

Supplementary Data

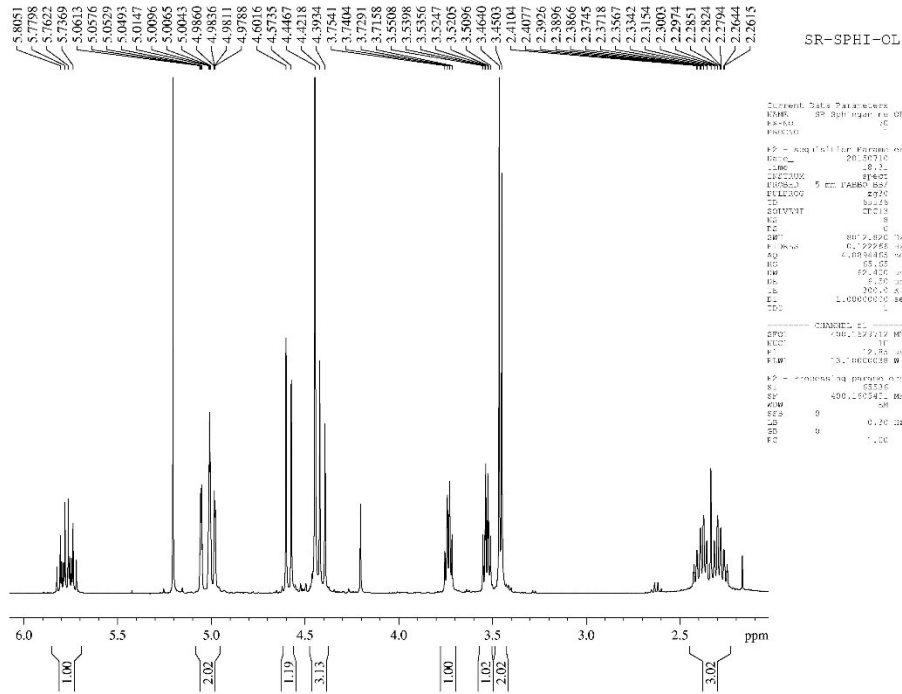
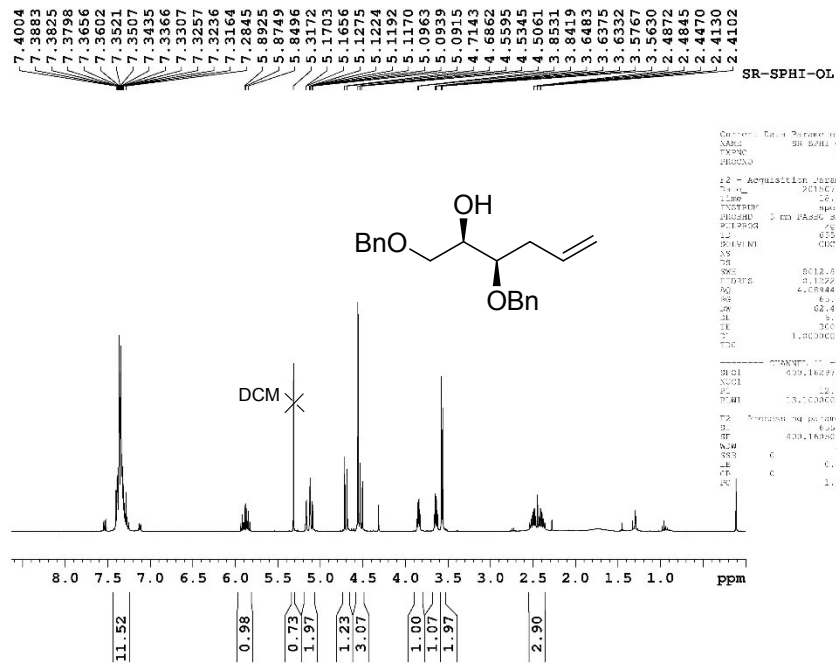
‘Chiron’ approach to stereoselective synthesis of Sphinganine and unnatural Safingol, an antineoplastic and antipsoriatic agent

Somireddy Kundooru, Pintu Das and Arun K. Shaw*

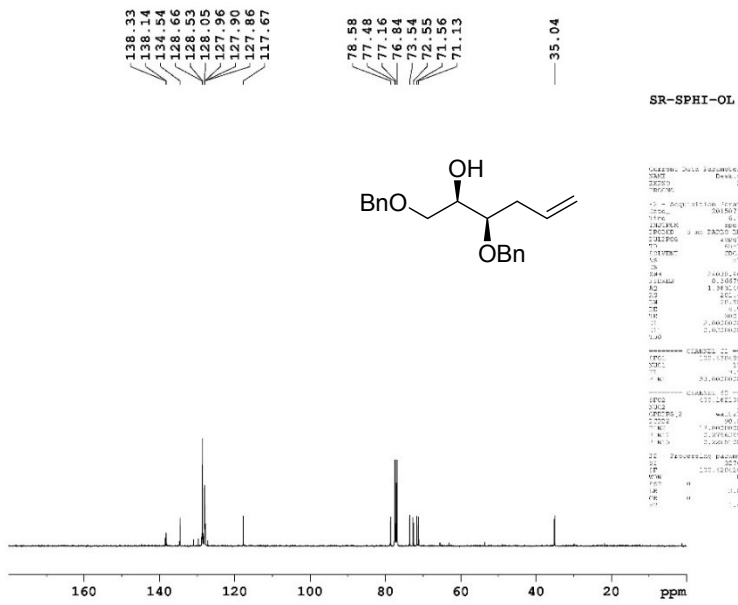
Division of Medicinal and Process Chemistry, CSIR-Central Drug Research Institute, Lucknow 226 031, India.

Contents:

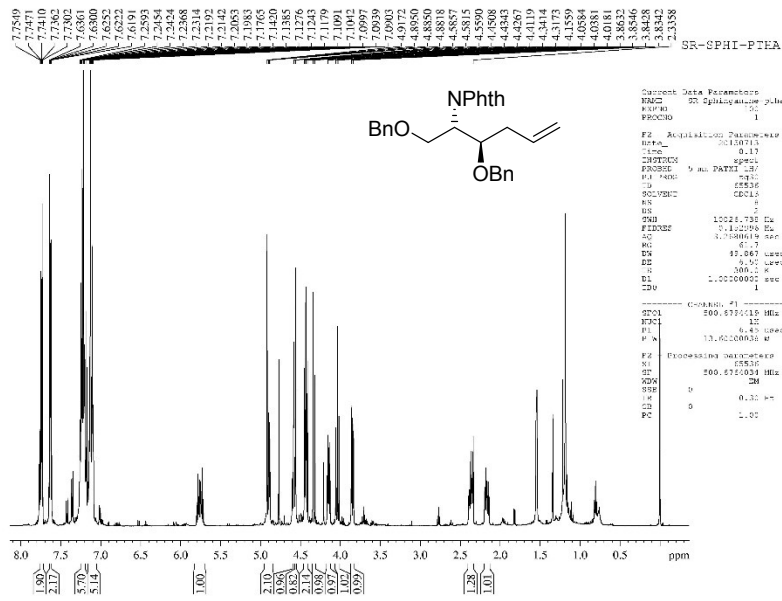
| | |
|---|--------------|
| 1. ¹ H NMR data of Compound 4 | Page No – 2 |
| 2. ¹³ C NMR data of Compound 4 | Page No – 3 |
| 3. ¹ H data of Compound 5 | Page No – 3 |
| 4. ¹ H and ¹³ C data of Compound 5 | Page No – 4 |
| 5. ¹ H data of Compound 7 | Page No – 5 |
| 6. ¹³ C data of Compound 7 | Page No – 6 |
| 7. ¹ H data of Compound 8 | Page No – 6 |
| 8. ¹ H and ¹³ C data of Compound 8 | Page No – 7 |
| 9. ¹ H and ¹³ C data of Compound 1 | Page No – 8 |
| 10. ¹ H data of Compound 12 | Page No – 9 |
| 11. ¹³ C data of Compound 12 | Page No – 10 |
| 12. ¹ H data of Compound 13 | Page No – 10 |
| 13. ¹ H and ¹³ C data of Compound 13 | Page No – 11 |
| 14. ¹ H data of Compound 15 | Page No – 12 |
| 15. ¹³ C data of Compound 15 | Page No – 12 |
| 16. ¹ H data of Compound 16 | Page No – 13 |
| 17. ¹ H and ¹³ C data of Compound 16 | Page No – 14 |
| 18. ¹ H and ¹³ C data of Compound 17 | Page No – 15 |
| 19. HRMS Spectra of compounds 4 and 5 | Page No – 16 |
| 20. HRMS Spectra of compounds 7 and 8 | Page No – 17 |
| 21. HRMS Spectra of compounds 1(Sphinganine) and 12 | Page No – 18 |
| 22. HRMS Spectra of compounds 13 and 15 | Page No – 19 |
| 23. HRMS Spectra of compounds 16 and 17(Safingol) | Page No – 20 |



