

Supporting Information

Novel Stereoselective Syntheses of *N*-Octyl- β -Valienamine (NOV) and *N*-Octyl-4-*epi*- β -Valienamine (NOEV) from (–)-Shikimic Acid

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^a Engineering Research Center of Pharmaceutical Process Chemistry of the Ministry of Education, East China University of Science and Technology, 130 Mei-Long Road, Shanghai 200237, P. R. China.

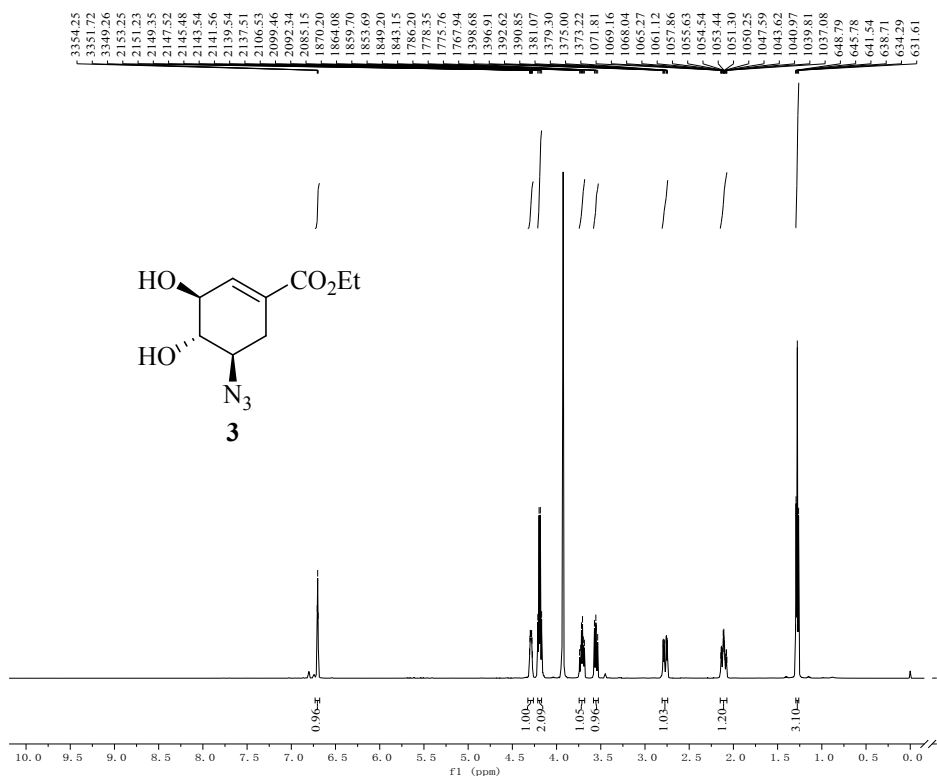
^b Shanghai Qingping Pharmaceutical Co. Ltd., 397 Zhao-Jiang Road, Baihe Town, Qingpu District, Shanghai 201710, P. R. China.

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¹H and ¹³C NMR Spectra of All Compounds..... S2-S15

¹H NMR Spectrum (500 MHz, CD₃COCD₃) of Compound 3:



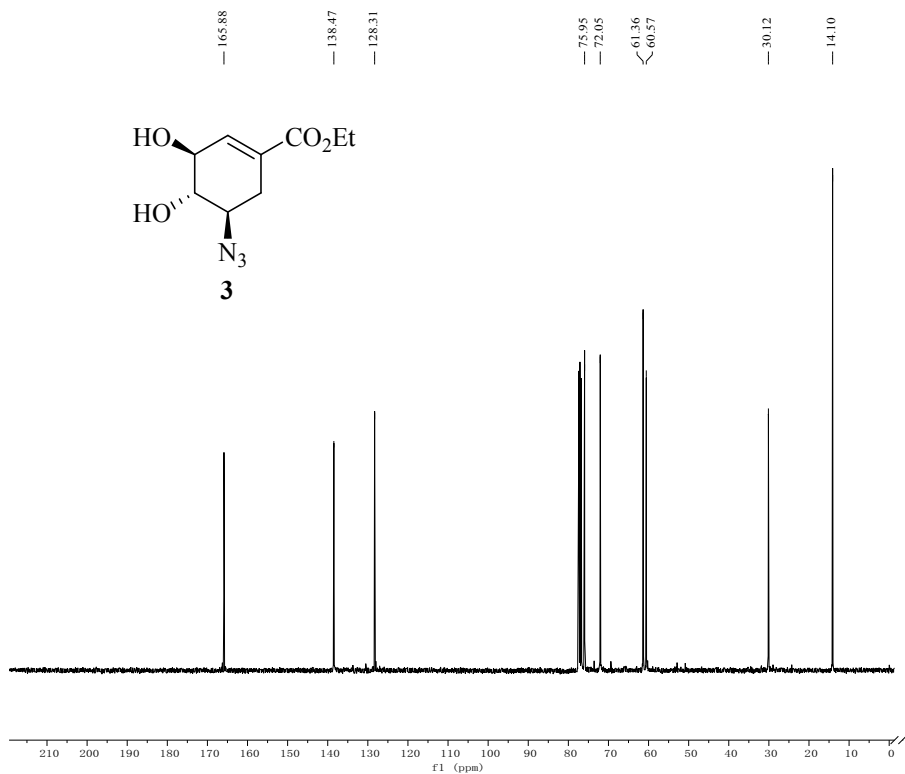
Current Data Parameters
 NAME SXX-qp-11
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130411
 Time 12.36
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT Acetone
 NS 8
 DS 0
 SWH 15015.015 Hz
 FIDRES 0.229111 Hz
 AQ 2.1824322 sec
 RG 16
 DW 33.300 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.0000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 10.50 usec
 PL -4.00 dB
 SFO1 500.1304556 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1299007 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00

¹³C NMR Spectrum (100 MHz, CDCl₃) of Compound 3:

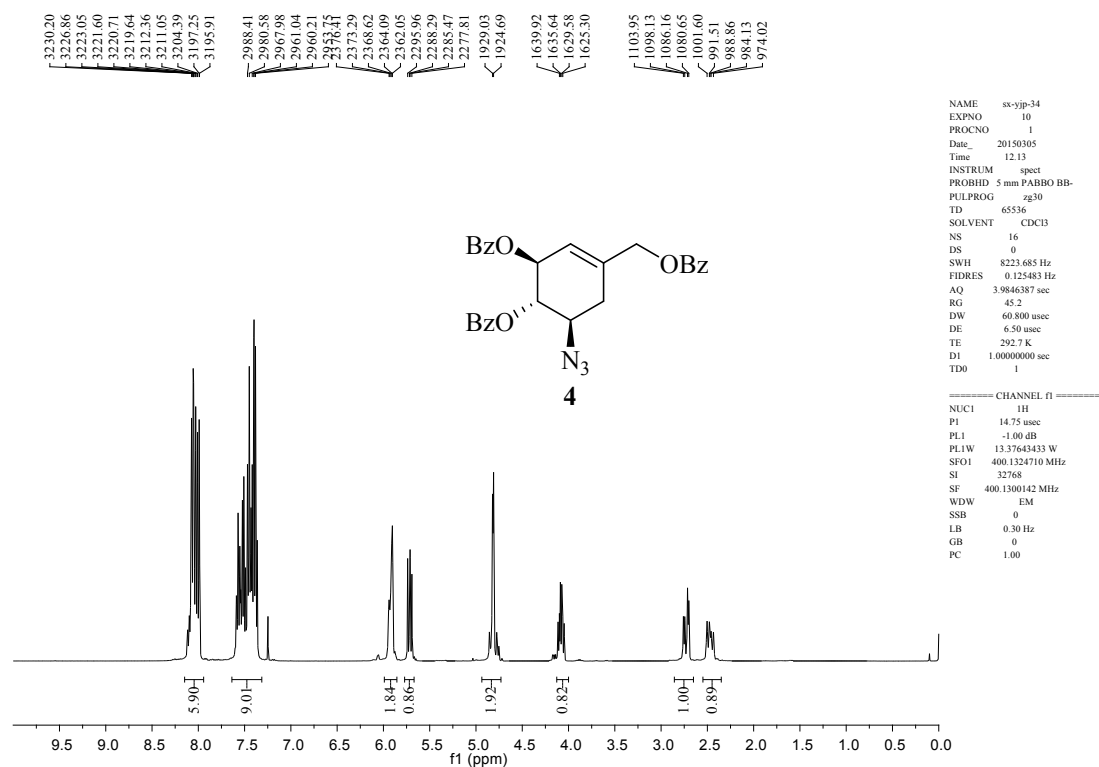


NAME sxx-qp-11
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 PROCNO 1
 Date_ 20121114
 Time 4.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 400
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 295.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

