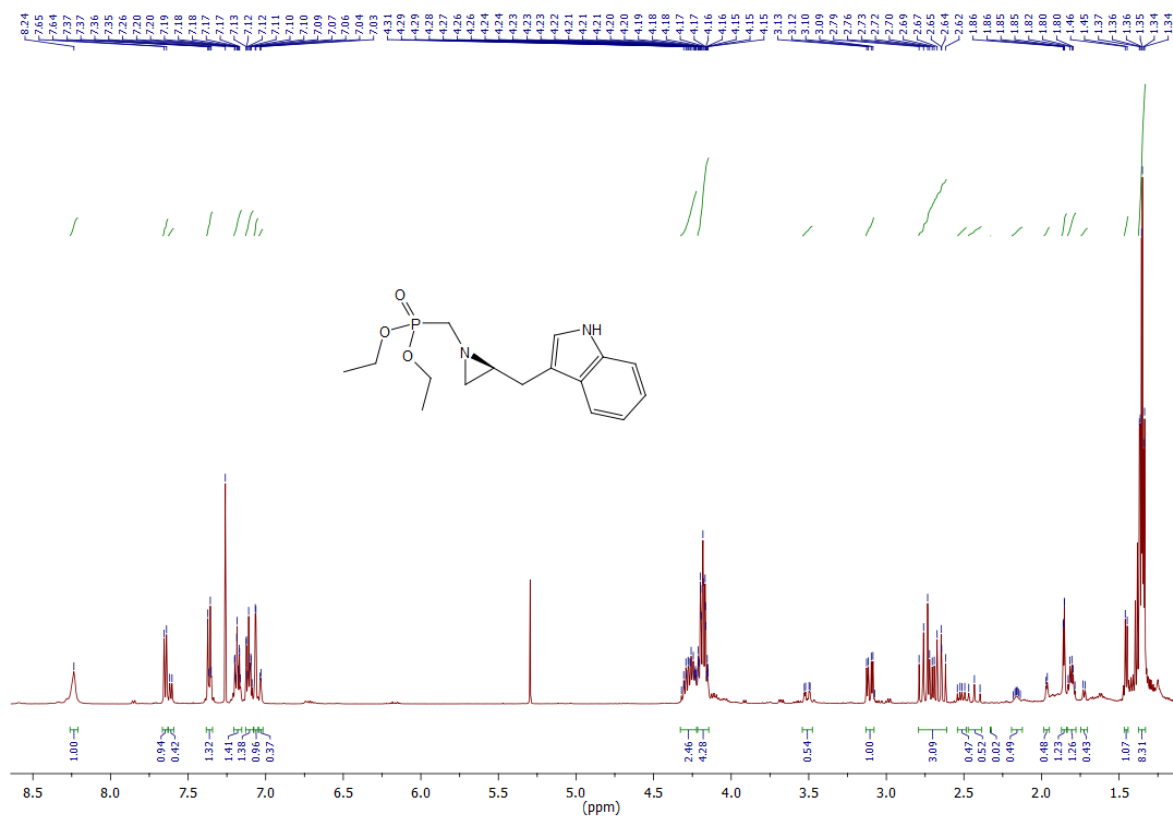
RMN $^{31}\text{P}\{^1\text{H}\}$

-24.19

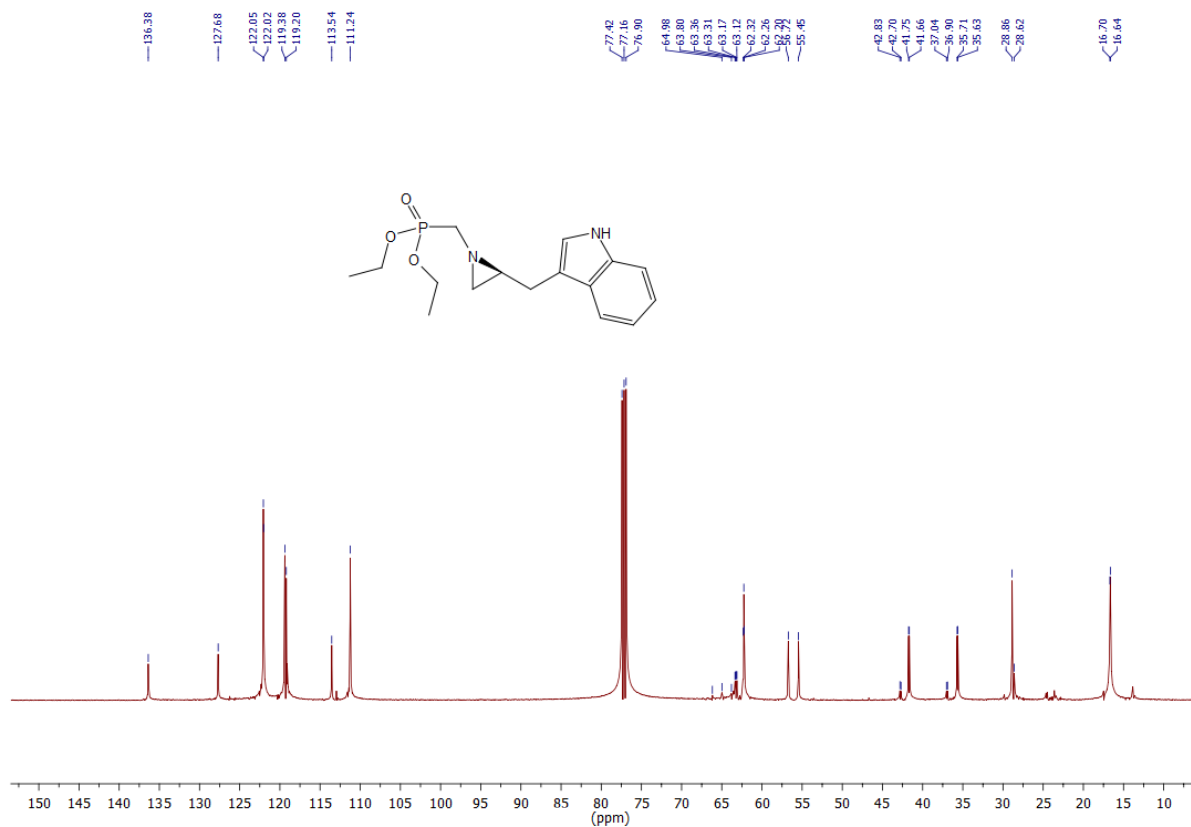


Diethyl (S)-((2-((1*H*-indol-3-yl)methyl)aziridin-1-yl)methyl)phosphonate – **2f**

RMN ¹H



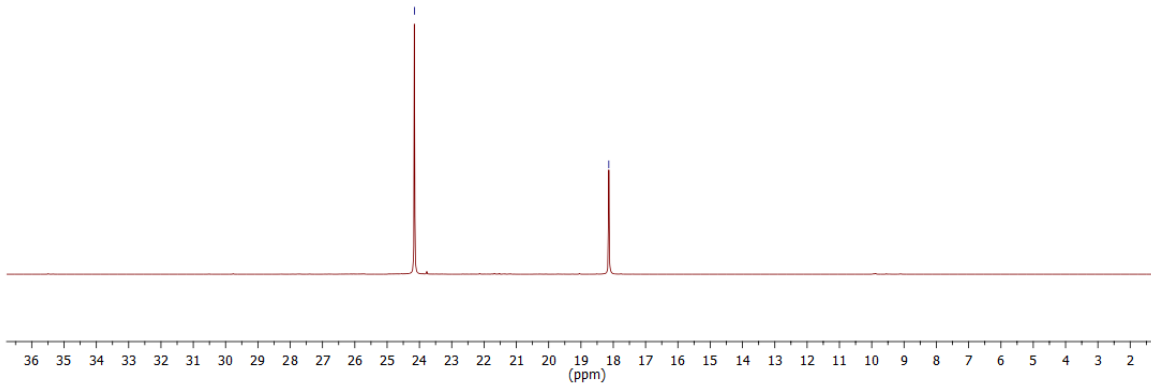
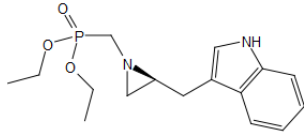
RMN ¹³C{¹H}



