

Supporting Information

First Stereoselective Total Synthesis of Brevipolide M

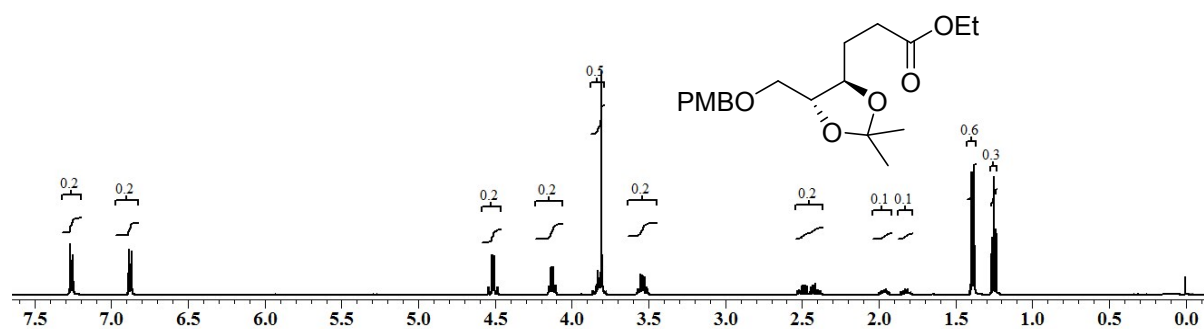
Kasa Shiva Raju and Gowravaram Sabitha*

Natural Products Chemistry Division and CSIR-Indian Institute of Chemical Technology,
Hyderabad 500007, India.

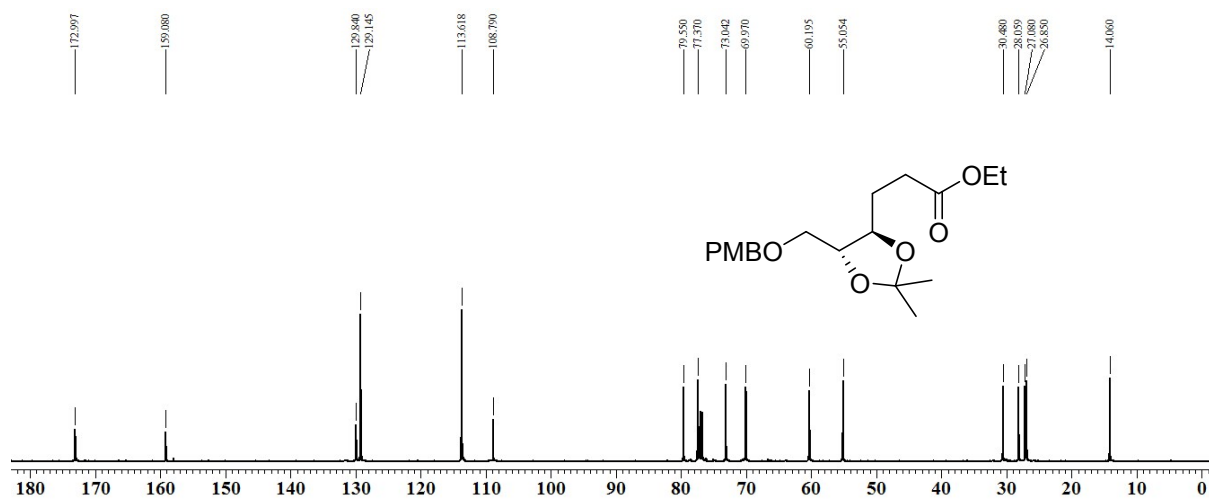
Corresponding author: Tel.: +91-40-27191629; fax: +91-40-27160512

e-mail: gowravaramsr@yahoo.com, sabitha@iict.res.in

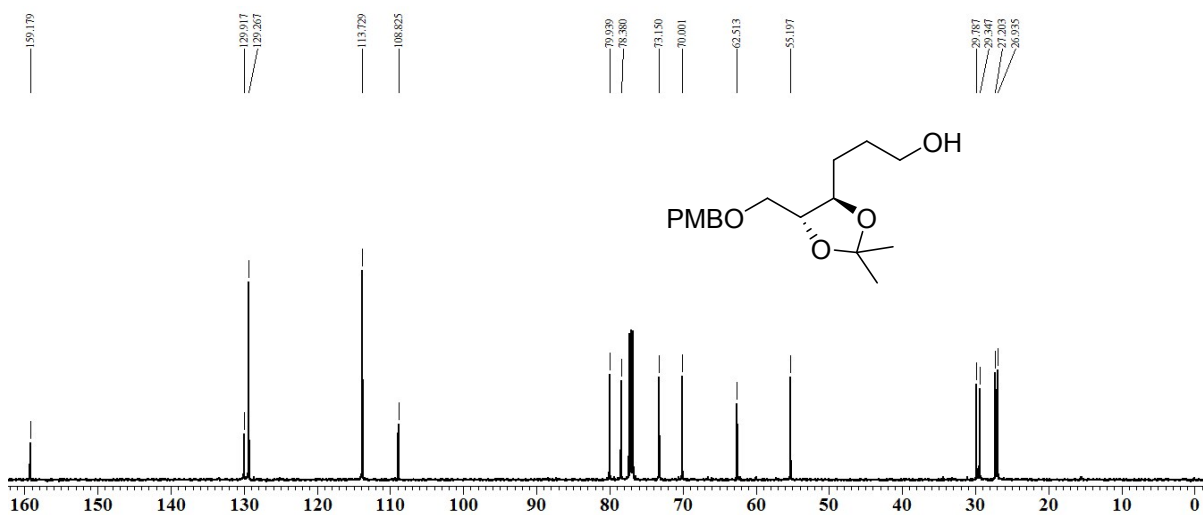
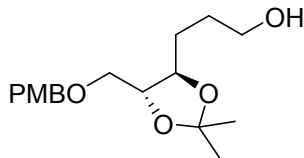
1. ^1H NMR and ^{13}C NMR Spectra of All Compounds	2 – 18
2. HPLC of Compound 29	19

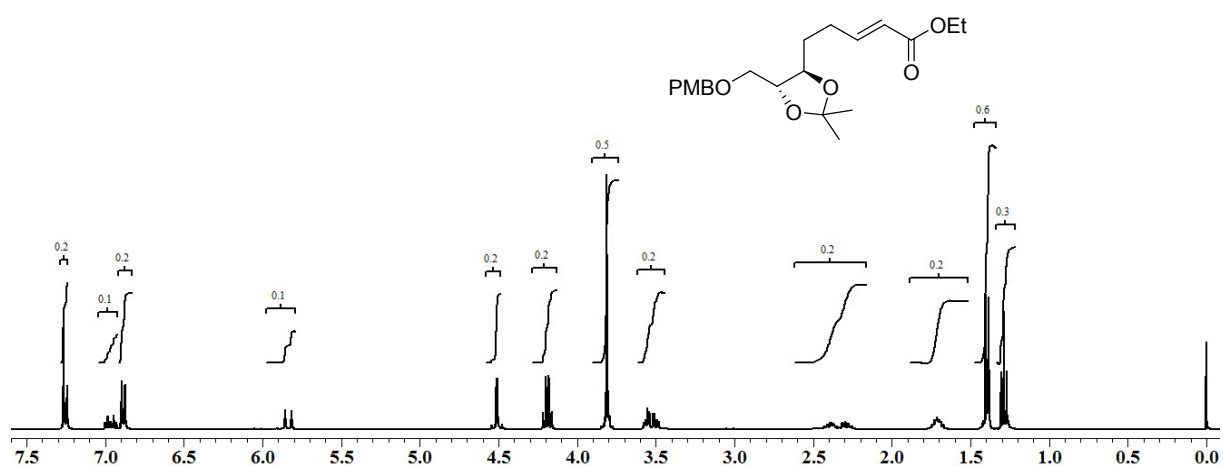


¹H NMR SPECTRUM (500 MHz, CDCl₃)