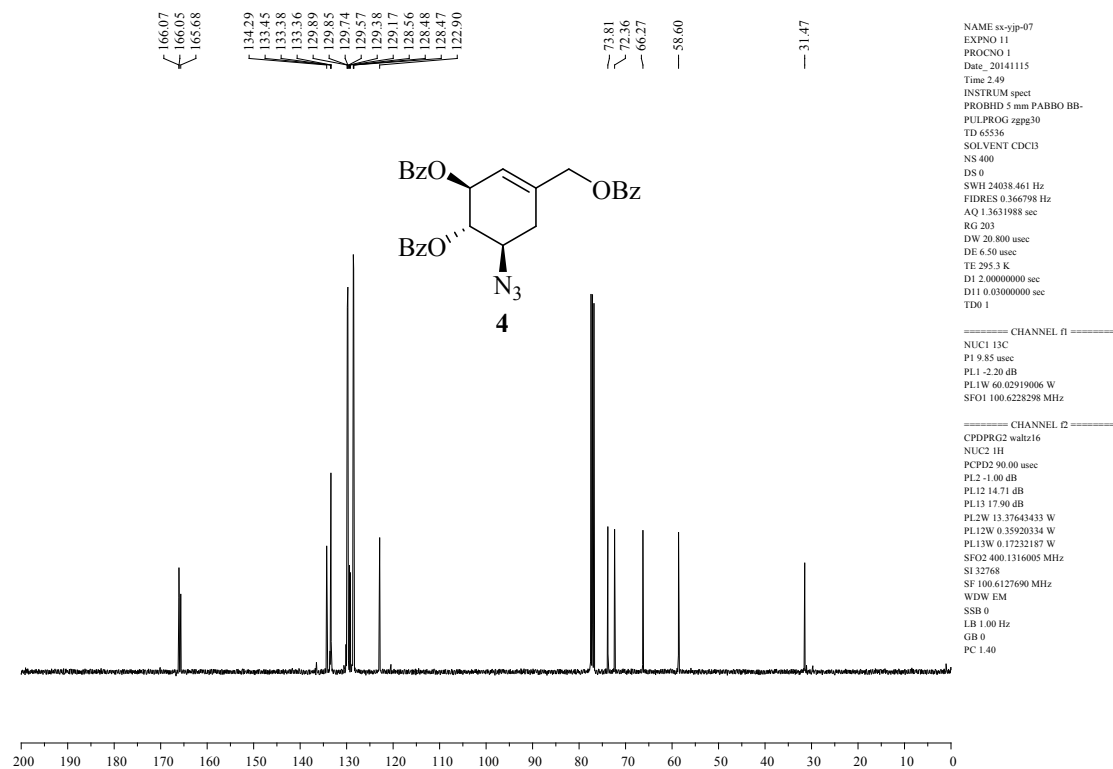
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 P1 9.85 usec
 PL1 -2.20 dB
 PL1W 60.02919006 W
 SFO1 100.6228298 MHz

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 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -1.00 dB
 PL12 14.71 dB
 PL13 17.90 dB
 PL2W 13.37643433 W
 PL12W 0.35920334 W
 PL13W 0.17232187 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

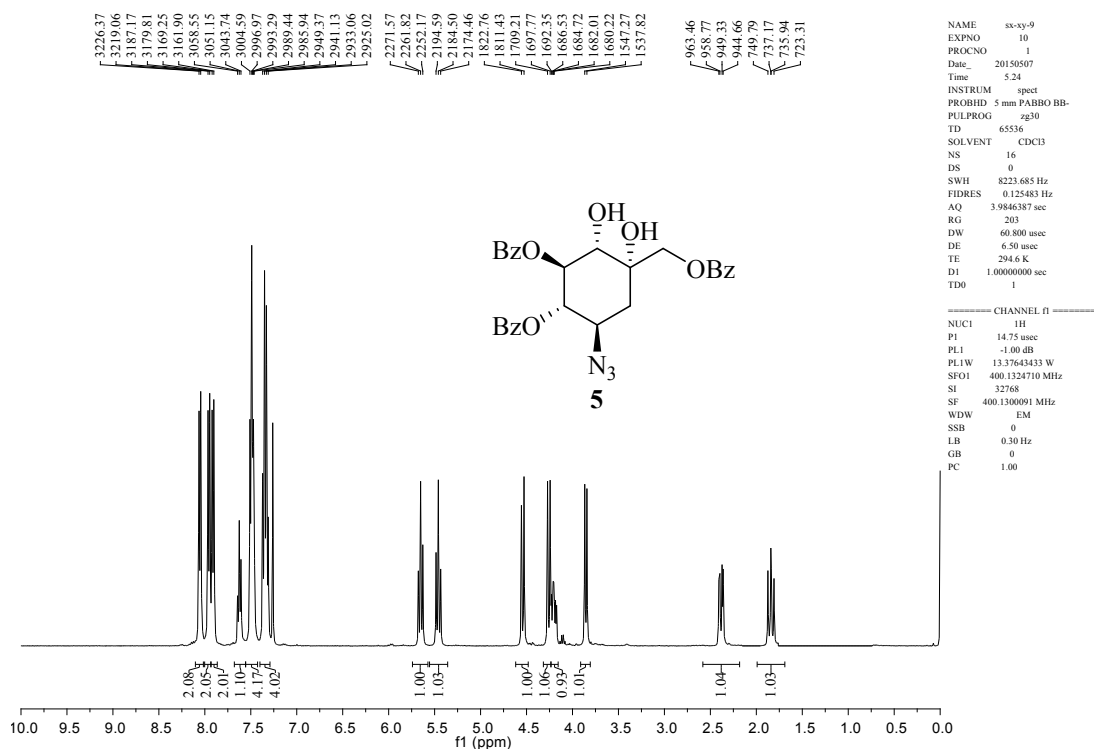
¹H NMR (400 MHz, CDCl₃) spectrum of compound 4:



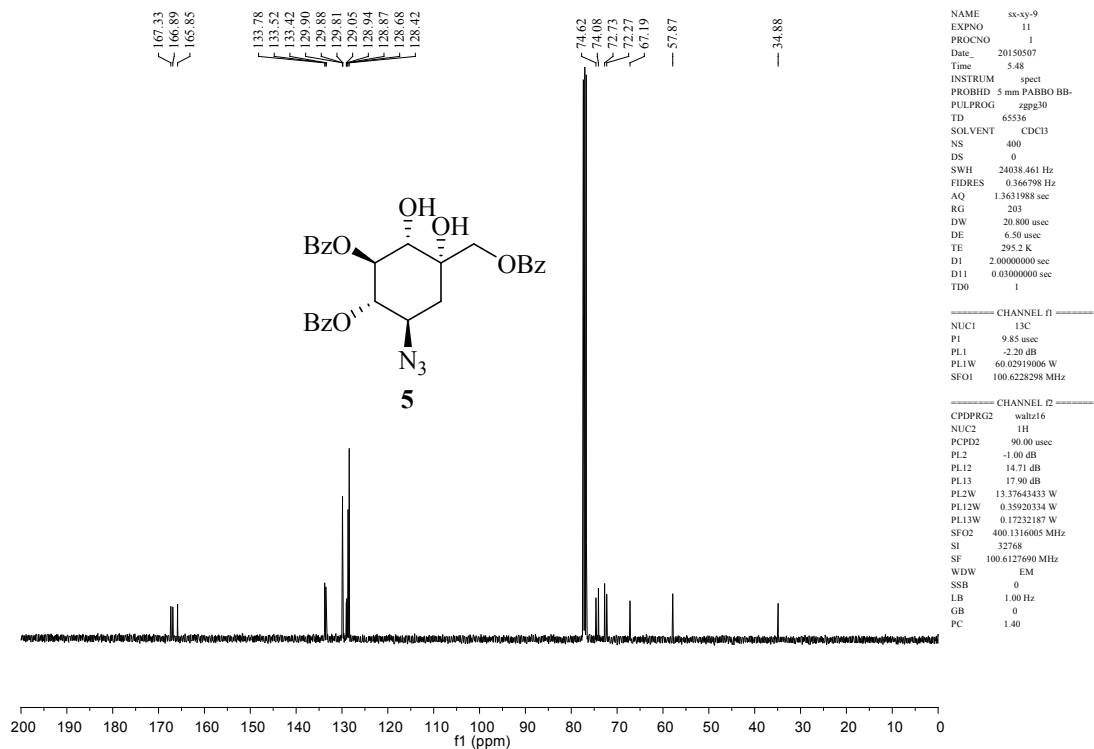
¹³C NMR (100 MHz, CDCl₃) spectrum of compound 4:



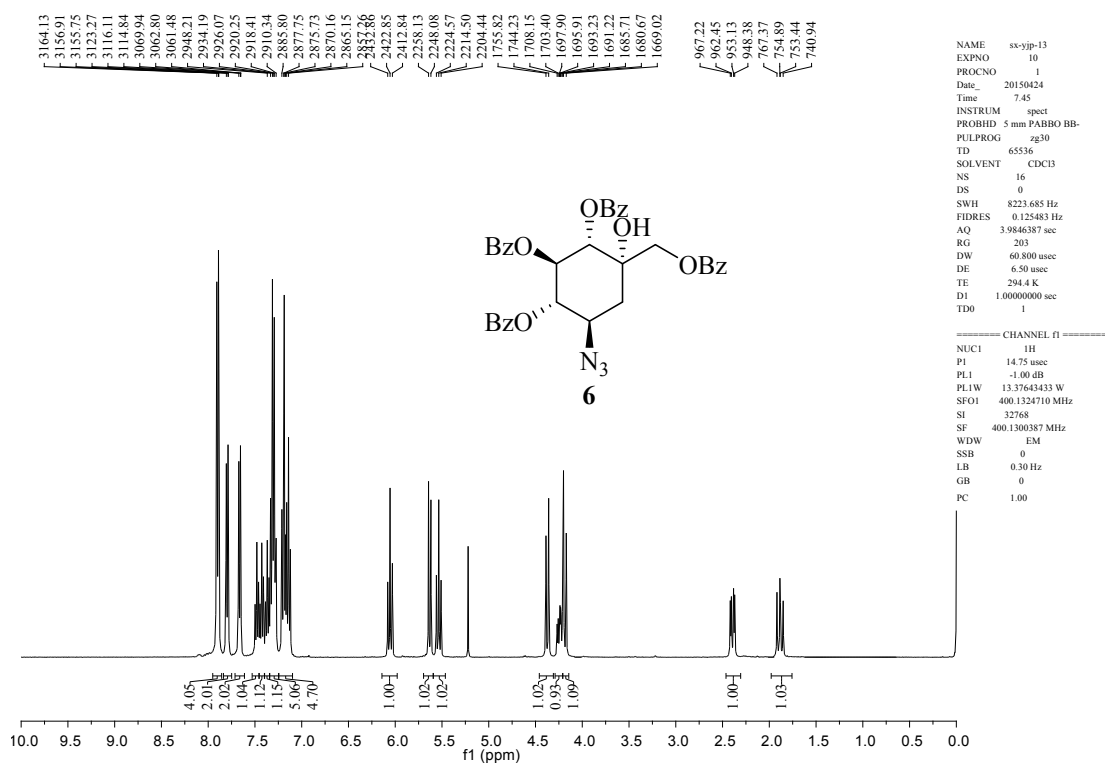
¹H NMR (400 MHz, CDCl₃) of spectrum of compound **5**:



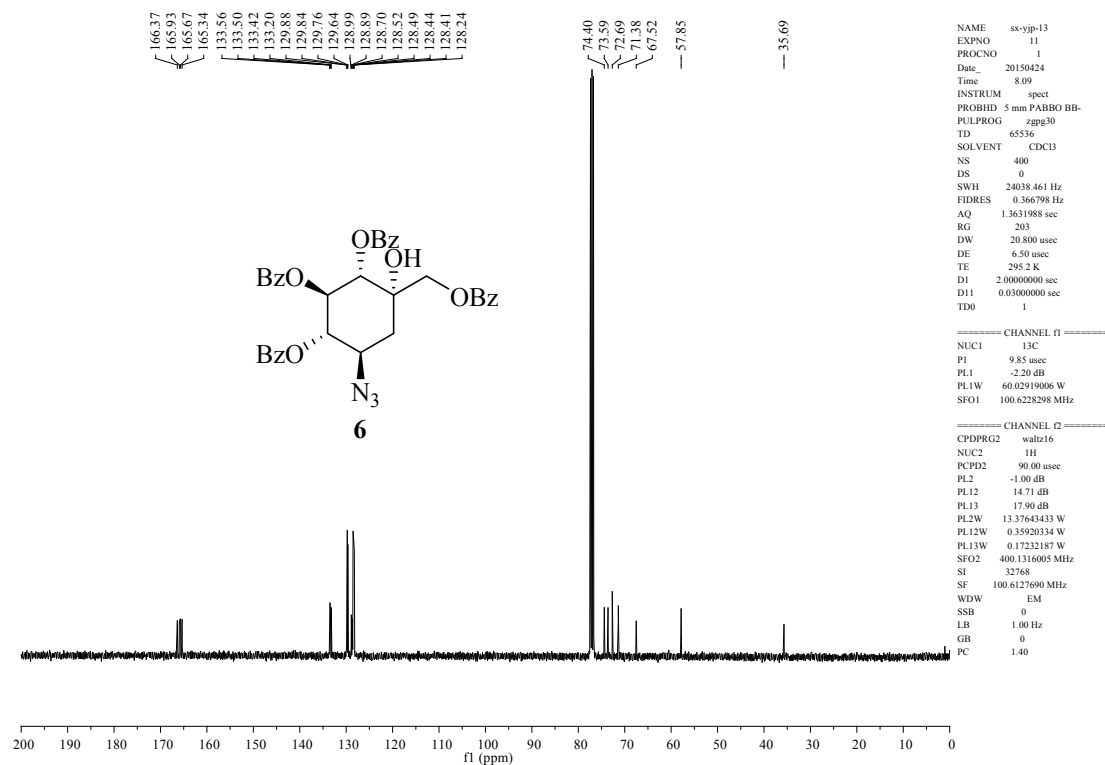
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **5**:



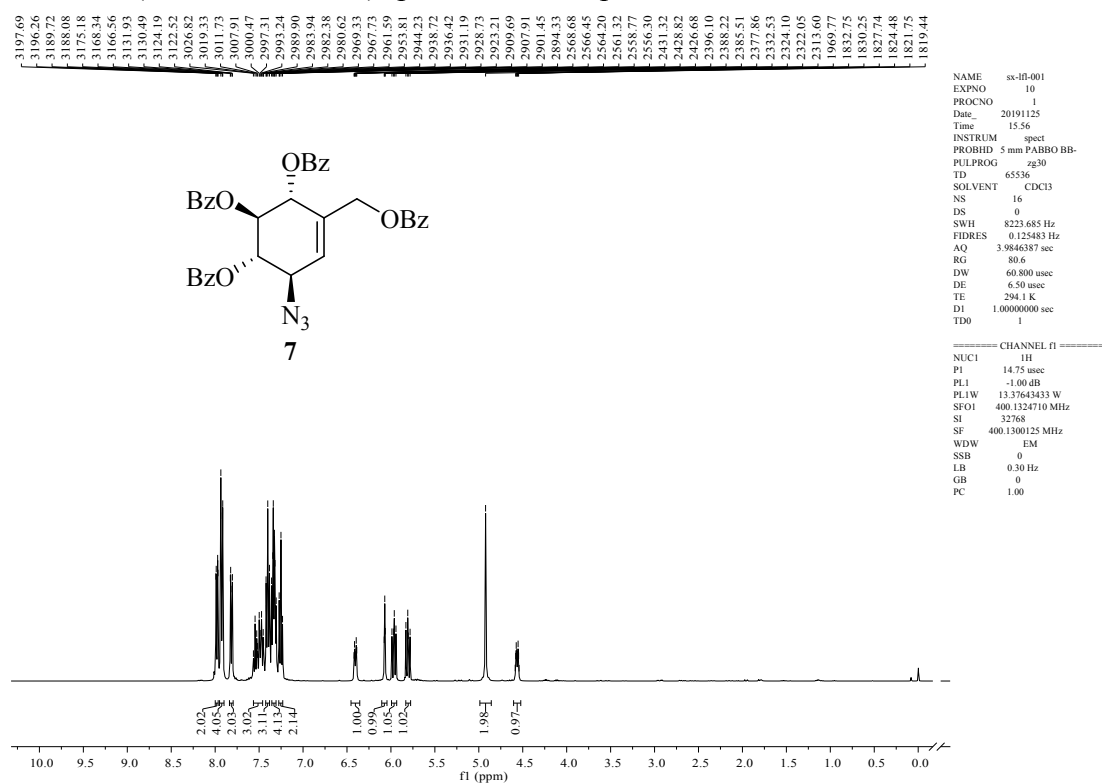
¹H NMR (400 MHz, CDCl₃) spectrum of compound **6**:



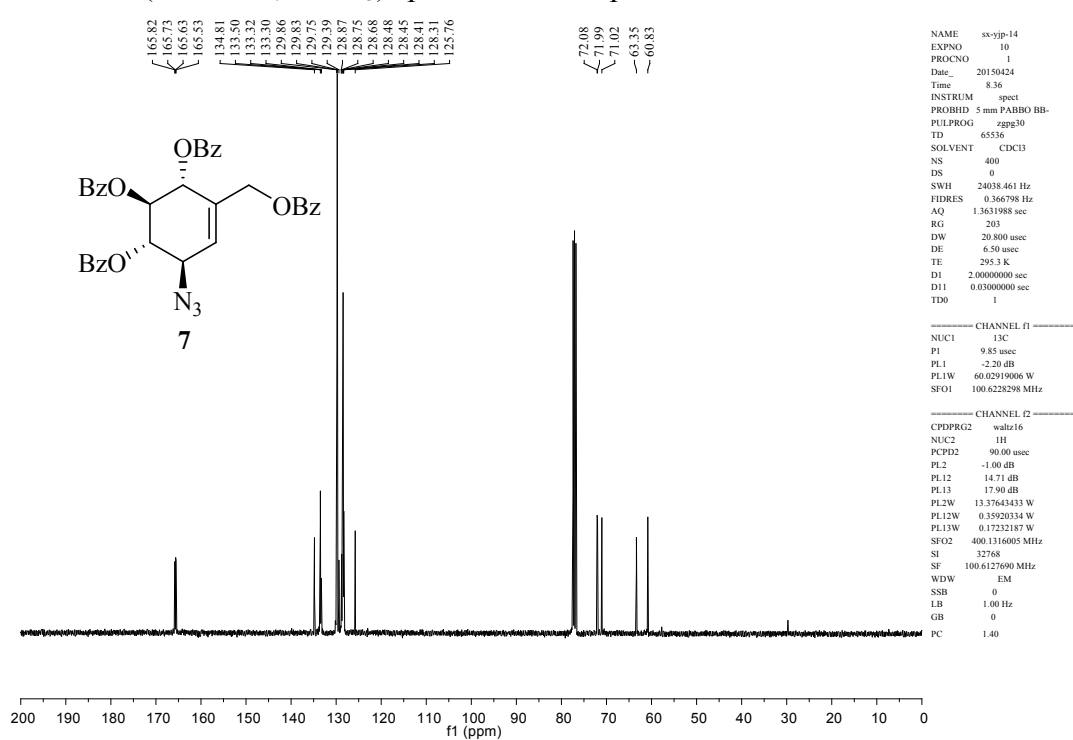
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **6**:



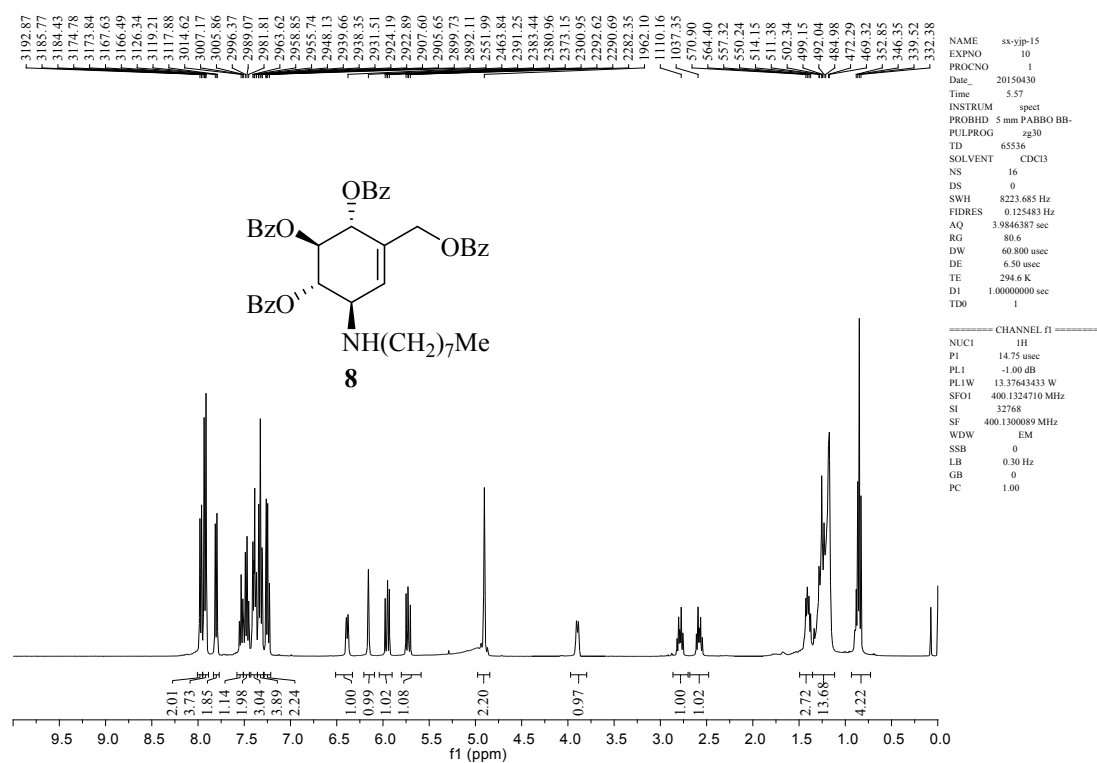
¹H NMR (400 MHz, CDCl₃) spectrum of compound 7:



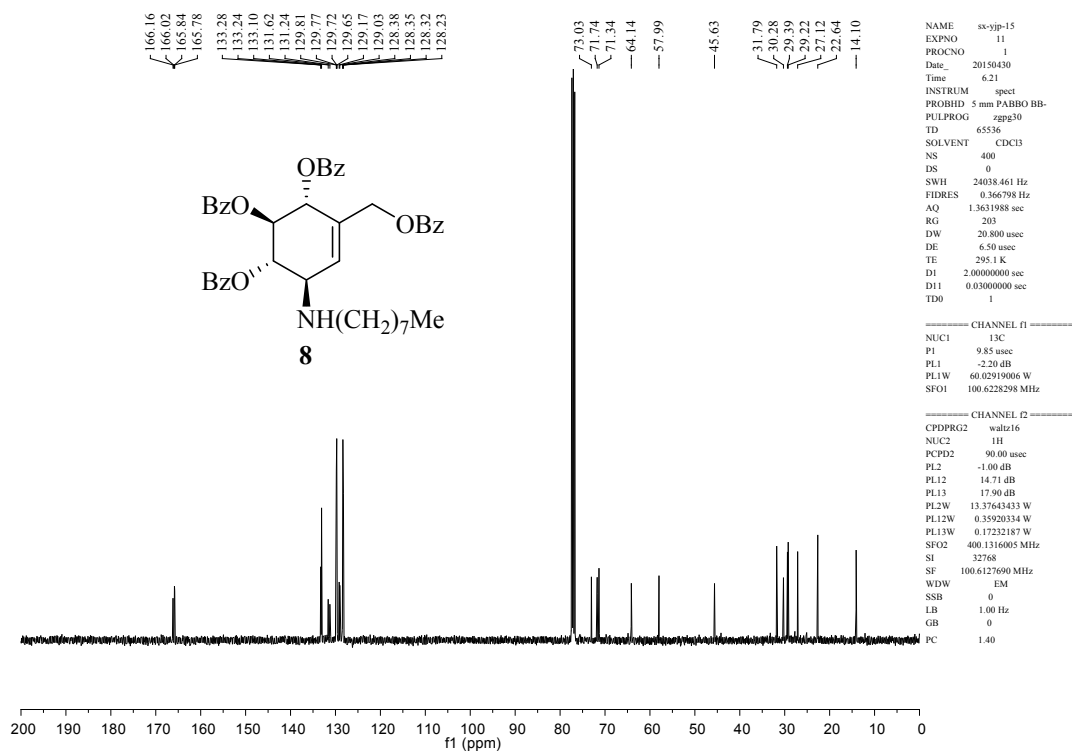
¹³C NMR (100 MHz, CDCl₃) spectrum of compound 7:



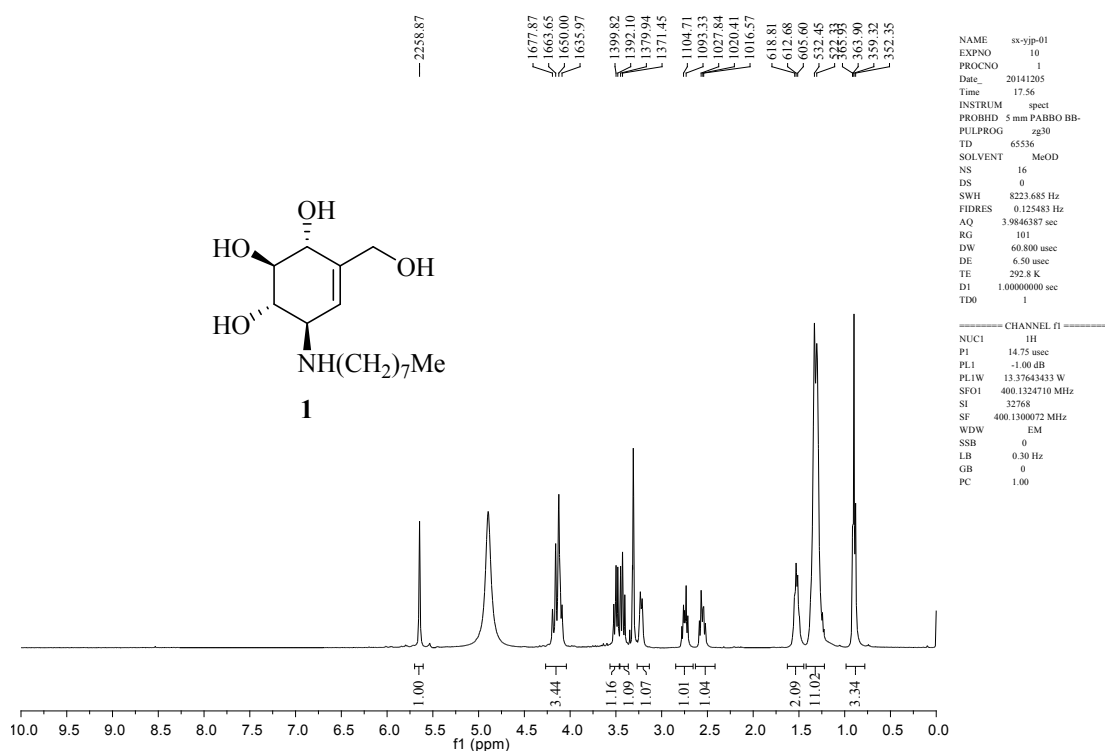
¹H NMR (400 MHz, CDCl₃) spectrum of compound **8**:



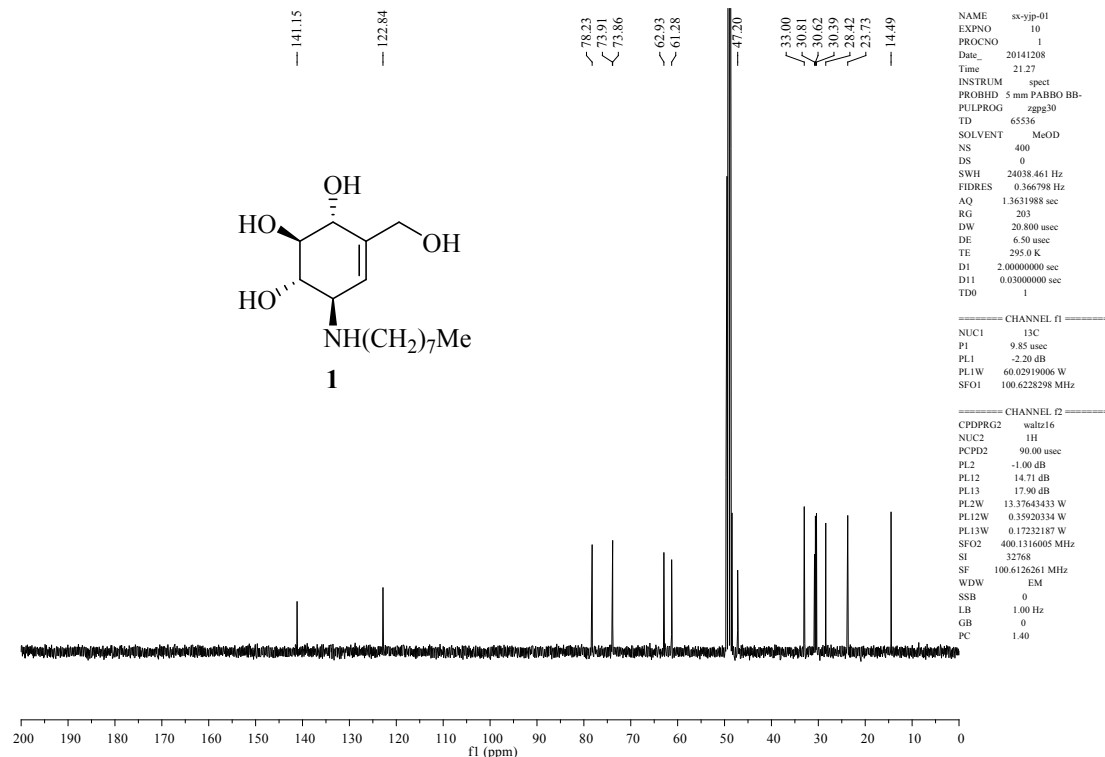
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **8**:



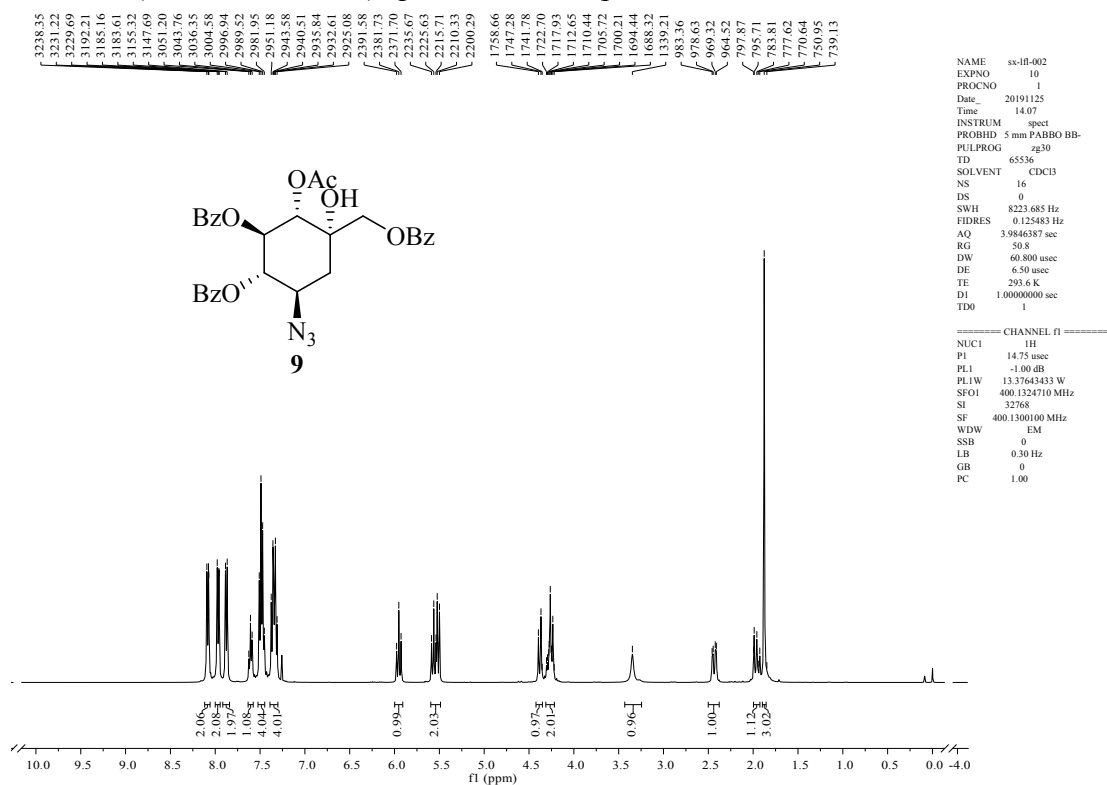
¹H NMR (400 MHz, CD₃OD) spectrum of NOV 1:



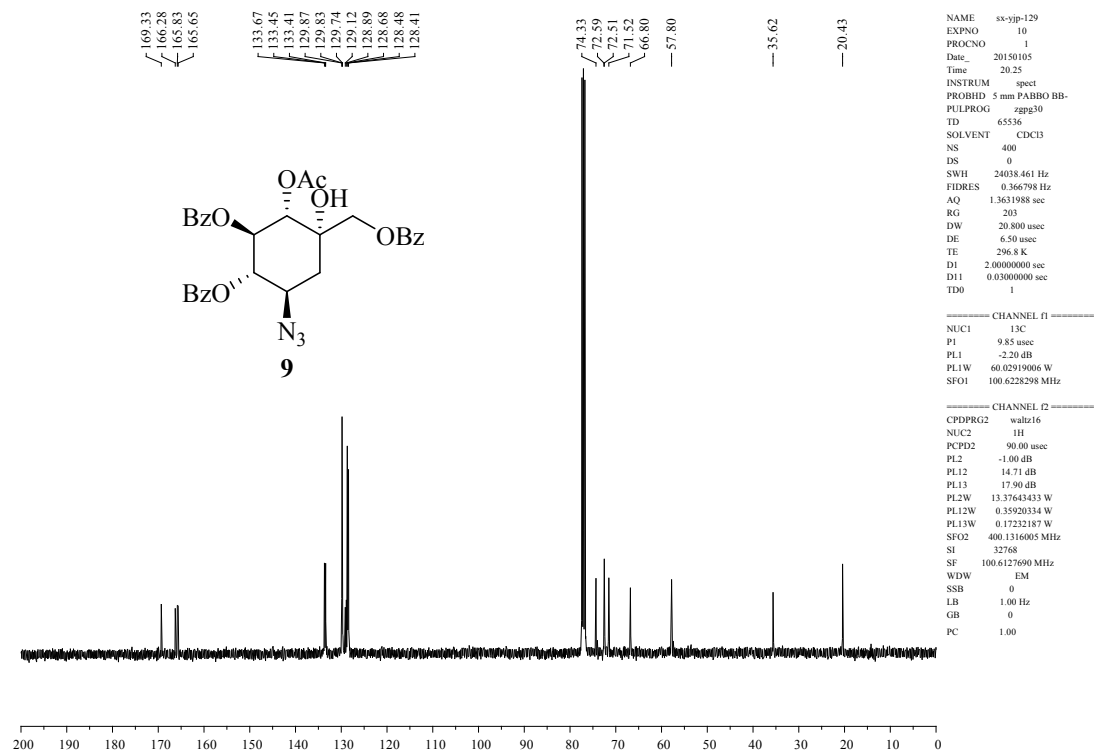
¹³C NMR (100 MHz, CD₃OD) spectrum of NOV 1:



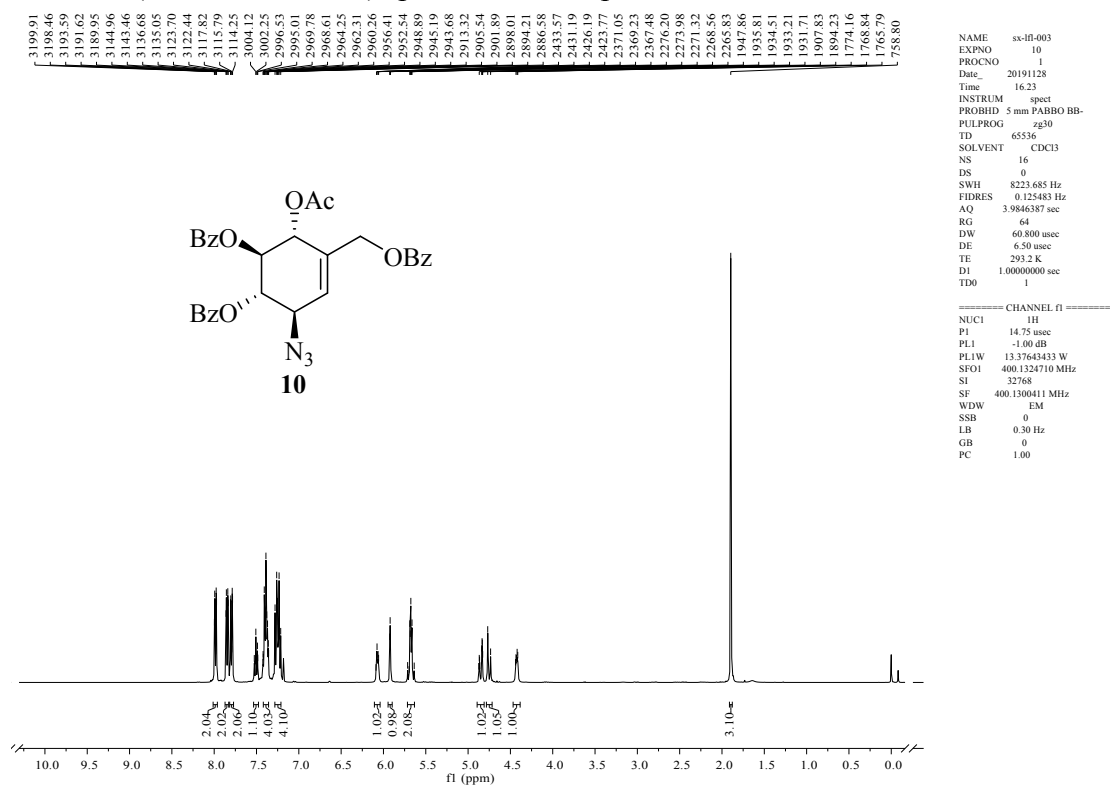
¹H NMR (400 MHz, CDCl₃) spectrum of compound **9**:



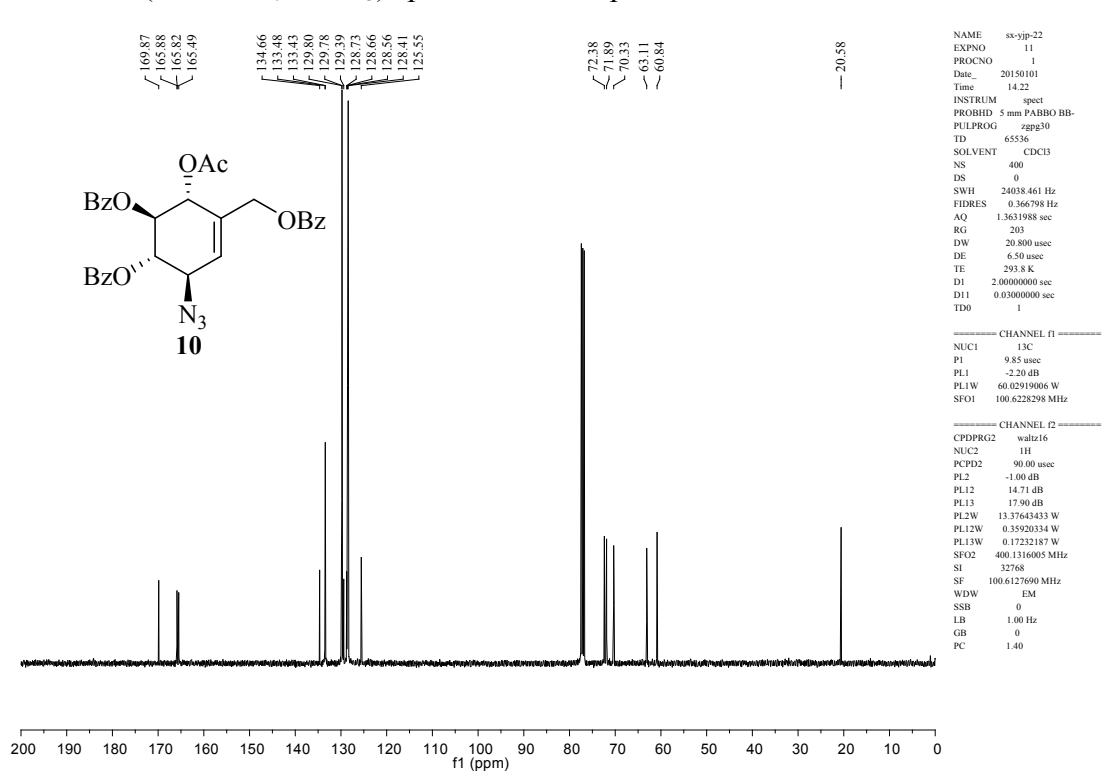
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **9**:



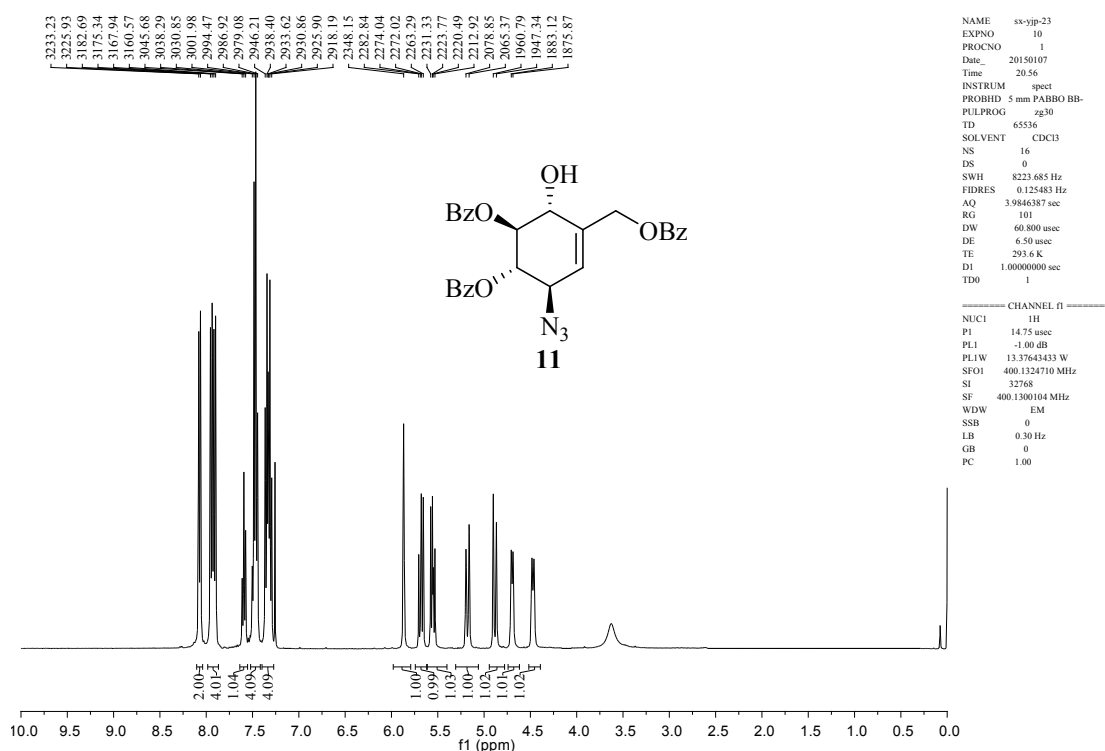
¹H NMR (400 MHz, CDCl₃) spectrum of compound **10**:



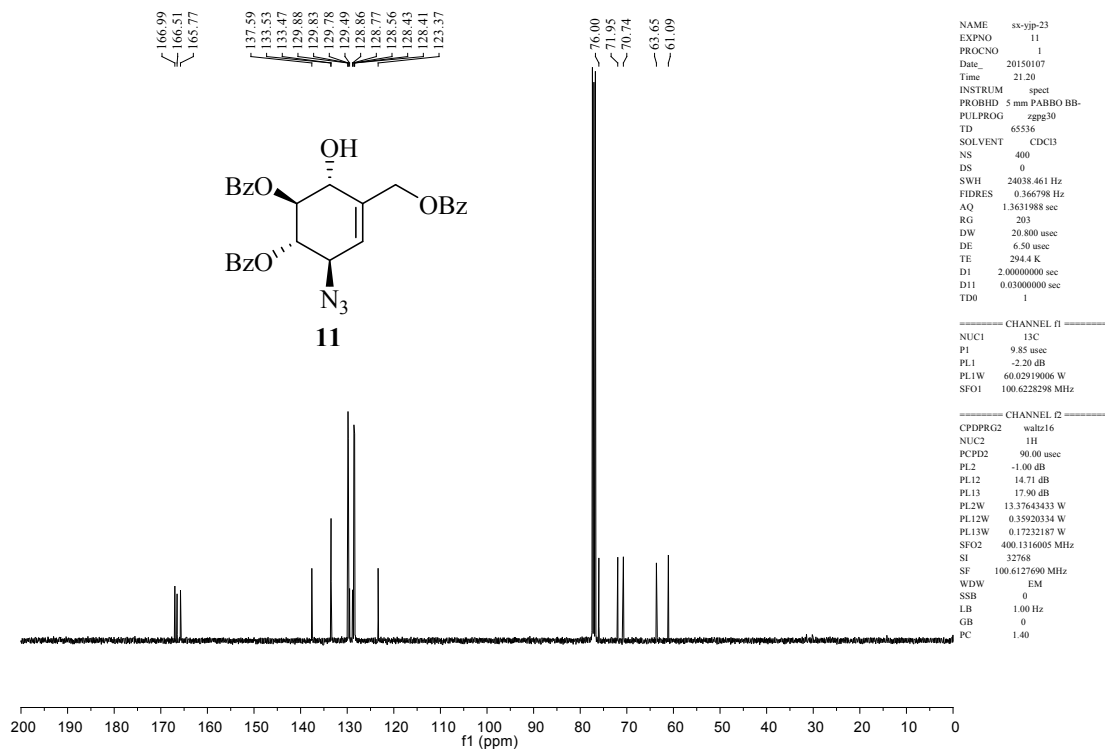
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **10**:



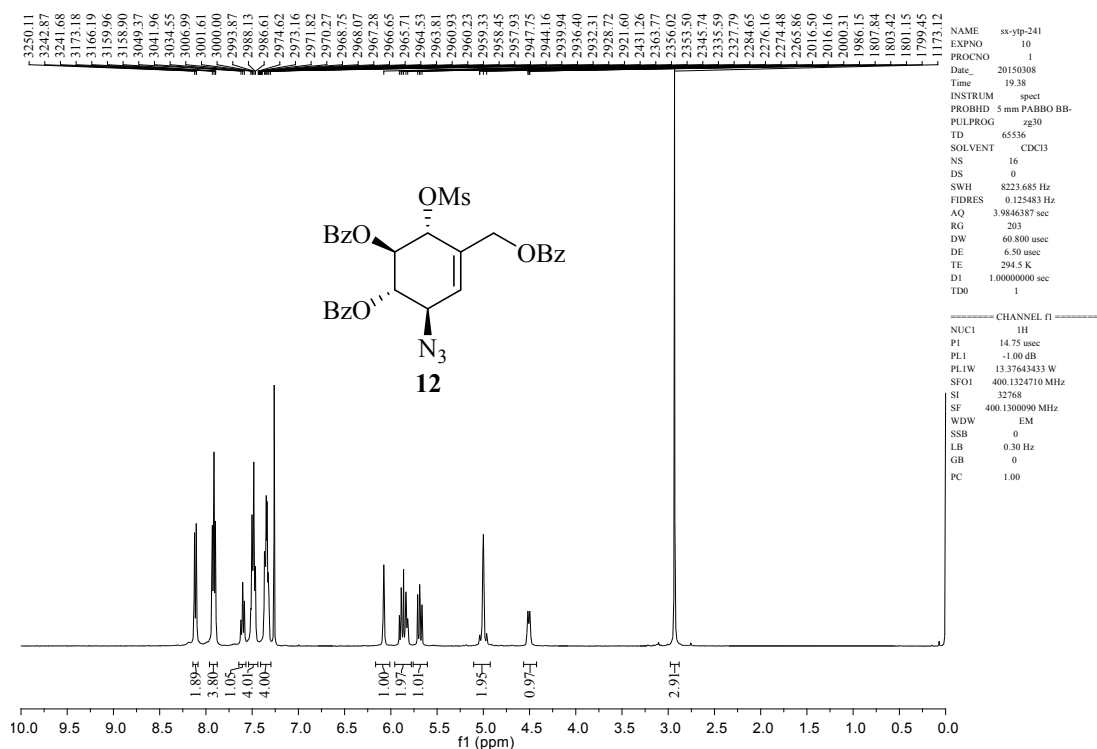
¹H NMR (400 MHz, CDCl₃) spectrum of compound **11**:



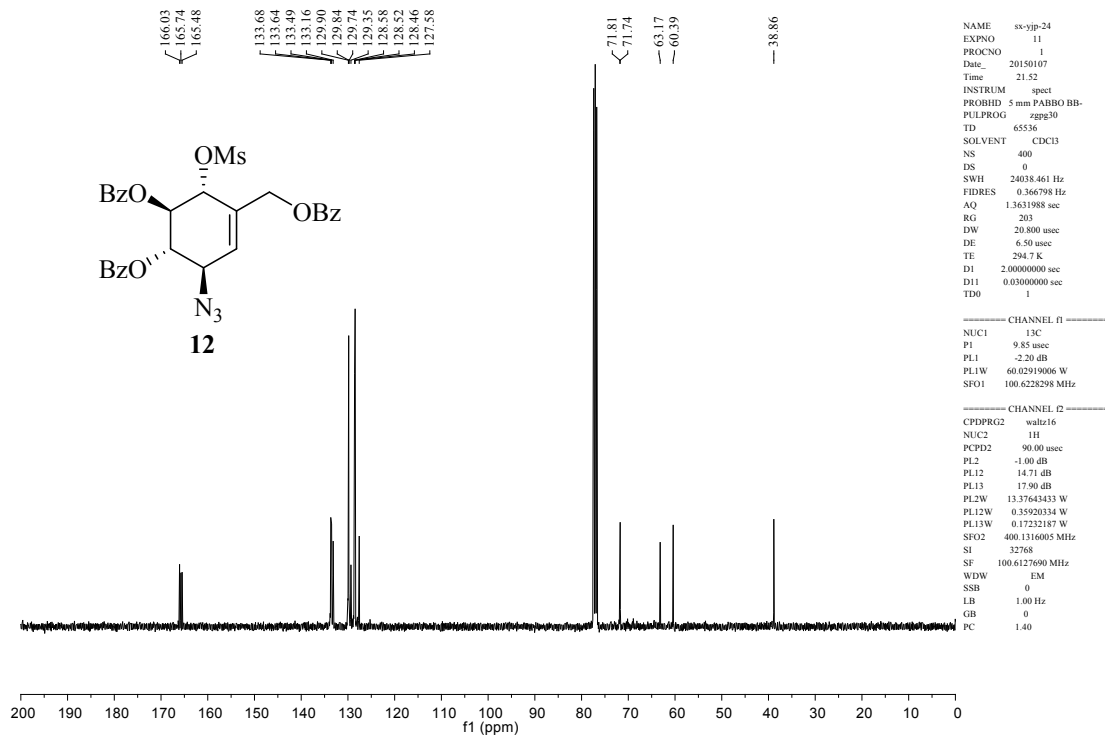
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **11**:



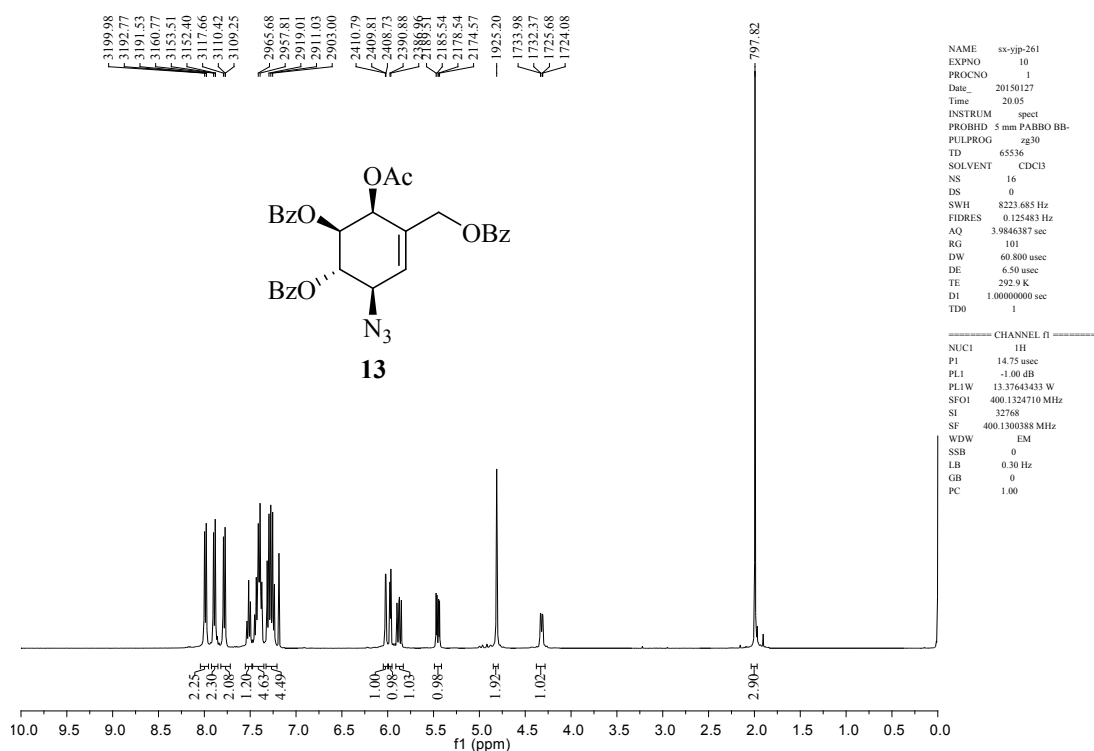
¹H NMR (400 MHz, CDCl₃) spectrum of compound **12**:



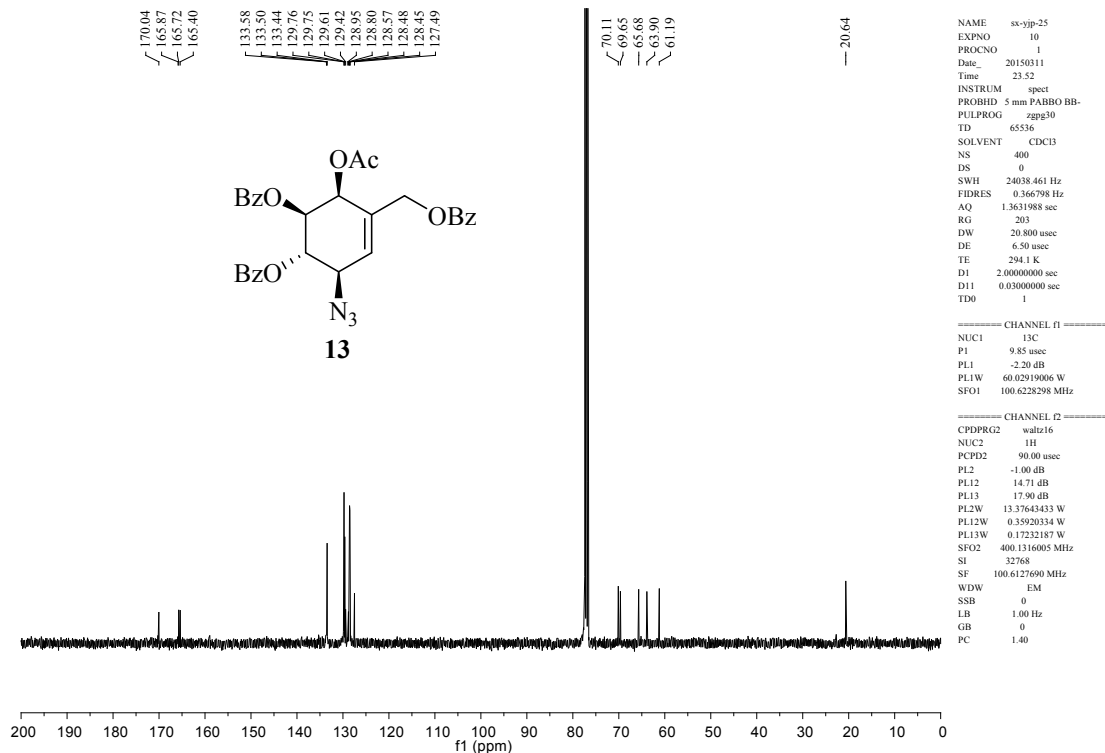
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **12**:



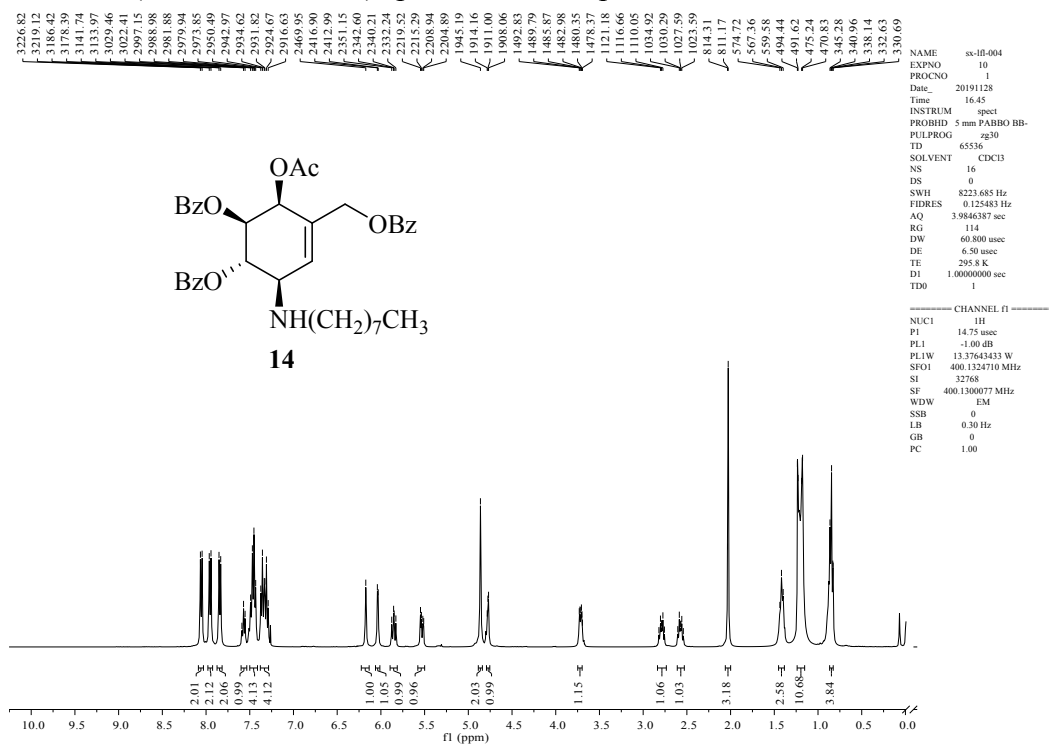
¹H NMR (400 MHz, CDCl₃) spectrum of compound **13**:



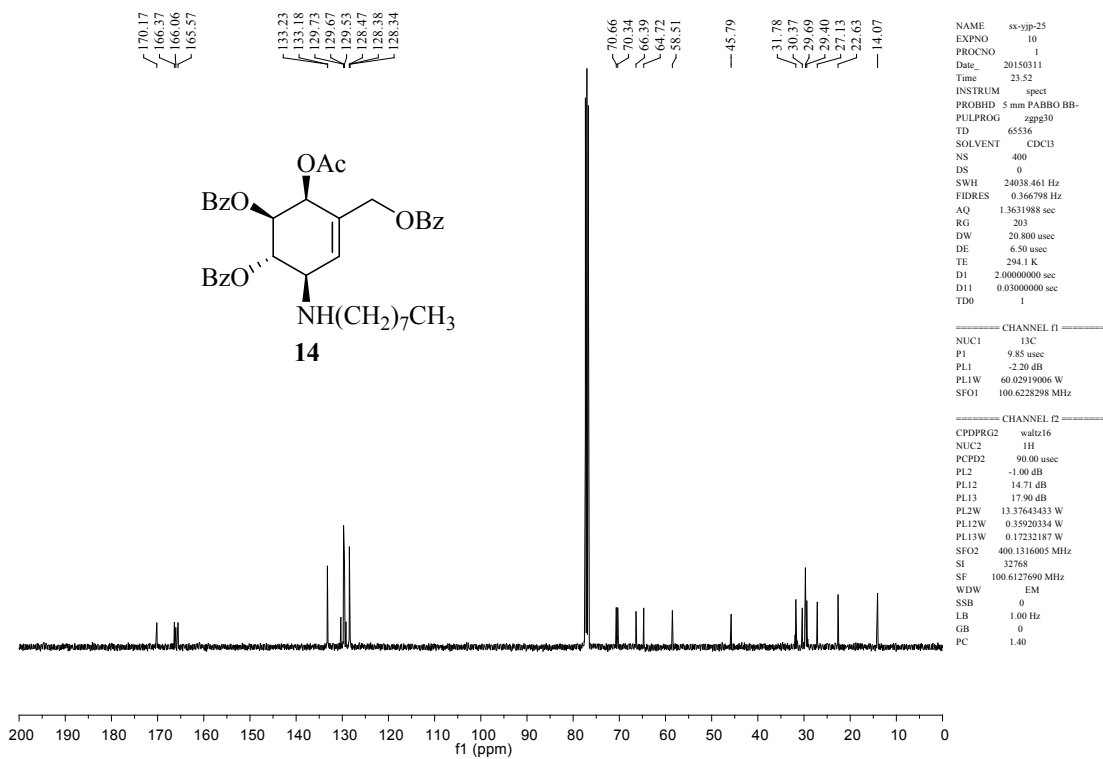
¹³C NMR (100 MHz, CDCl₃) spectrum of compound **13**:



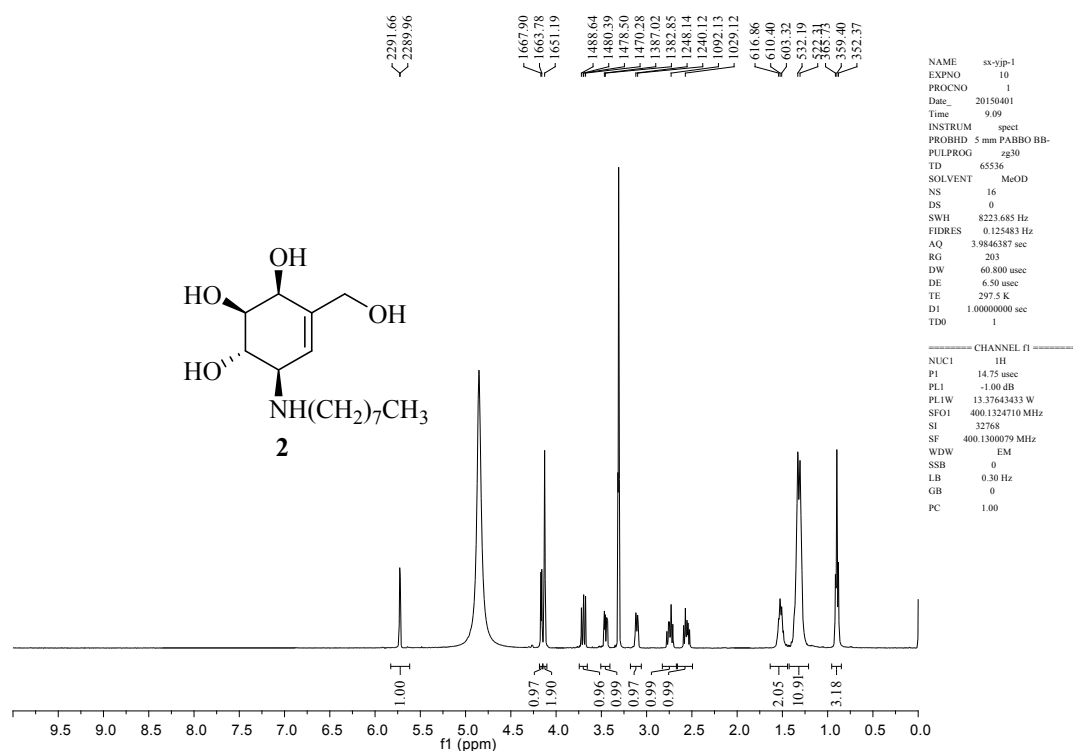
¹H NMR (400 MHz, CDCl₃) spectrum of compound **14**:



¹³C NMR (100 MHz, CDCl₃) spectrum of compound **14**:



¹H NMR (400 MHz, CD₃OD) spectrum of NOEV 2:



¹³C NMR (100 MHz, CD₃OD) spectrum of NOEV 2:

