

Supporting Information for

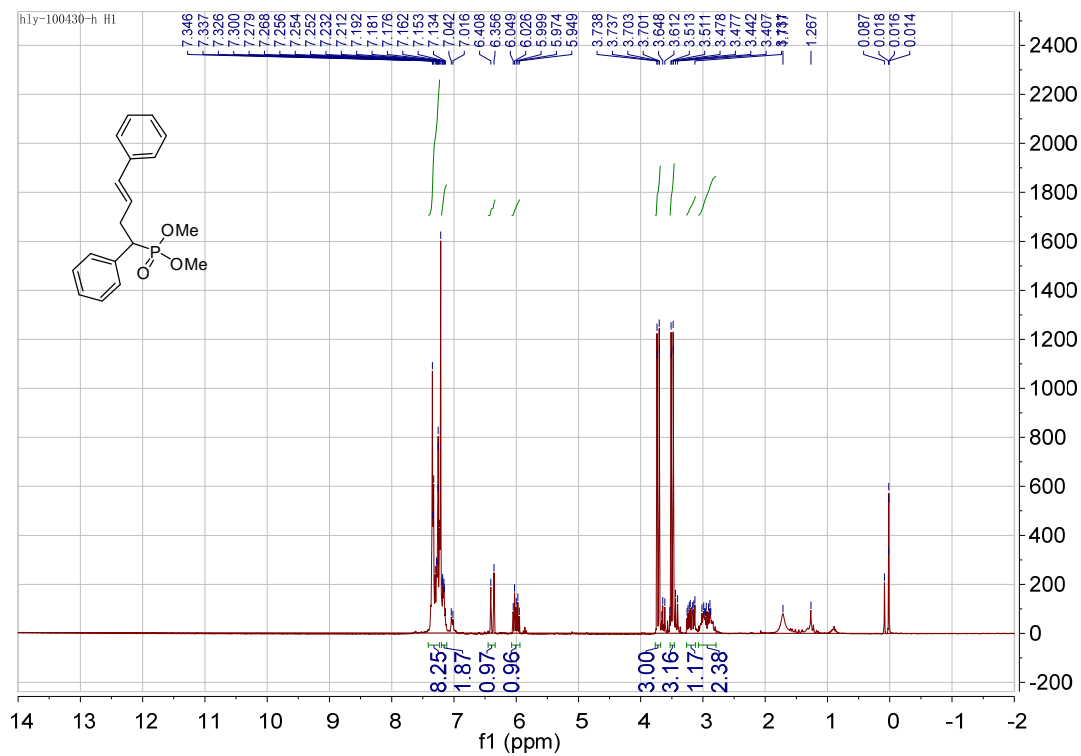
Synthesis of phostones via DABCO-catalyzed bromocyclization of alkenylphosphonic acid monoesters

Haiyang Wang,^a Liye Huang,^a Xiaohui Cao,^a Dacheng Liang and Ai-Yun Peng^{a*}

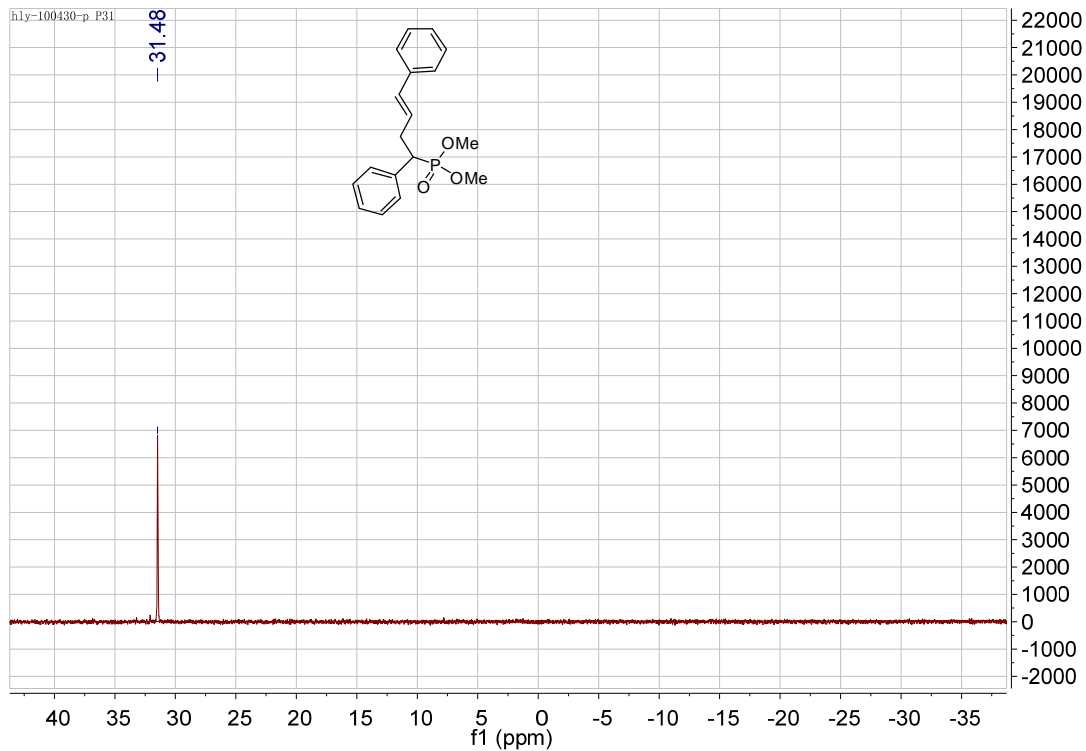
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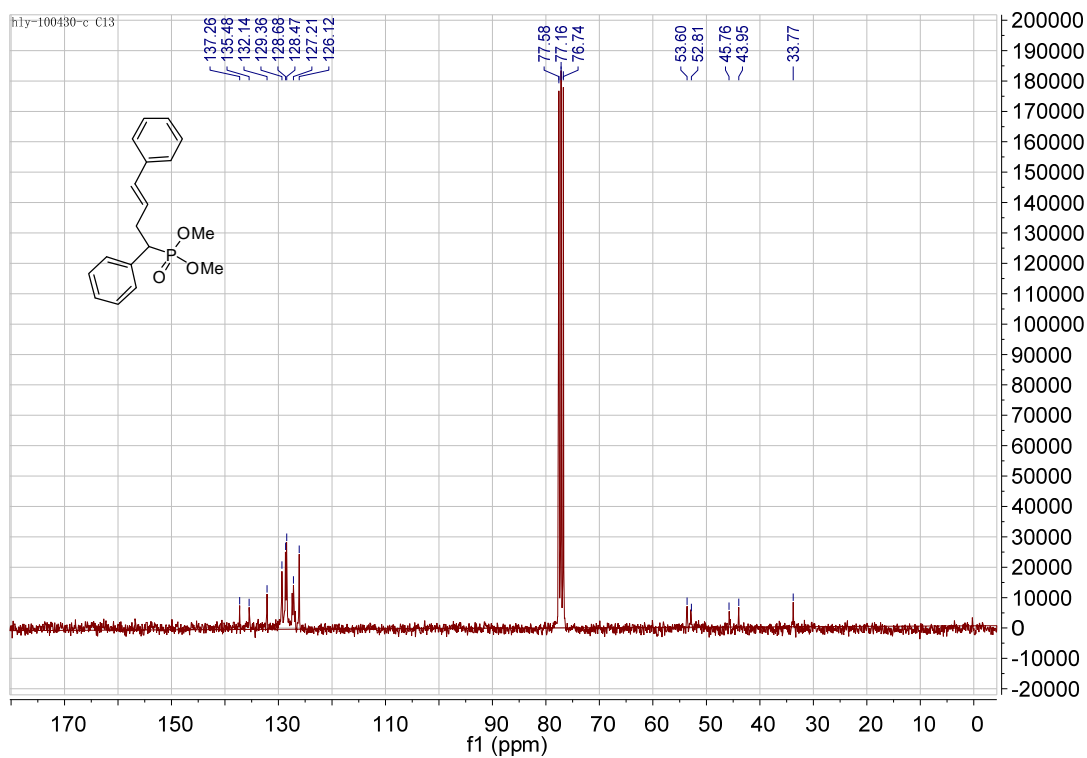
¹H NMR (300 MHz, CDCl₃) of **4a**



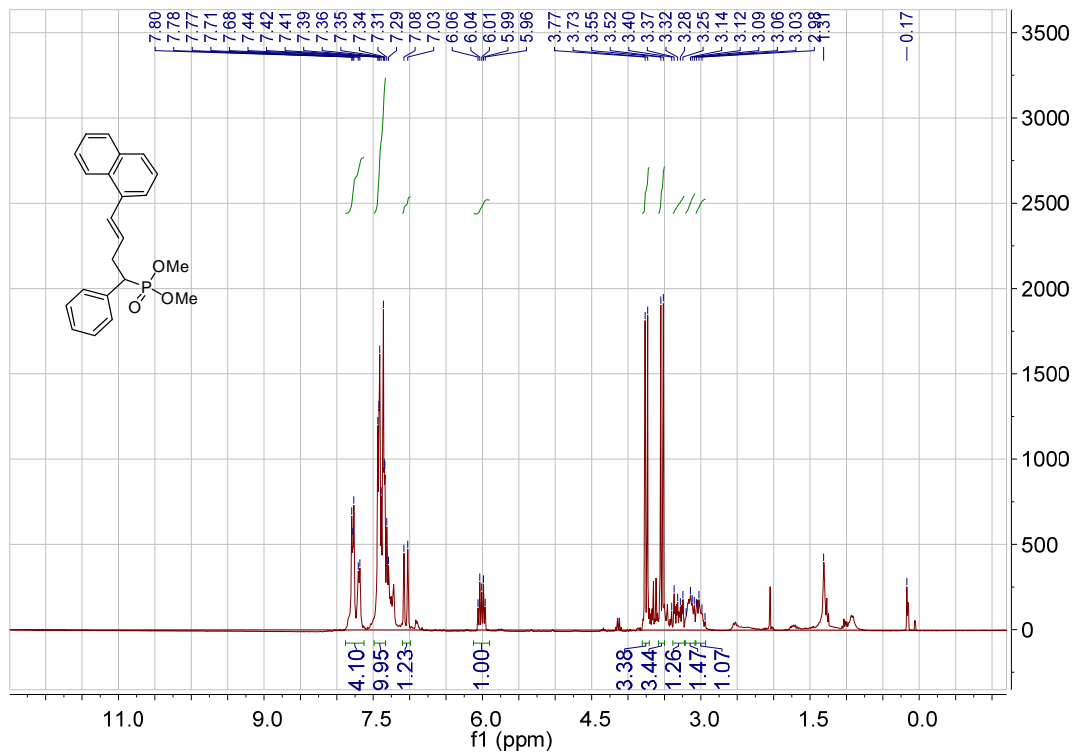
³¹P NMR (121 MHz, CDCl₃) of **4a**



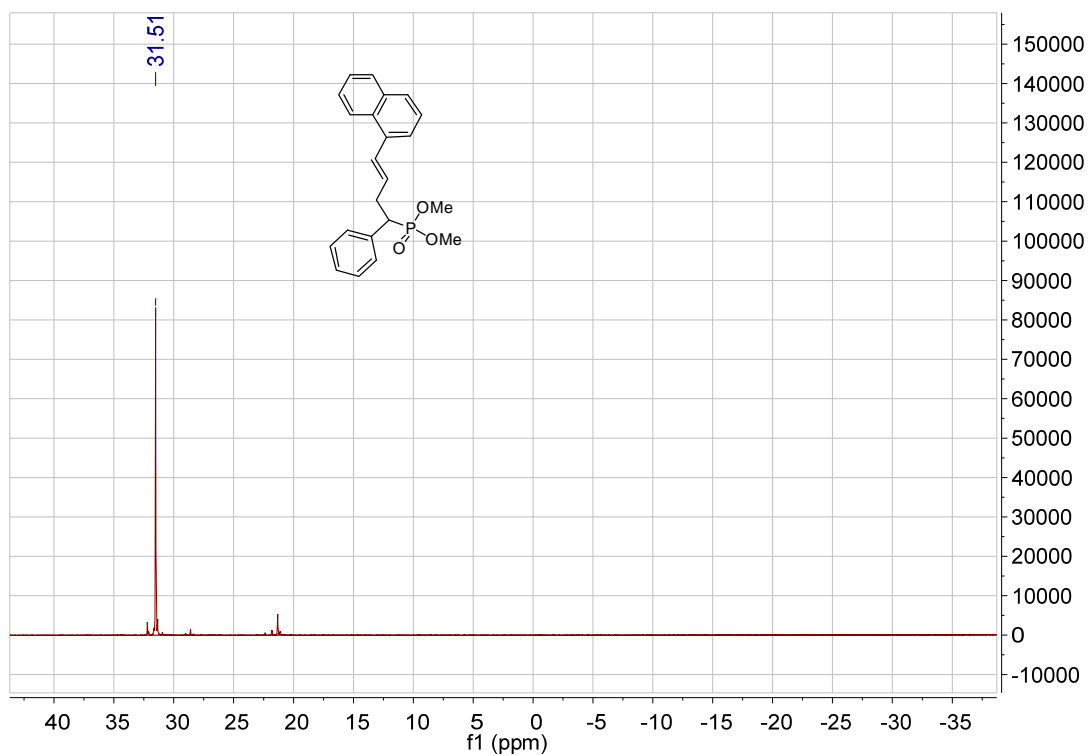
¹³C NMR (75 MHz, CDCl₃) of **4a**



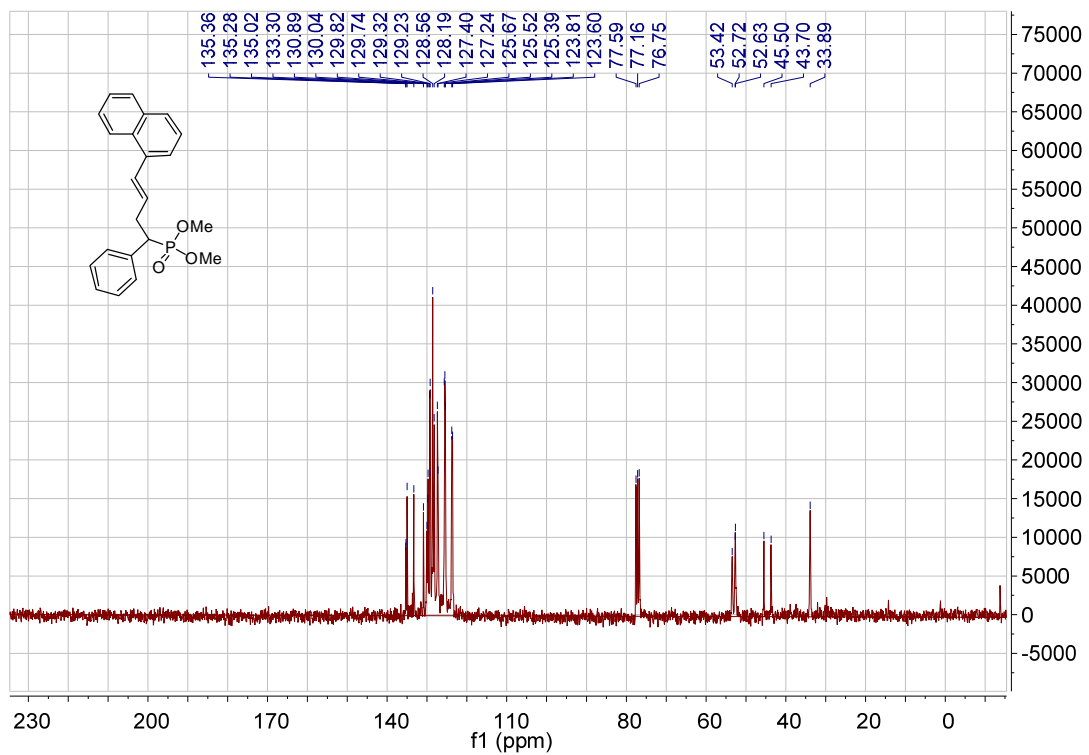
¹H NMR (300 MHz, CDCl₃) of **4b**



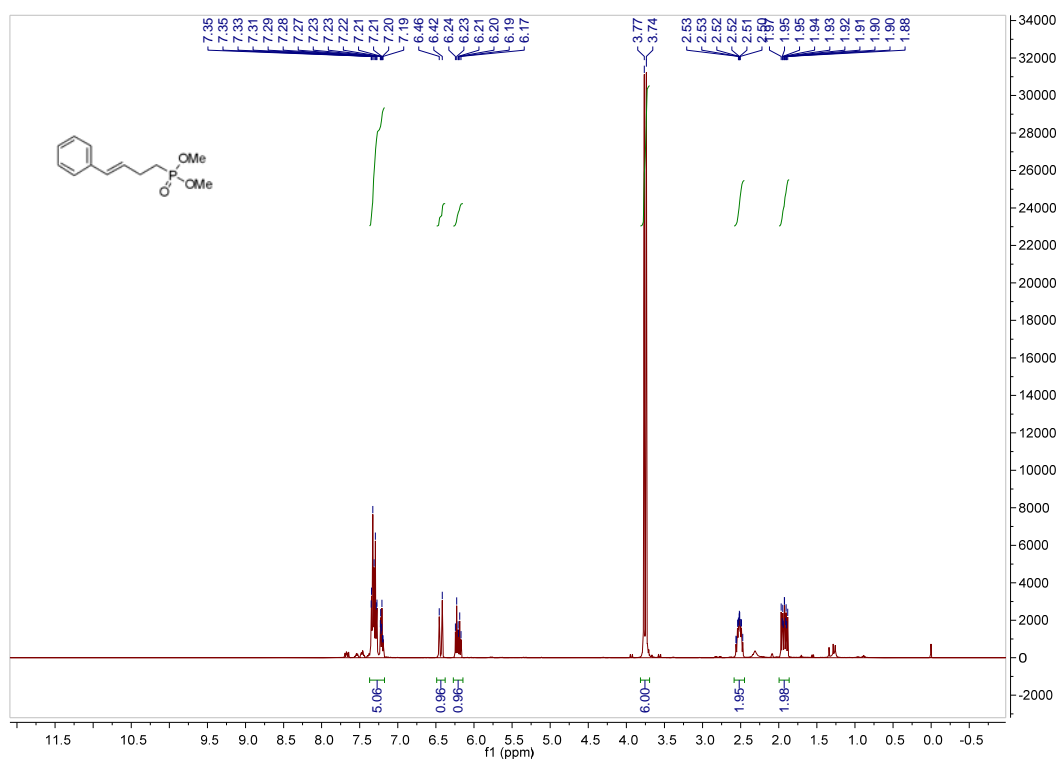
³¹P NMR (121 MHz, CDCl₃) of **4b**



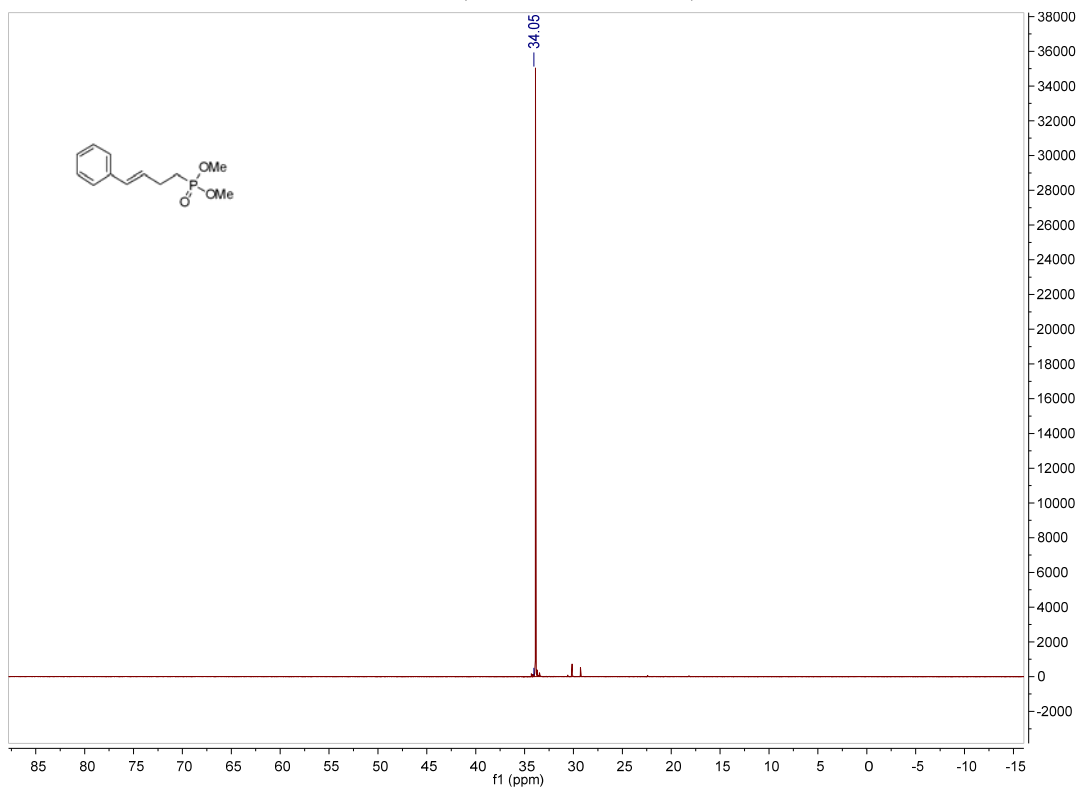
¹³C NMR (75 MHz, CDCl₃) of **4b**



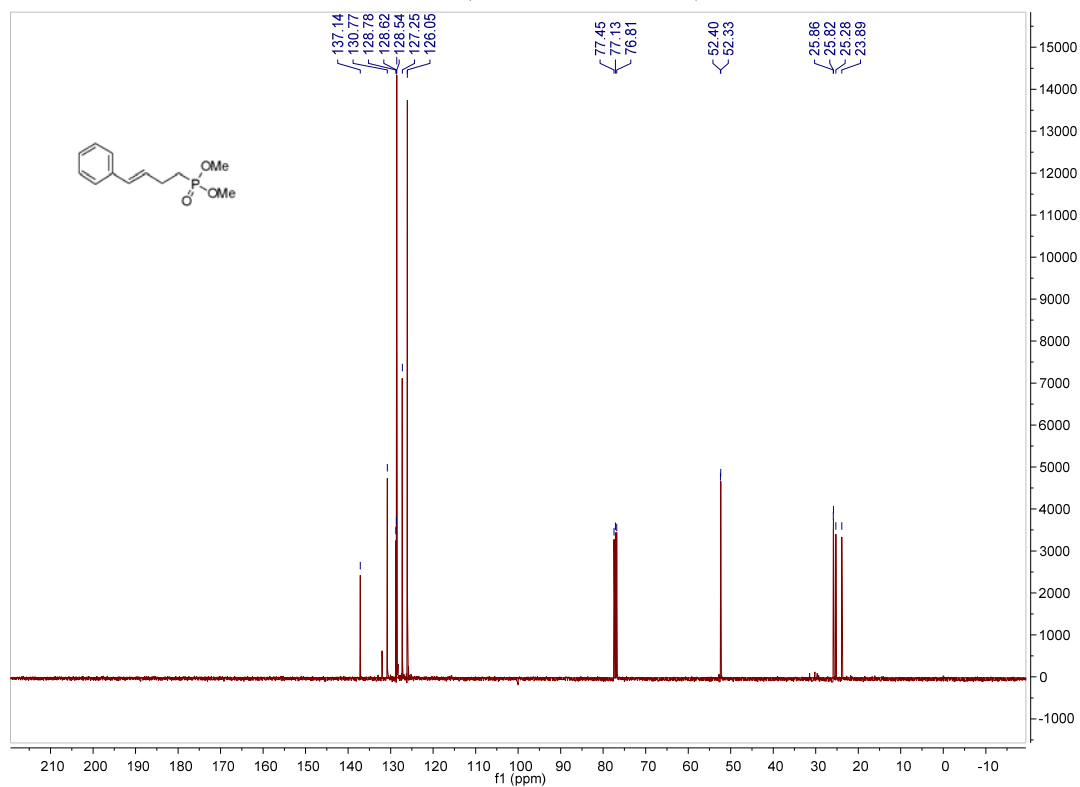
¹H NMR (400 MHz, CDCl₃) of **4c**



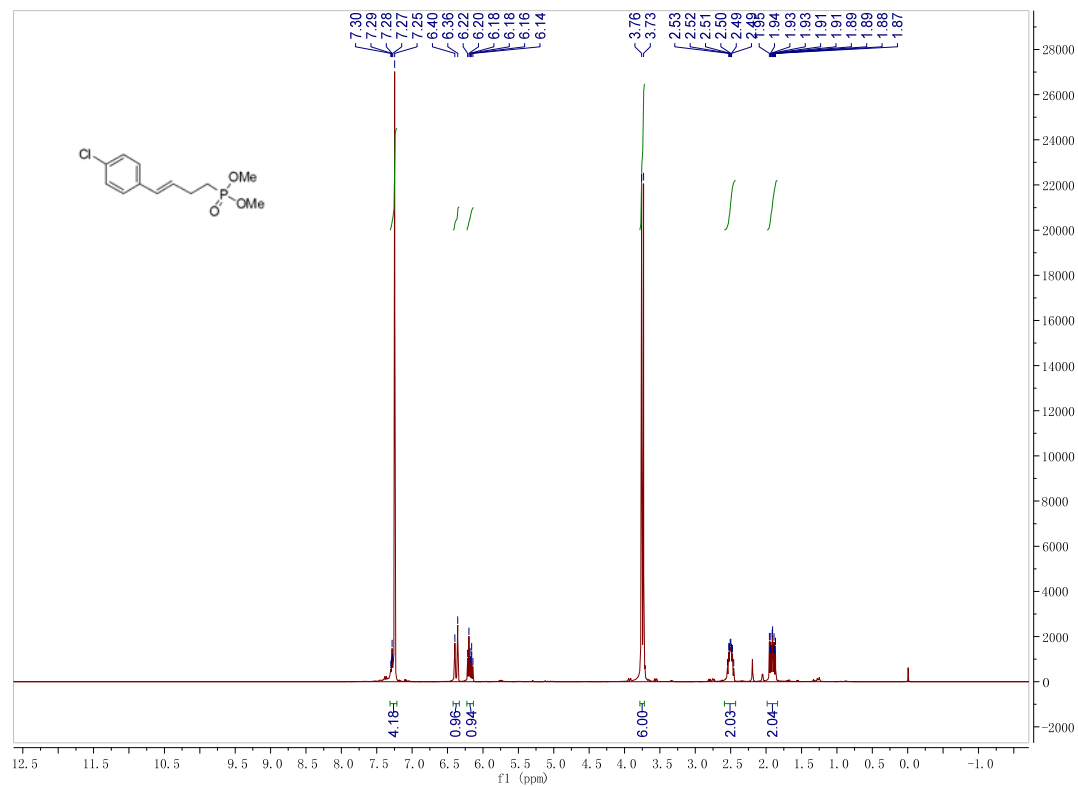
³¹P NMR (162 MHz, CDCl₃) of **4c**



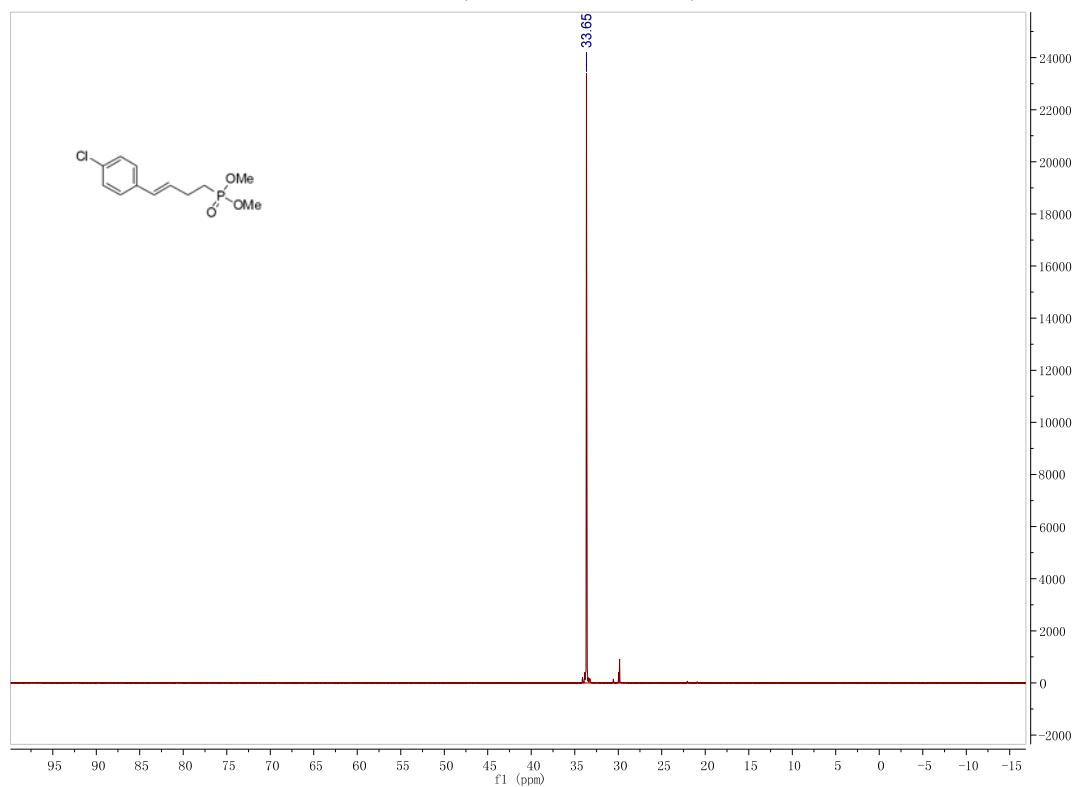
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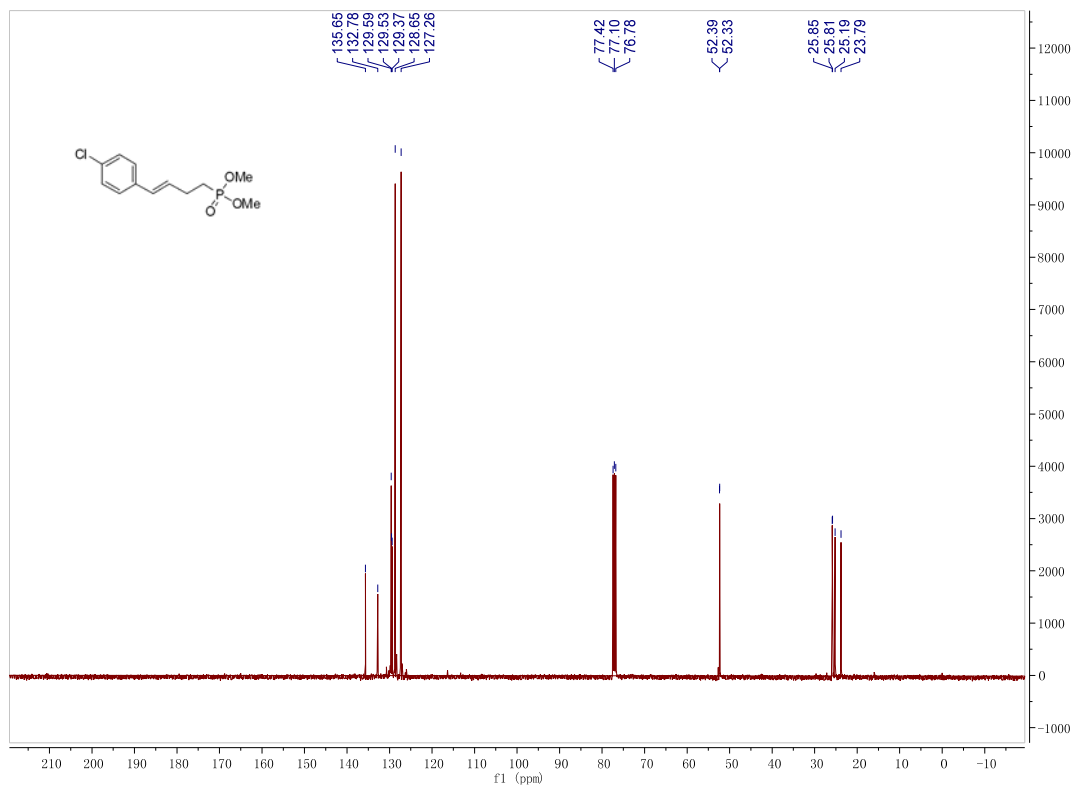
¹H NMR (400 MHz, CDCl₃) of **4d**



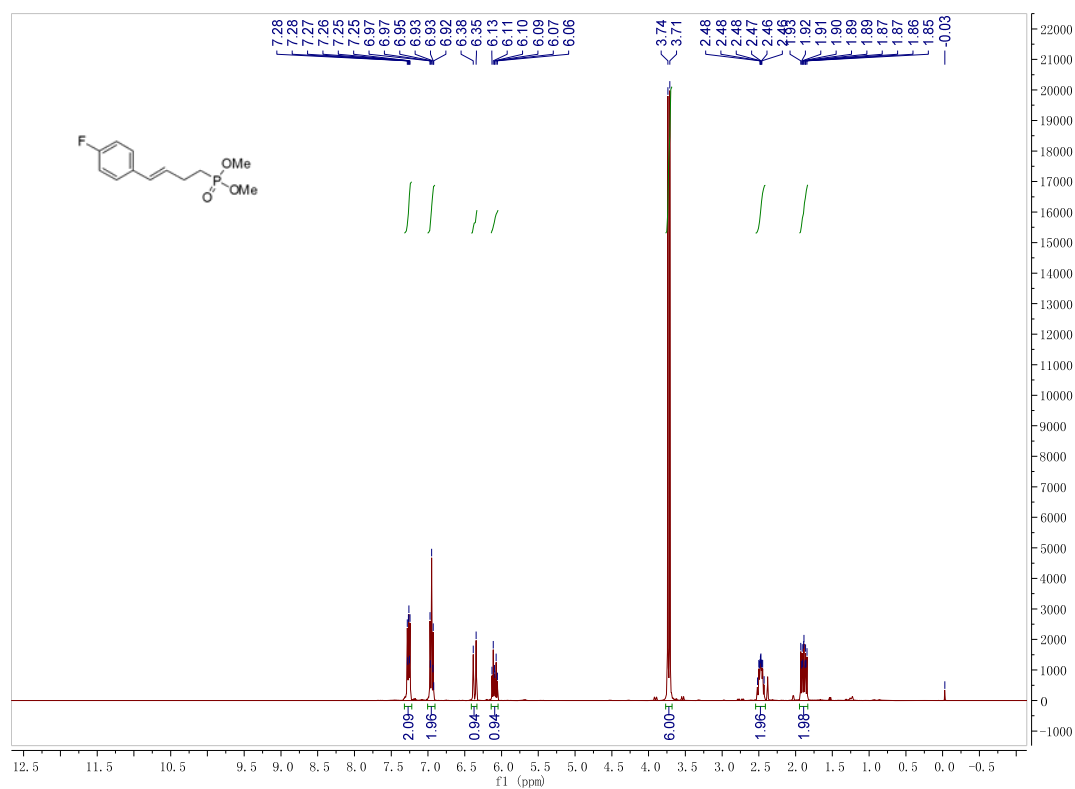
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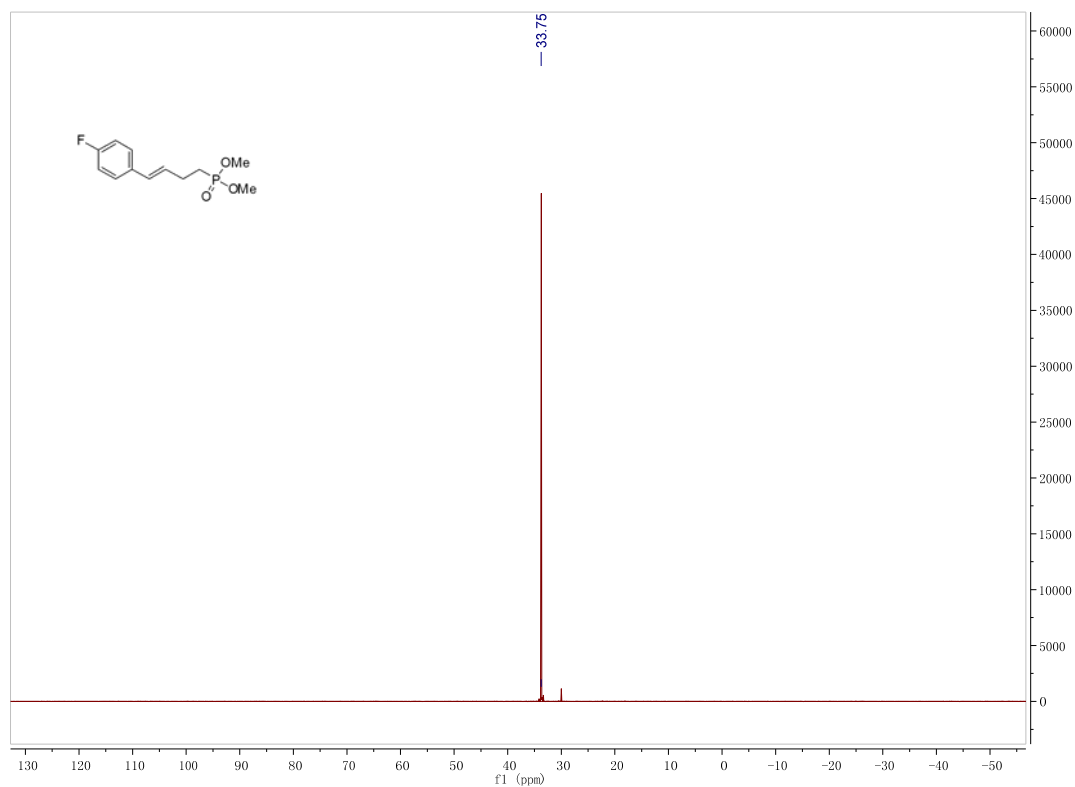
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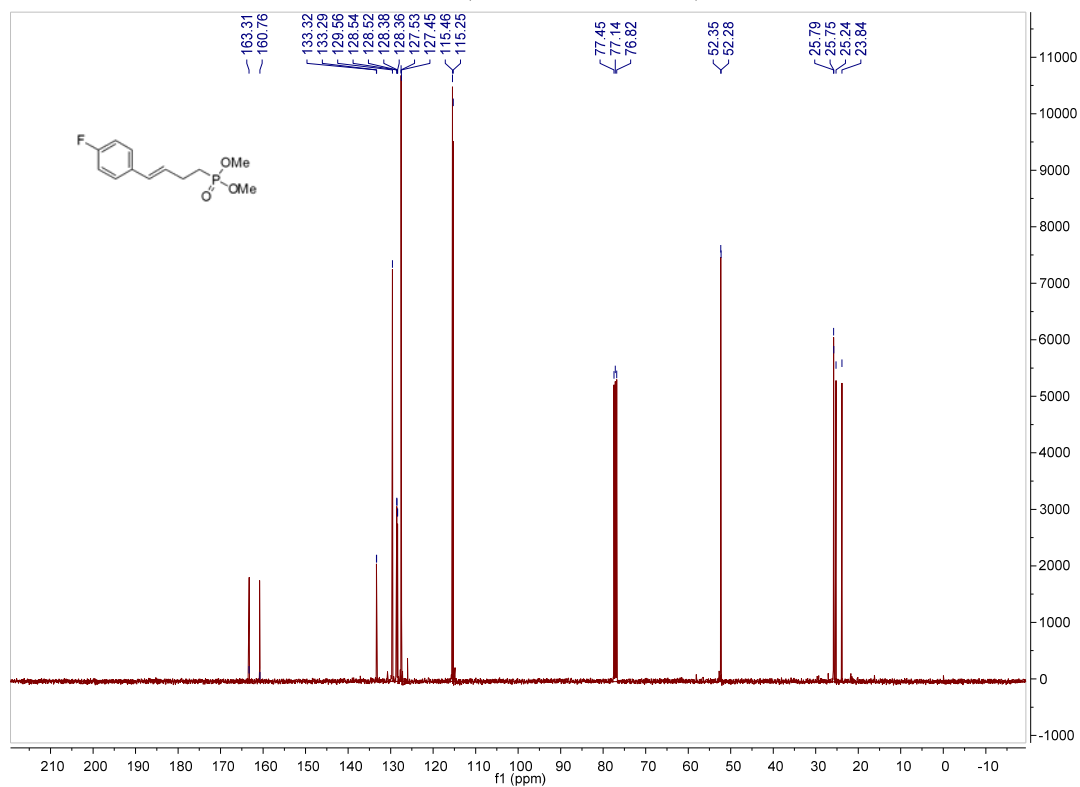
¹H NMR (400 MHz, CDCl₃) of **4e**



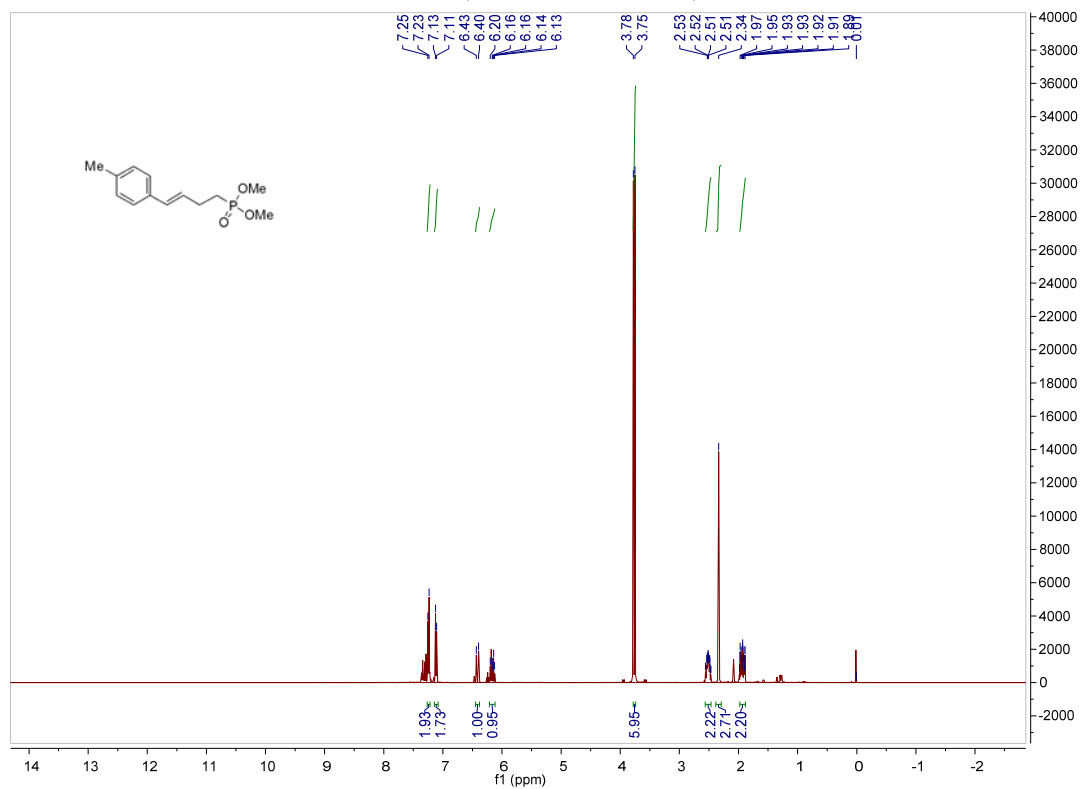
³¹P NMR (162 MHz, CDCl₃) of **4e**



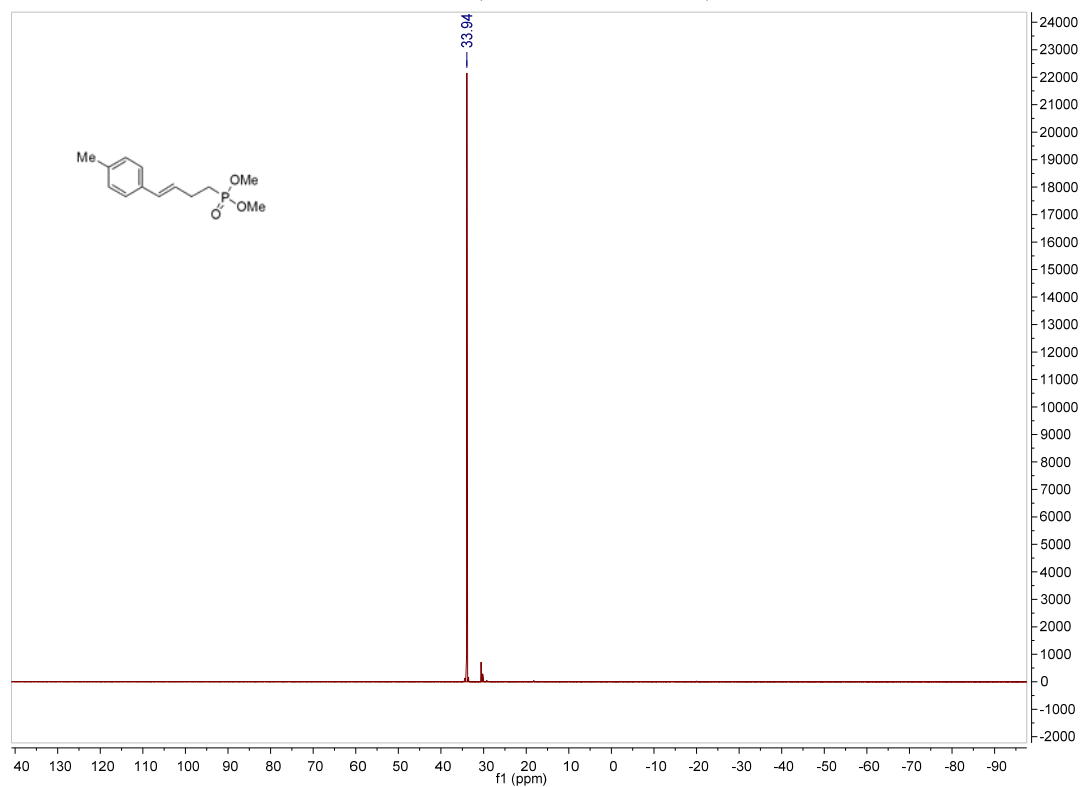
^{13}C NMR (101 MHz, CDCl_3) of **4e**



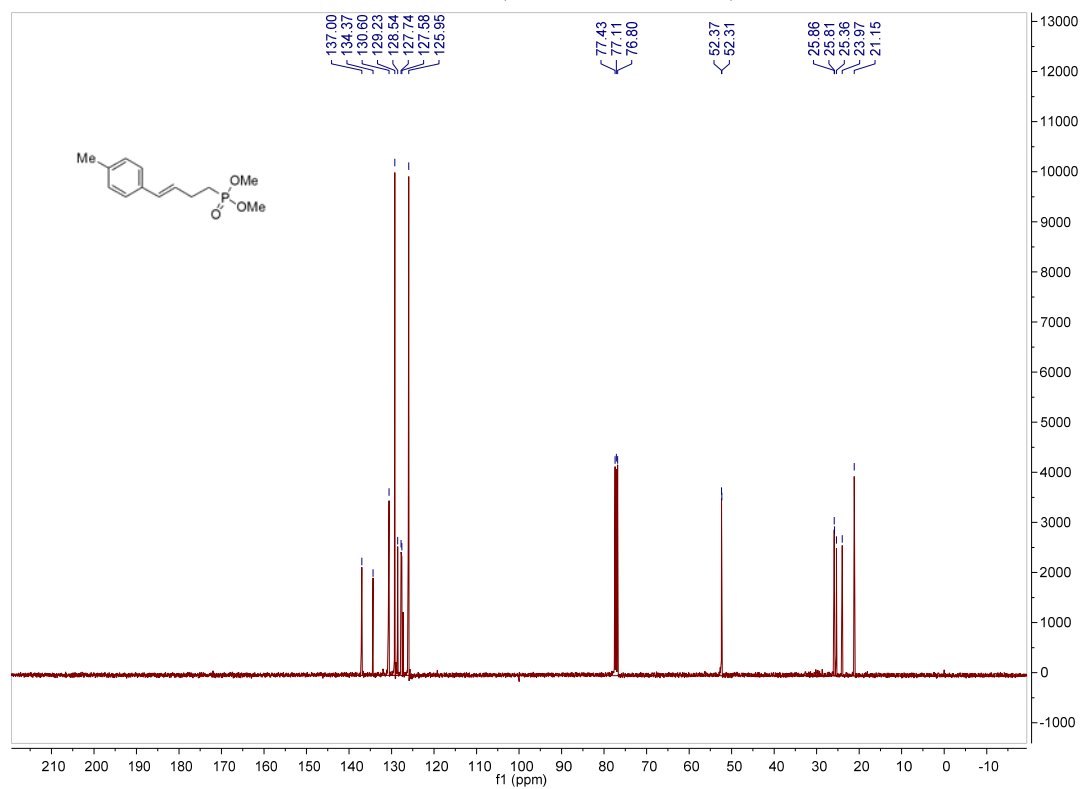
^1H NMR (400 MHz, CDCl_3) of **4f**



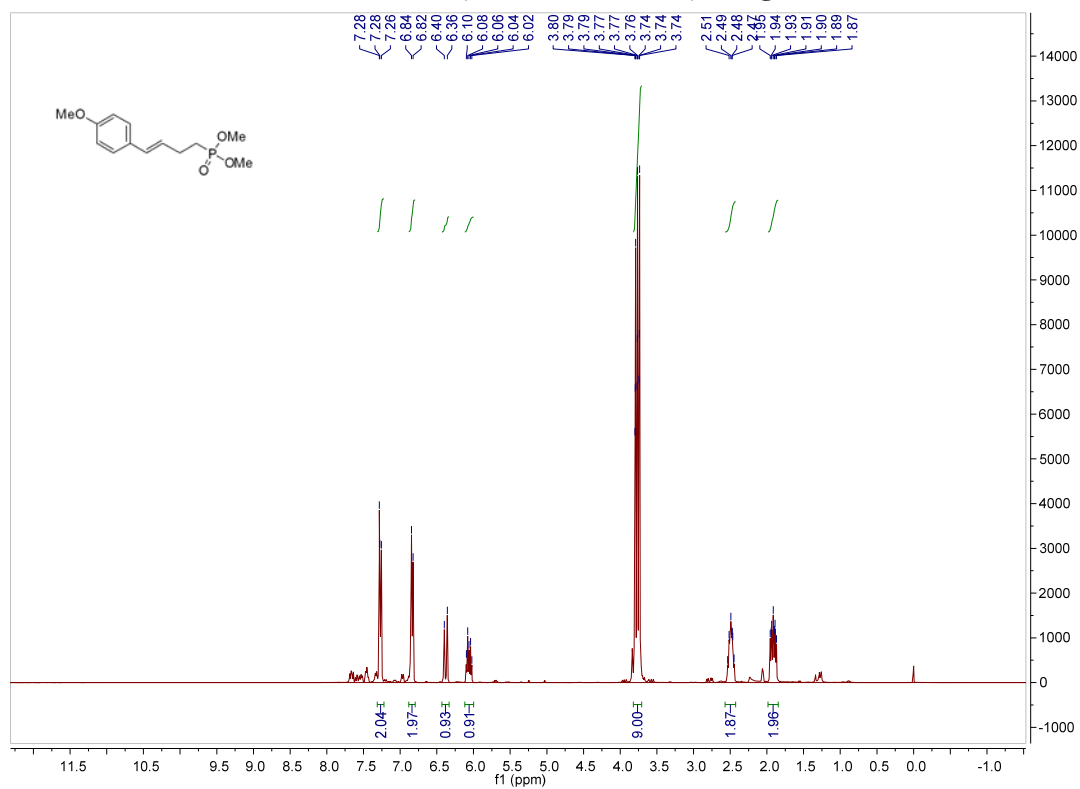
^{31}P NMR (162 MHz, CDCl_3) of **4f**



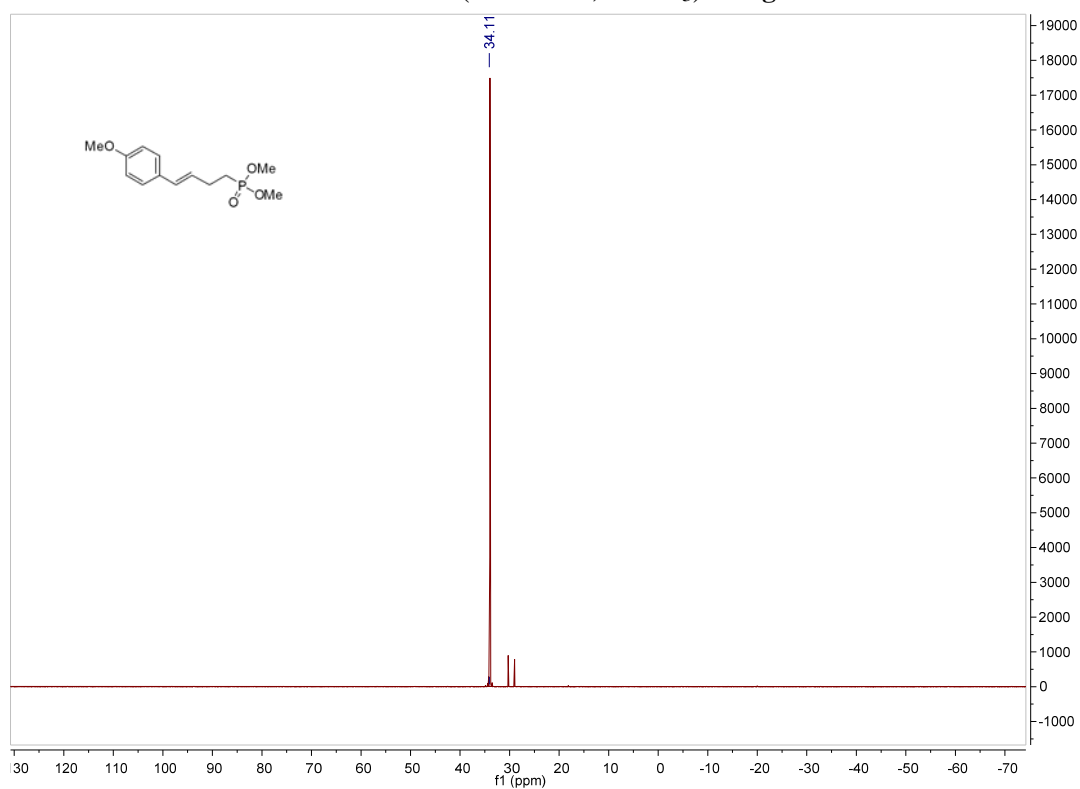
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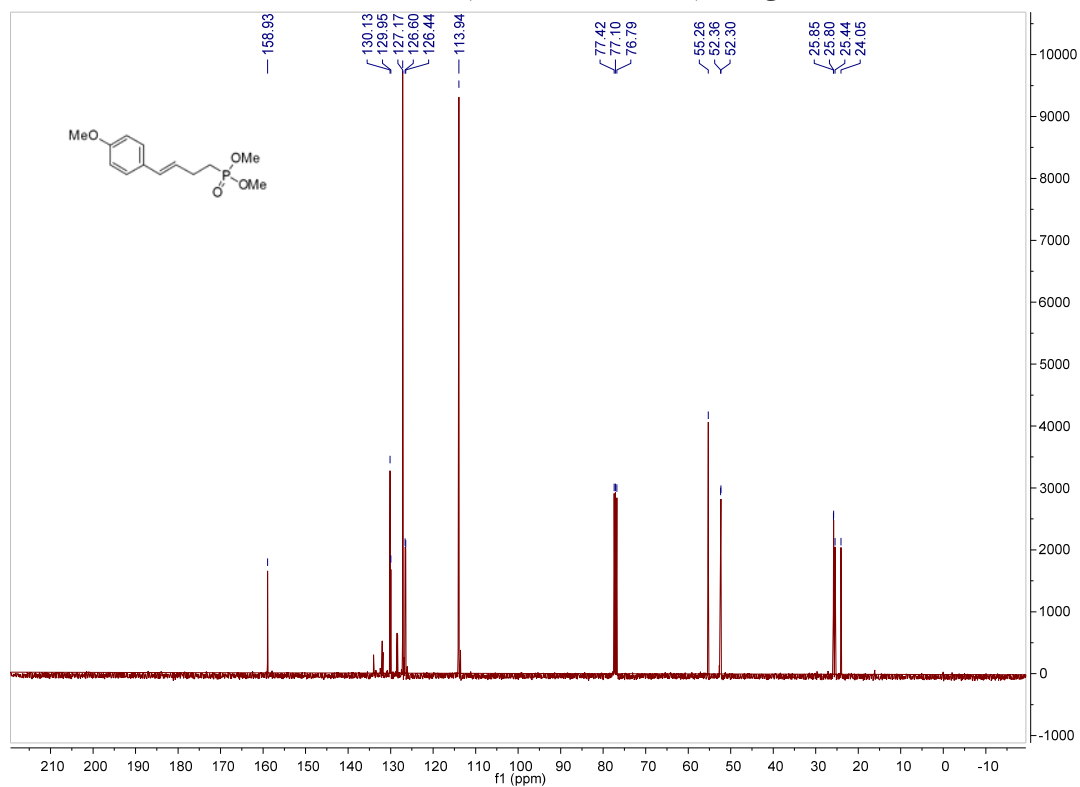
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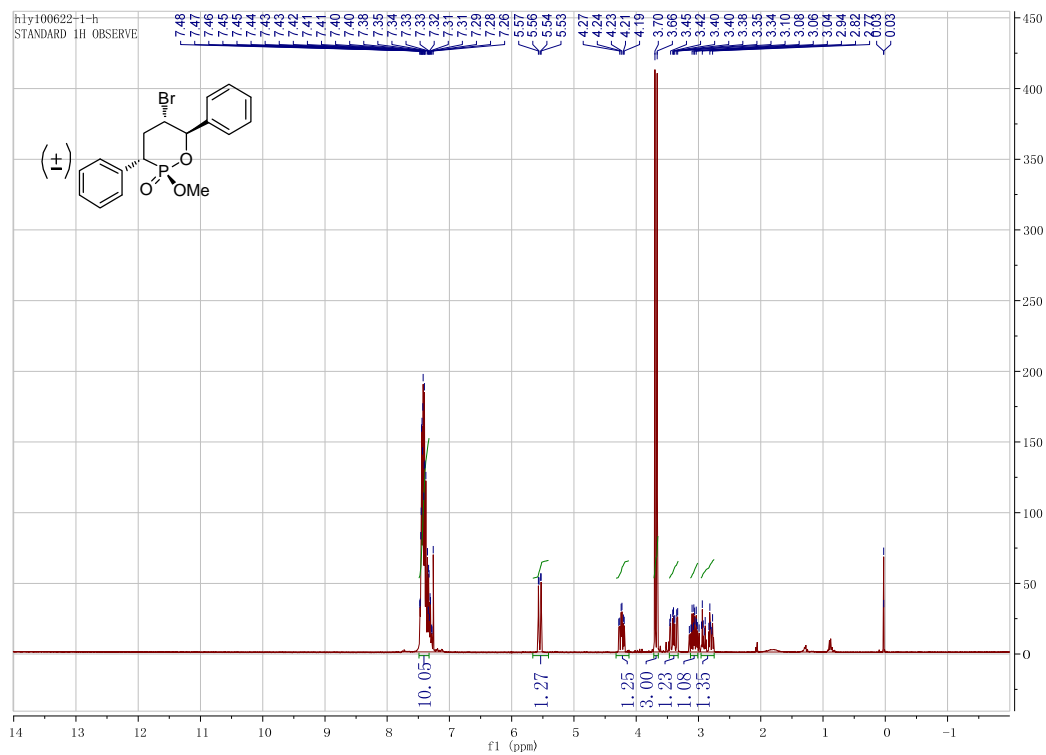
^{31}P NMR (162 MHz, CDCl_3) of **4g**



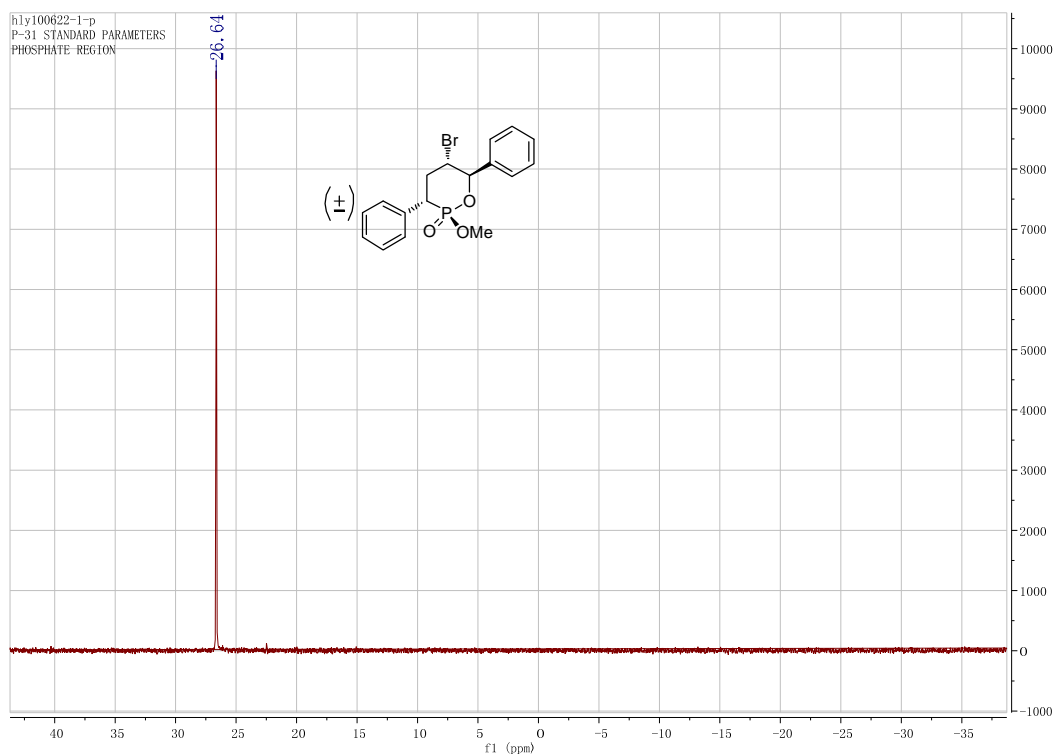
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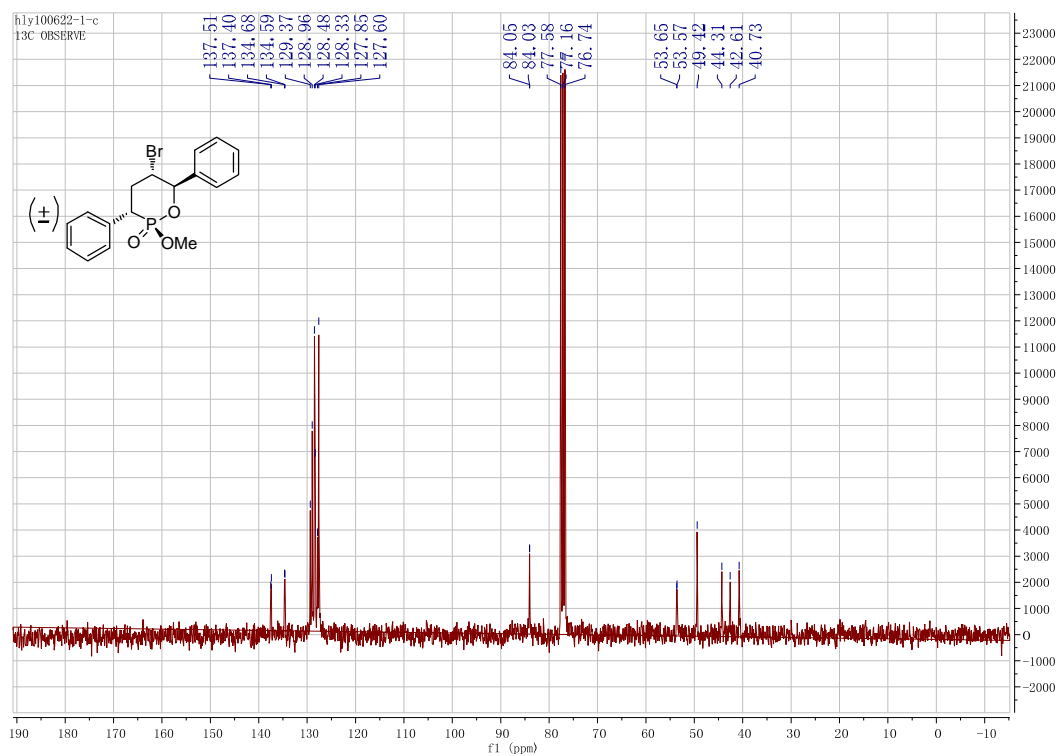
¹H NMR (300 MHz, CDCl₃) of **6aa**



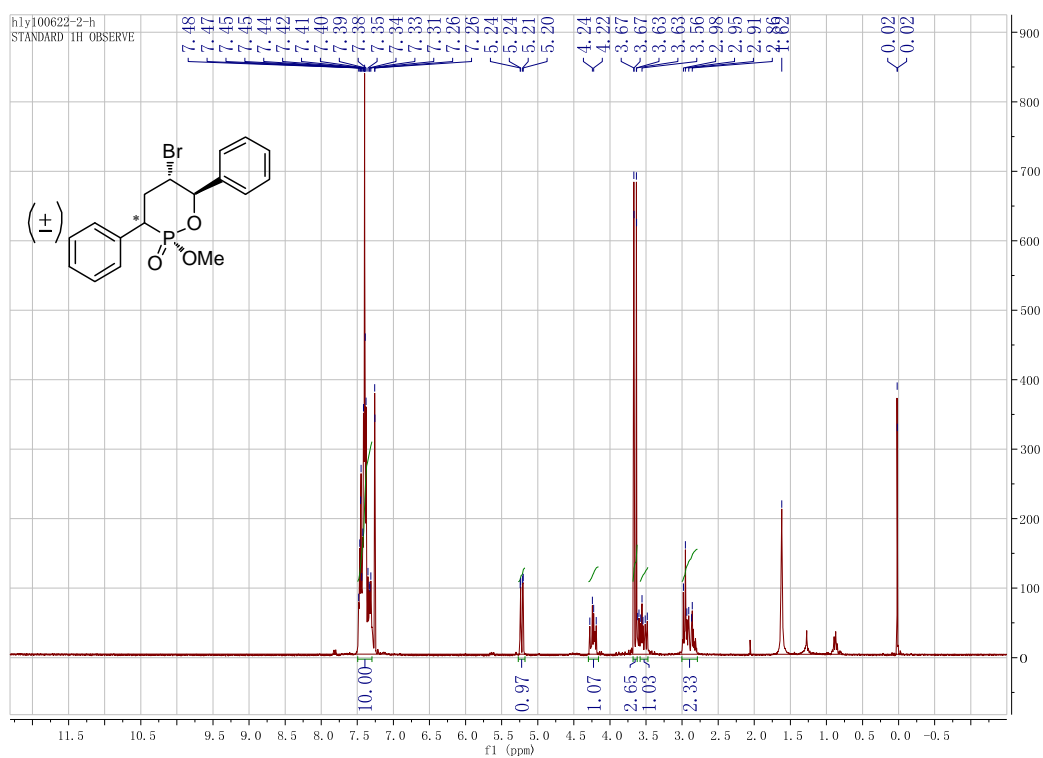
^{31}P NMR (121 MHz, CDCl_3) of **6aa**



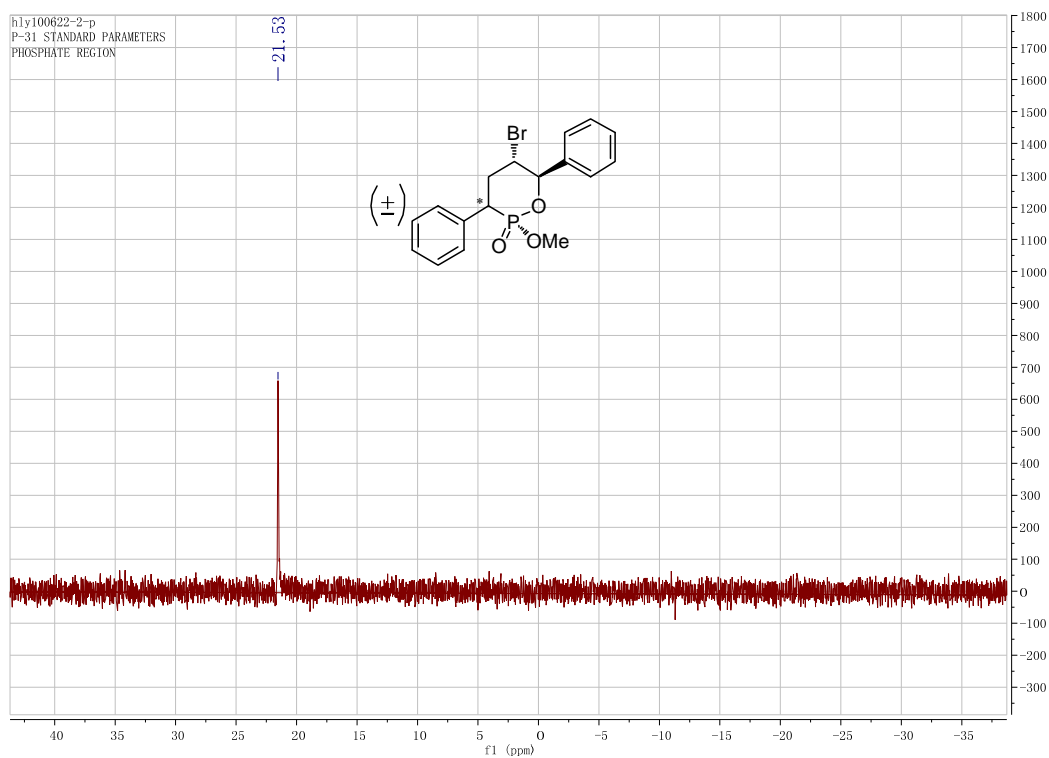
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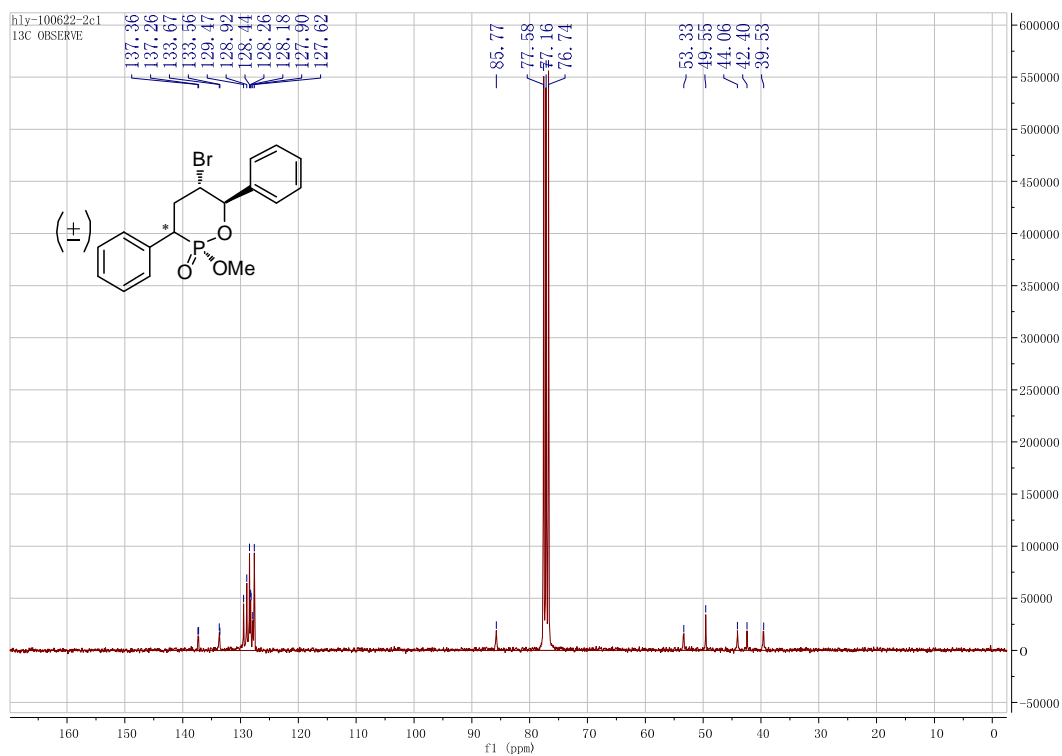
^1H NMR (300 MHz, CDCl_3) of **6ab**



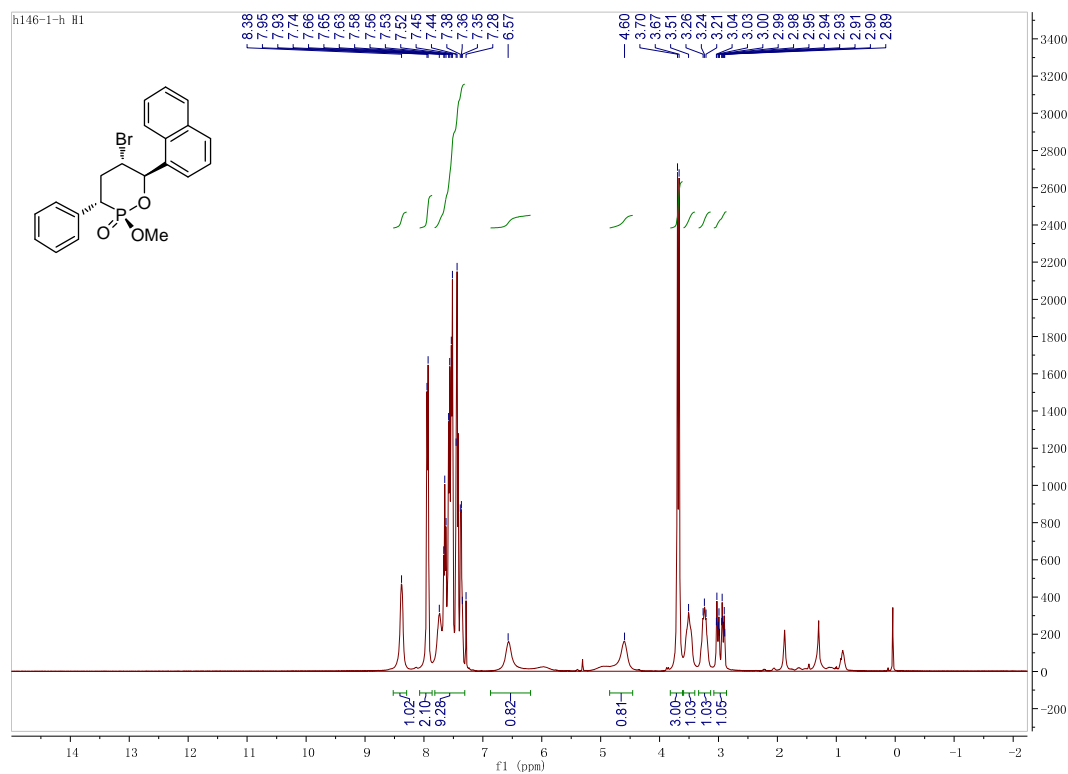
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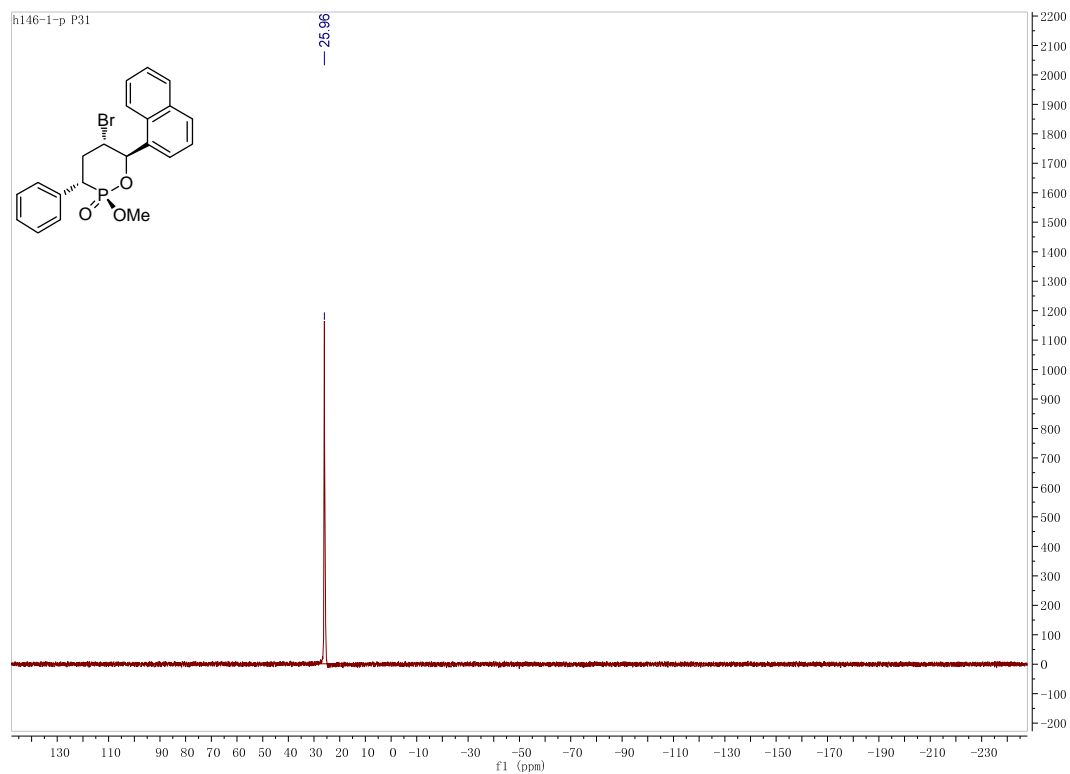
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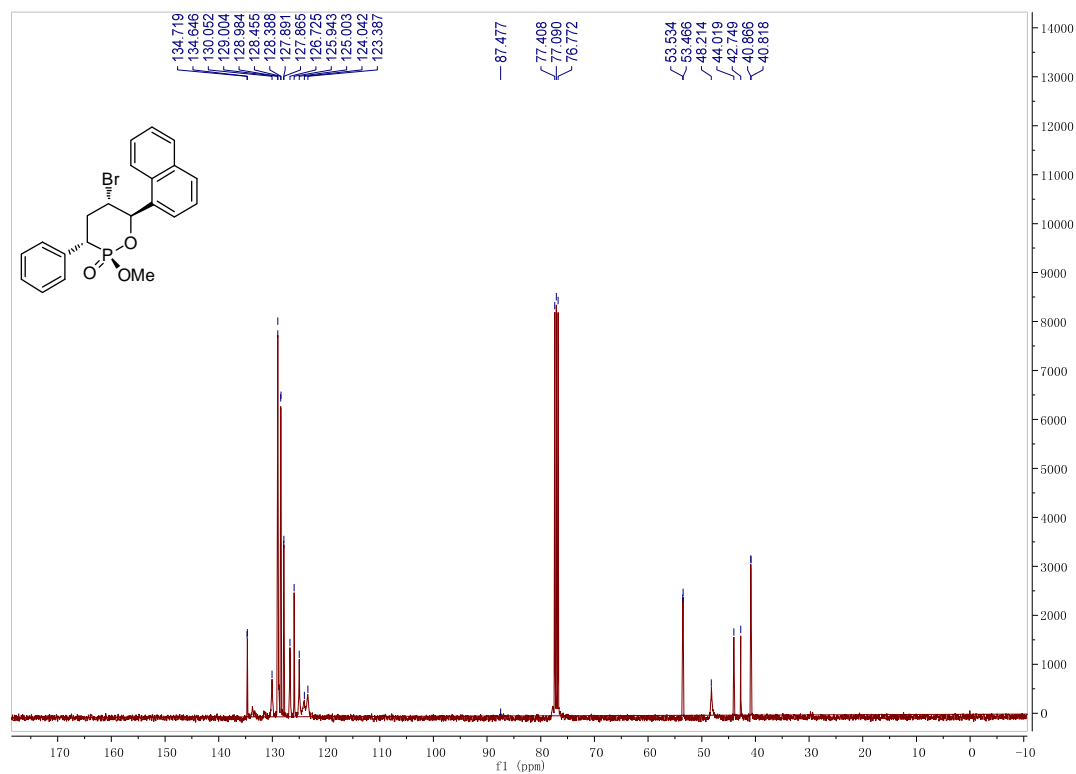
^1H NMR (400 MHz, CDCl_3) of **6ba**



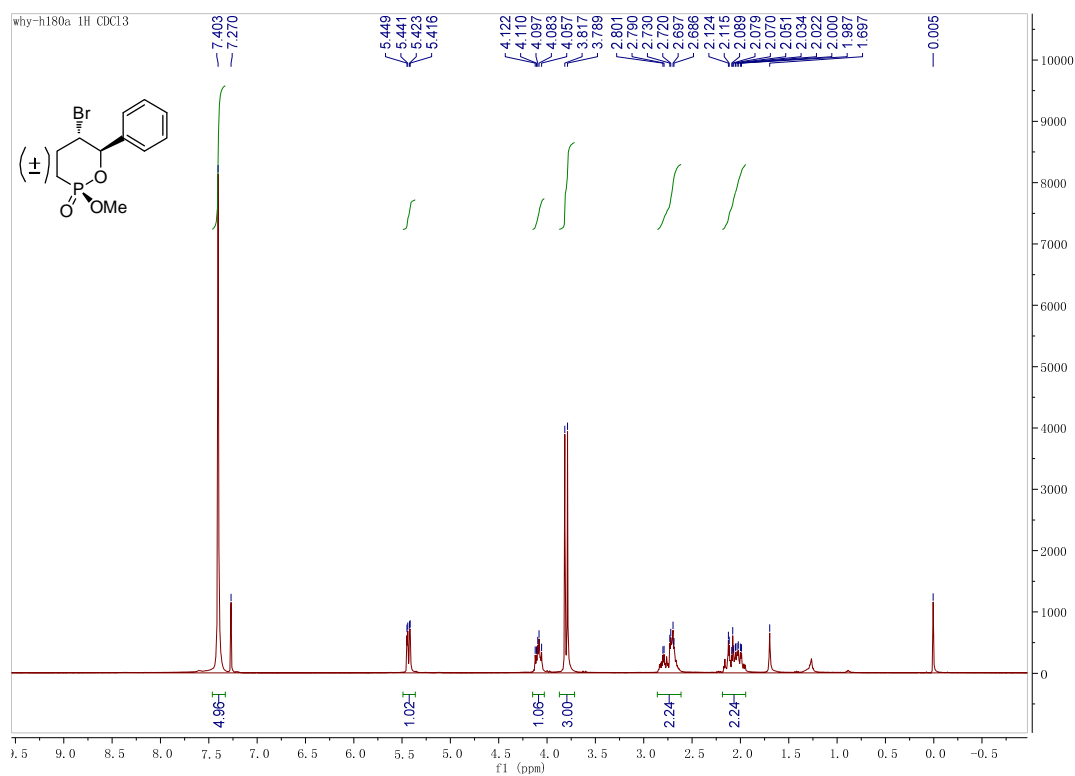
^{31}P NMR (162 MHz, CDCl_3) of **6ba**



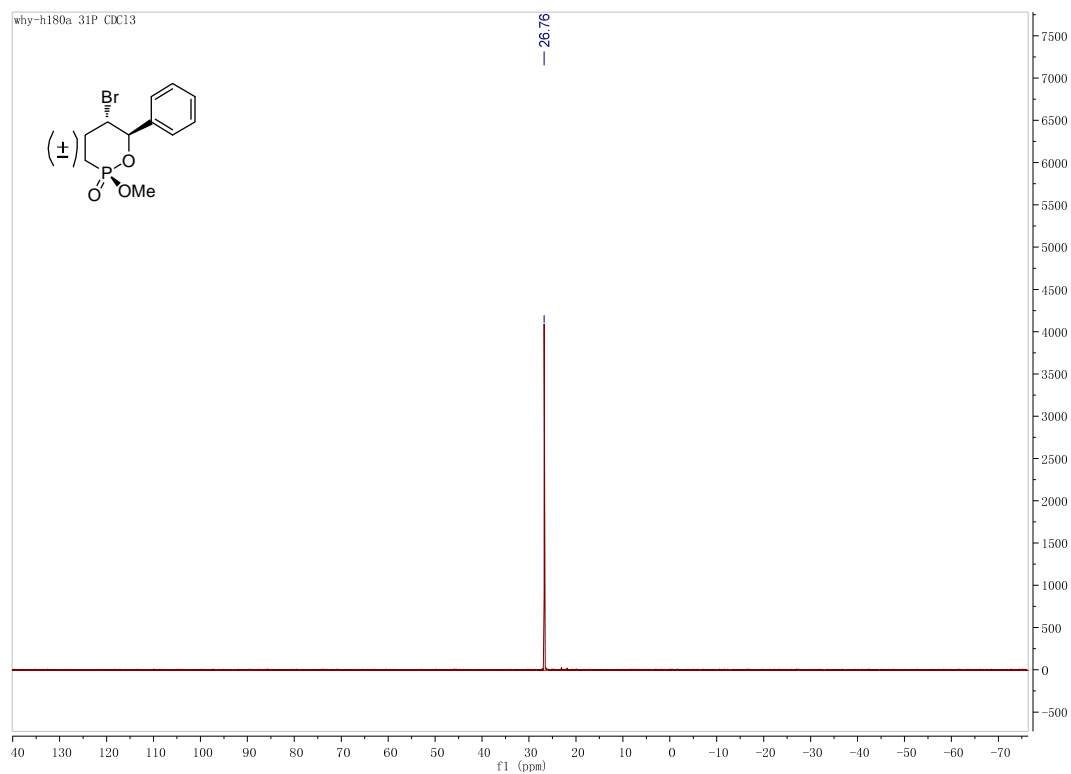
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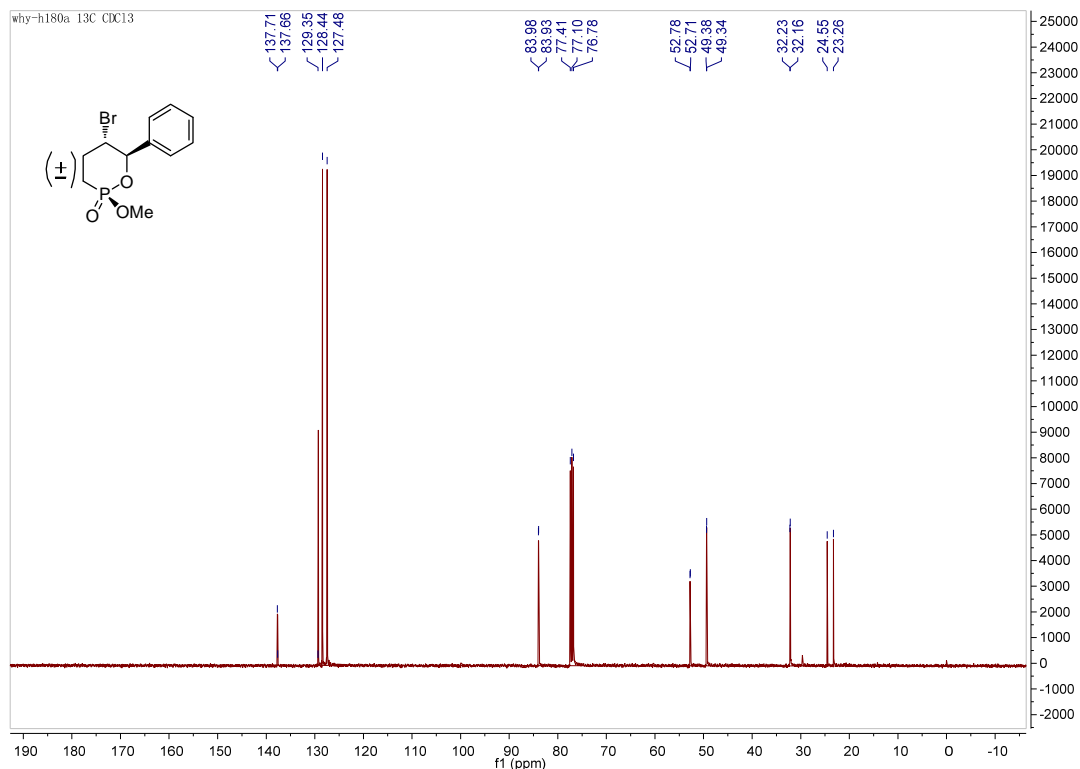
¹H NMR (400 MHz, CDCl₃) of **6ca**



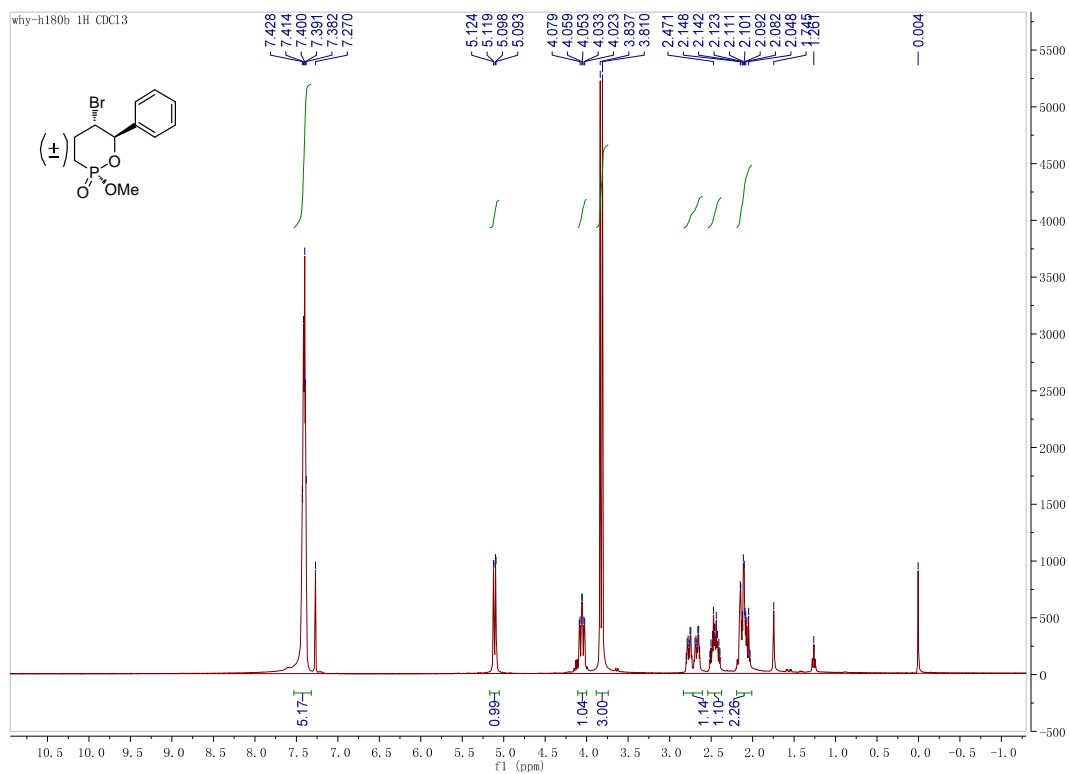
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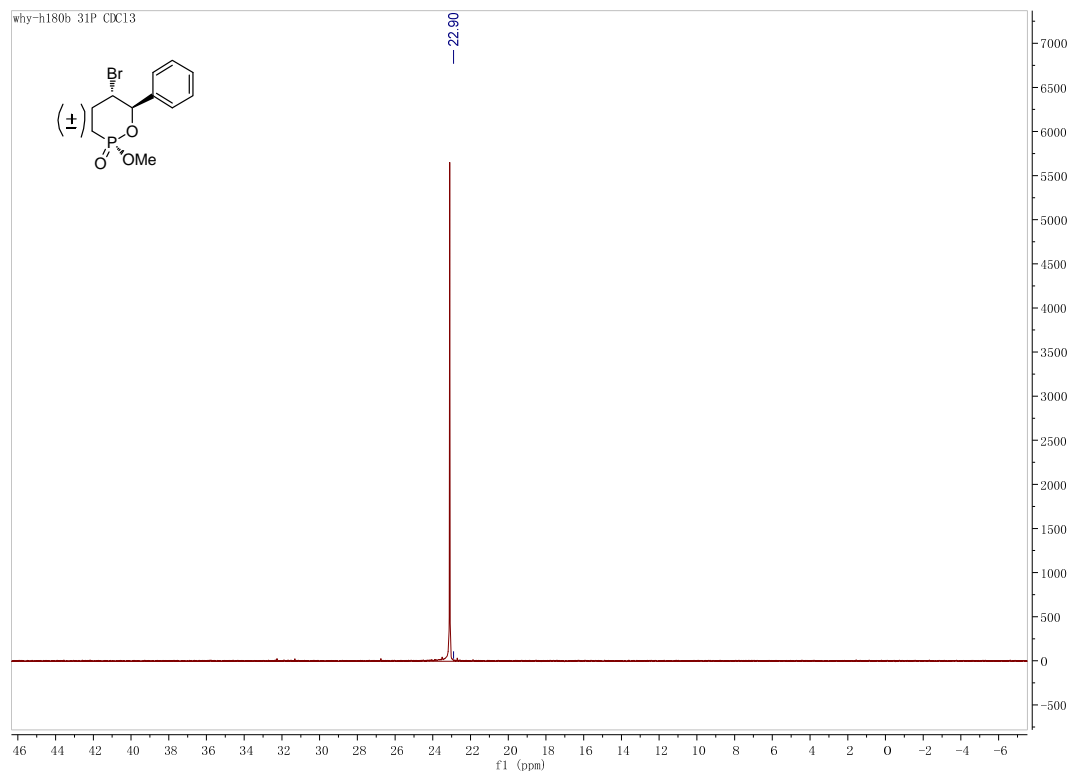
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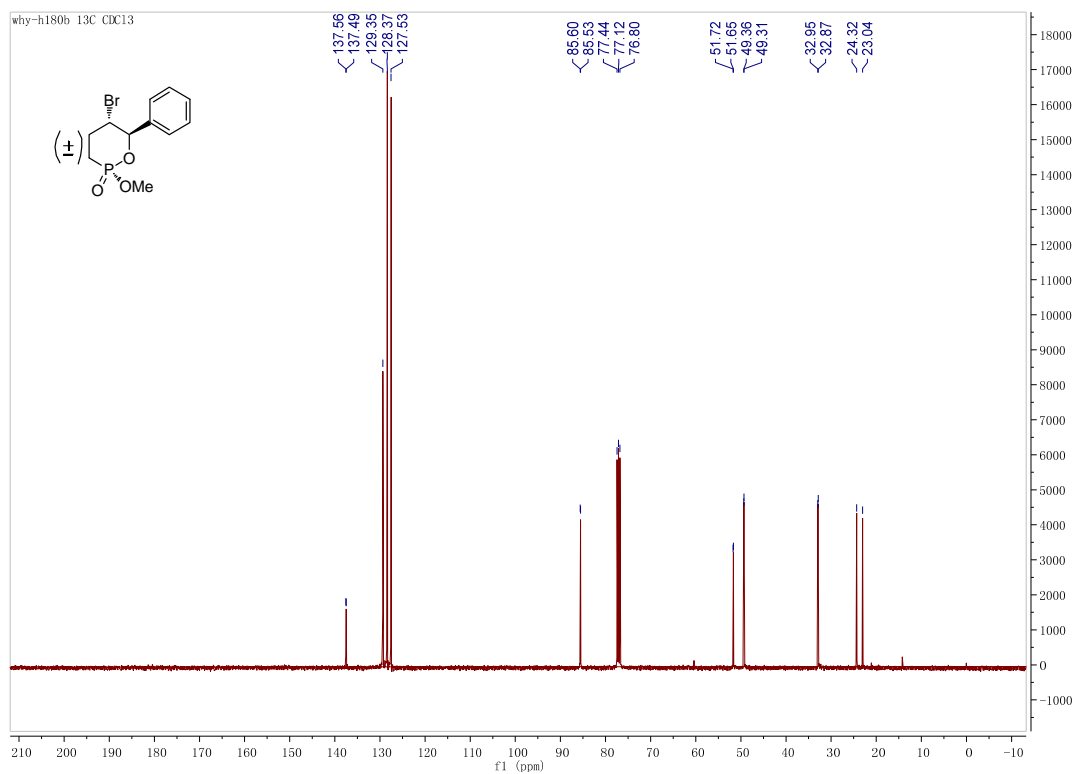
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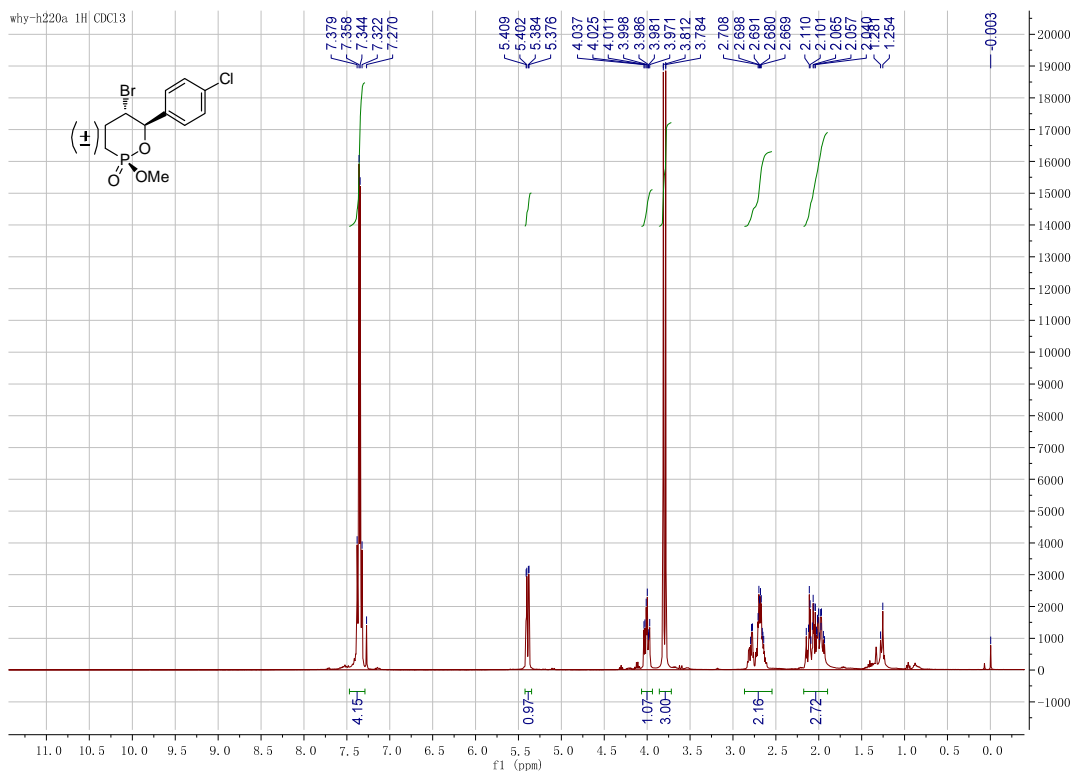
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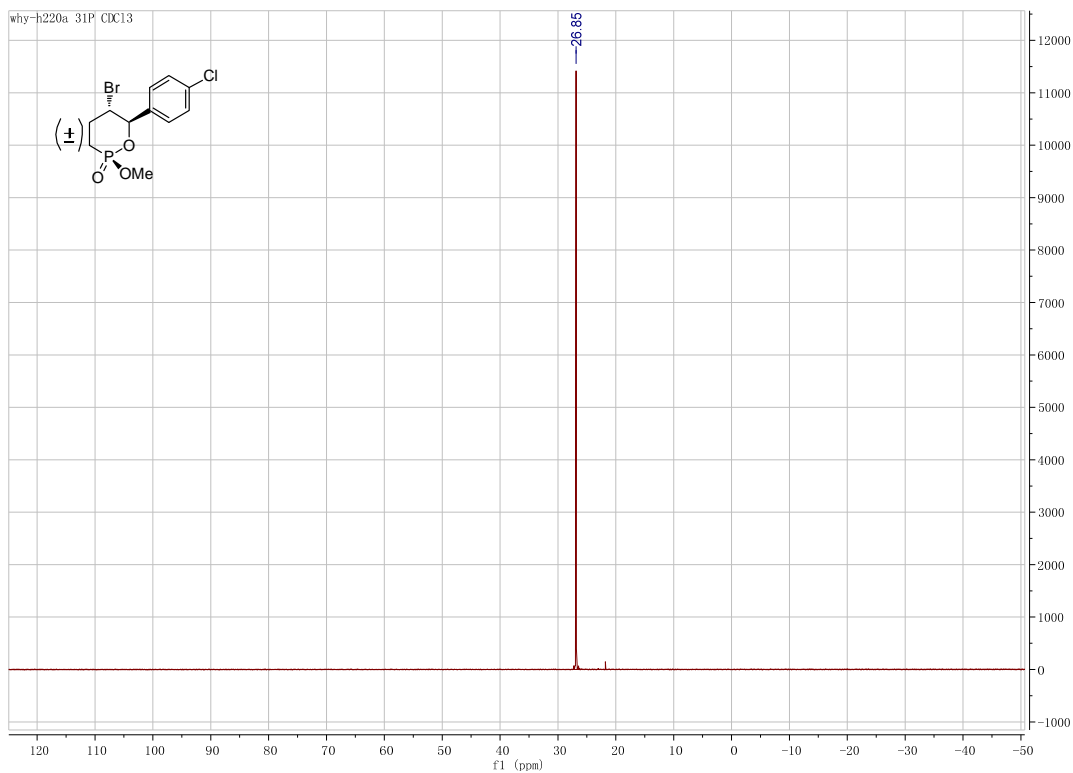
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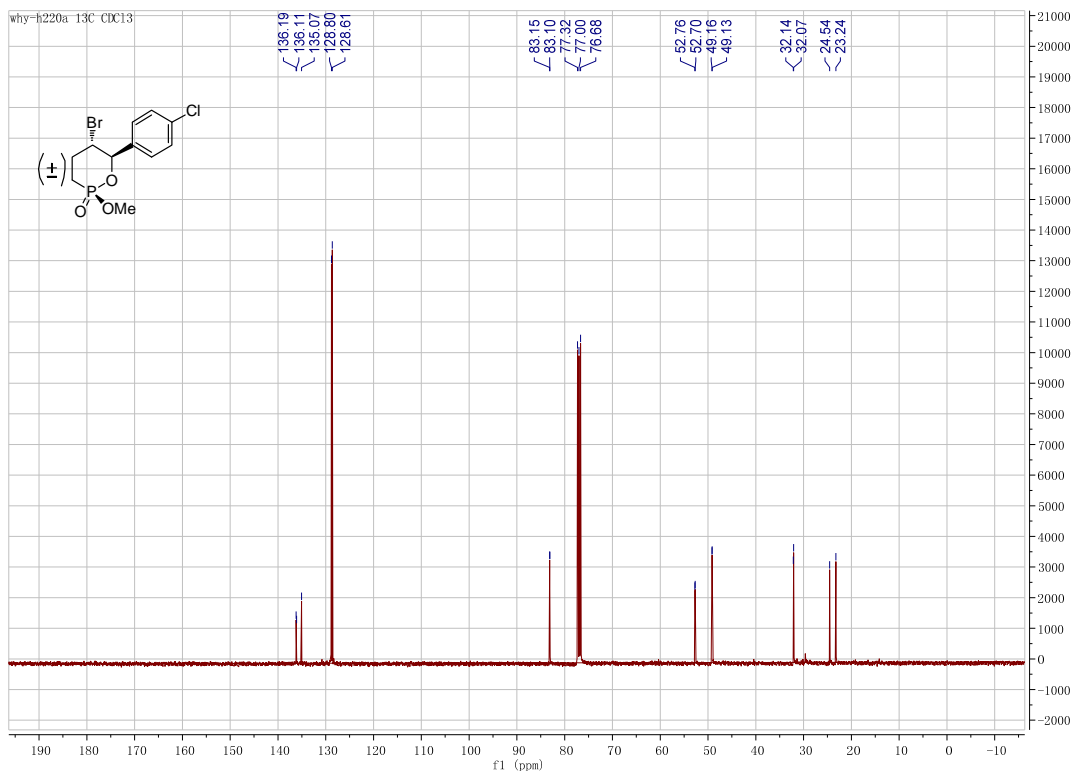
^1H NMR (400 MHz, CDCl_3) of **6da**



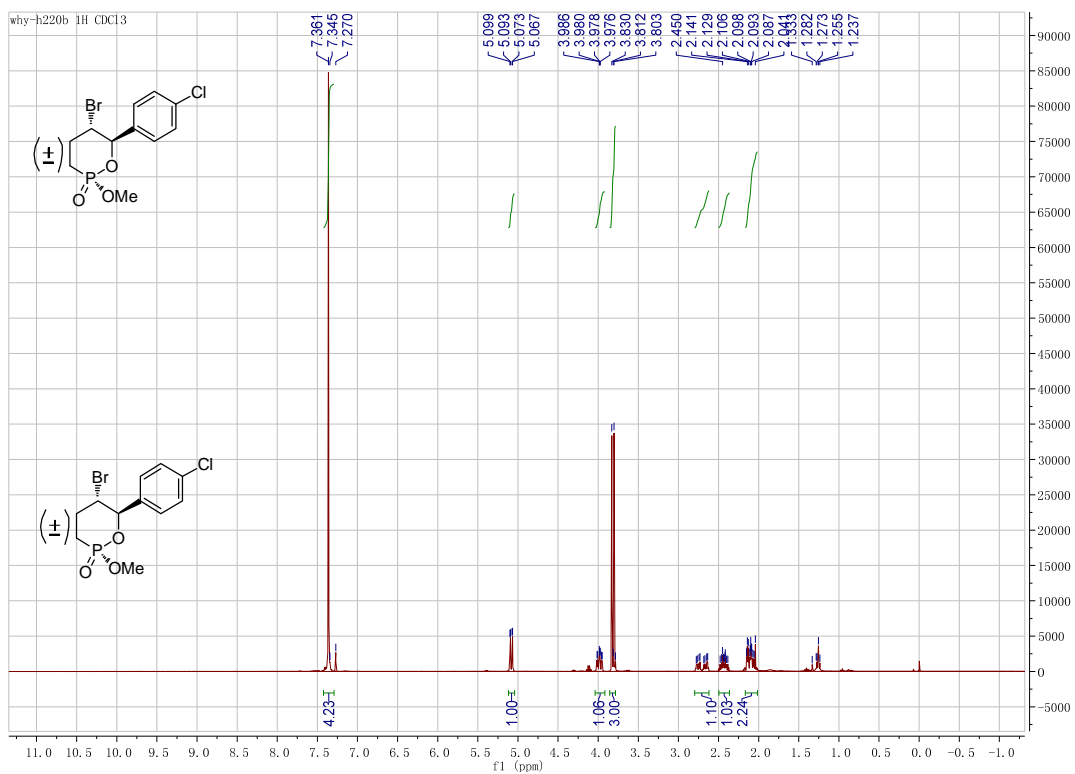
^{31}P NMR (162 MHz, CDCl_3) of **6da**



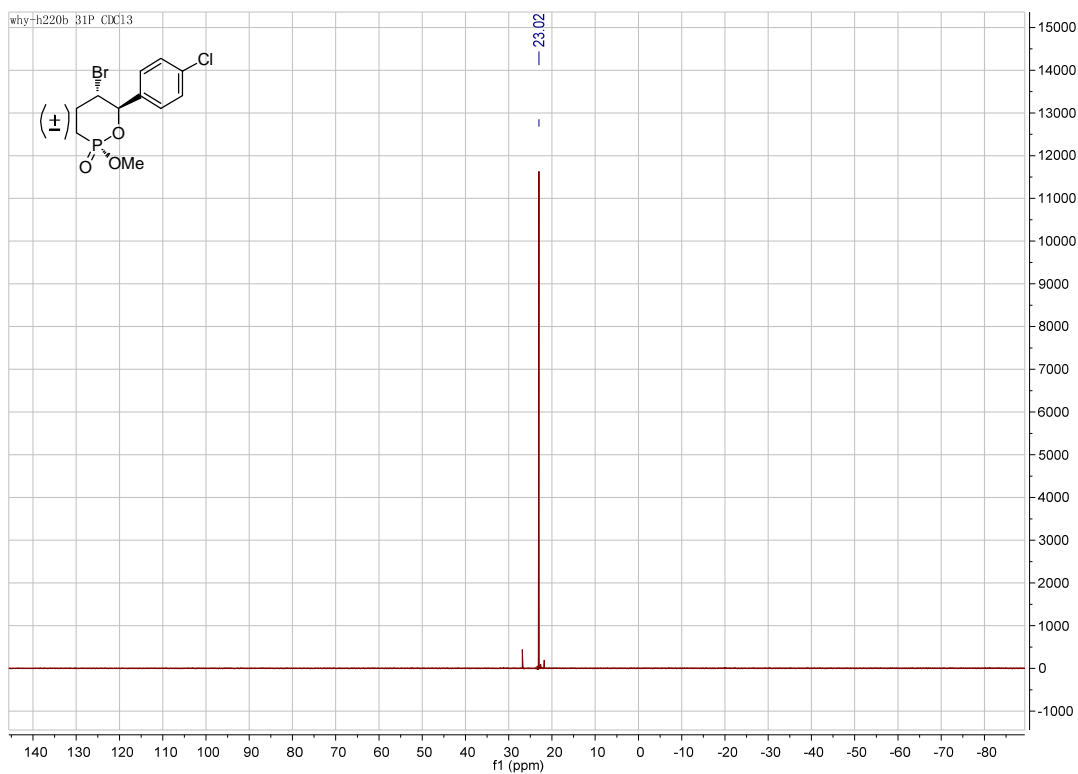
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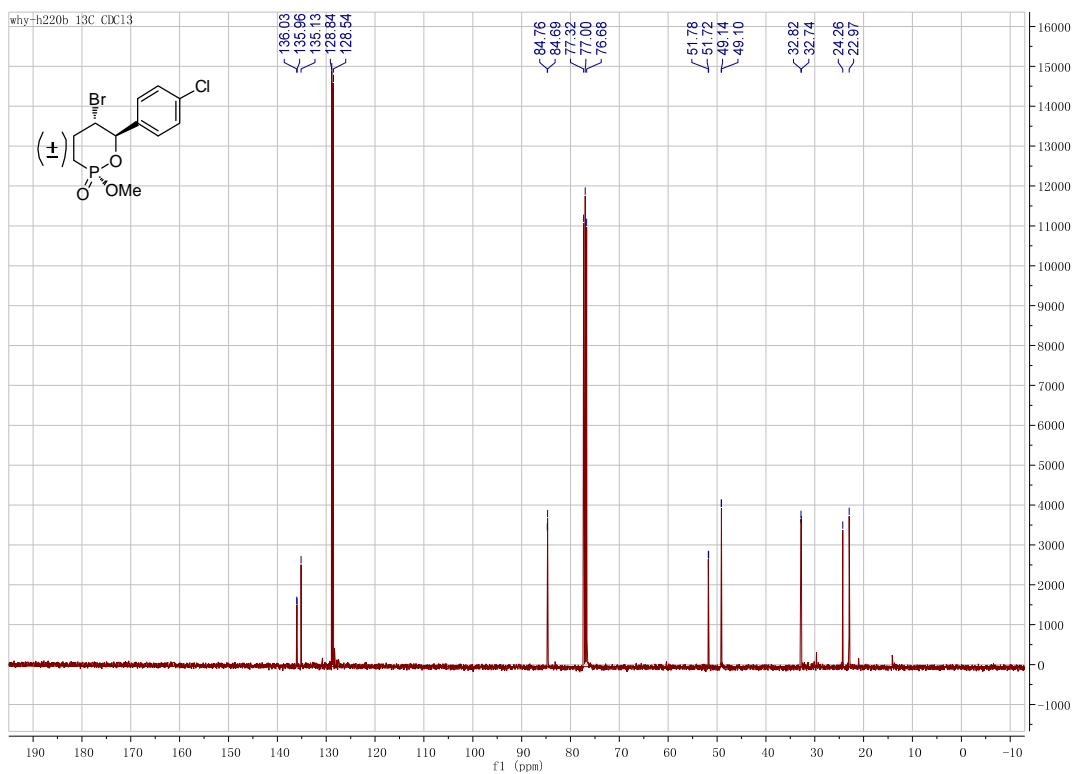
¹H NMR (400 MHz, CDCl₃) of **6db**



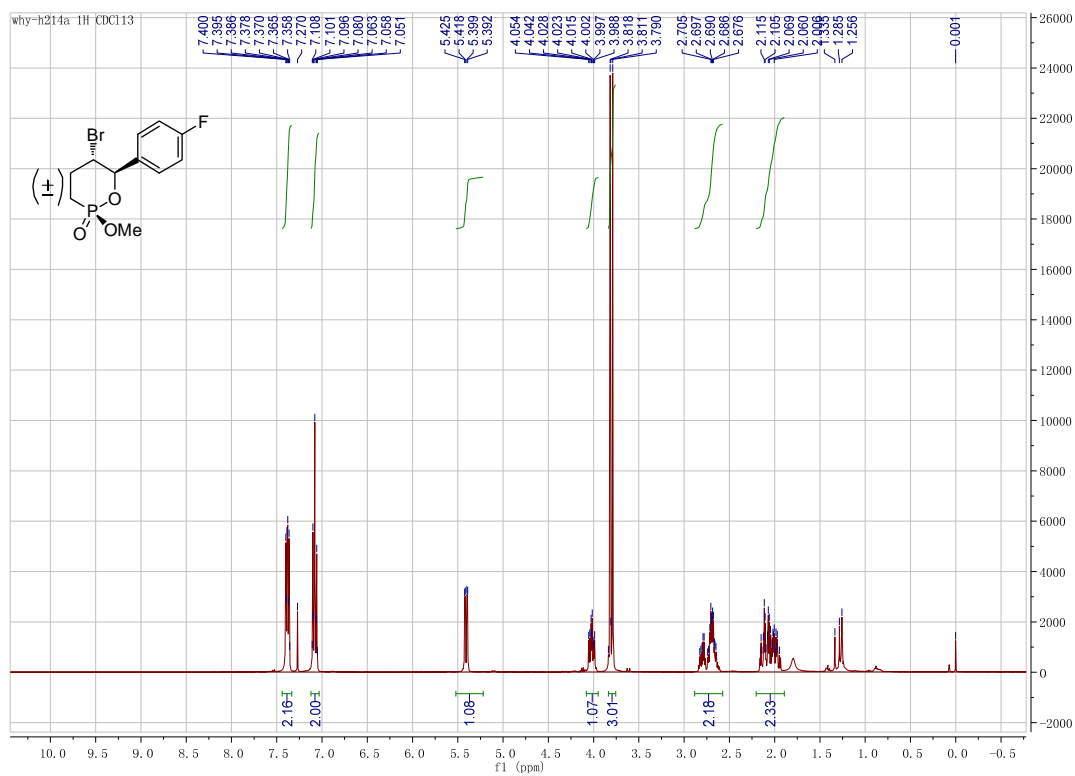
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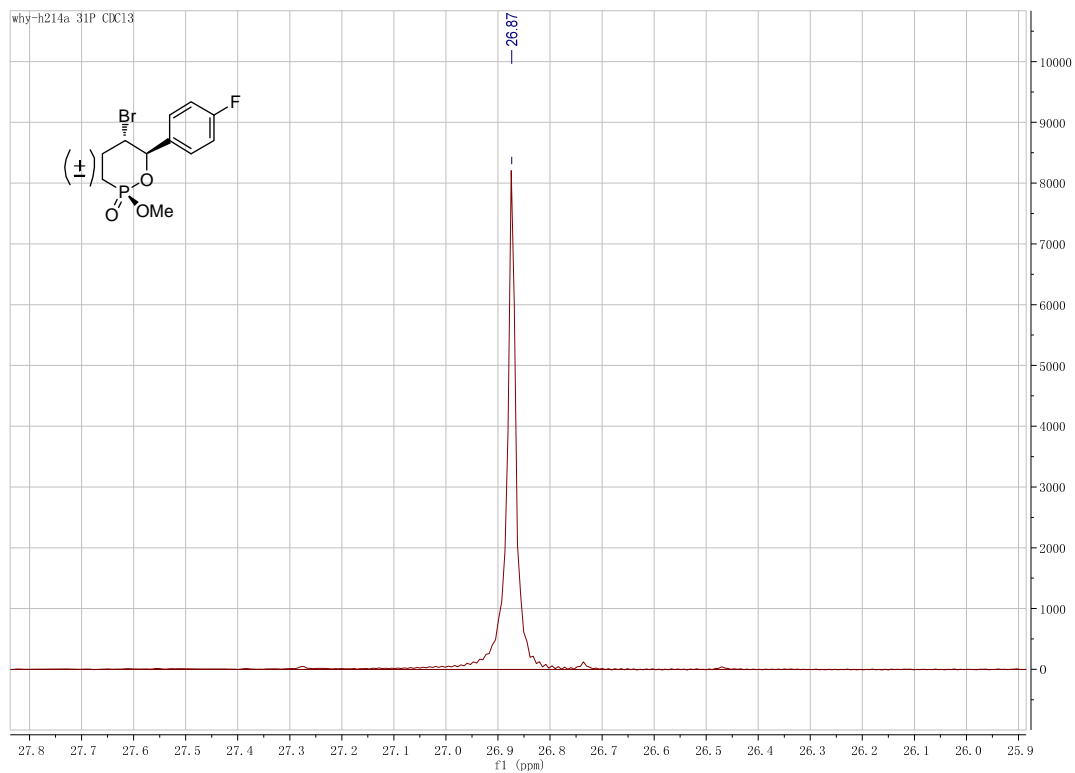
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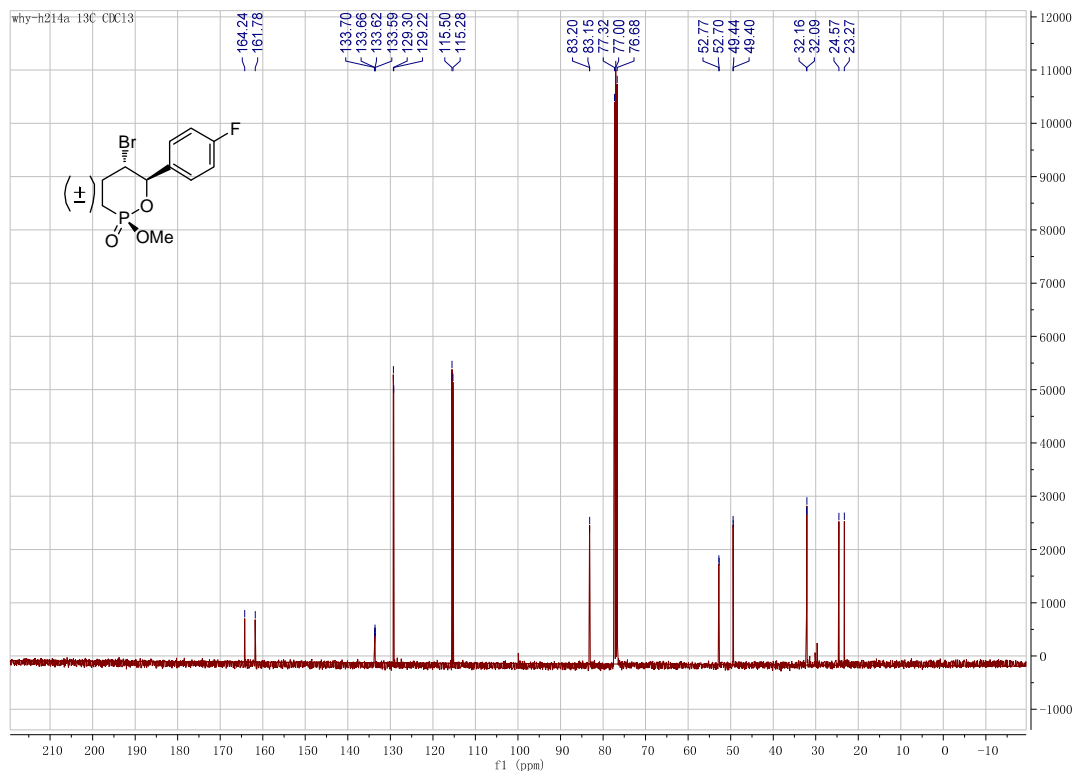
^1H NMR (400 MHz, CDCl_3) of **6ea**



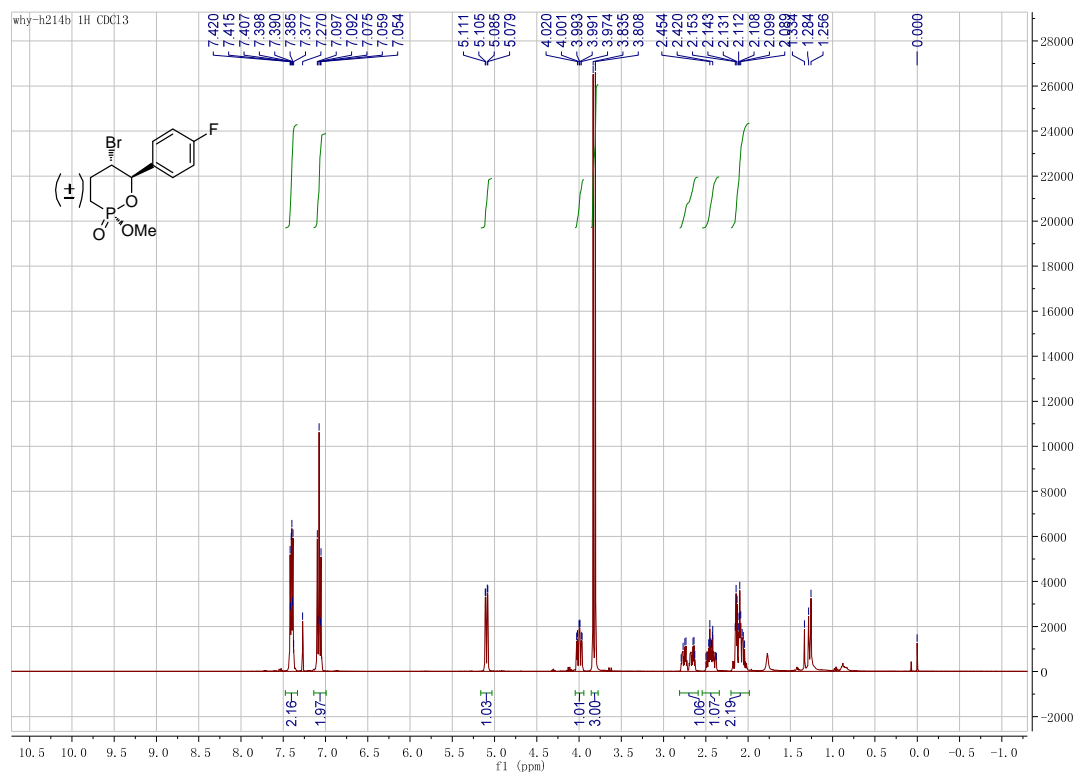
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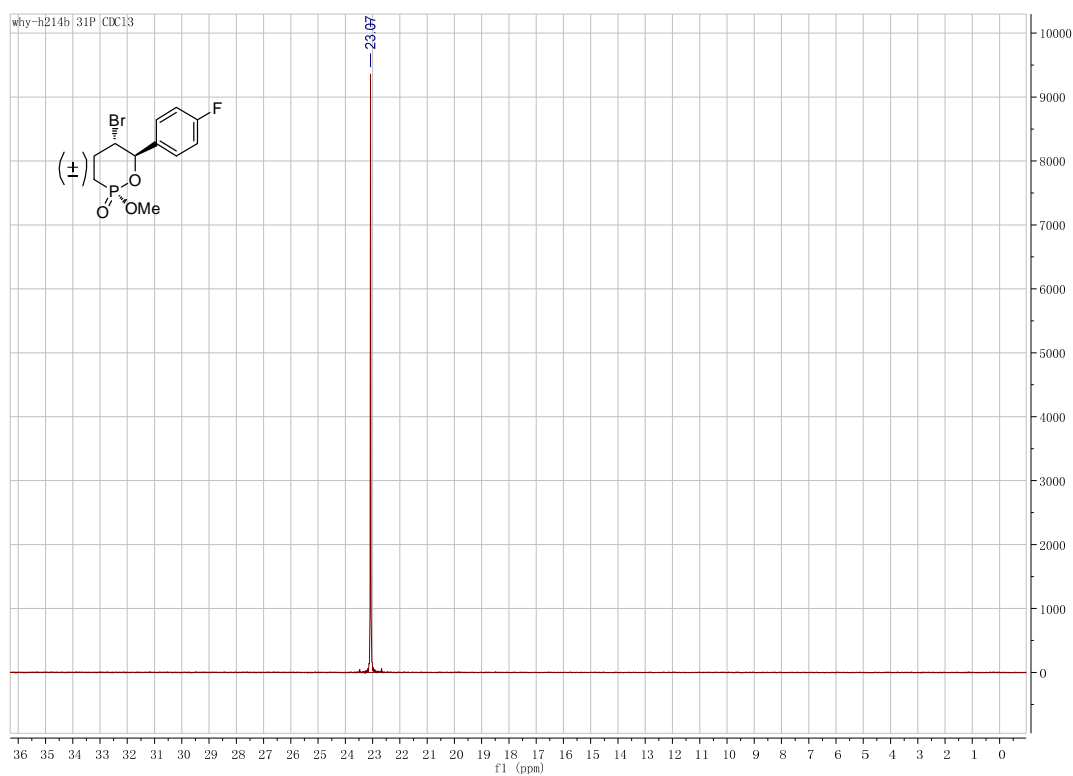
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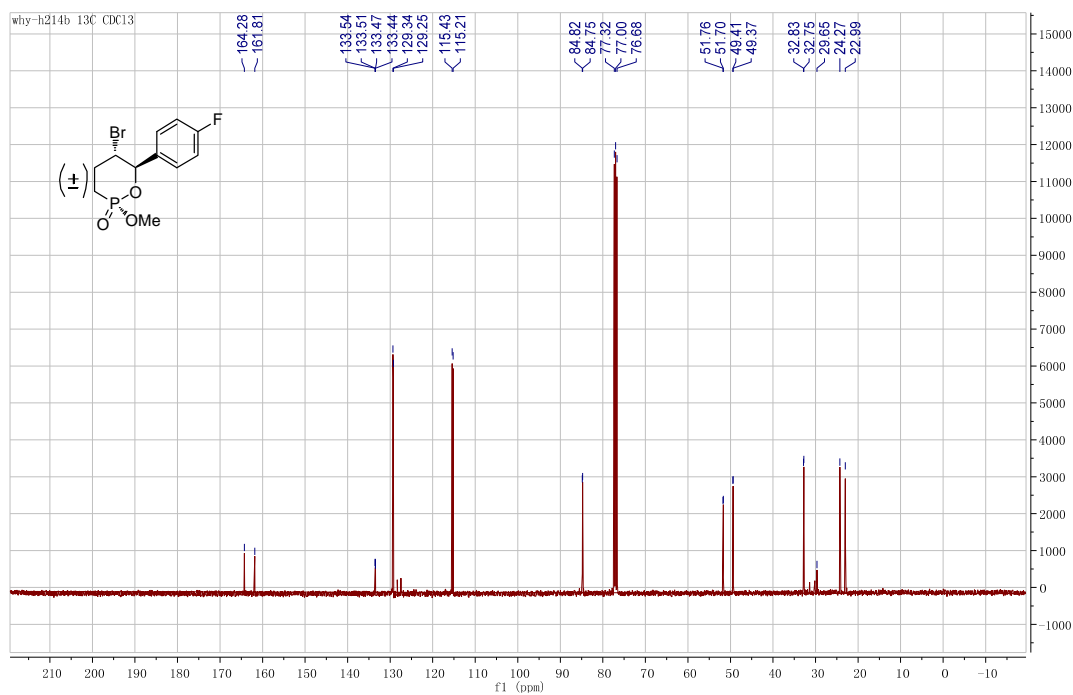
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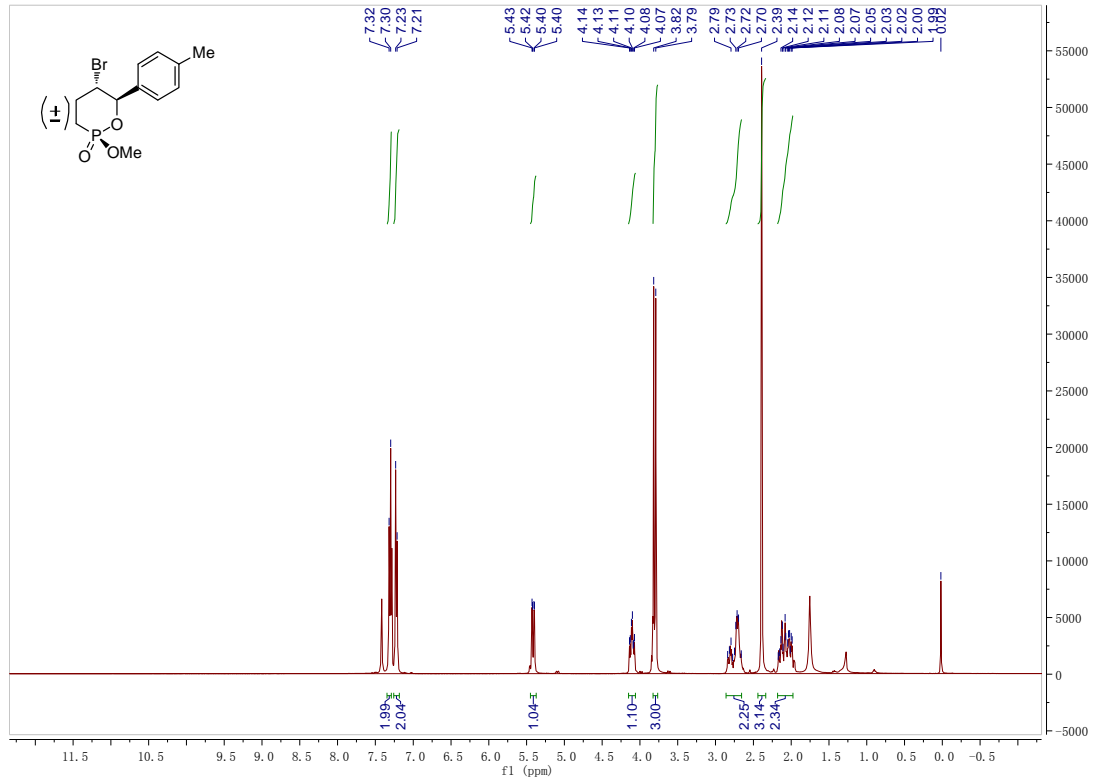
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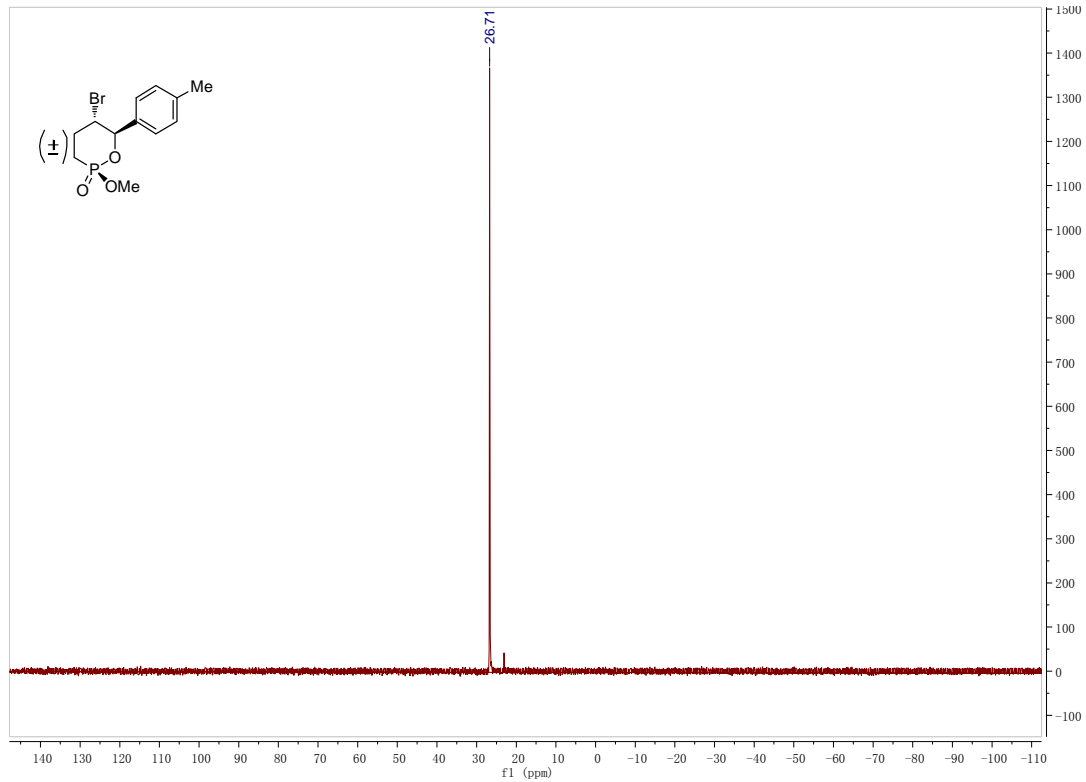
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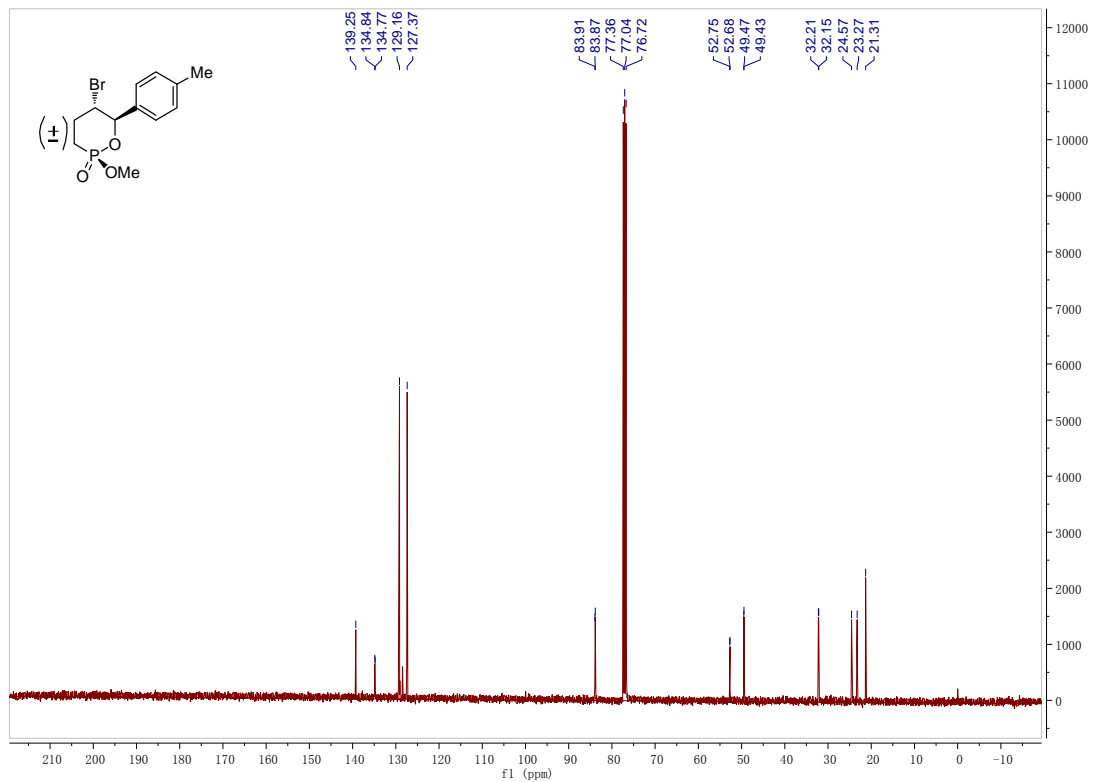
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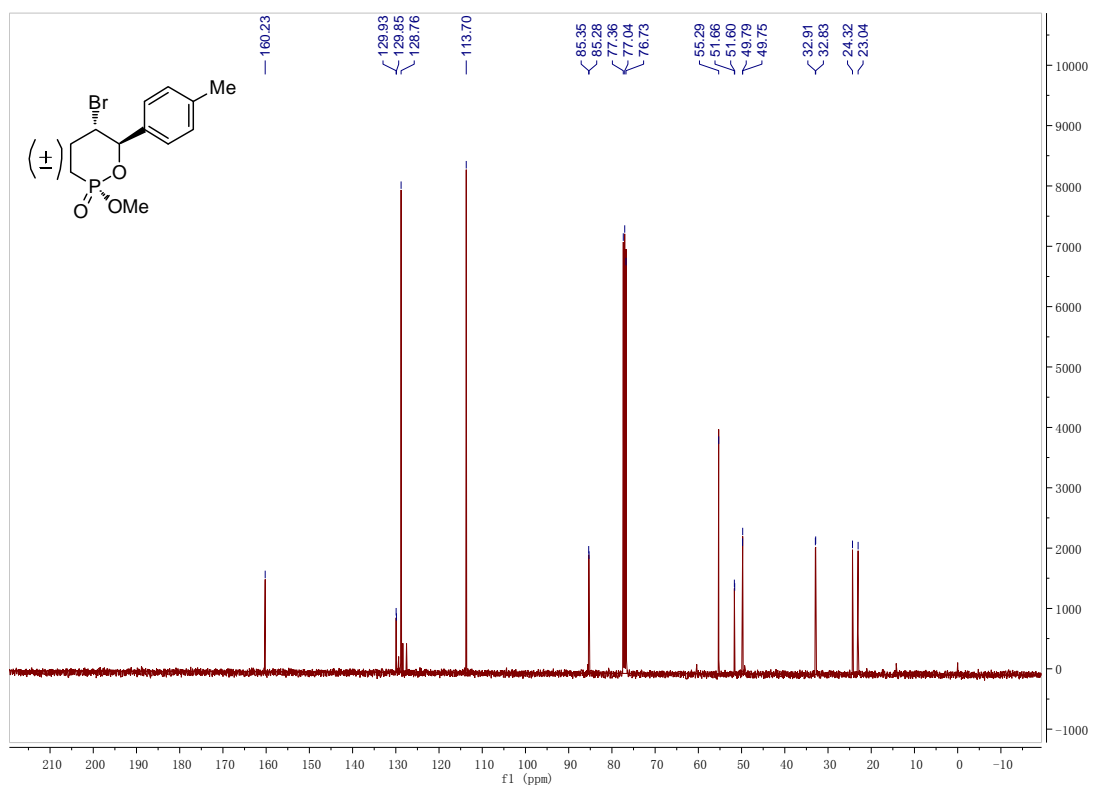
^{31}P NMR (162 MHz, CDCl_3) of **6fa**