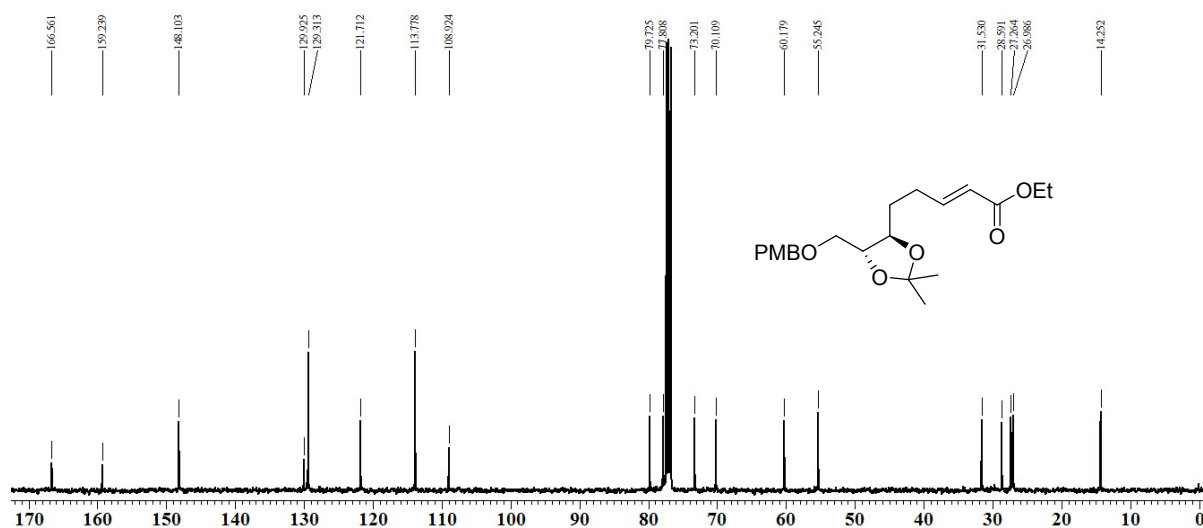


¹³C NMR SPECTRUM (100 MHz, CDCl₃)

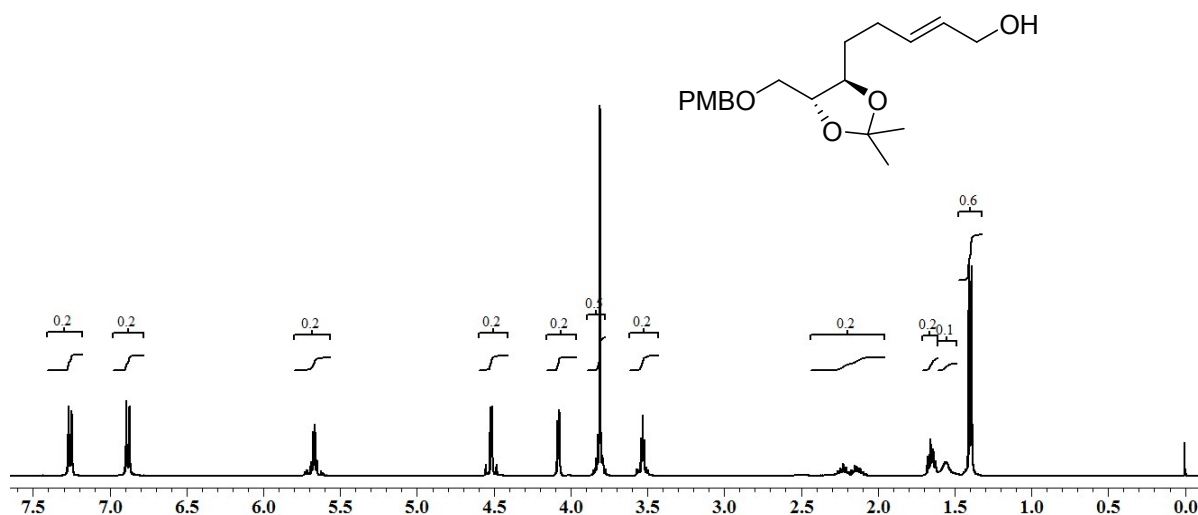




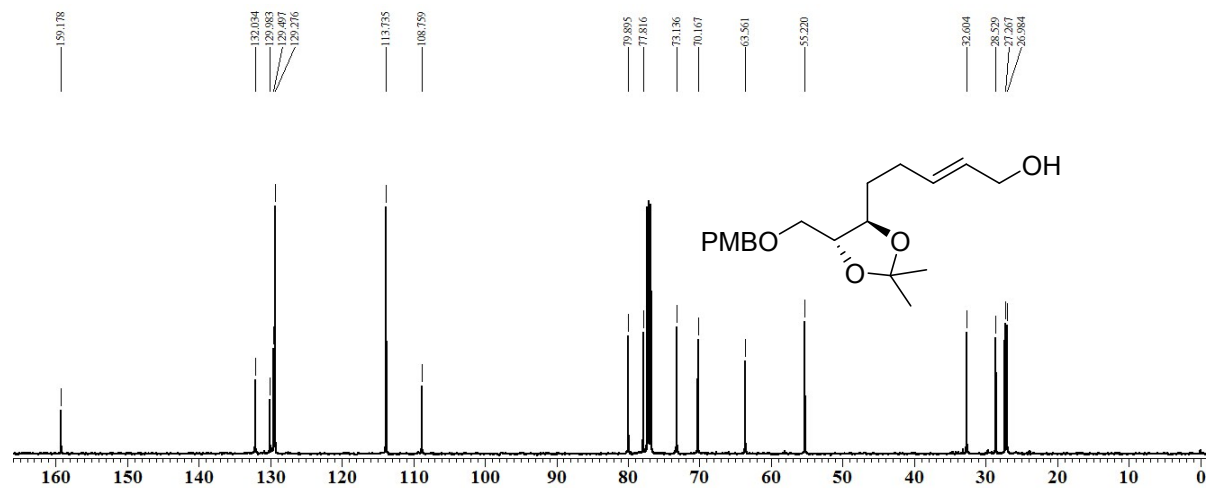
¹H NMR SPECTRUM (400 MHz, CDCl₃)



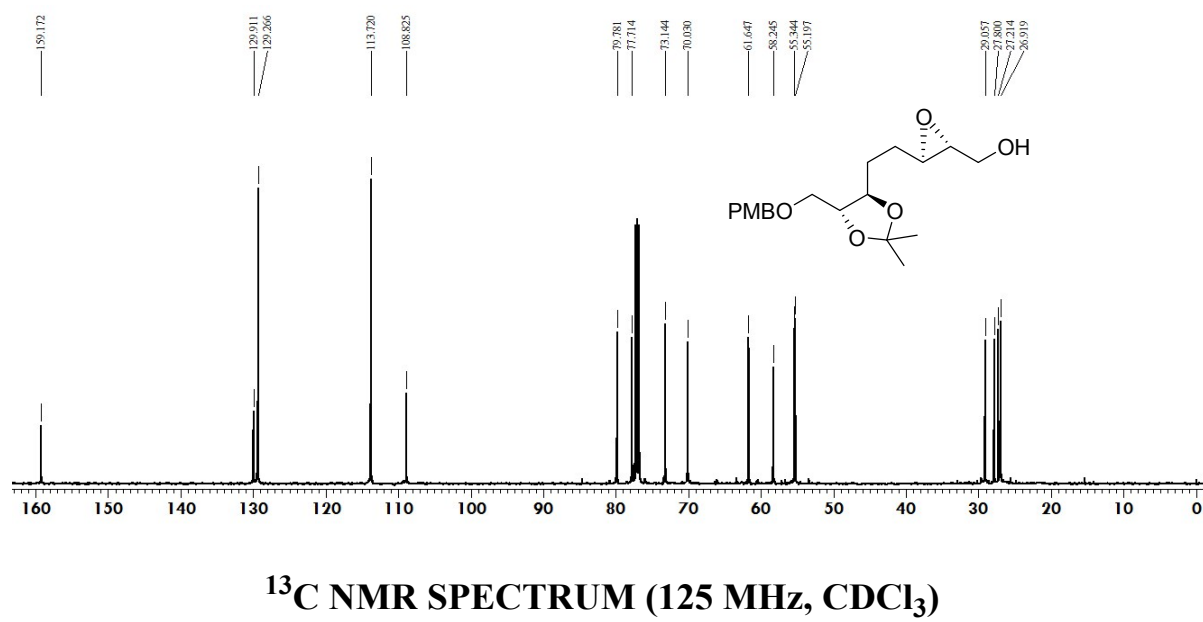
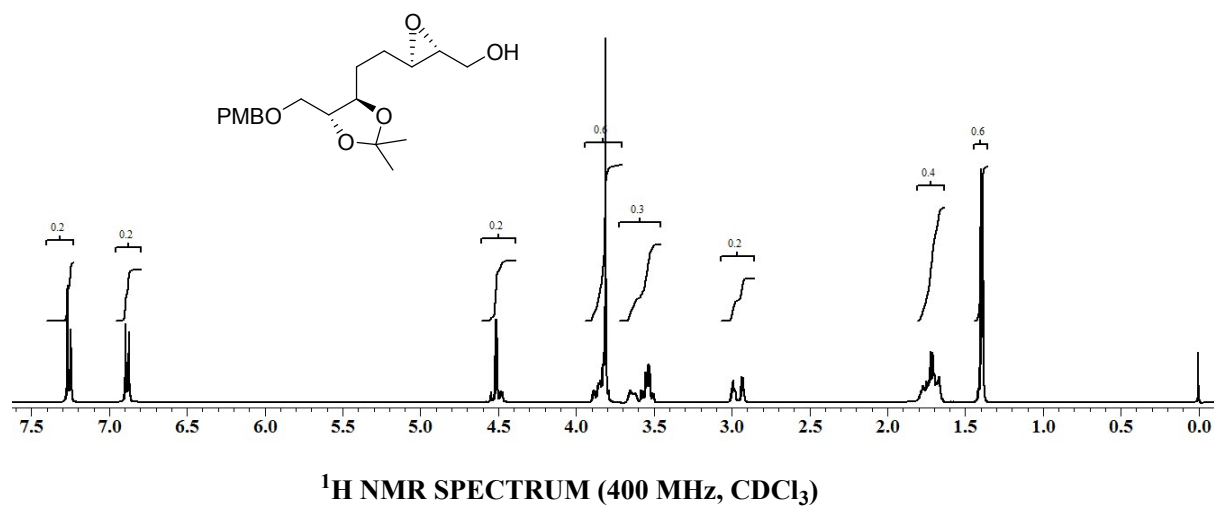
¹³C NMR SPECTRUM (100 MHz, CDCl₃)

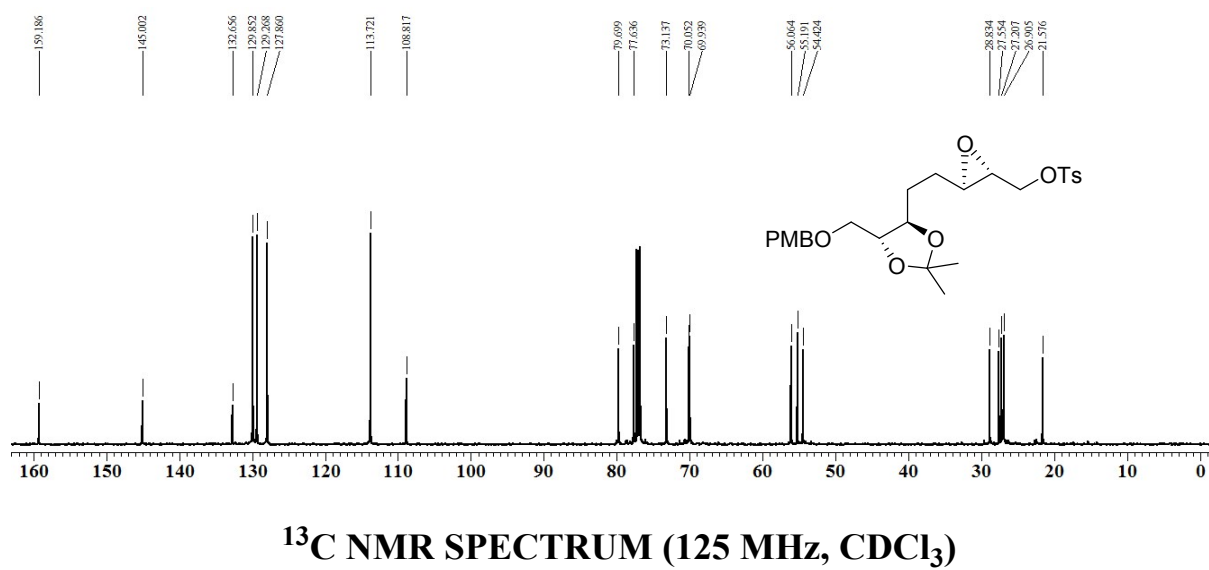
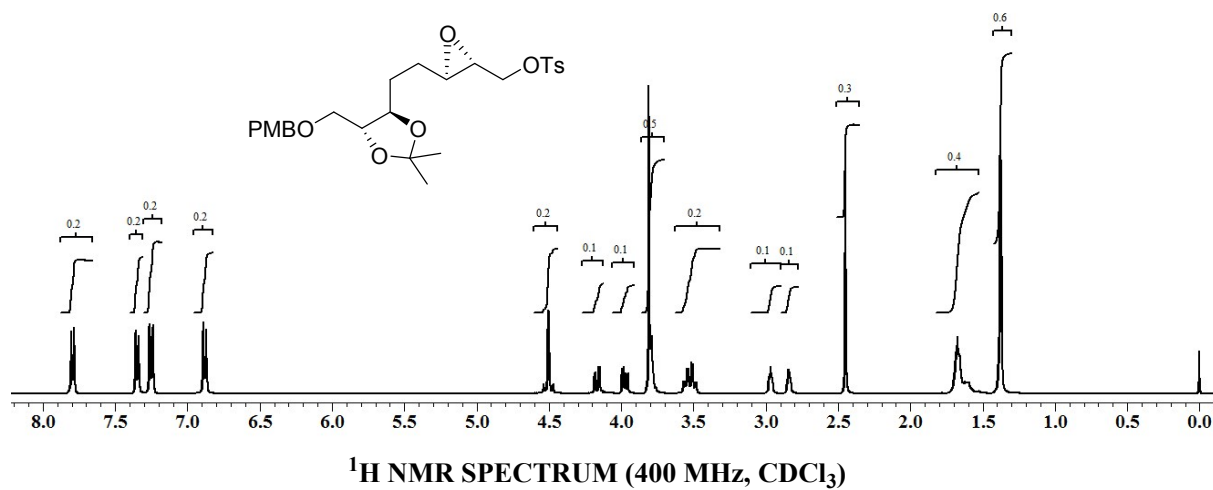


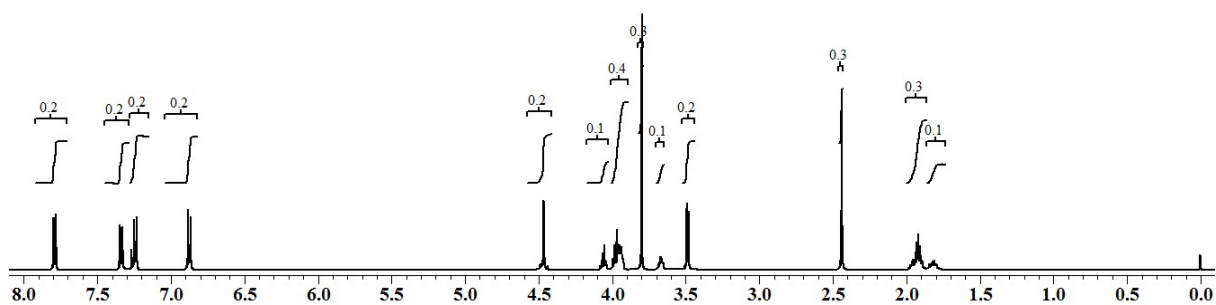
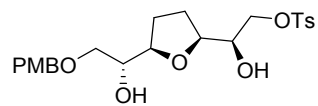
¹H NMR SPECTRUM (400 MHz, CDCl₃)



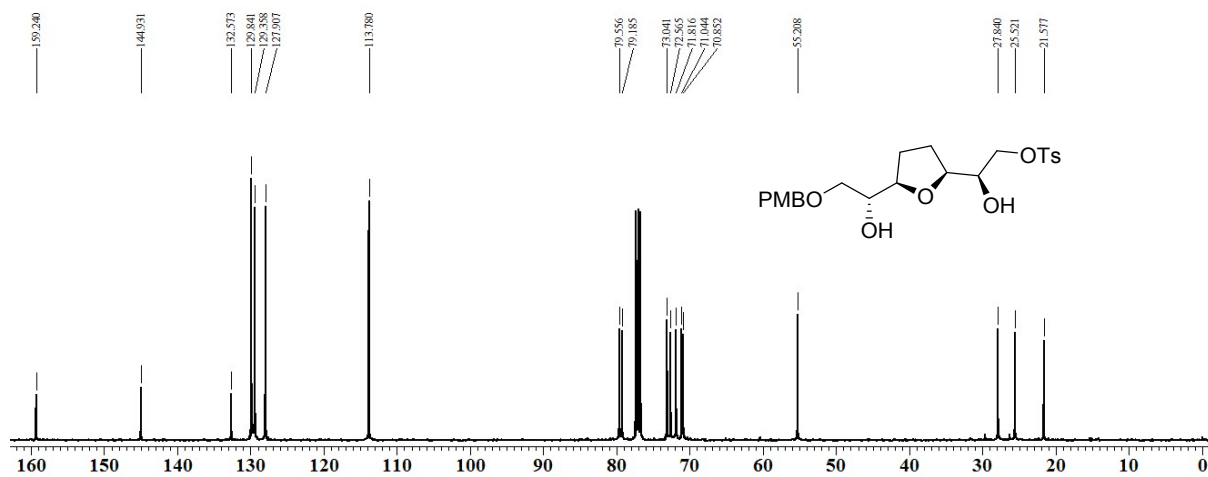
¹³C NMR SPECTRUM (125 MHz, CDCl₃)



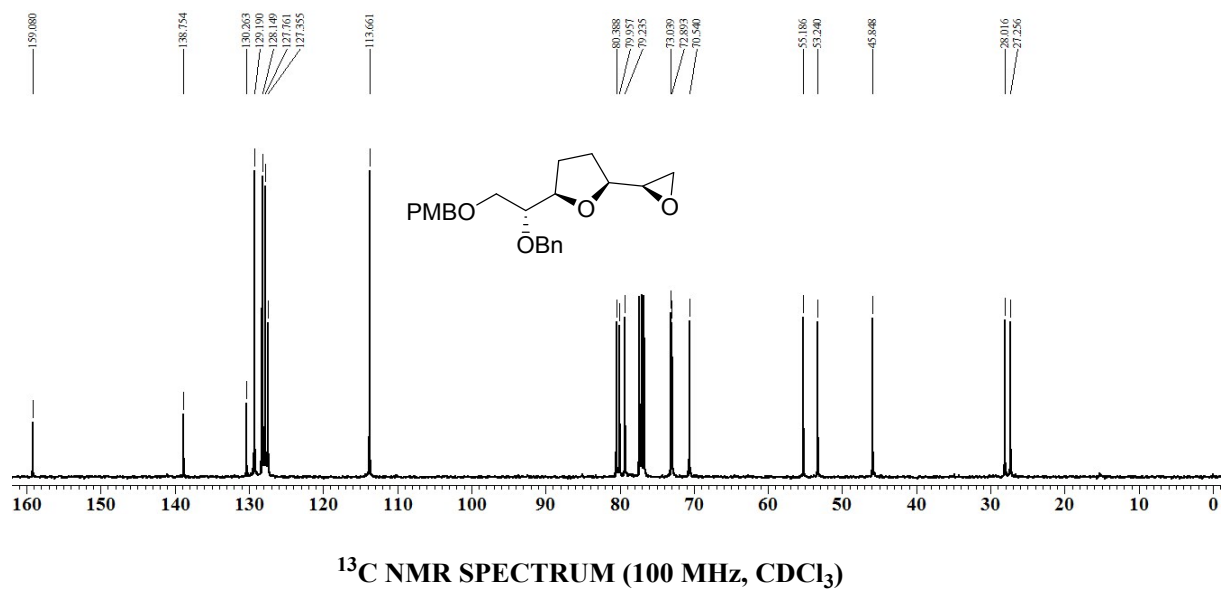
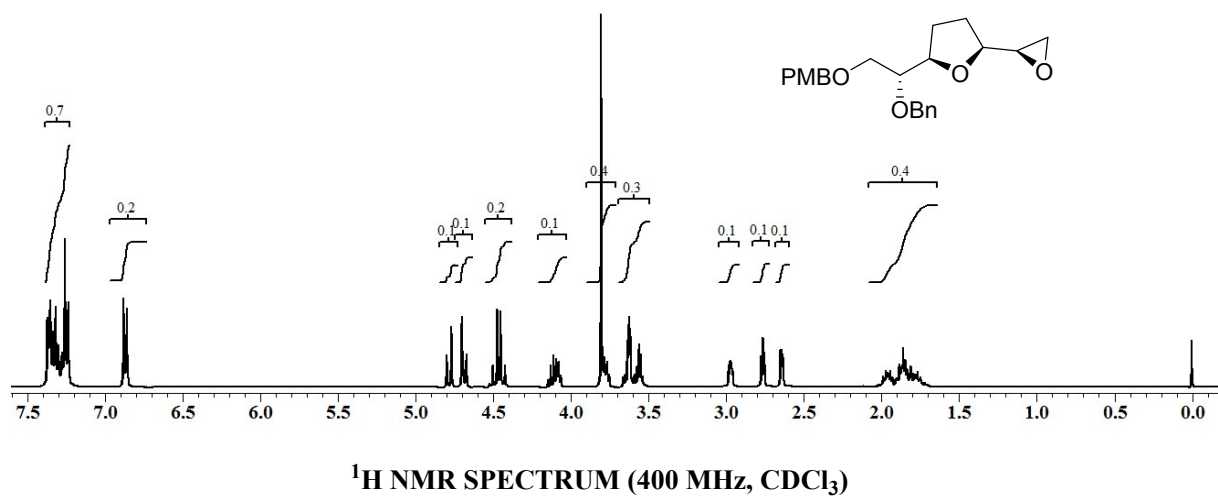


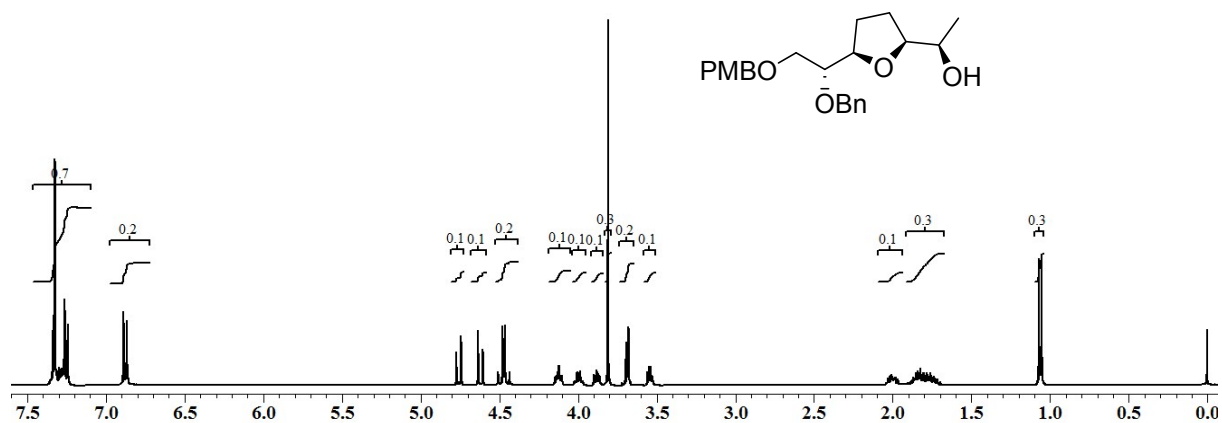


^1H NMR SPECTRUM (400 MHz, CDCl_3)

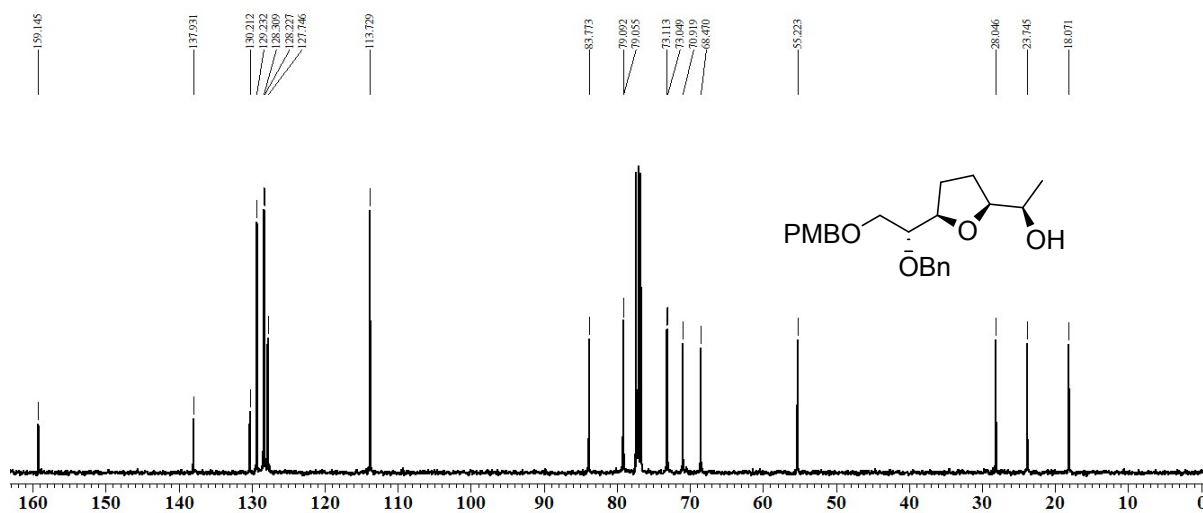


^{13}C NMR SPECTRUM (100 MHz, CDCl_3)

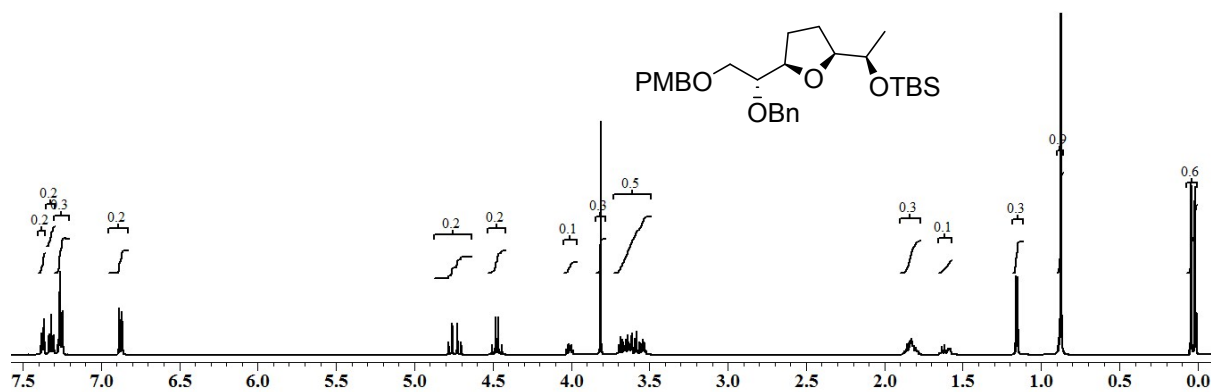




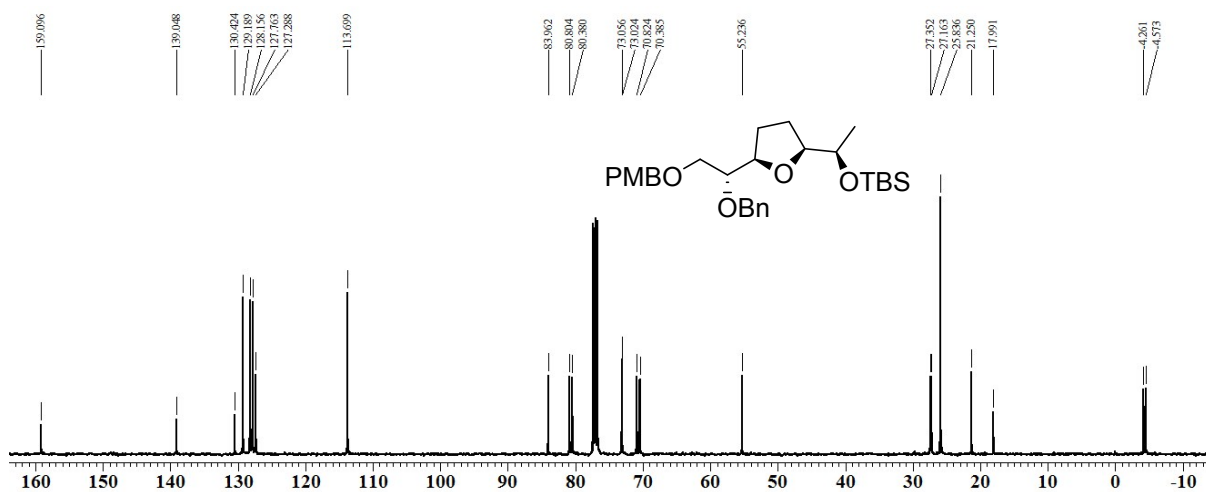
^1H NMR SPECTRUM (400 MHz, CDCl_3)



^{13}C NMR SPECTRUM (100 MHz, CDCl_3)

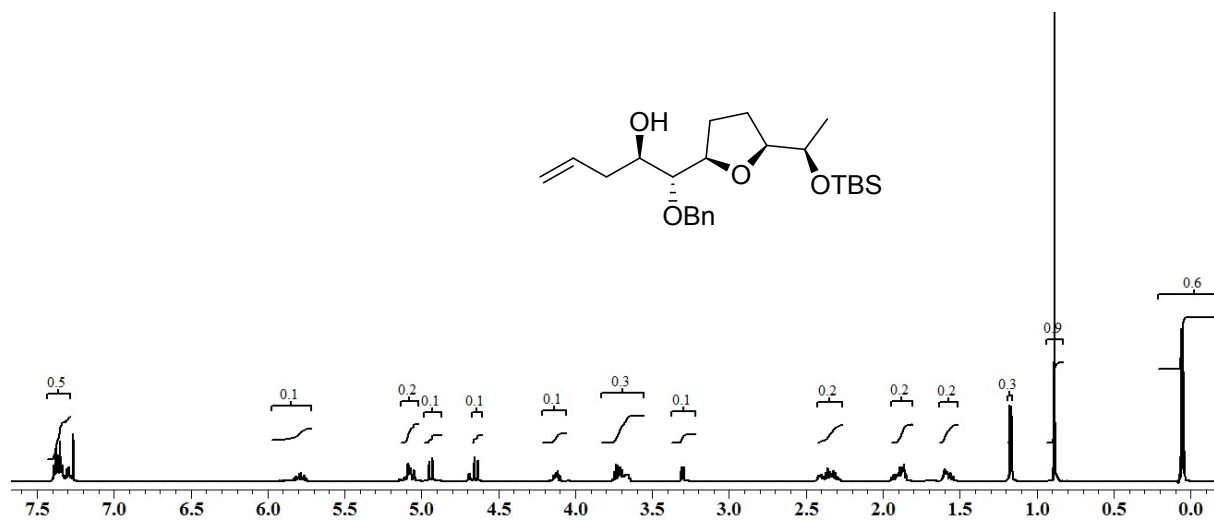


¹H NMR SPECTRUM (500 MHz, CDCl₃)

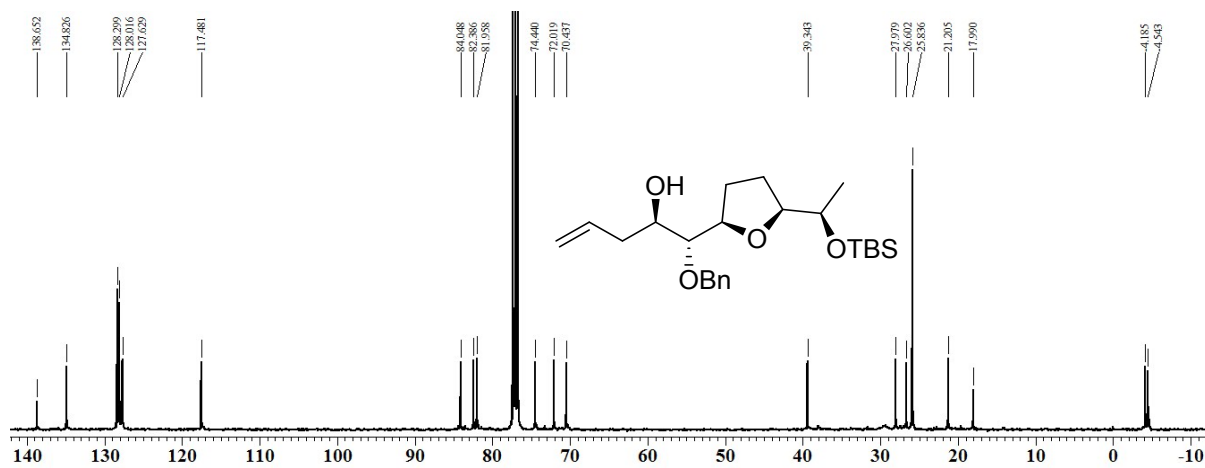


¹³C NMR SPECTRUM (100 MHz, CDCl₃)

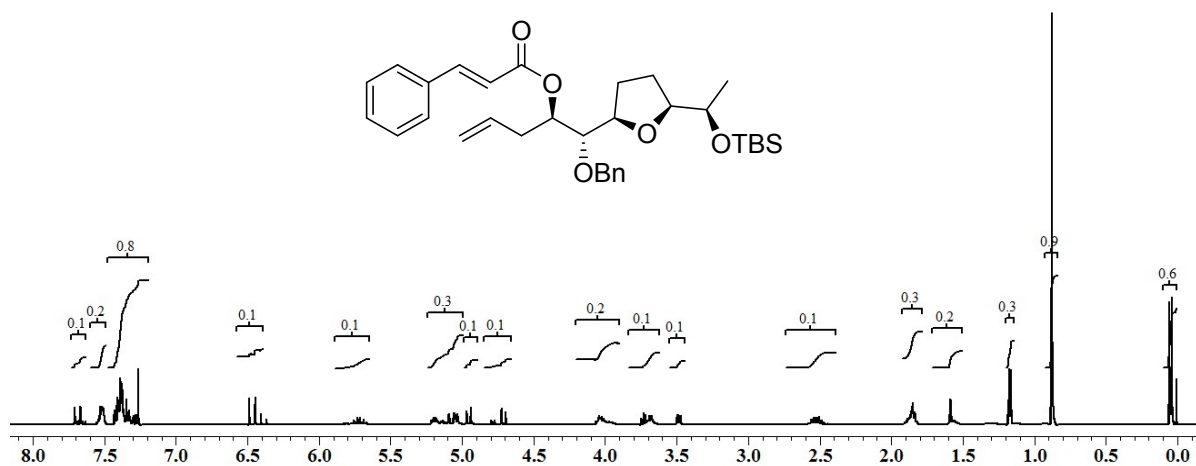




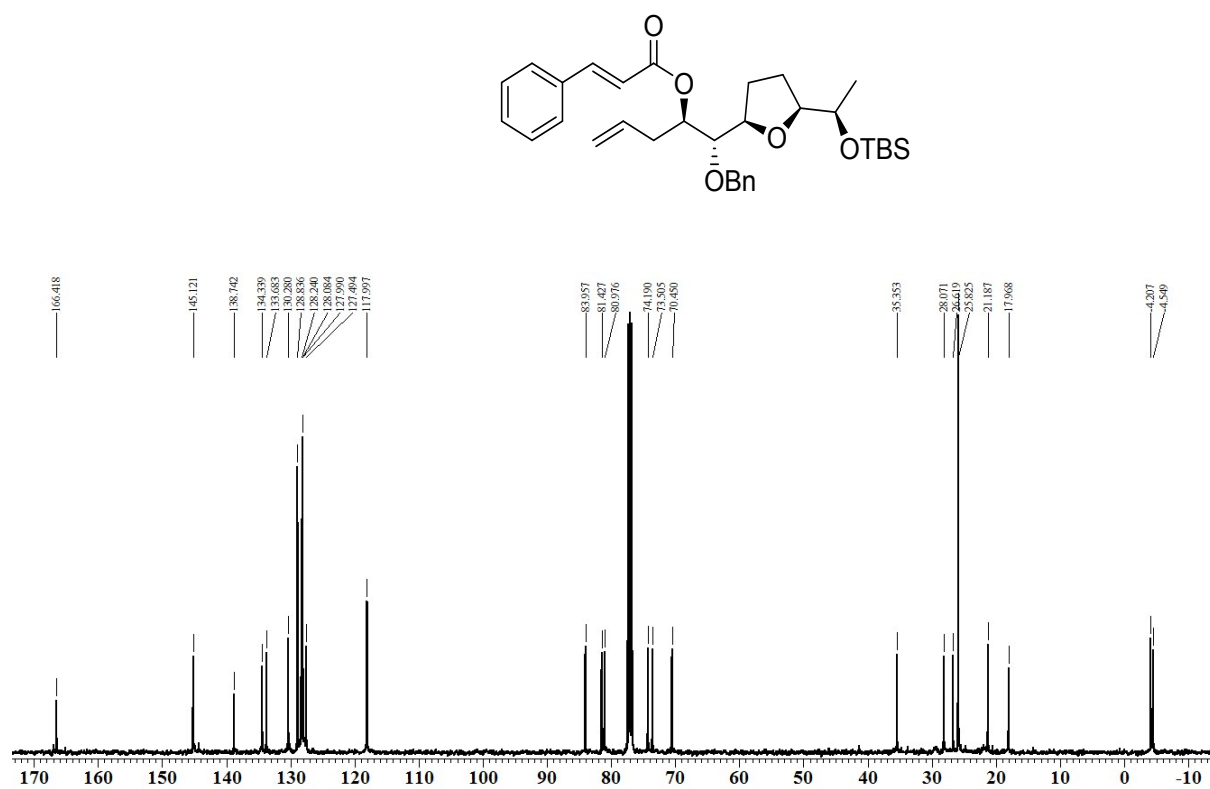
¹H NMR SPECTRUM (500 MHz, CDCl₃)



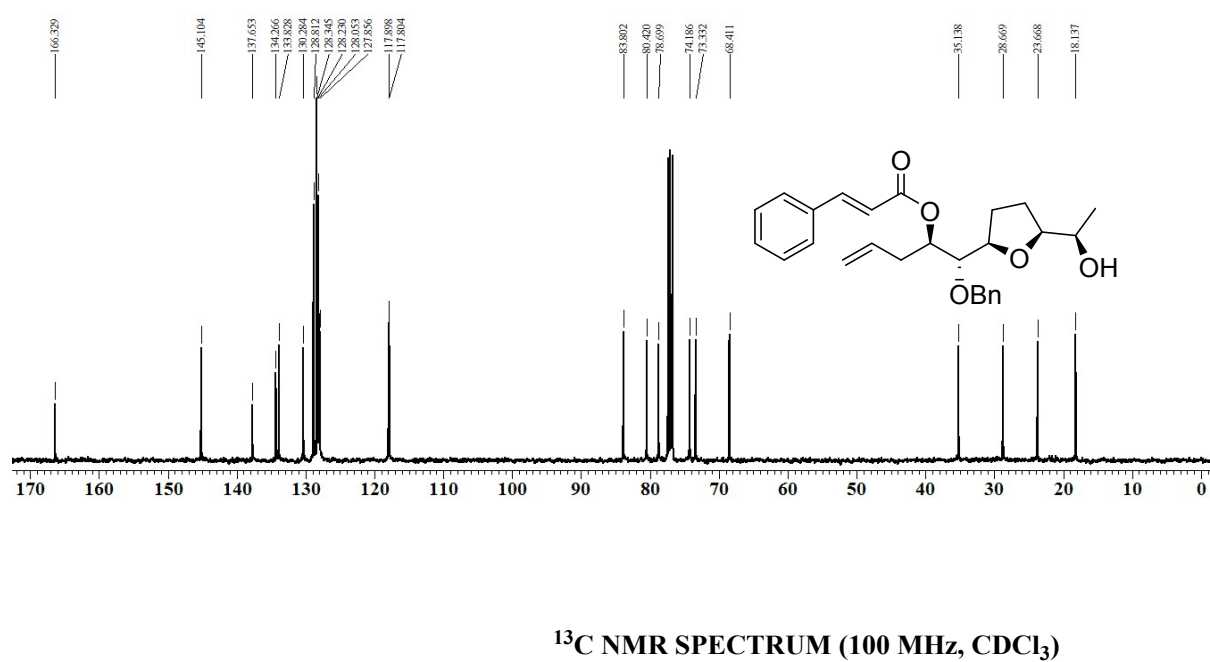
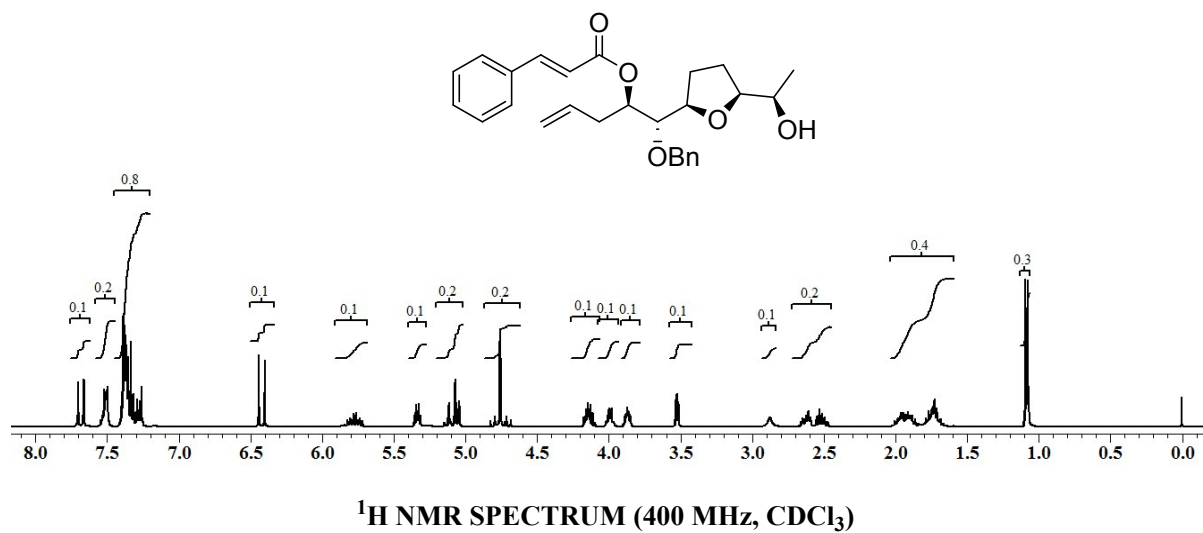
¹³C NMR SPECTRUM (100 MHz, CDCl₃)

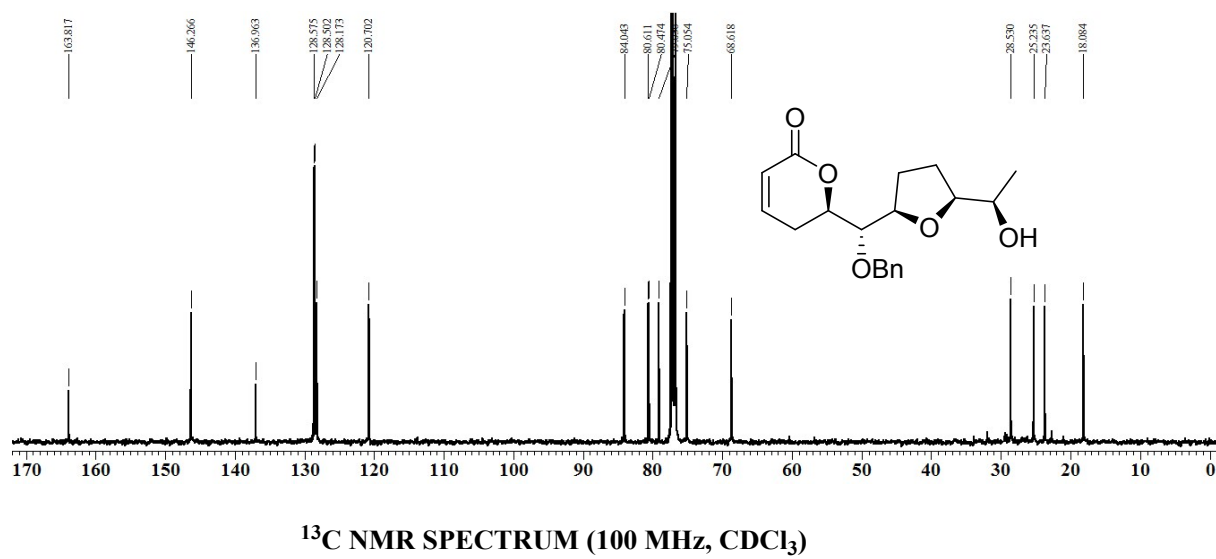
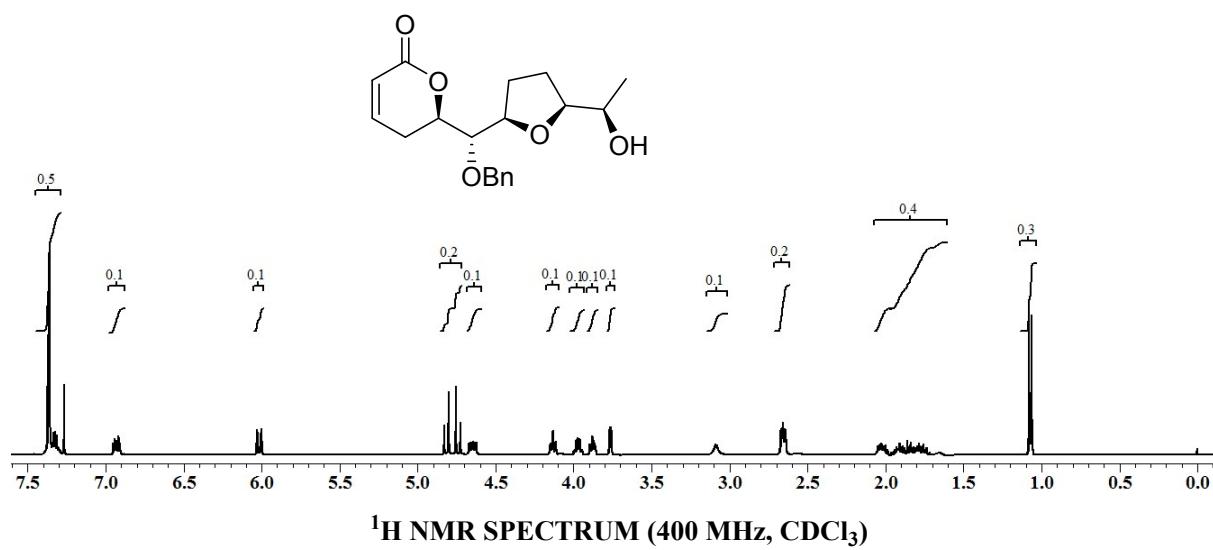


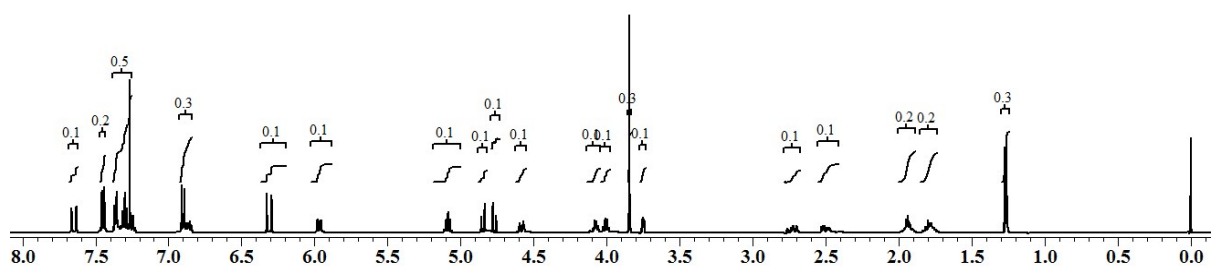
¹H NMR SPECTRUM (400 MHz, CDCl₃)



¹³C NMR SPECTRUM (100 MHz, CDCl₃)

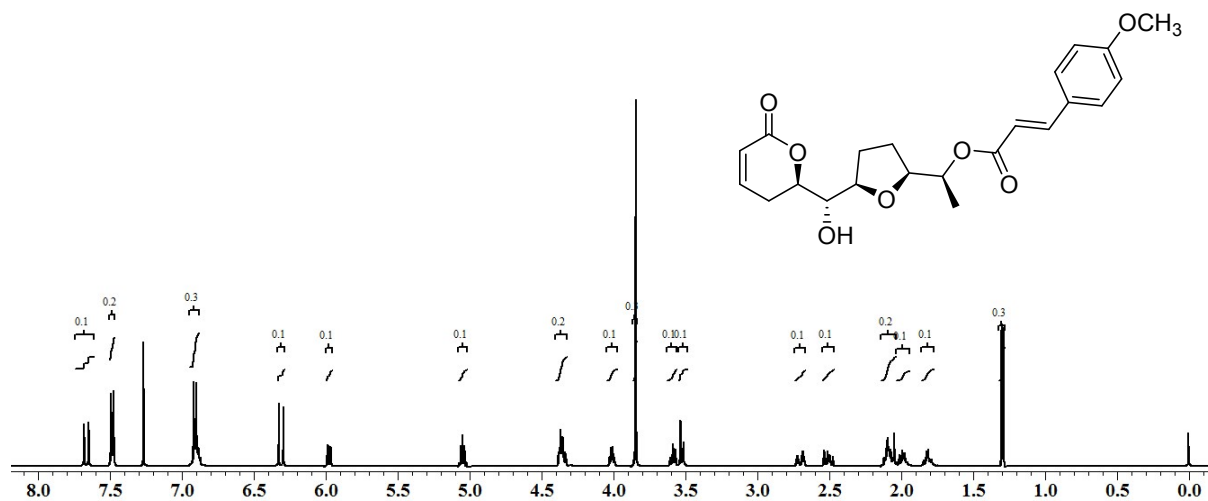




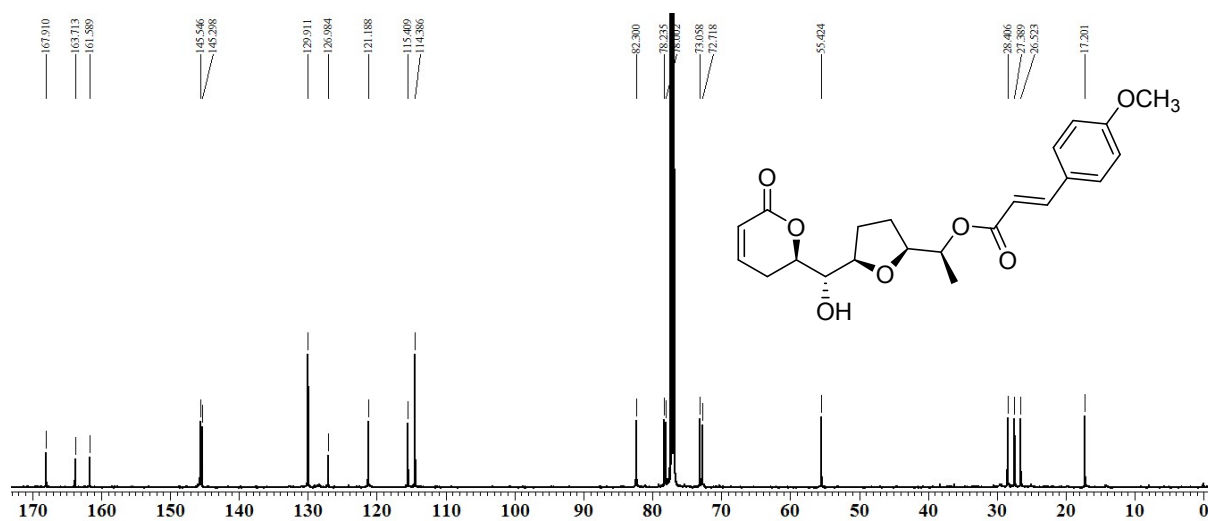


Chemical structure of compound 10 is shown. The structure is a complex molecule containing a cyclohexanone, a furanose ring, a benzylidene acetal, and a p-methoxyphenyl group. The peaks are labeled with their corresponding chemical shifts: 166.763, 163.993, 161.361, 146.388, 144.501, 138.201, 129.737, 128.779, 127.880, 127.571, 127.662, 126.545, 115.763, 114.392, 81.848, 81.424, 80.157, 74.704, 72.296, 55.362, 28.526, 27.847, 24.923, and 16.619.

^{13}C NMR SPECTRUM (100 MHz, CDCl_3)



¹H NMR SPECTRUM (500 MHz, CDCl₃)



¹³C NMR SPECTRUM (125 MHz, CDCl₃)

HPLC of Compound 29

+

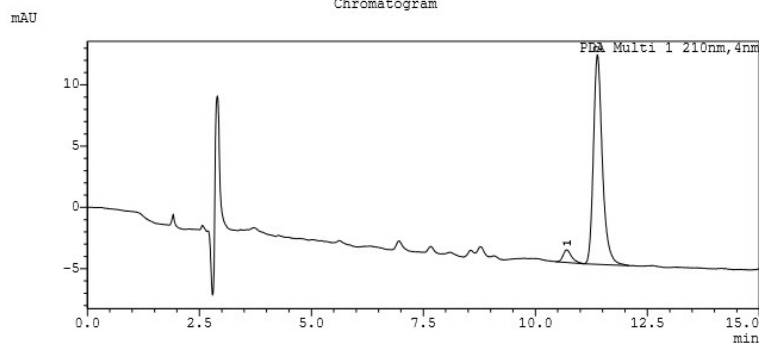


LC-MS DATA REPORT

HCY-DNPC

Sample Code : GSR-OH-420
 Data File : 120617.2.1cd
 Method : LC-MS ISOCRATIC.lcm
 Injection Volume : 5
 Date Acquired : 6/12/2017 11:25:26 AM
 Report File : LC-MS Data Report.lsr
 Chromatographic Conditions : Column:LUNA C8 (250 X 4.6mm, 5.0µ)
 Mobile Phase: 90 %ACN IN 0.1 % FA
 Flow Rate: 1.0 mL/min

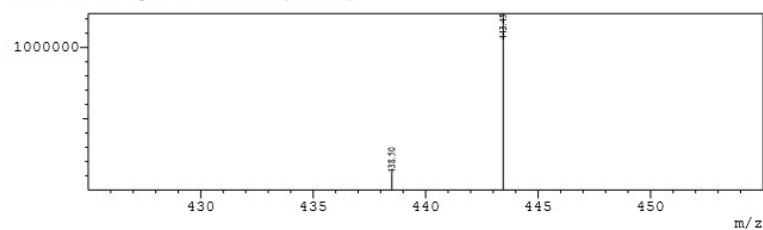
Chromatogram



PDA Ch1 210nm

Peak#	Ret. Time	Peak Start	Peak End	Area	Area%
1	10.700	10.453	11.072	13679	5.418
2	11.385	11.072	12.096	238772	94.582
Total				252451	100.000

Q1 Scan Positive+
 \$If\$(SpPrTab==SpPrTab)Spectrum Mode:Averaged 10.450-10.907(3801-3967)
 BG Mode:Averaged 0.000-9.988(1-3633)



Q1 Scan Positive+
 \$If\$(SpPrTab==SpPrTab)Spectrum Mode:Averaged 11.066-12.051(4025-4383)
 BG Mode:Averaged 0.000-10.841(1-3943)

HCY-DNPC