RMN $^{31}\text{P}\{^1\text{H}\}$

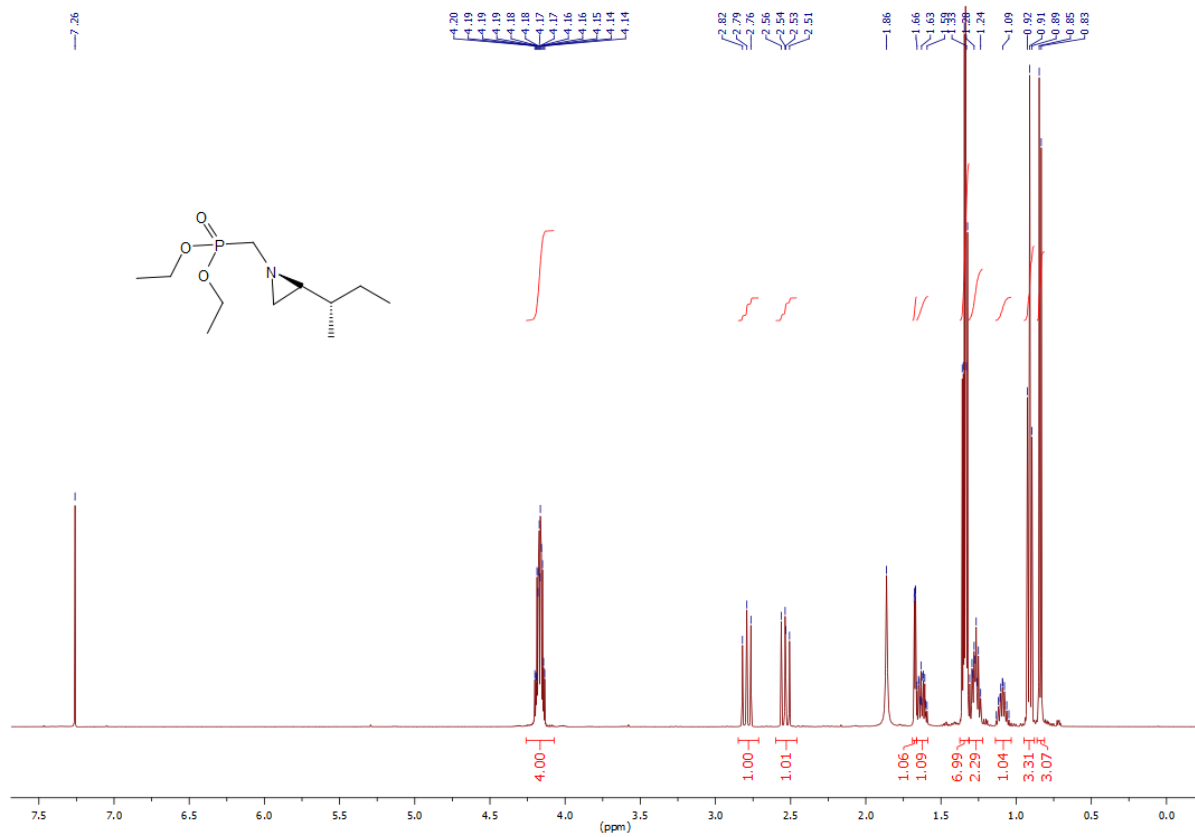
—24.16

—18.14

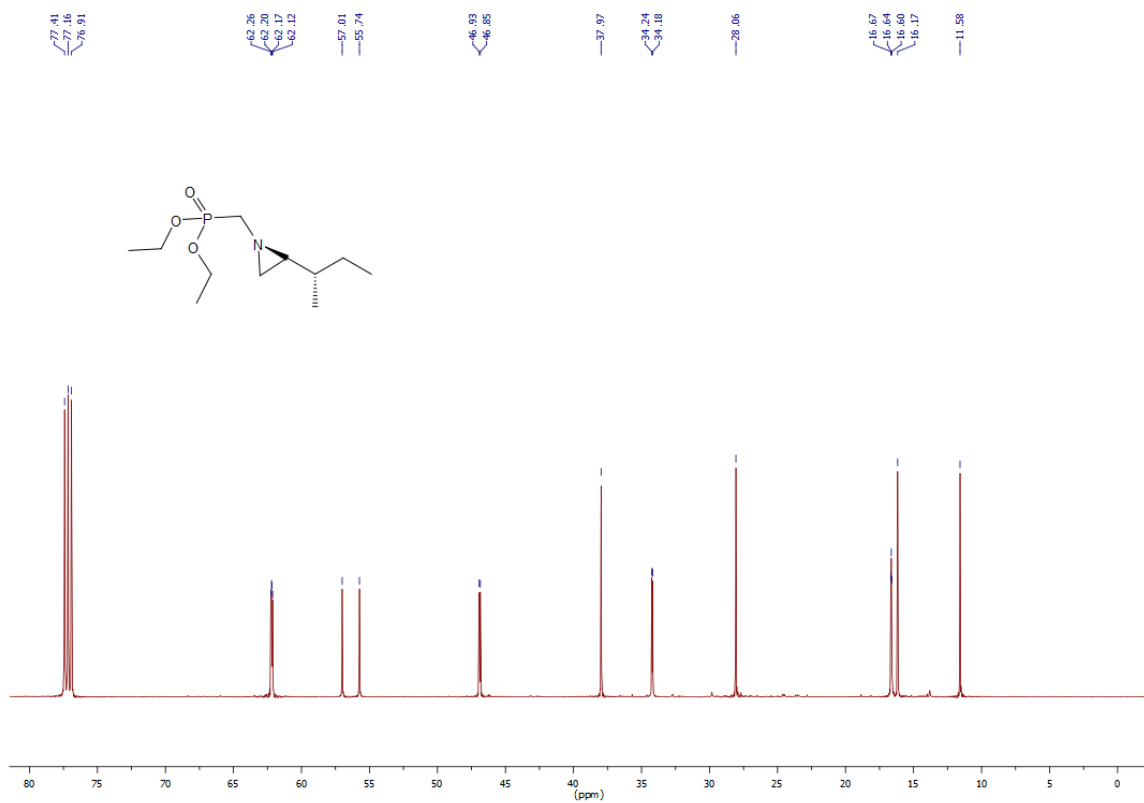


Diethyl (((S)-2-((S)-*sec*-butyl)aziridin-1-yl)methyl)phosphonate – **2h**

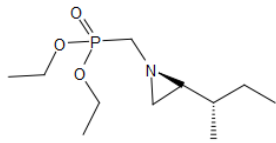
RMN ^1H



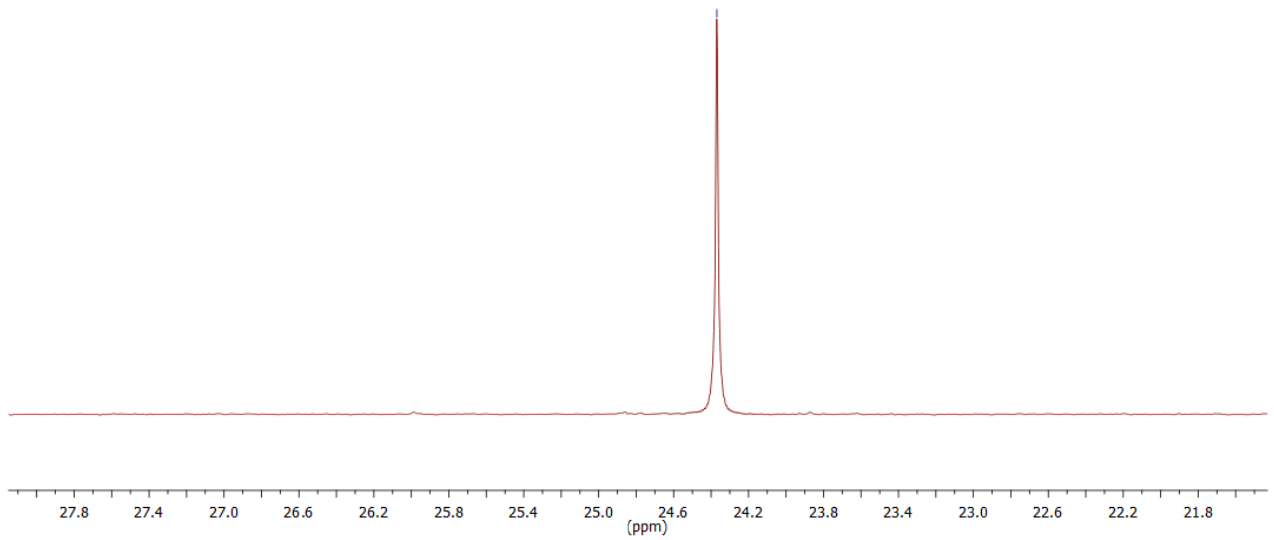
RMN $^{13}\text{C}\{^1\text{H}\}$



RMN $^{31}\text{P}\{^1\text{H}\}$

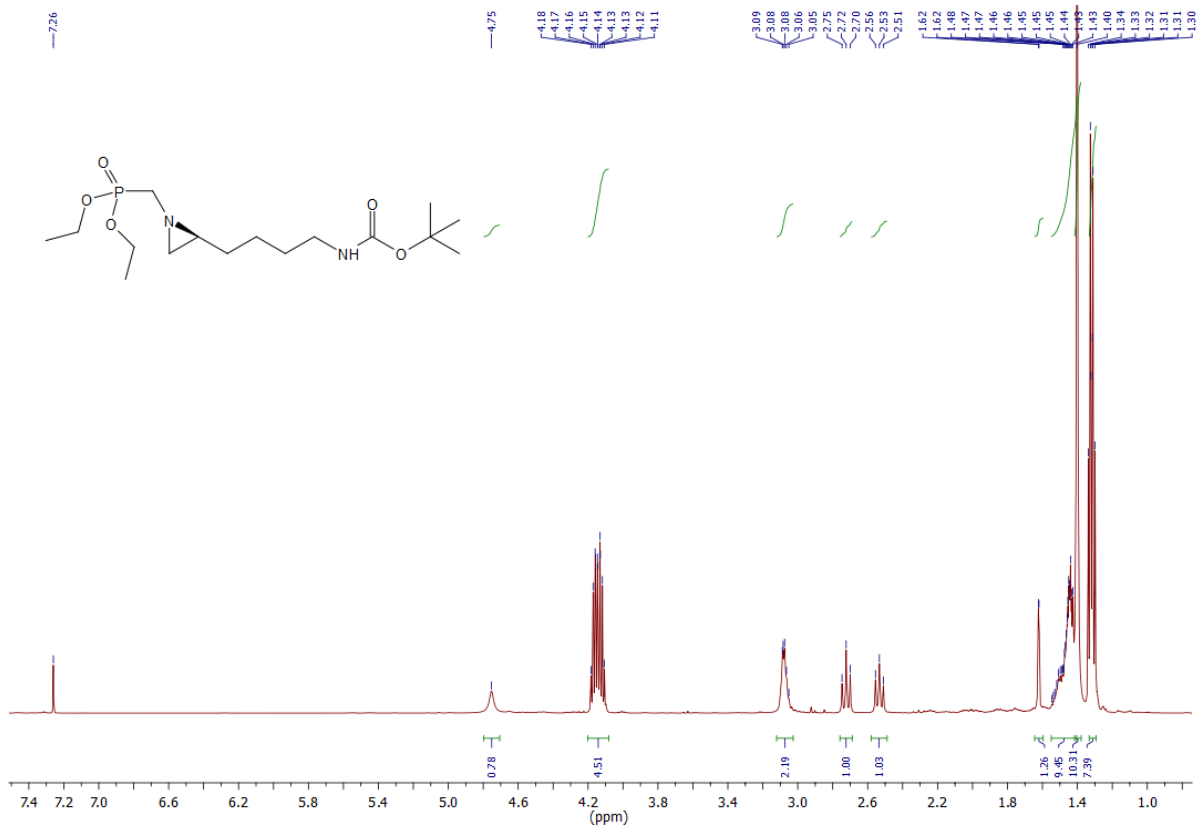


—24.37

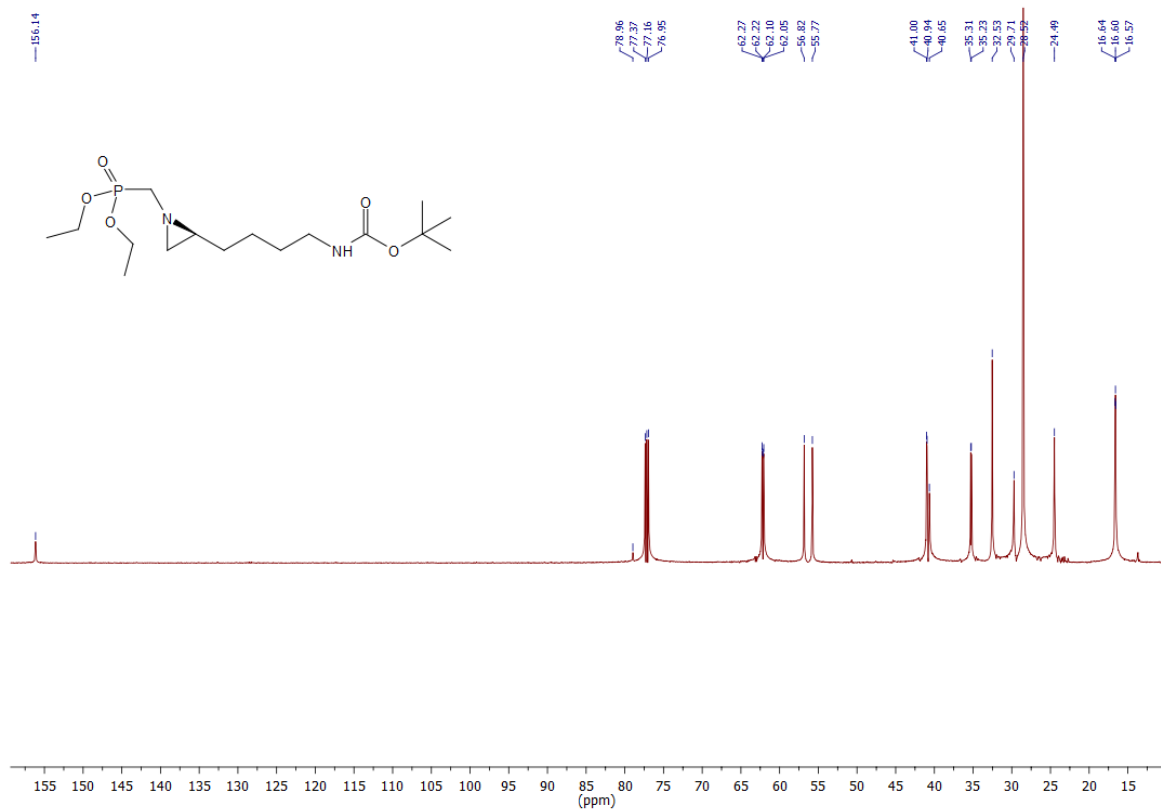


tert-Butyl (*S*)-(4-(1-((diethoxyphosphoryl)methyl)aziridin-2-yl)butyl)carbamate **2j**

RMN ¹H

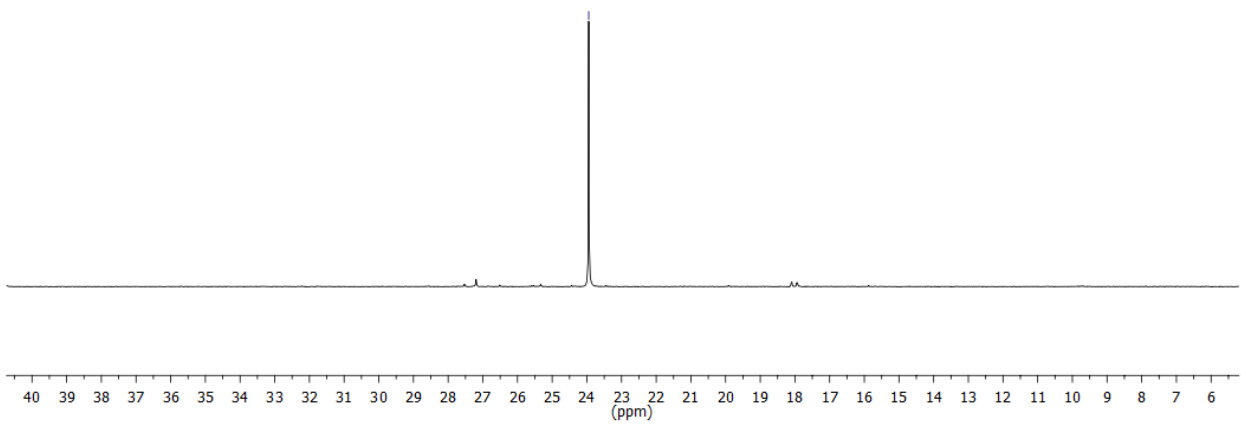
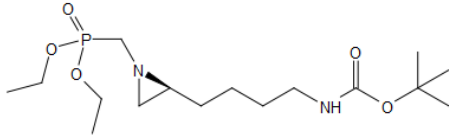


RMN ¹³C{¹H}



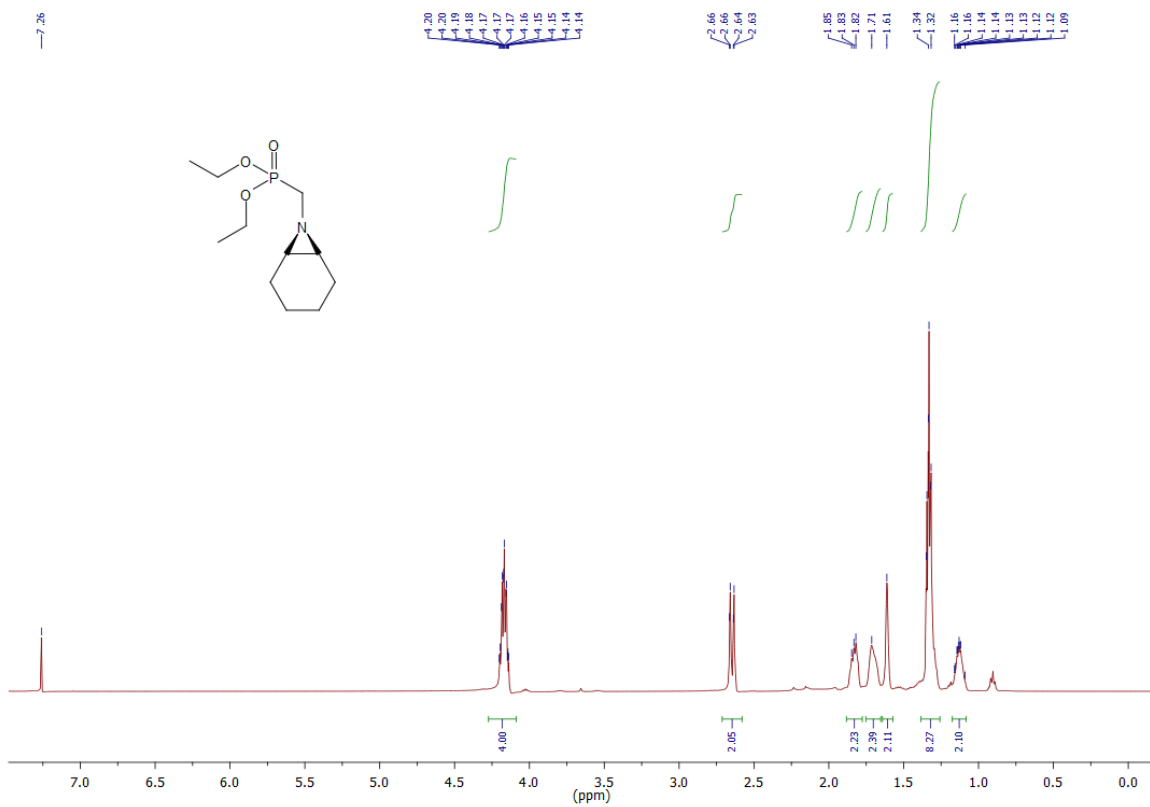
RMN $^{31}\text{P}\{^1\text{H}\}$

-23.95

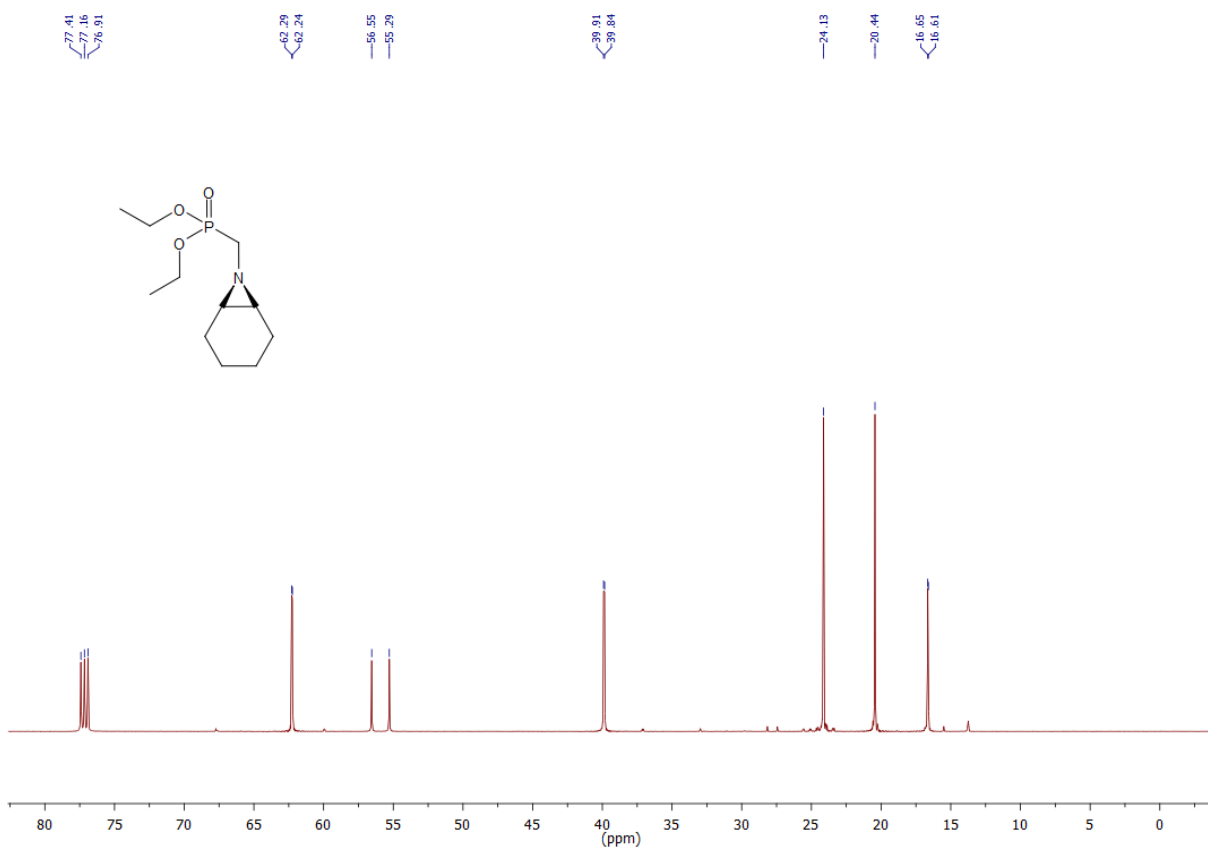


Diethyl (((1R,6S)-7-azabicyclo[4.1.0]heptan-7-yl)methylene)phosphonate (**21**)

RMN ^1H



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



RMN $^{31}\text{P}\{^1\text{H}\}$

24.46
24.40
24.38
24.36
24.32
24.29
24.22
24.18