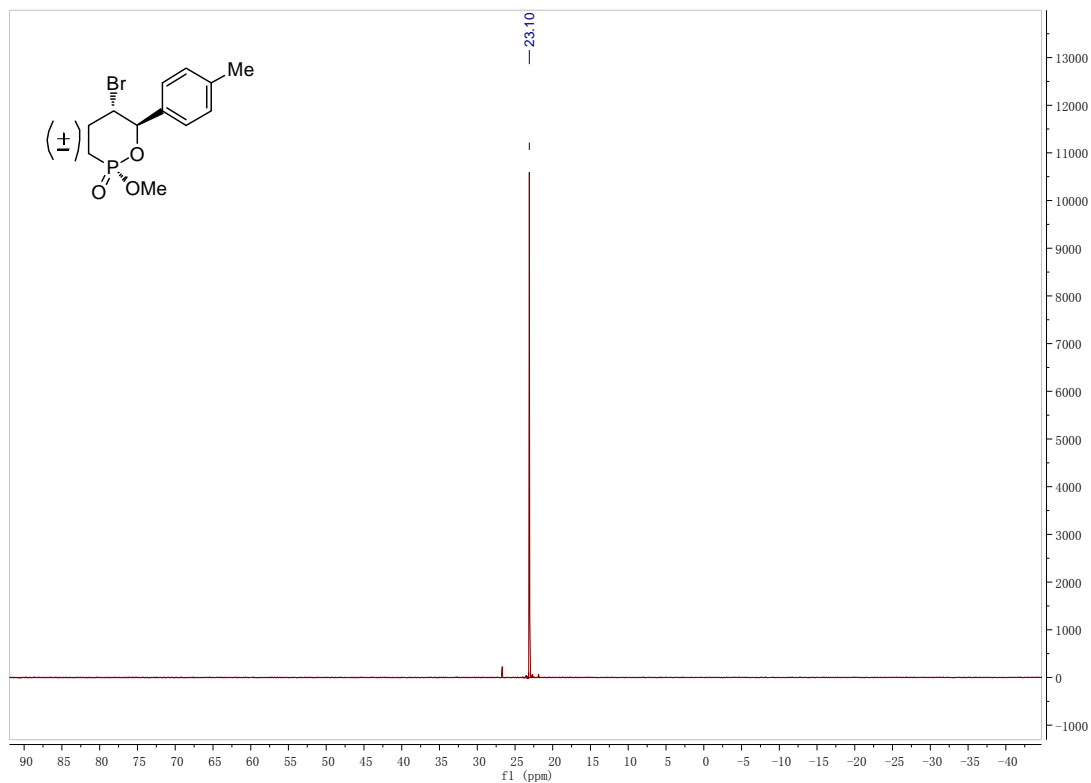
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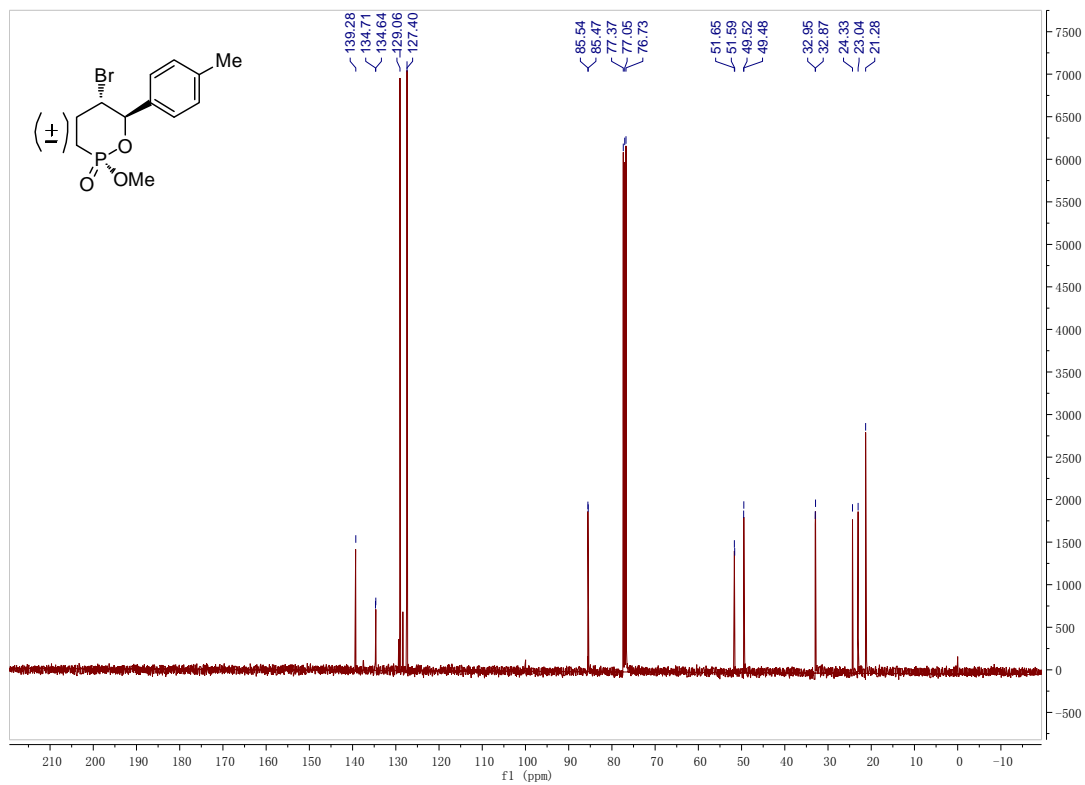
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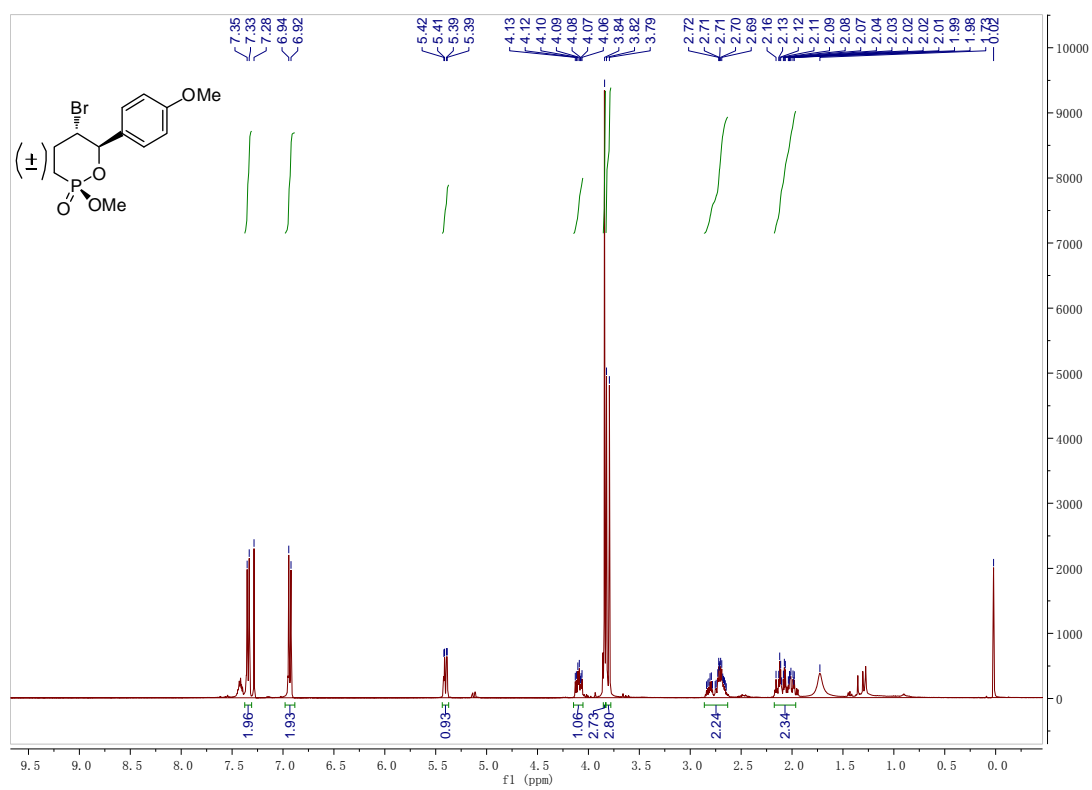
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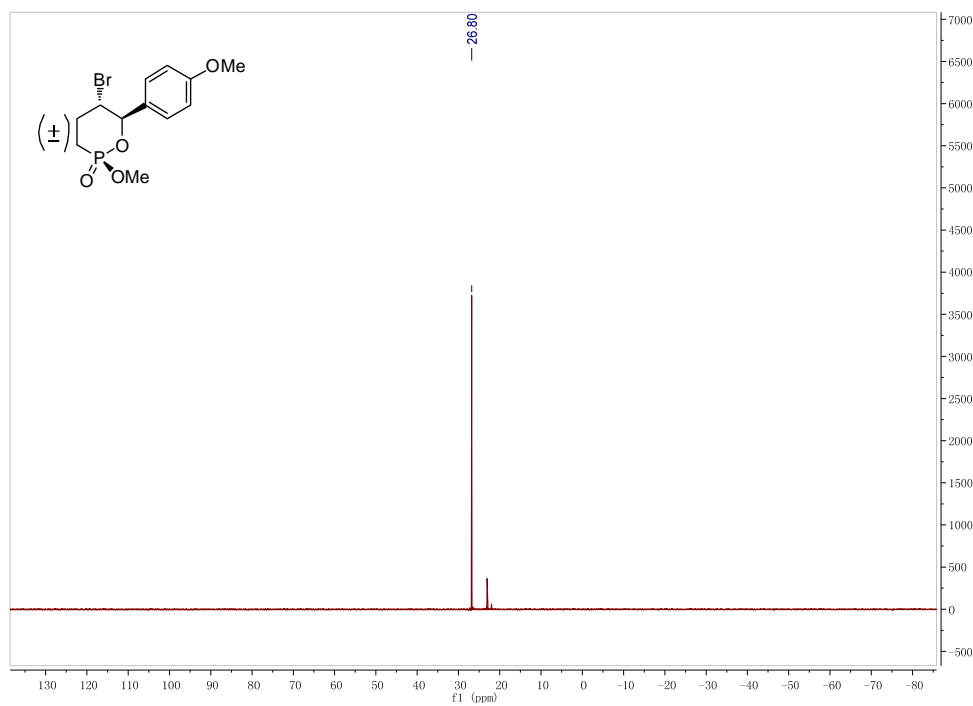
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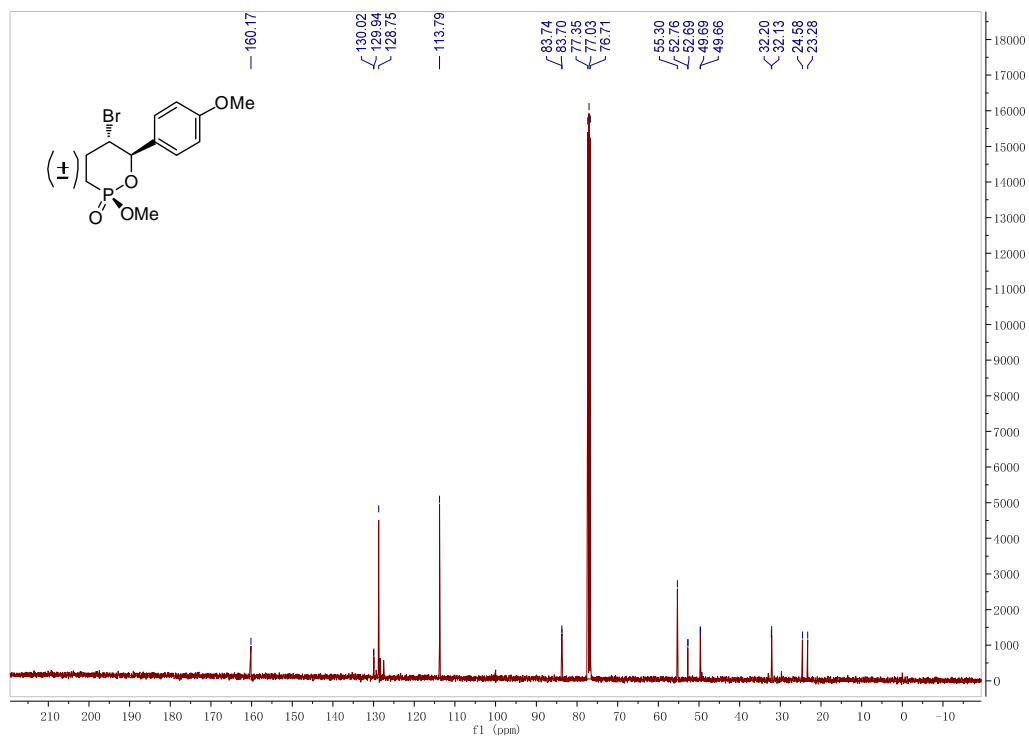
^1H NMR (400 MHz, CDCl_3) of **6ga**



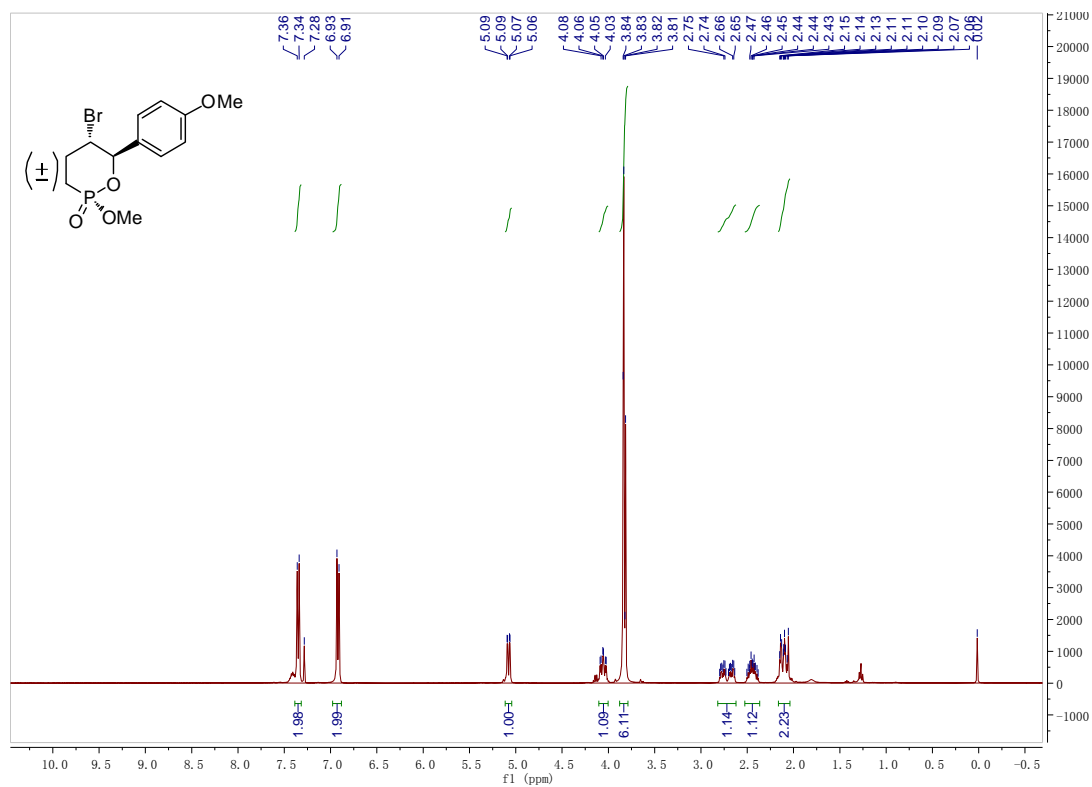
^{31}P NMR (162 MHz, CDCl_3) of **6ga**



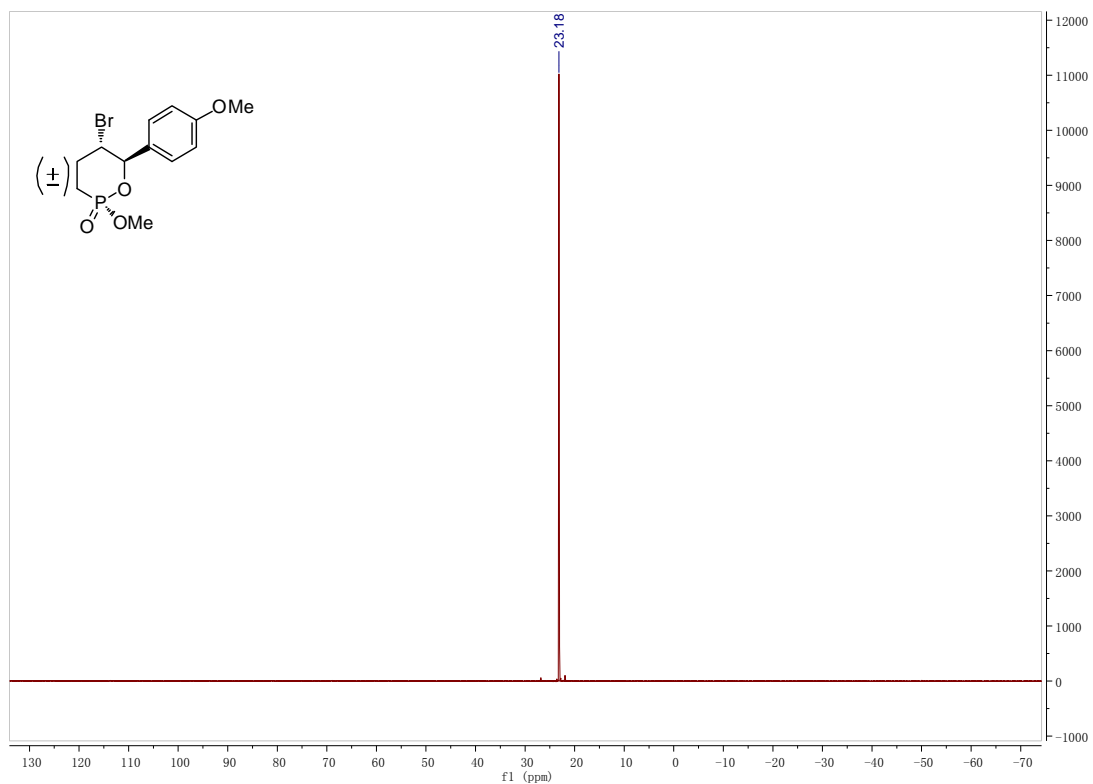
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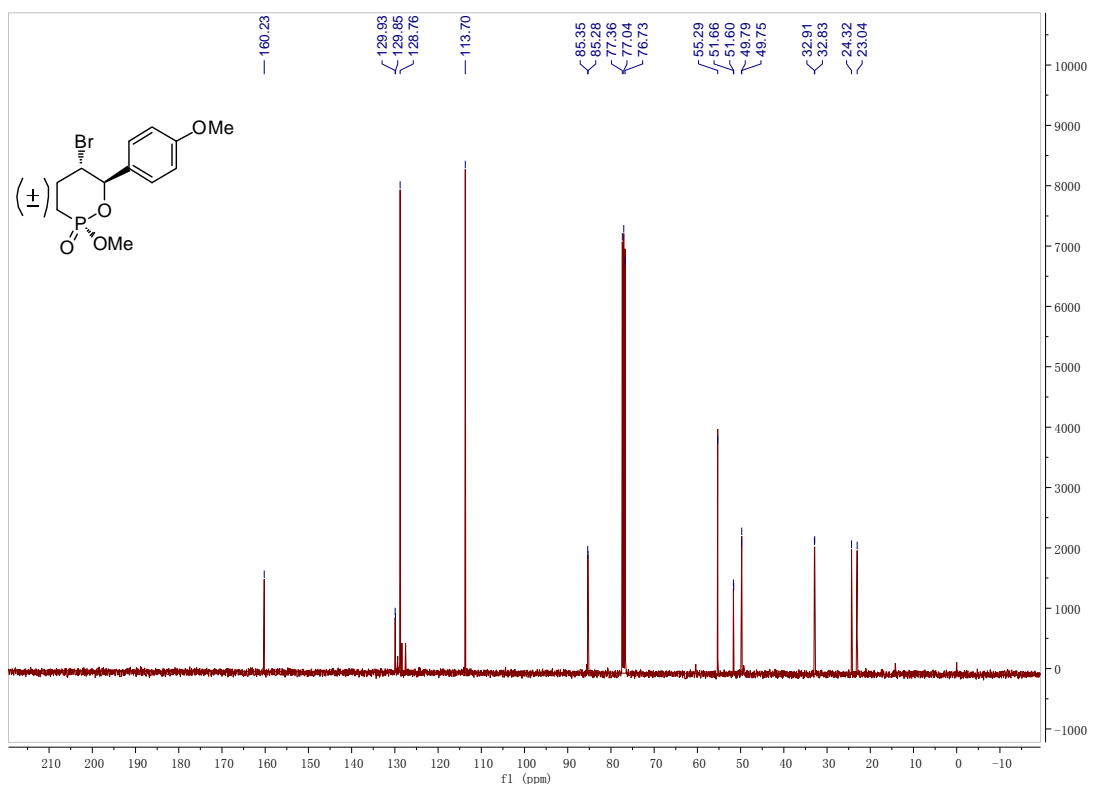
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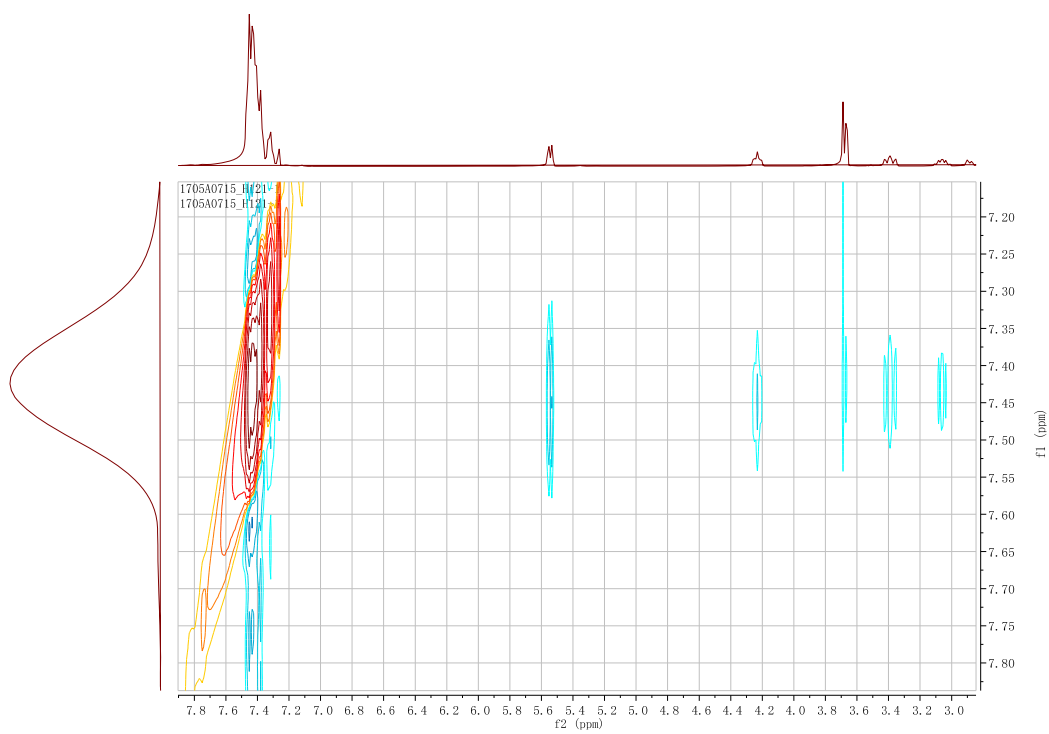
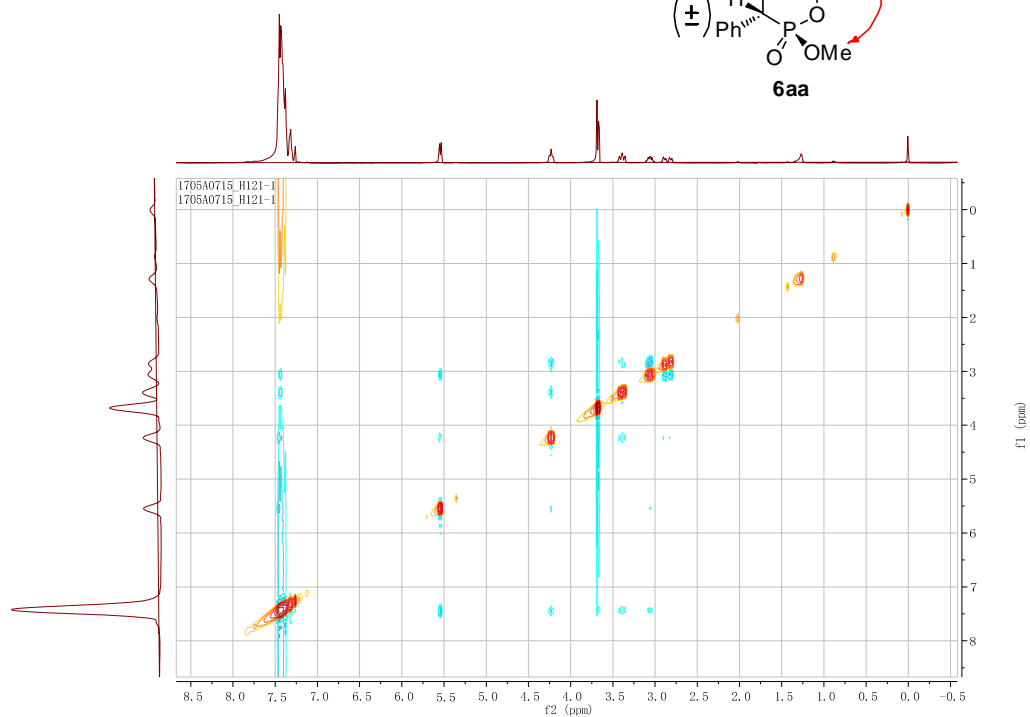
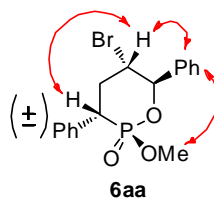
³¹P NMR (162 MHz, CDCl₃) of **6b**



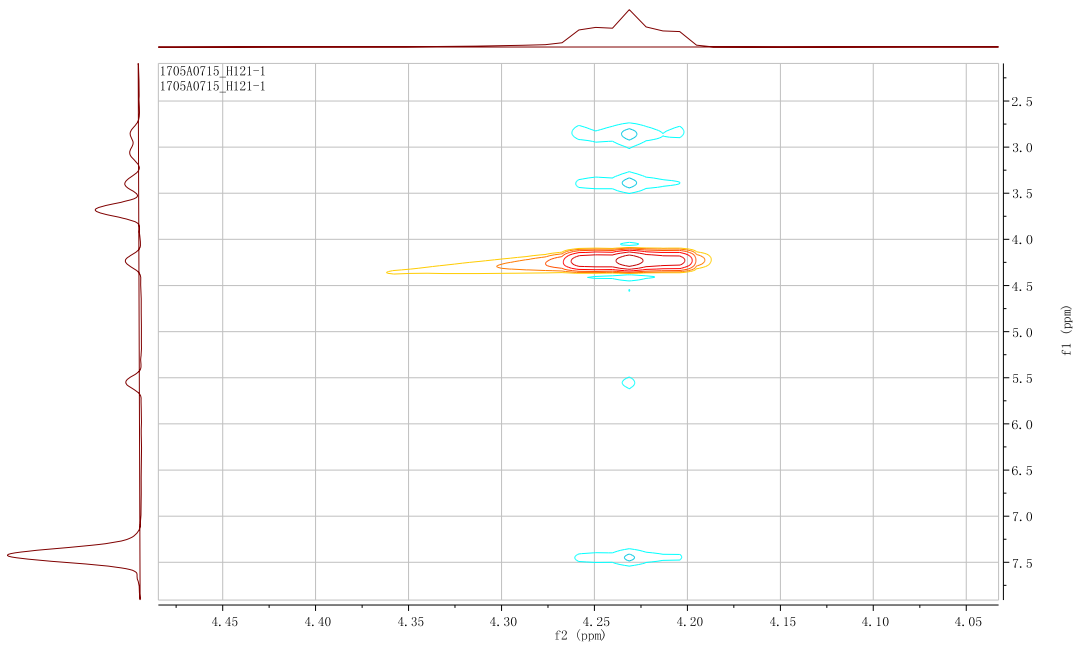
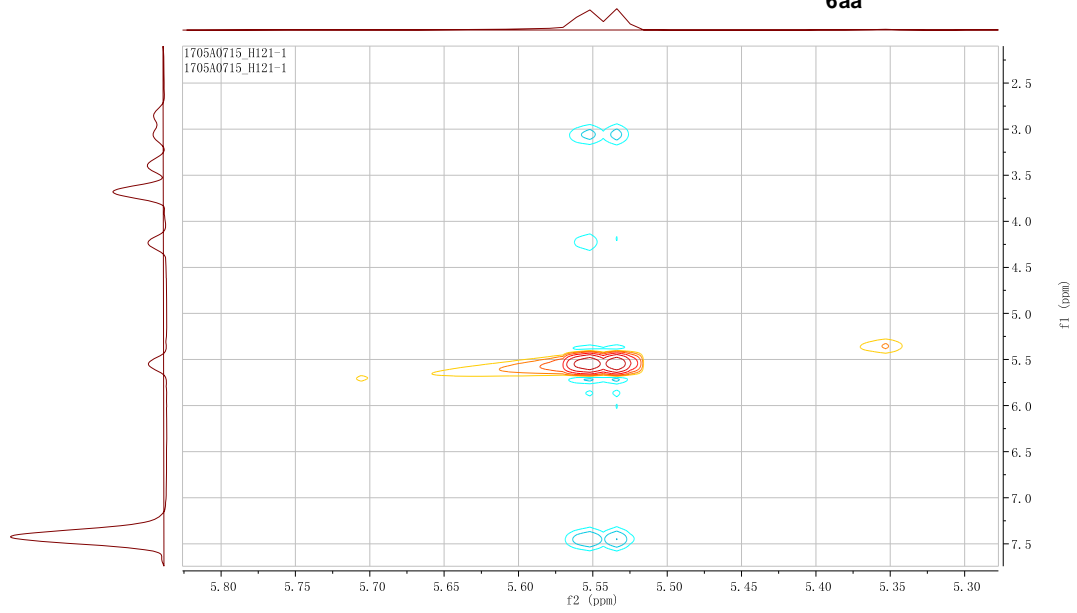
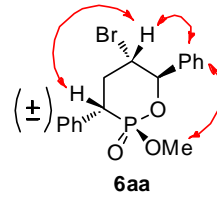
¹³C NMR (101 MHz, CDCl₃) of **6b**



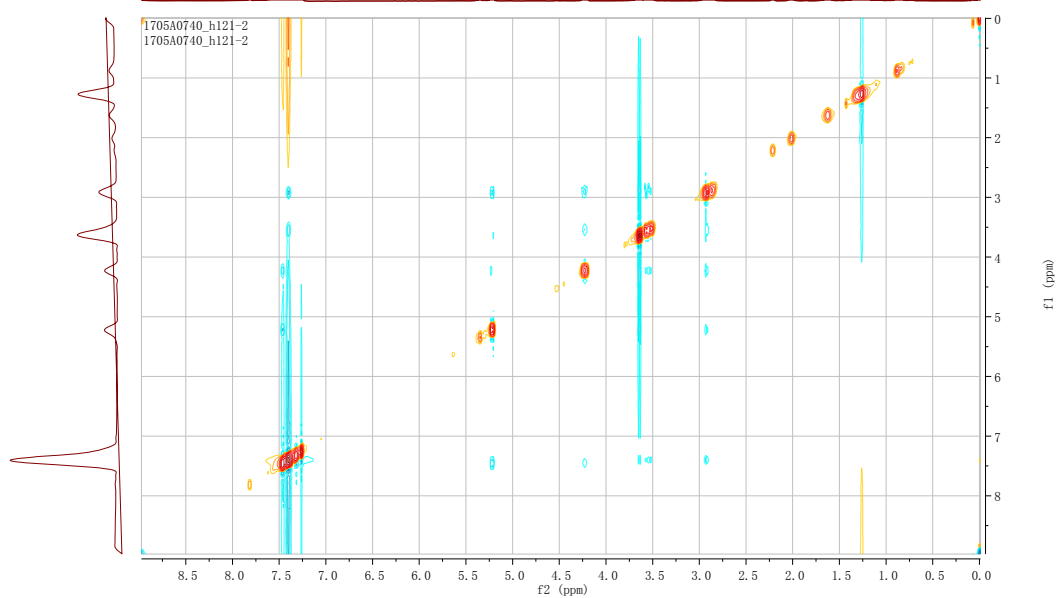
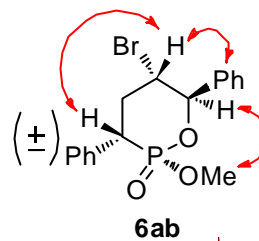
NOE spectra for 6aa



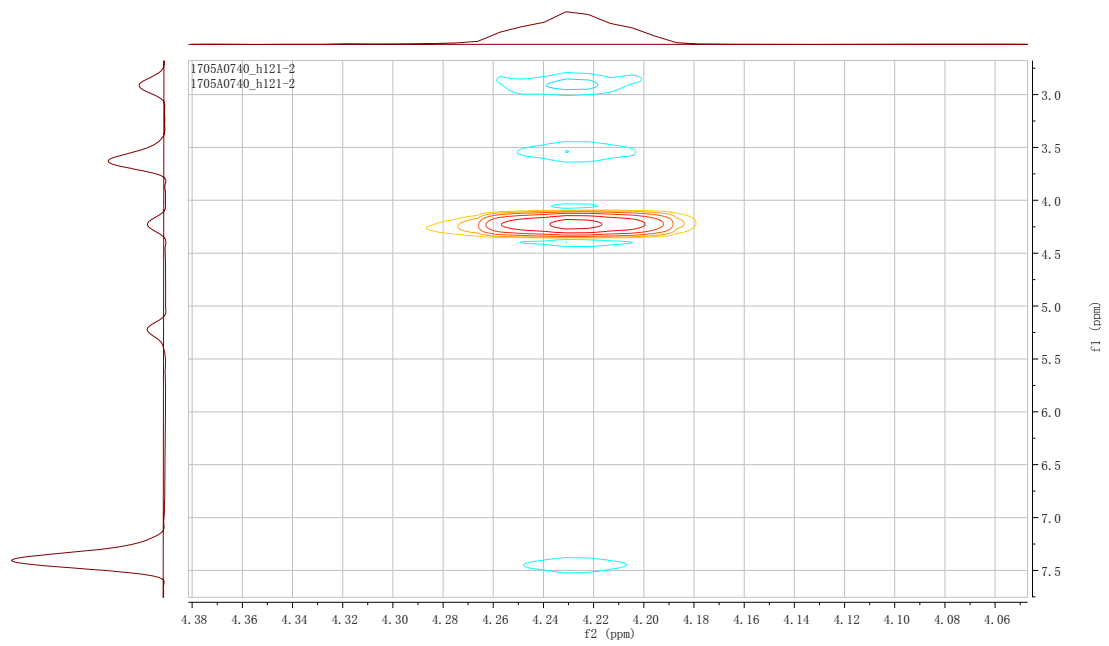
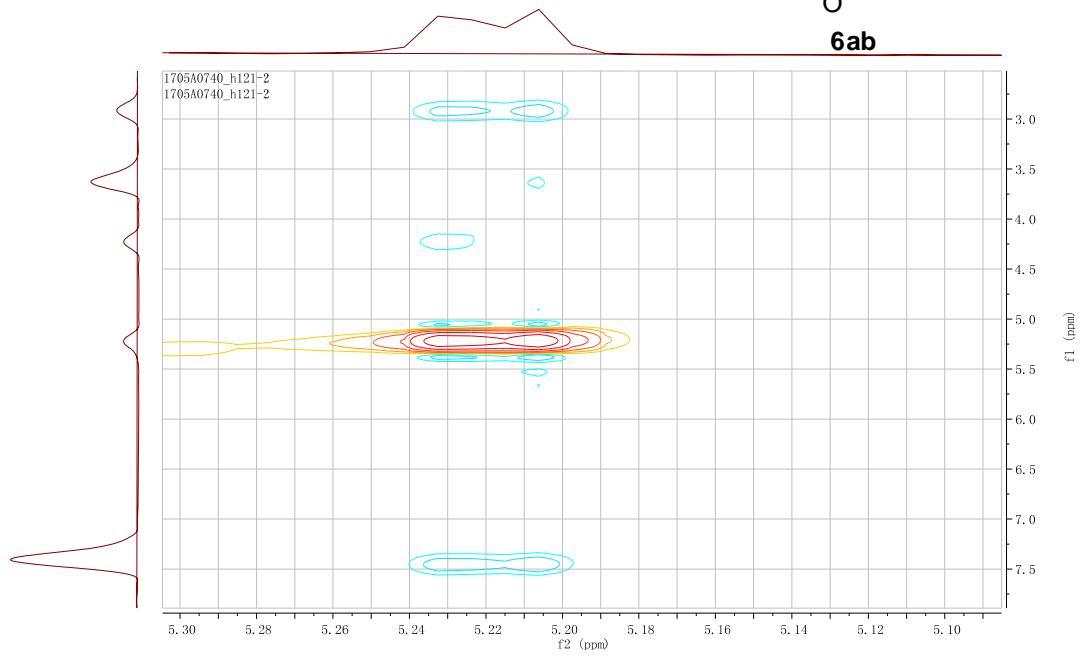
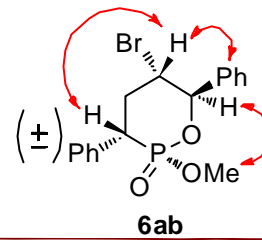
NOE spectra for 6aa



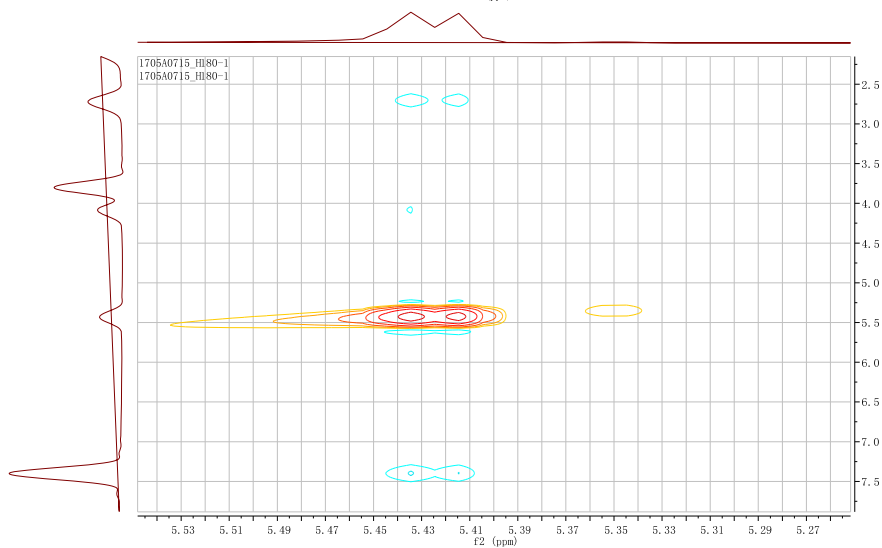
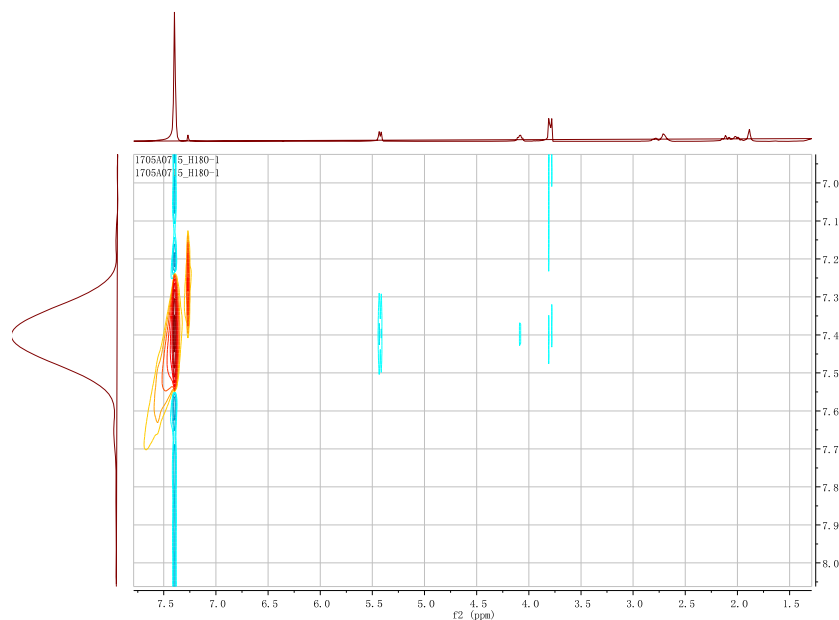
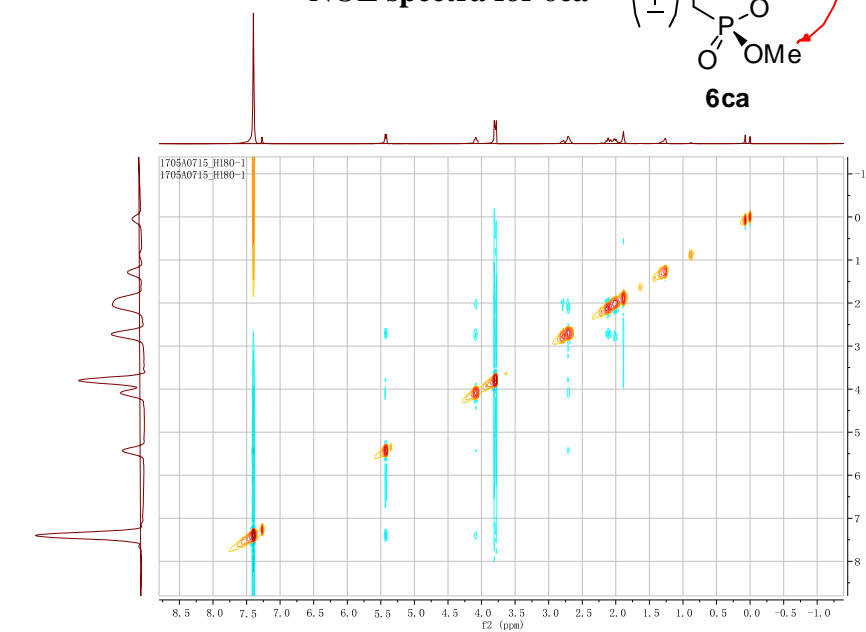
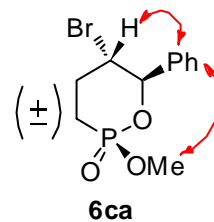
NOE spectra for 6ab



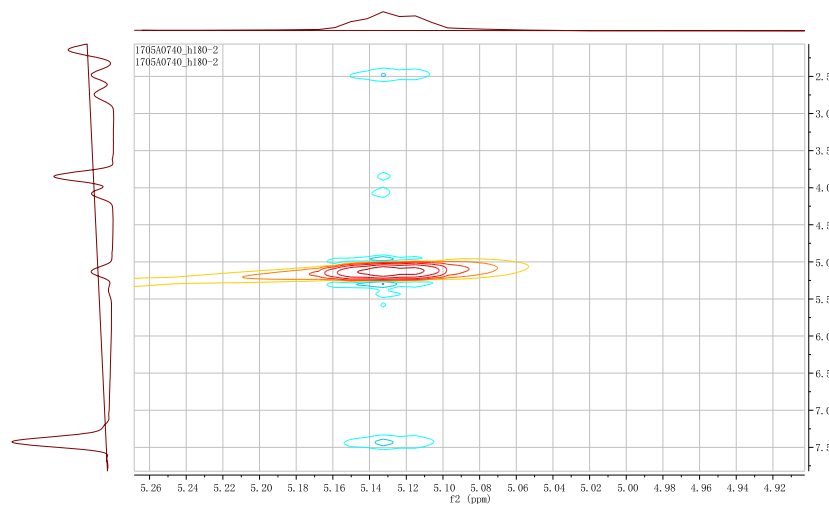
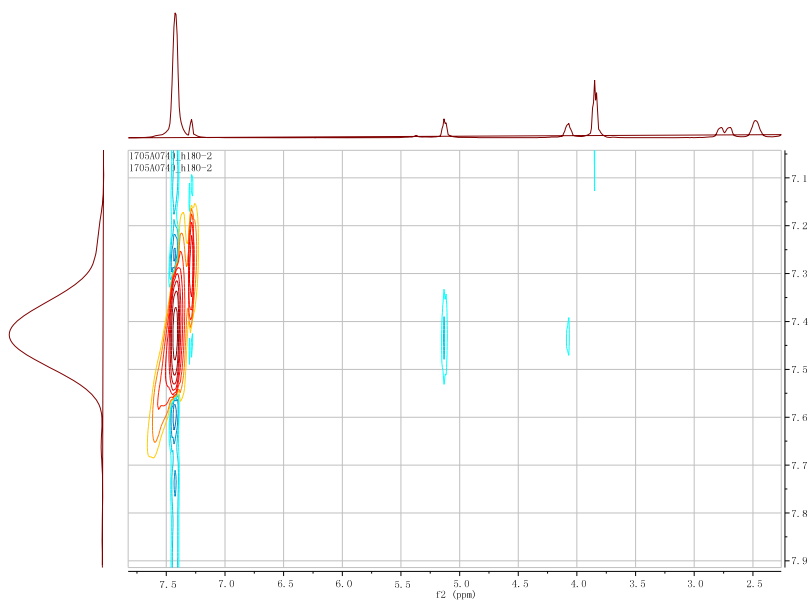
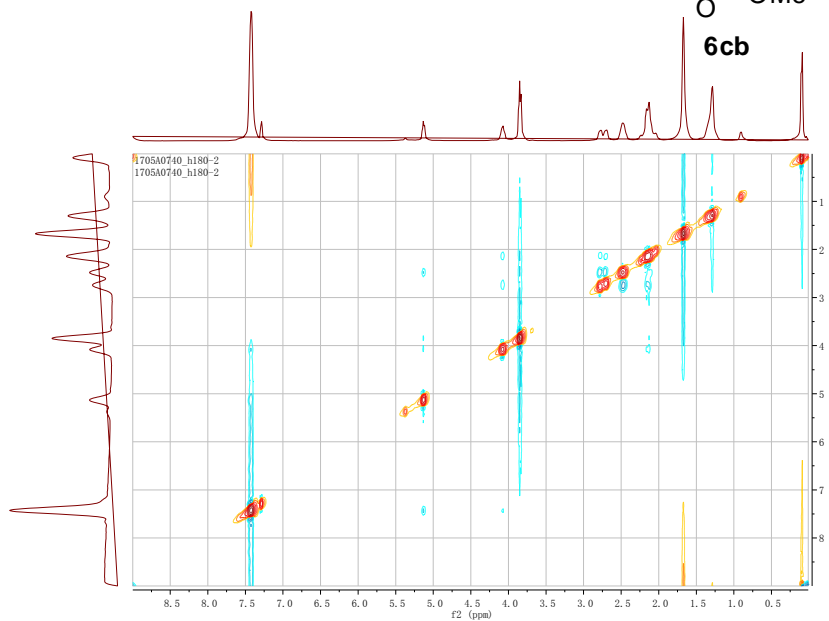
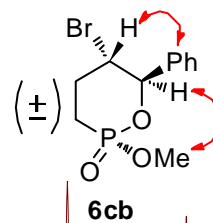
NOE spectra for 6ab



NOE spectra for 6ca



NOE spectra for 6cb



The X-Ray crystallography of 6ba

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) A

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: A

Bond precision: C-C = 0.0105 A Wavelength=1.54178
Cell: a=5.4900(2) b=19.9165(6) c=18.1684(8)
 alpha=90 beta=94.993(4) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	1979.02(13)	1979.02(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H20 Br O3 P	?
Sum formula	C21 H20 Br O3 P	C21 H20 Br N0 O3 P
Mr	431.24	431.25
Dx, g cm-3	1.447	1.447
Z	4	4
Mu (mm-1)	3.738	3.738
F000	880.0	880.0
F000'	880.52	
h,k,lmax	6,22,20	6,22,20
Nref	2943	2938
Tmin,Tmax	0.428,0.474	
Tmin'	0.147	

Correction method= Not given

Data completeness= 0.998 Theta(max) = 59.995

R(reflections)= 0.0613(2417) wR2(reflections)= 0.1800(2938)

S = 1.074 Npar= 236

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