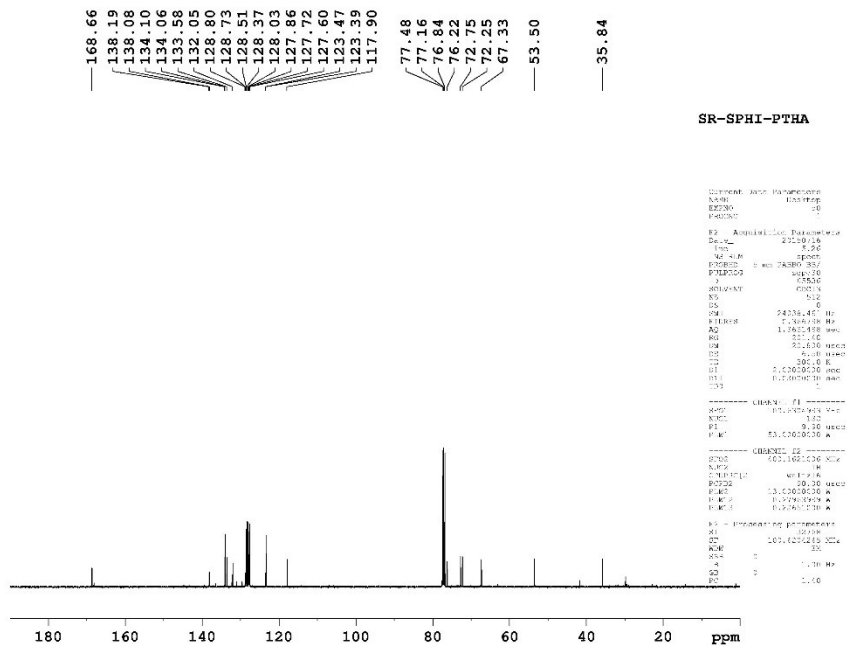
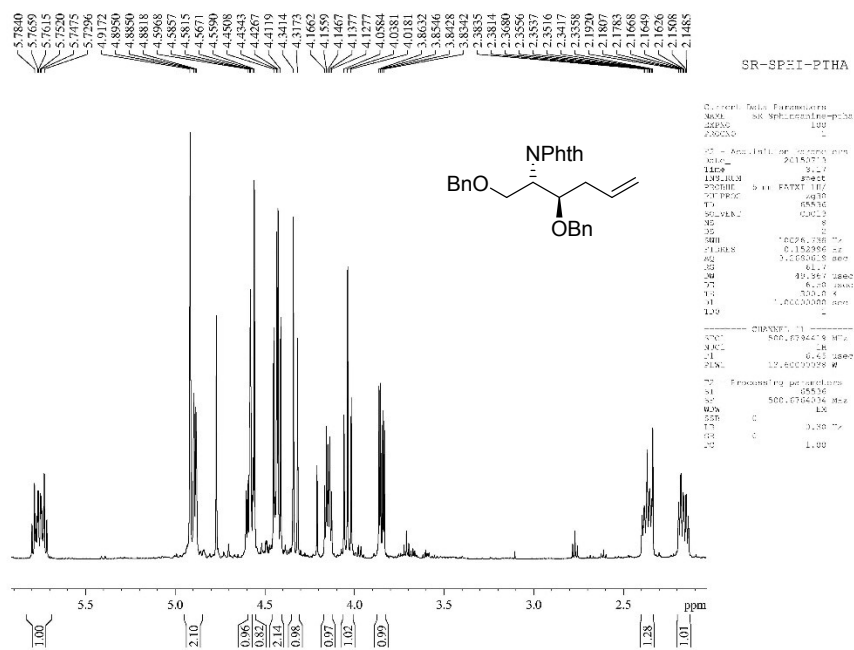
¹H NMR Spectra of Compound 4



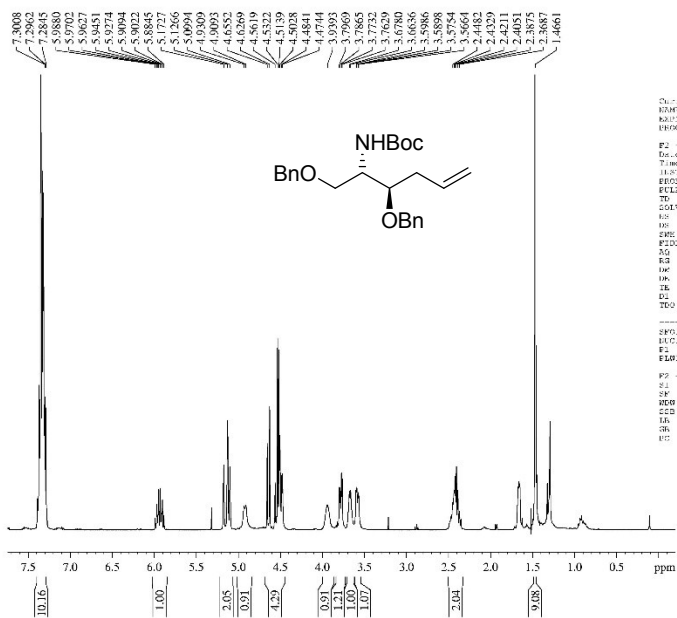
¹³C NMR Spectrum of Compound 4



¹H NMR Spectrum of Compound 5



¹H and ¹³C NMR Spectra of Compound 5



SR-SPHI-BOC

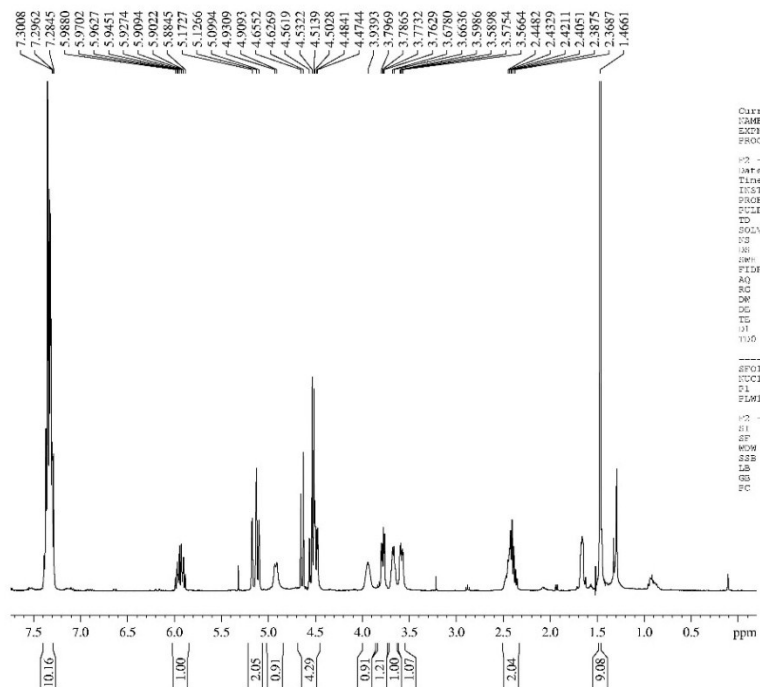
```

Current Data Parameters
NAME SR SPHI-BOC
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150717
Time 11:27
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 8
SWH 8012.820 Hz
FIDRES 0.122216 Hz
AQ 4.058443 sec
RG 65.55
DE 62.400 usec
TE 300.2 K
SI 1.00000000 sec
RG 1

===== CHANNEL f1 =====
SF01 400.162912 MHz
NUC1 1H
P1 13.20 usec
PL1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1605000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
EC 1.00
  
```



SR-SPHI-BOC

```

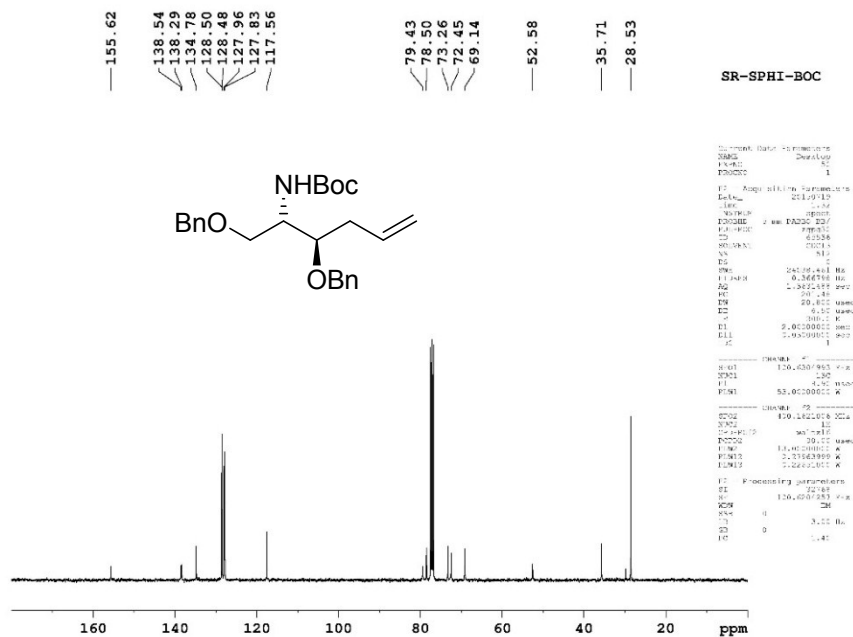
Current Data Parameters
NAME SR SPHI-BOC
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150717
Time 11:27
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 8
SWH 8012.820 Hz
FIDRES 0.122216 Hz
AQ 4.058443 sec
RG 65.55
DE 62.400 usec
TE 300.2 K
SI 1.00000000 sec
RG 1

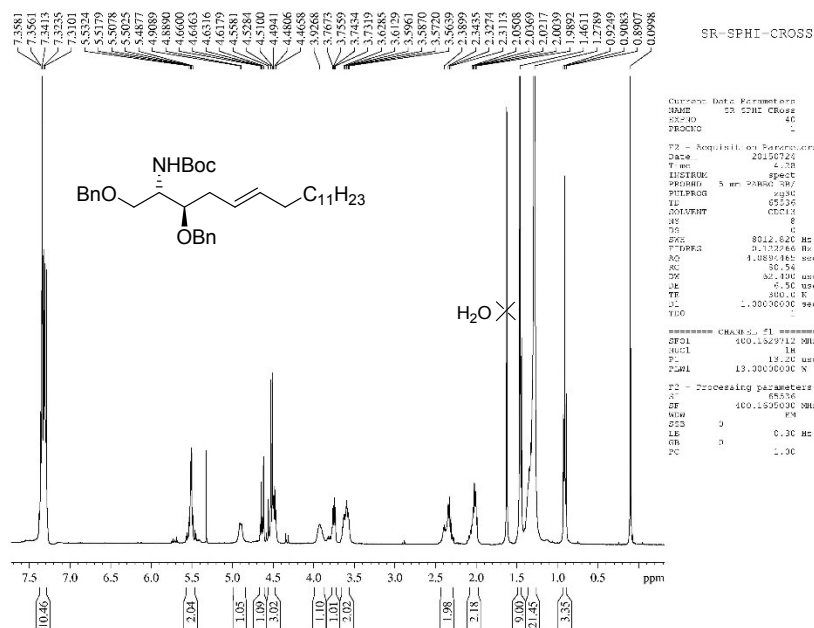
===== CHANNEL f1 =====
SF01 400.162912 MHz
NUC1 1H
P1 13.20 usec
PL1 13.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1605000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
EC 1.00
  
```

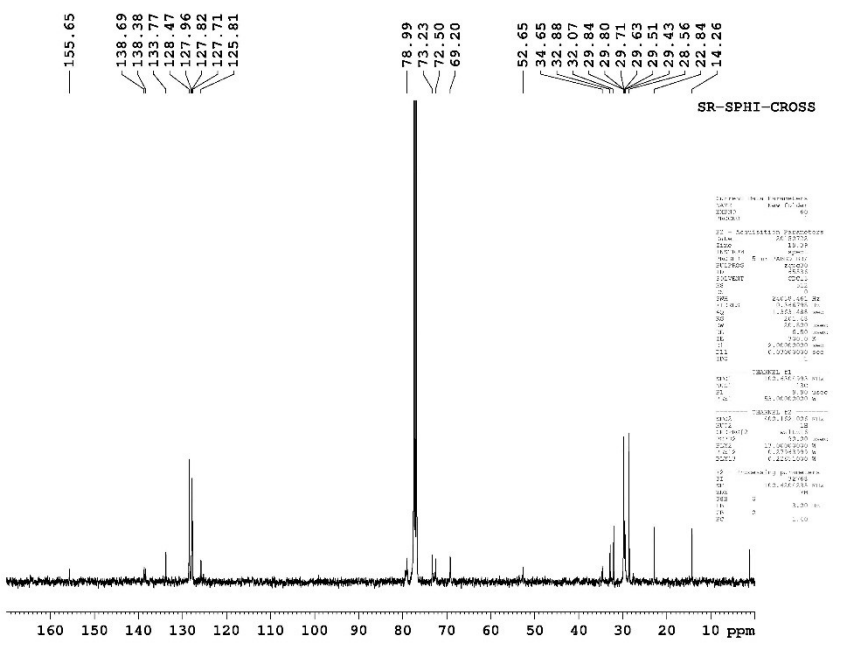
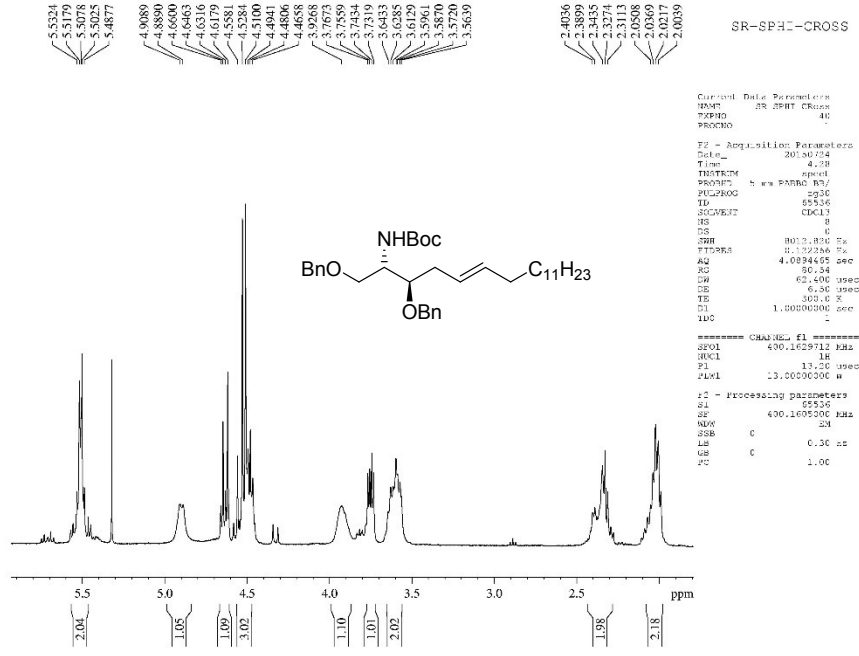
¹H NMR Spectra of Compound 7



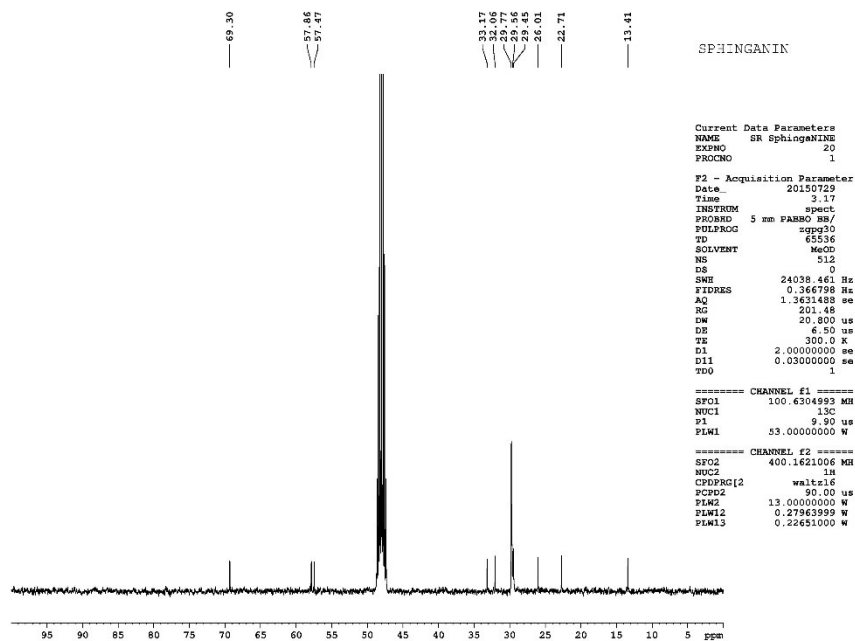
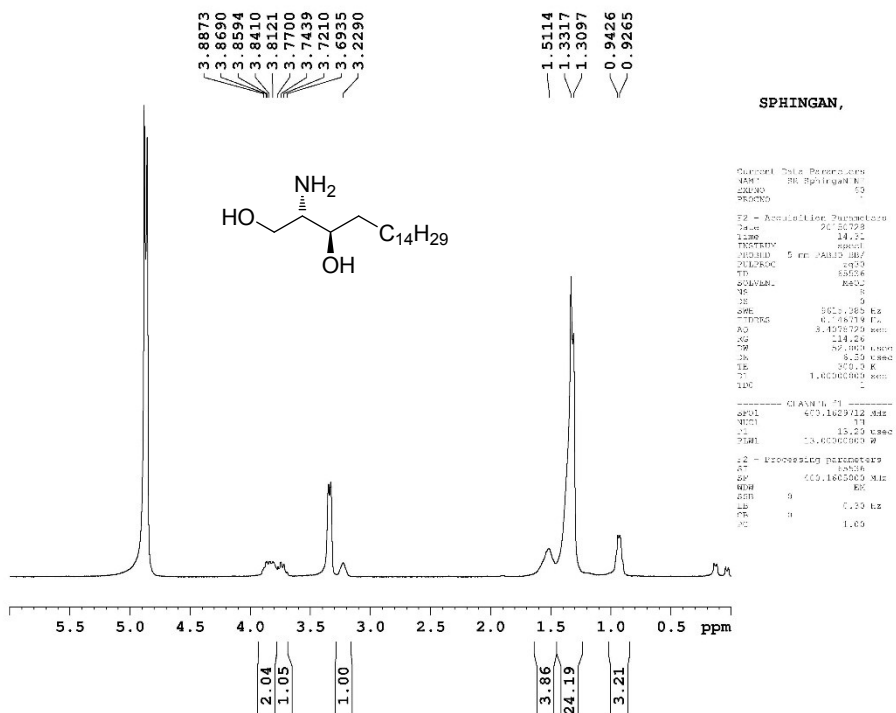
^{13}C NMR Spectrum of Compound 7



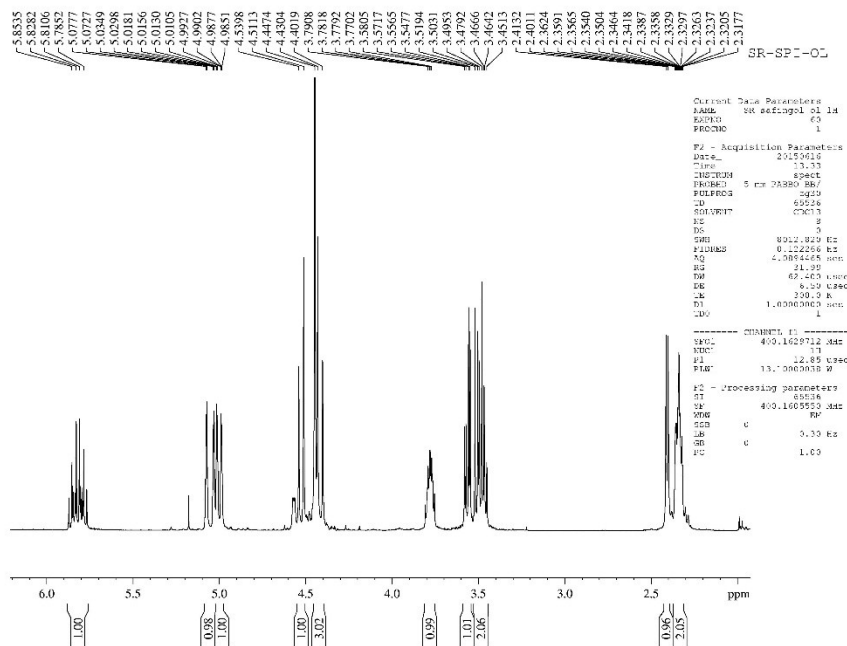
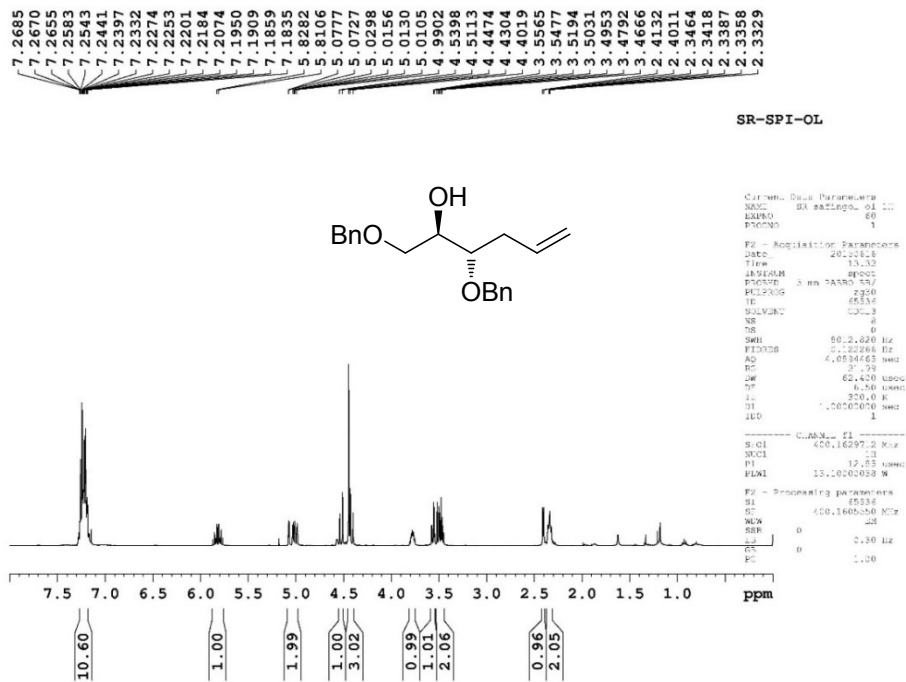
^1H NMR Spectra of Compound 8



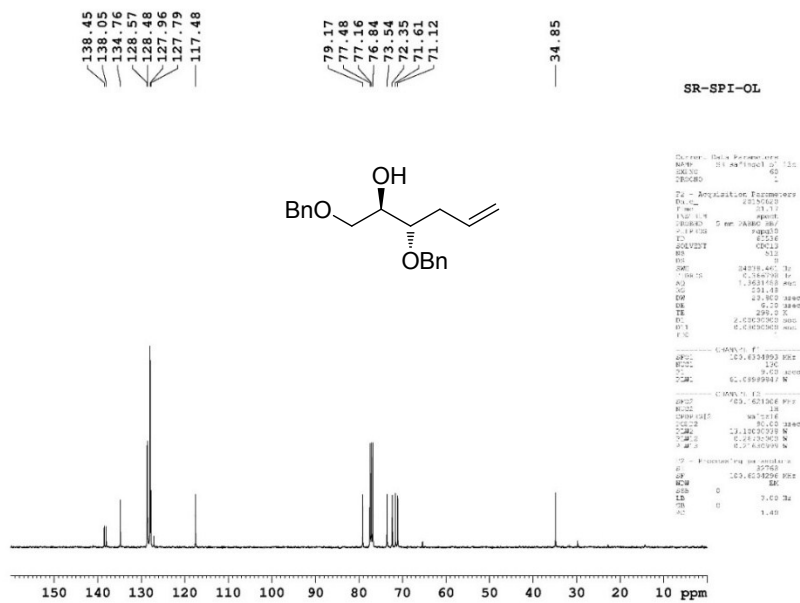
¹H and ¹³C NMR Spectra of Compound 8



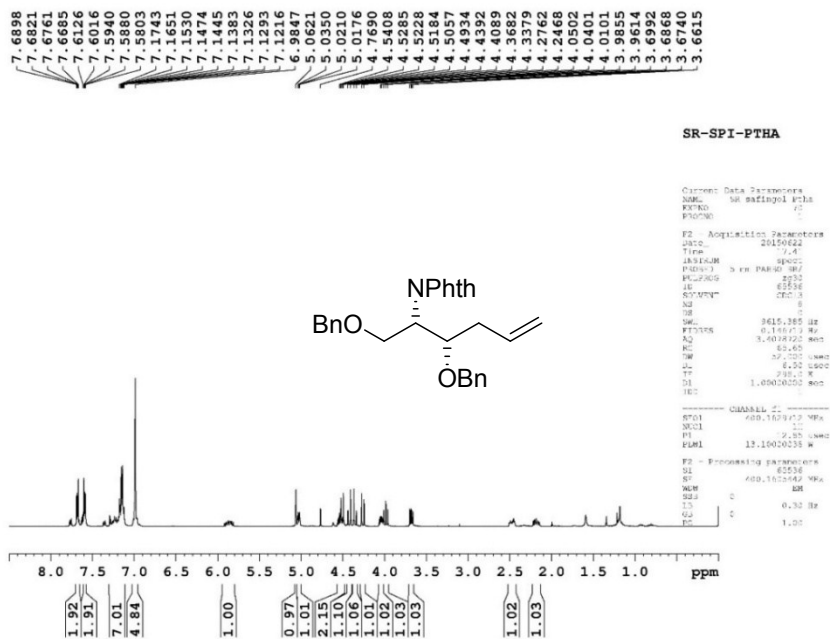
¹H and ¹³C NMR Spectra of Spinganine 1



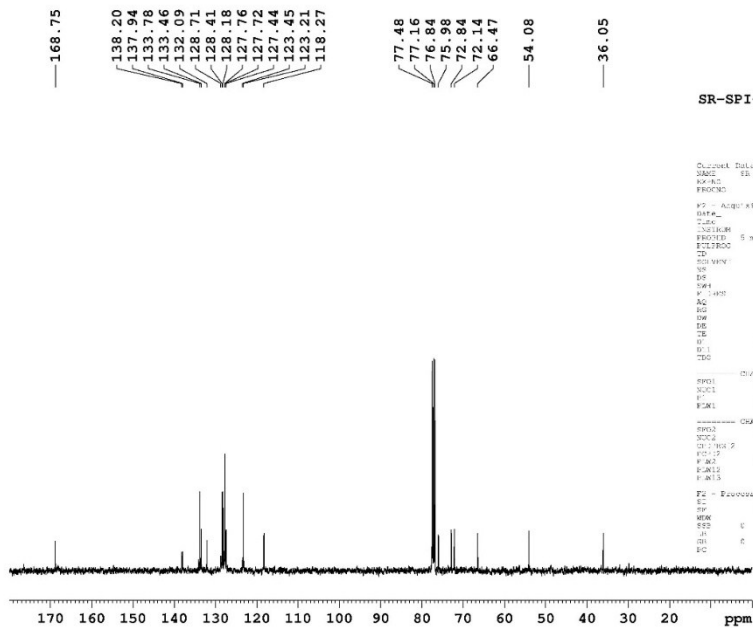
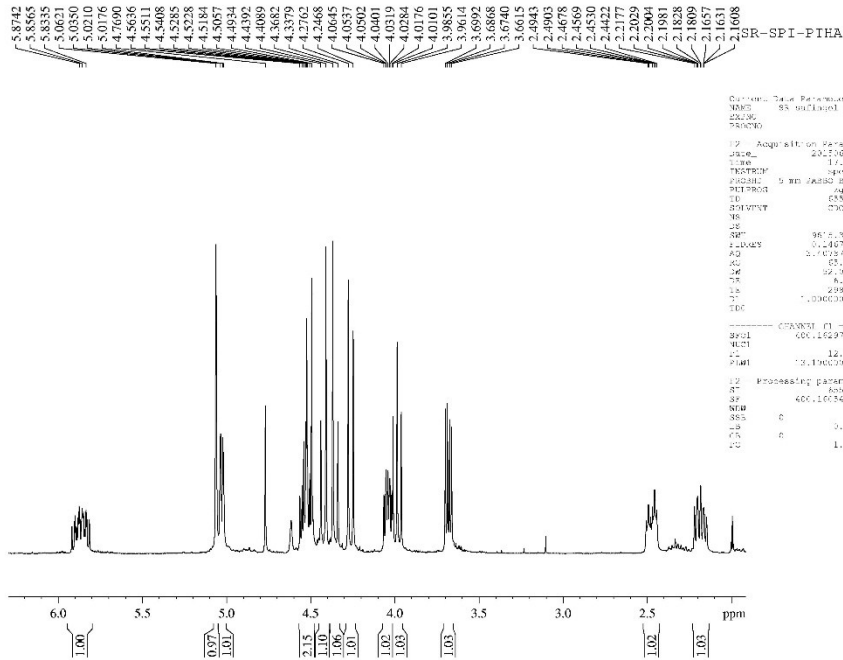
¹H NMR Spectra of Compound 12



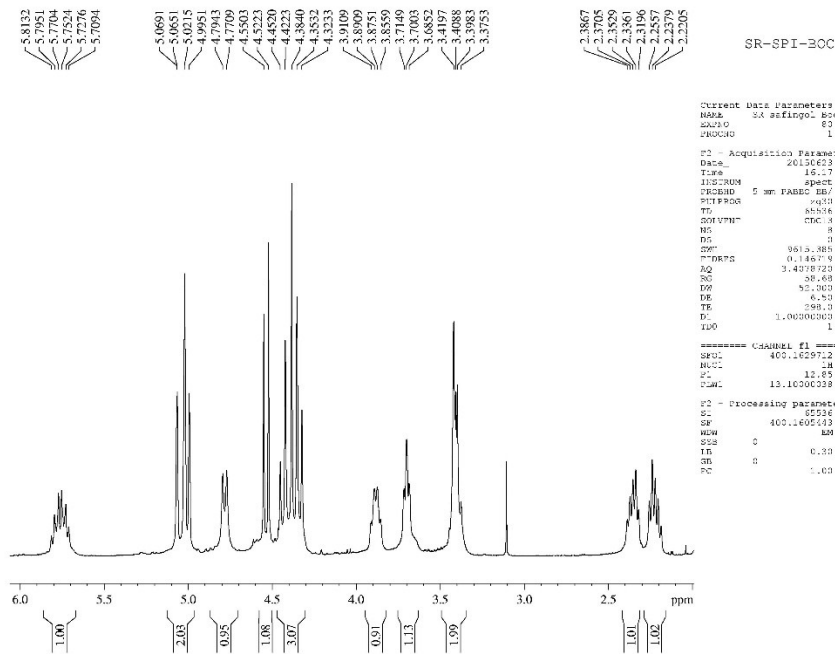
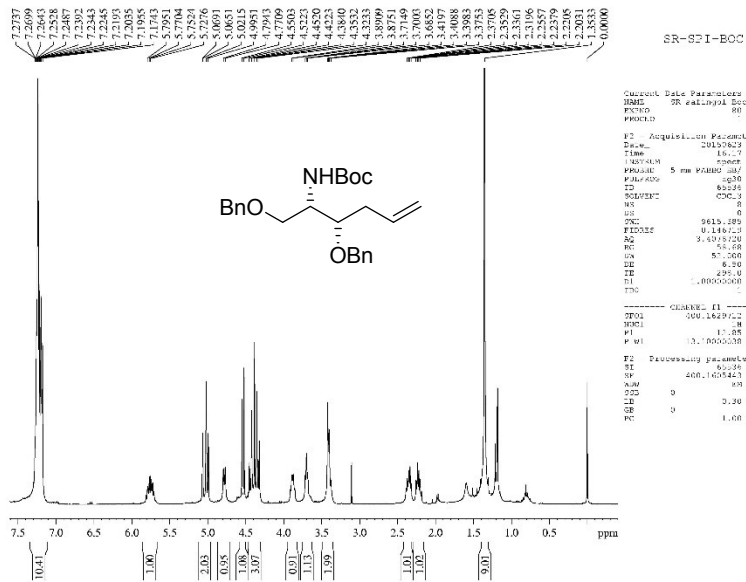
¹³C NMR Spectrum of Compound 12



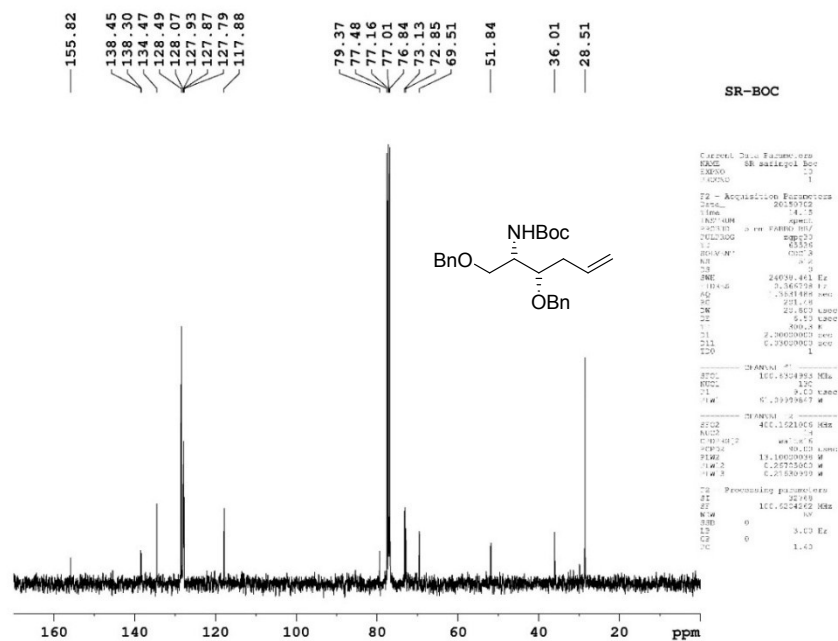
¹H NMR Spectrum of Compound 13



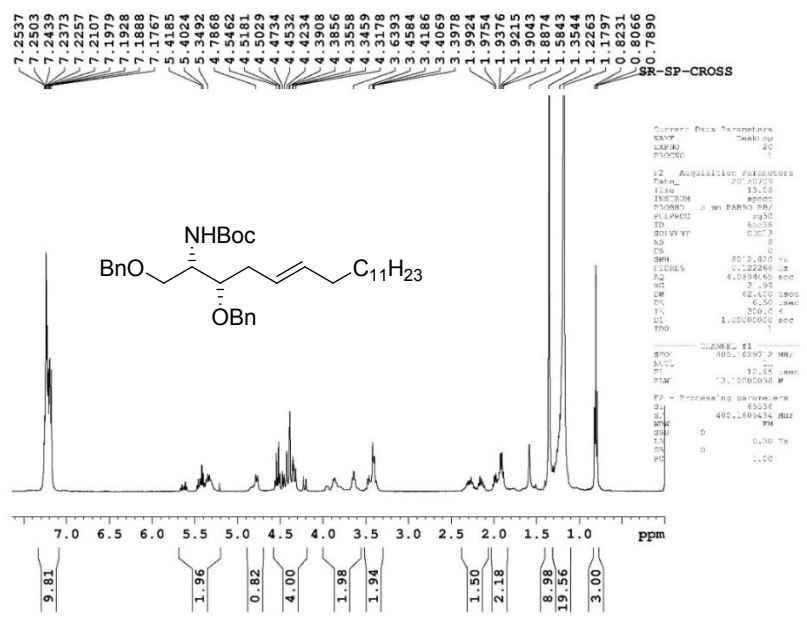
^1H and ^{13}C NMR Spectra of Compound 13



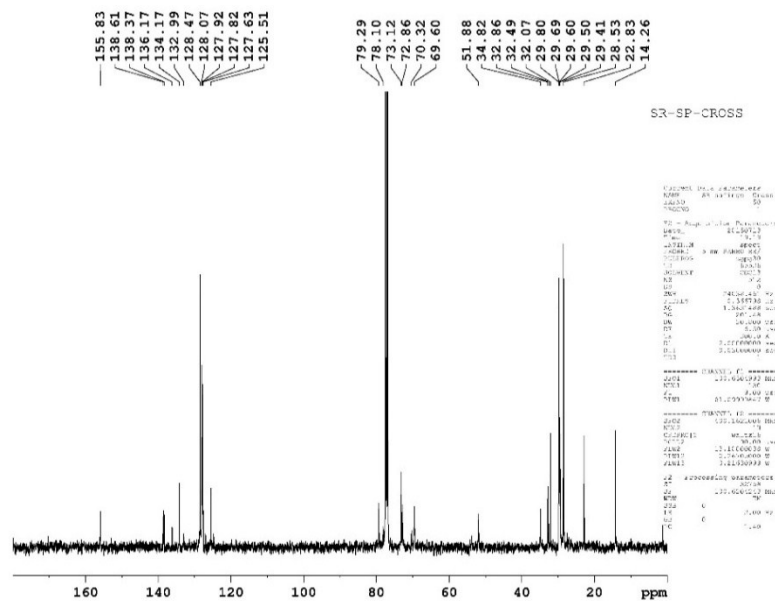
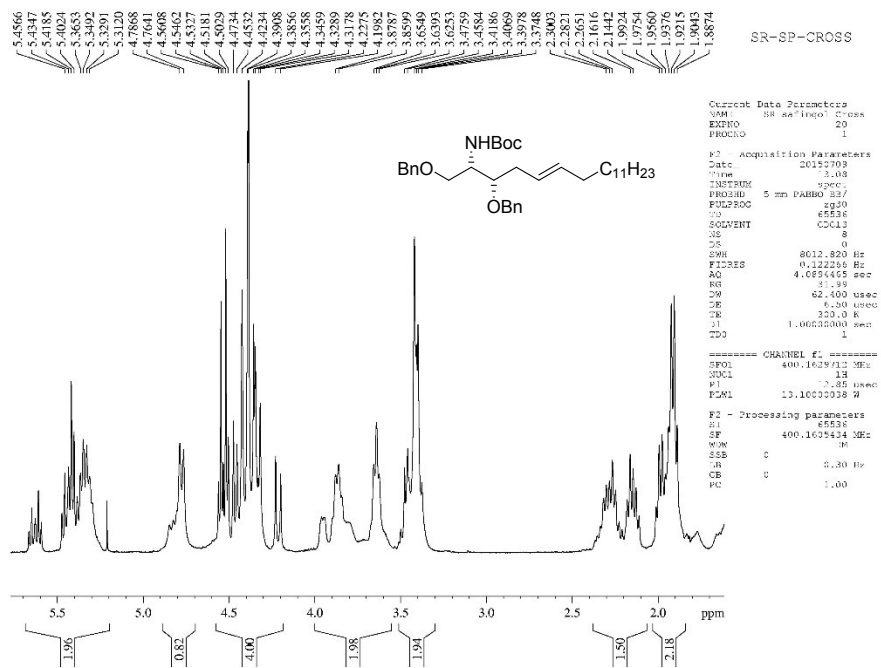
¹H NMR Spectra of Compound 15



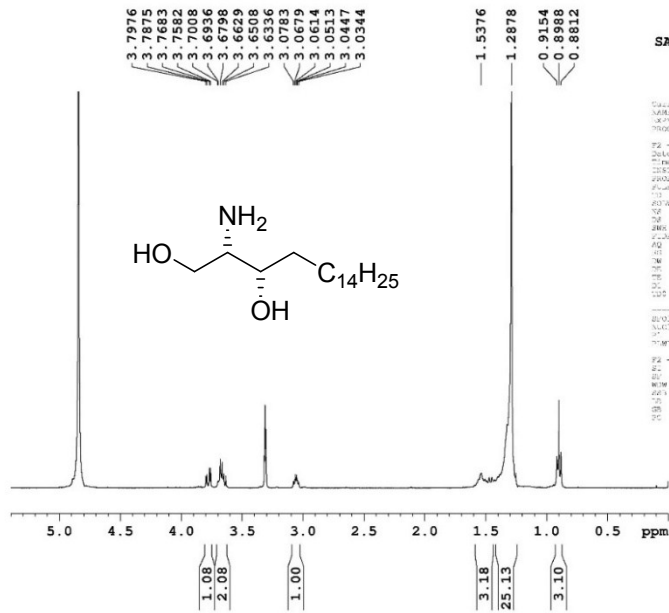
¹³CNMR Spectrum of Compound 15



¹H NMR Spectra of Compound 16



¹³C NMR Spectra of Compound 16

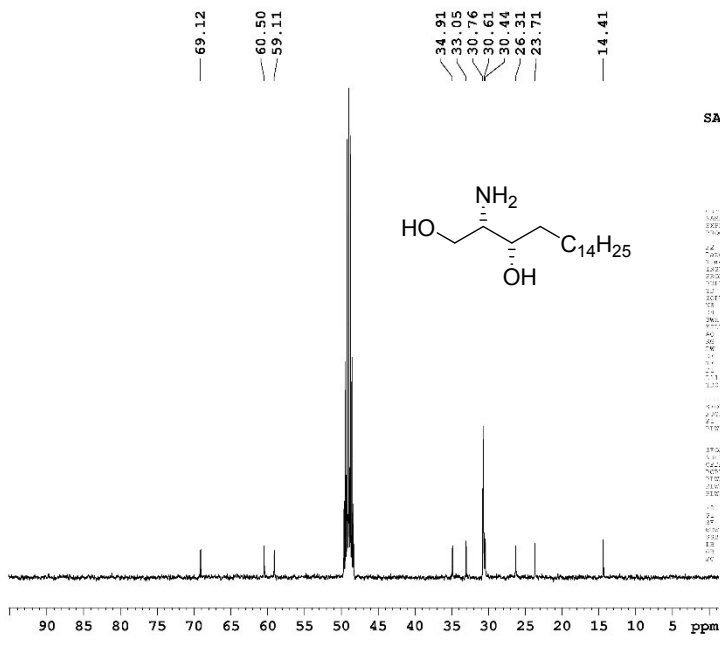


SAFINGOL-HCL

```

NAME: Safingol-HCL
EXPNO: 2
PROCNO: 1
PROCAM: 1
AQ: 0.10000000
RG: 327.50000000
SF: 300.13500000
WDW: EM
SSB: 0
LB: 3.00000000
GB: 0
PC: 1.00000000
SFO: 300.13500000
AQ: 0.10000000
RG: 327.50000000
SF: 300.13500000
WDW: EM
SSB: 0
LB: 3.00000000
GB: 0
PC: 1.00000000

```



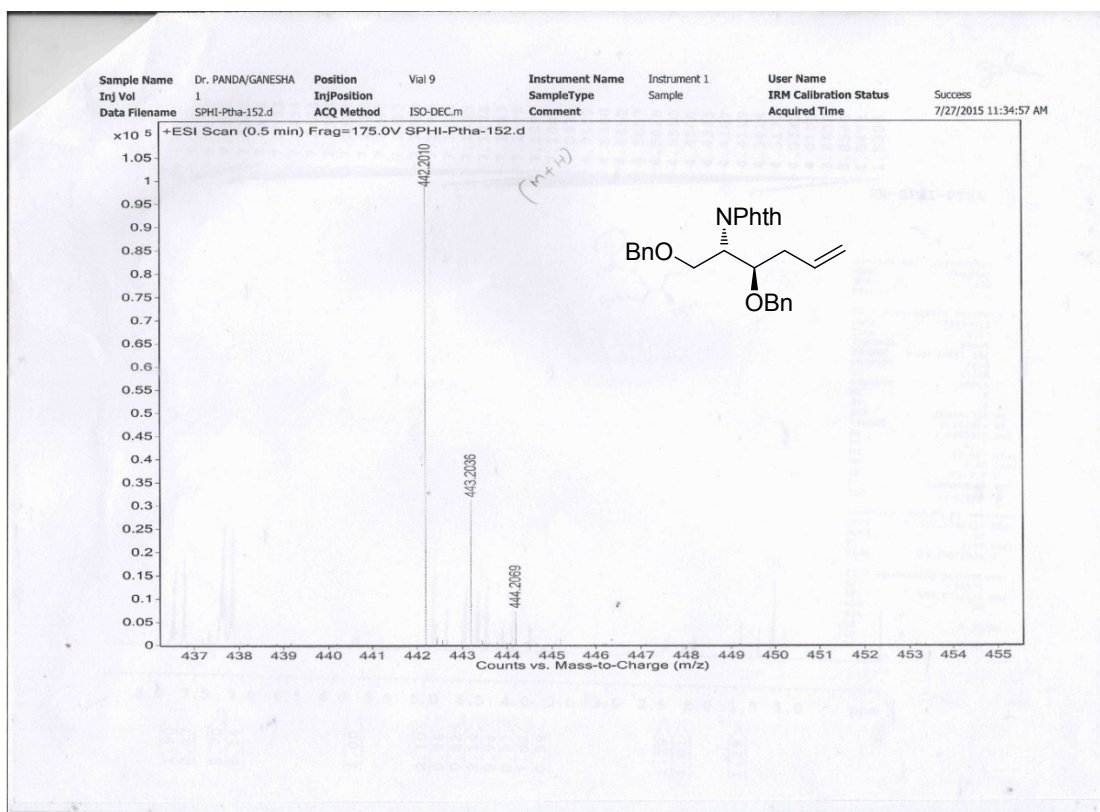
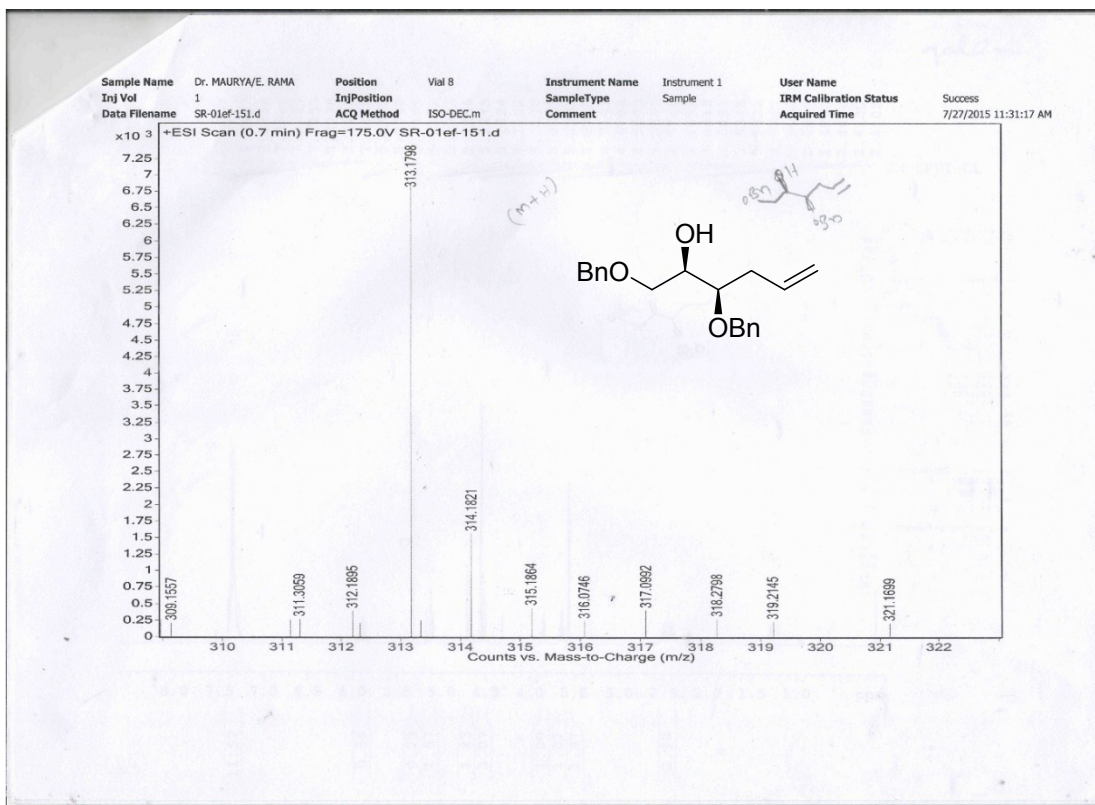
SAFINGOL-HCL

```

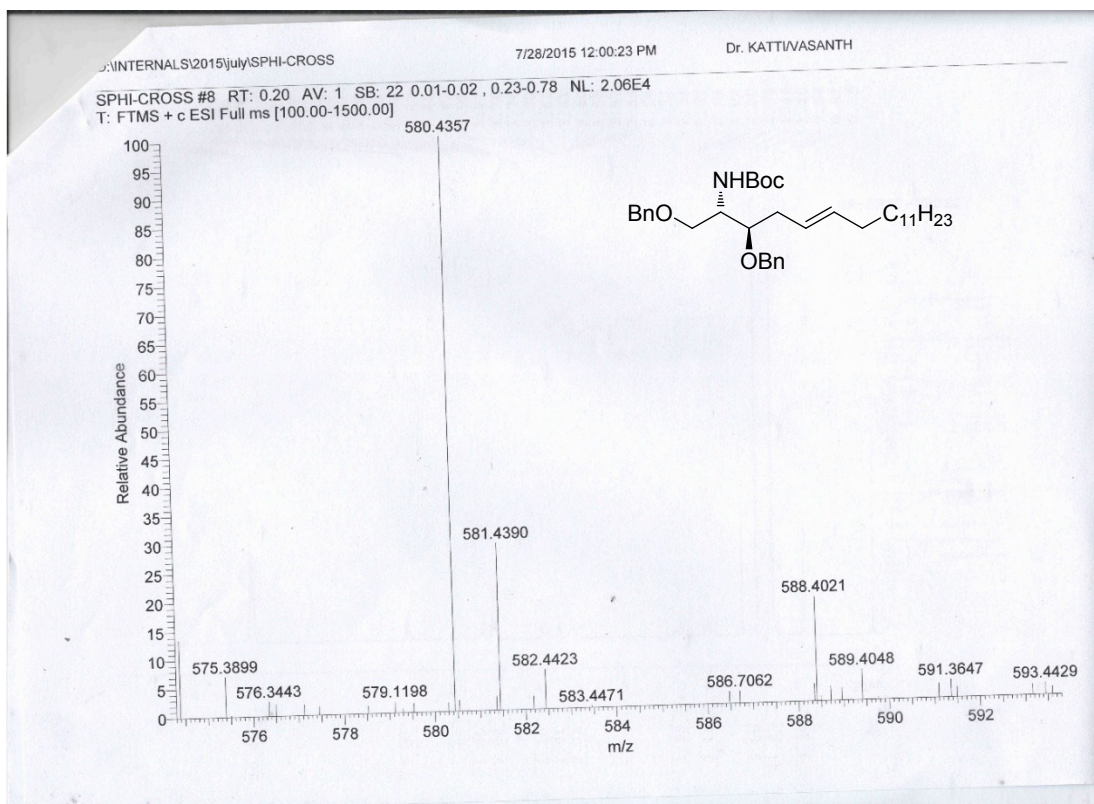
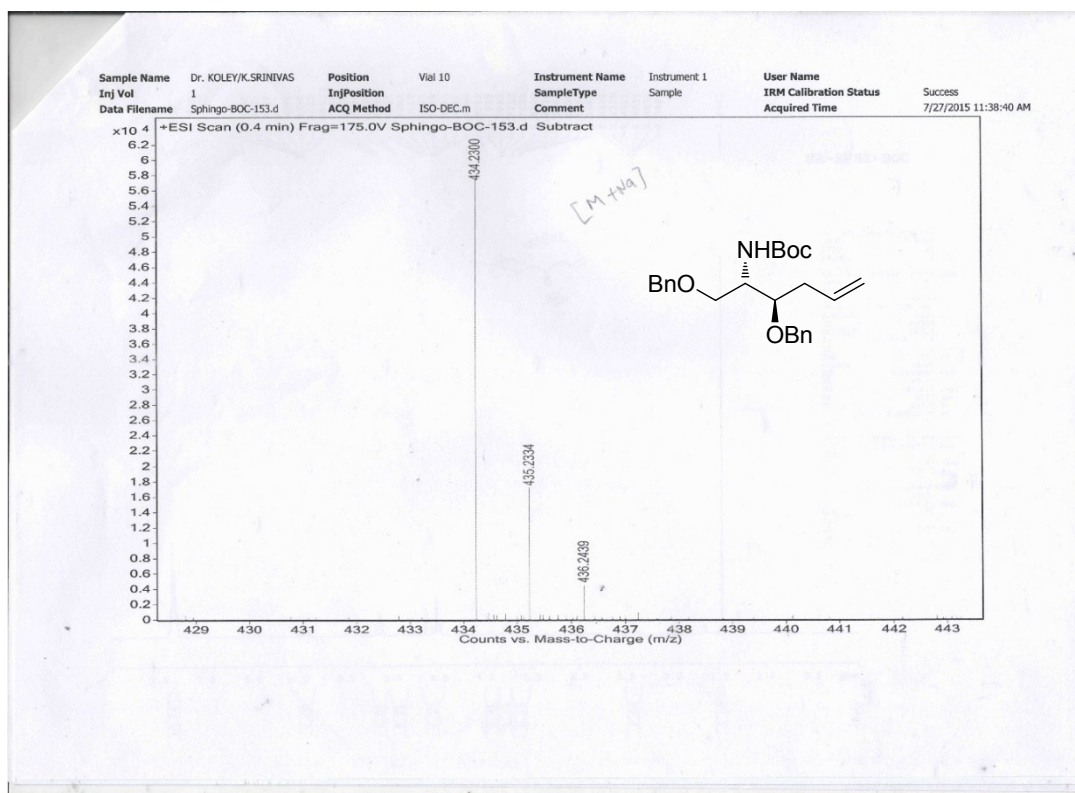
NAME: Safingol-HCL
EXPNO: 2
PROCNO: 1
PROCAM: 1
AQ: 0.10000000
RG: 327.50000000
SF: 300.13500000
WDW: EM
SSB: 0
LB: 3.00000000
GB: 0
PC: 1.00000000
SFO: 300.13500000
AQ: 0.10000000
RG: 327.50000000
SF: 300.13500000
WDW: EM
SSB: 0
LB: 3.00000000
GB: 0
PC: 1.00000000

```

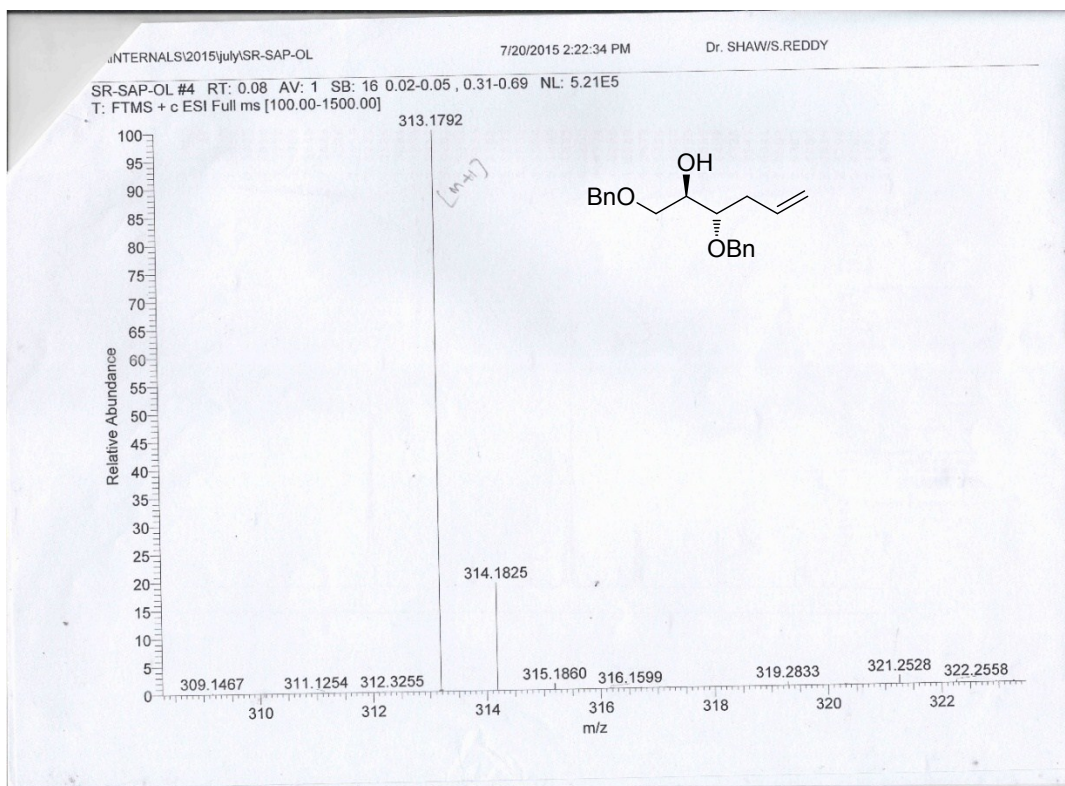
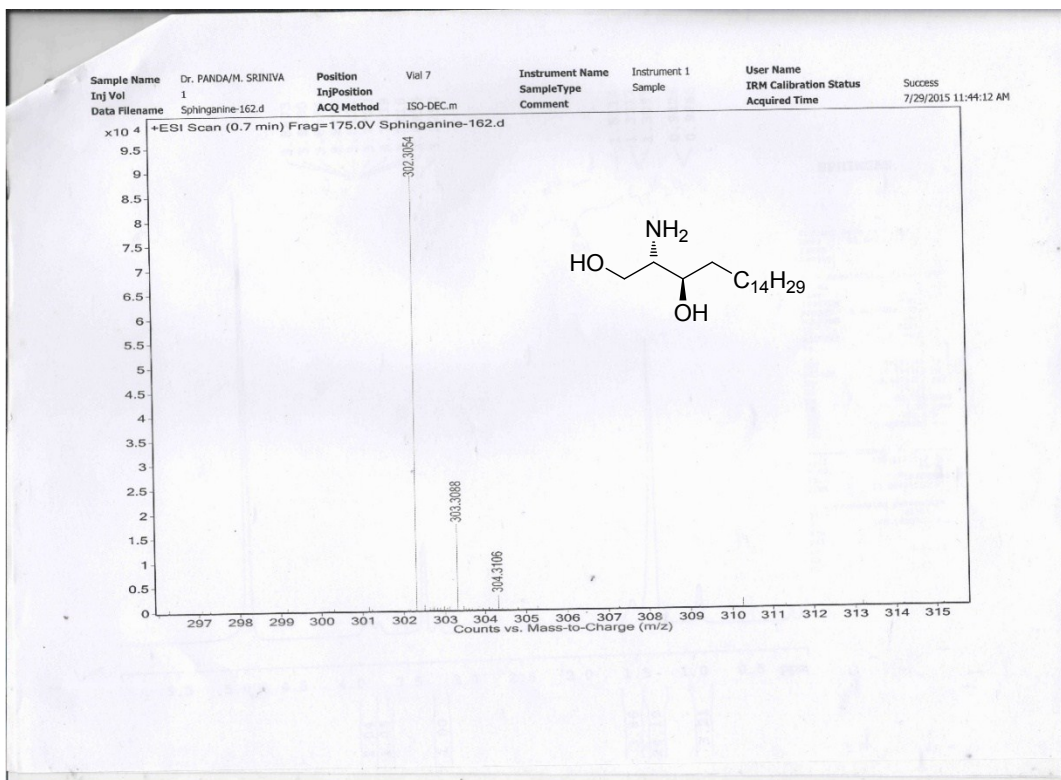
¹H and ¹³C NMR Spectra of Safingol 17



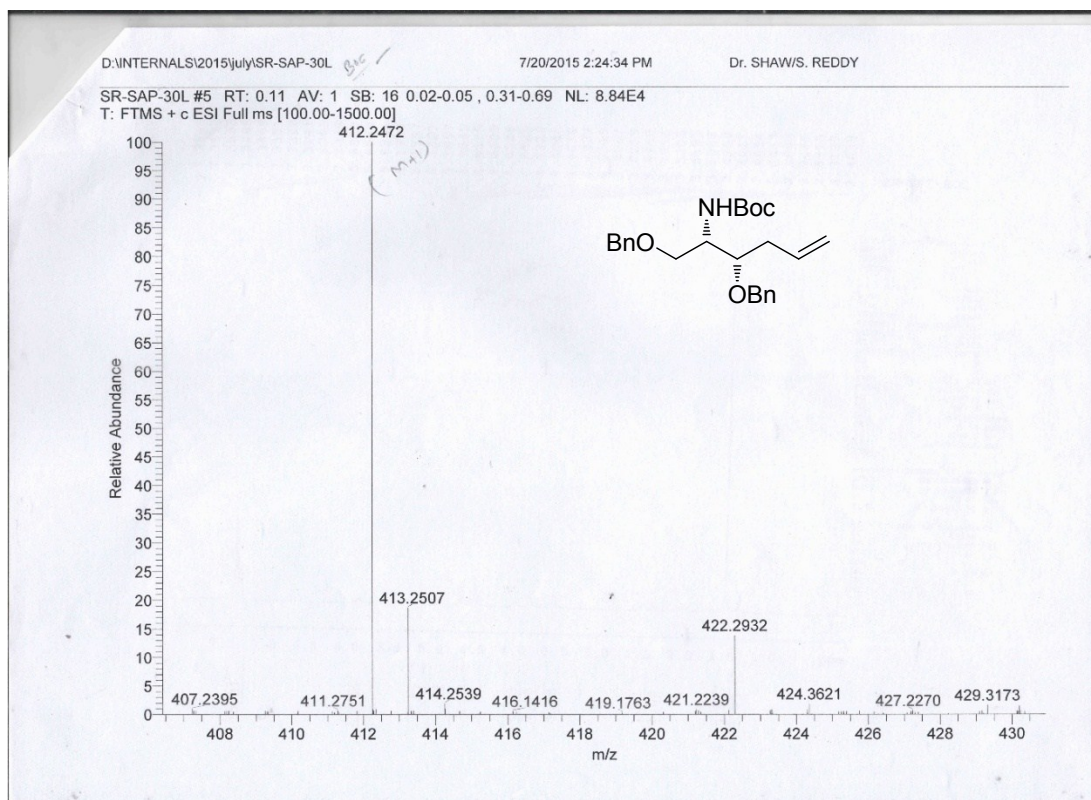
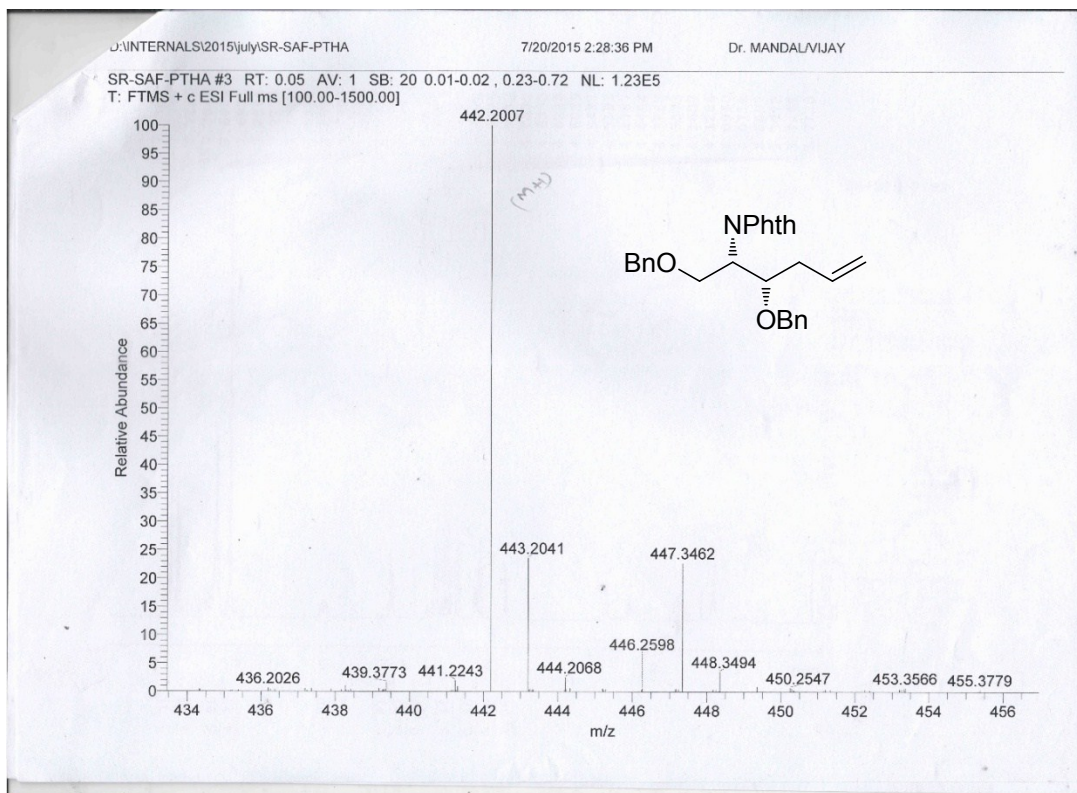
HRMS Spectra of compounds 4 and 5



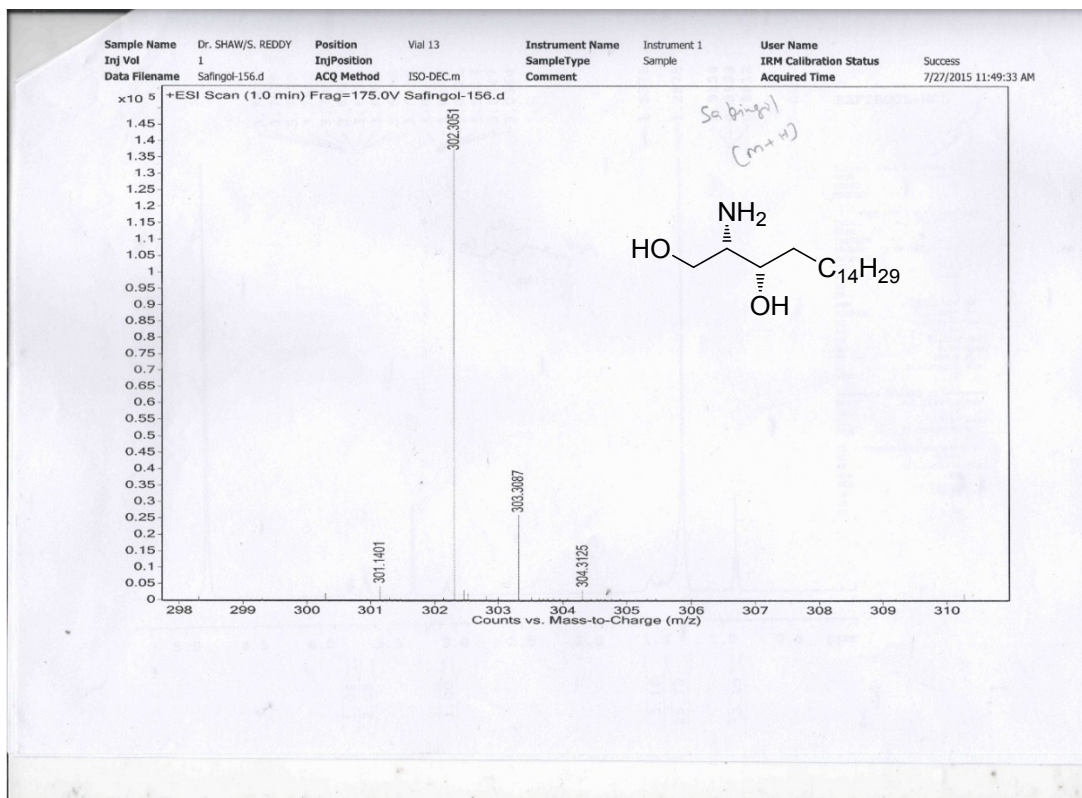
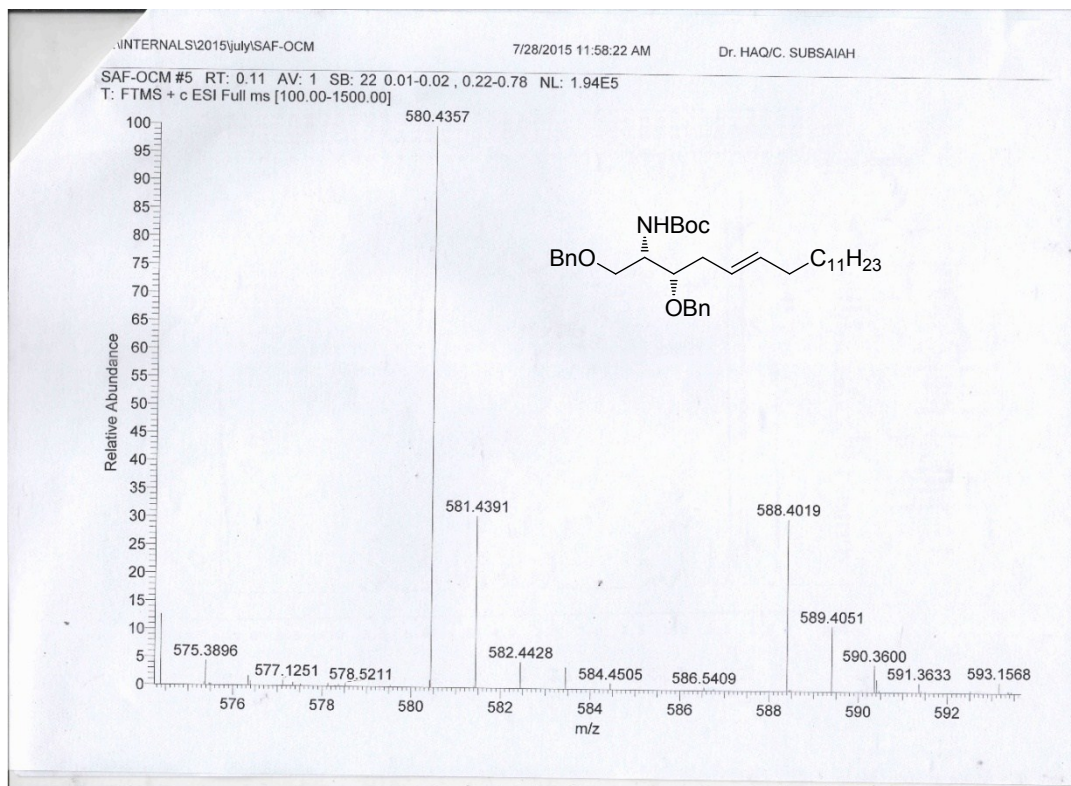
HRMS Spectra of compounds 7 and 8



HRMS Spectra of compounds 1(Sphinganine) and 12



HRMS Spectra of compounds 13 and 15



HRMS Spectra of compounds 16 and 17(Safingol)