

Synthesis of Dihydrogambirtannine by alkyne [2 + 2 + 2]-cyclootrimerisation

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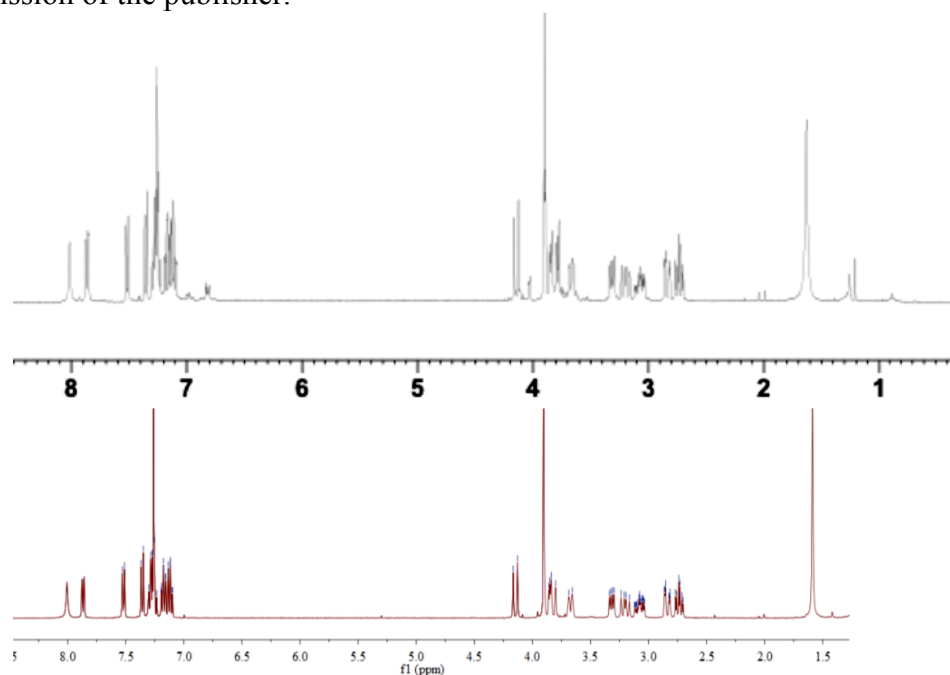
NMR spectroscopic data

comparison table	2
alcohol 6	3
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aldehyde 8	4
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dihydrogambirtannine 1	13

Dihydrogambirtannine Data Comparison

¹H NMR spectroscopic data.

Upper trace: synthetic material. Lower trace: reported, reproduced from reference 1 with the permission of the publisher.

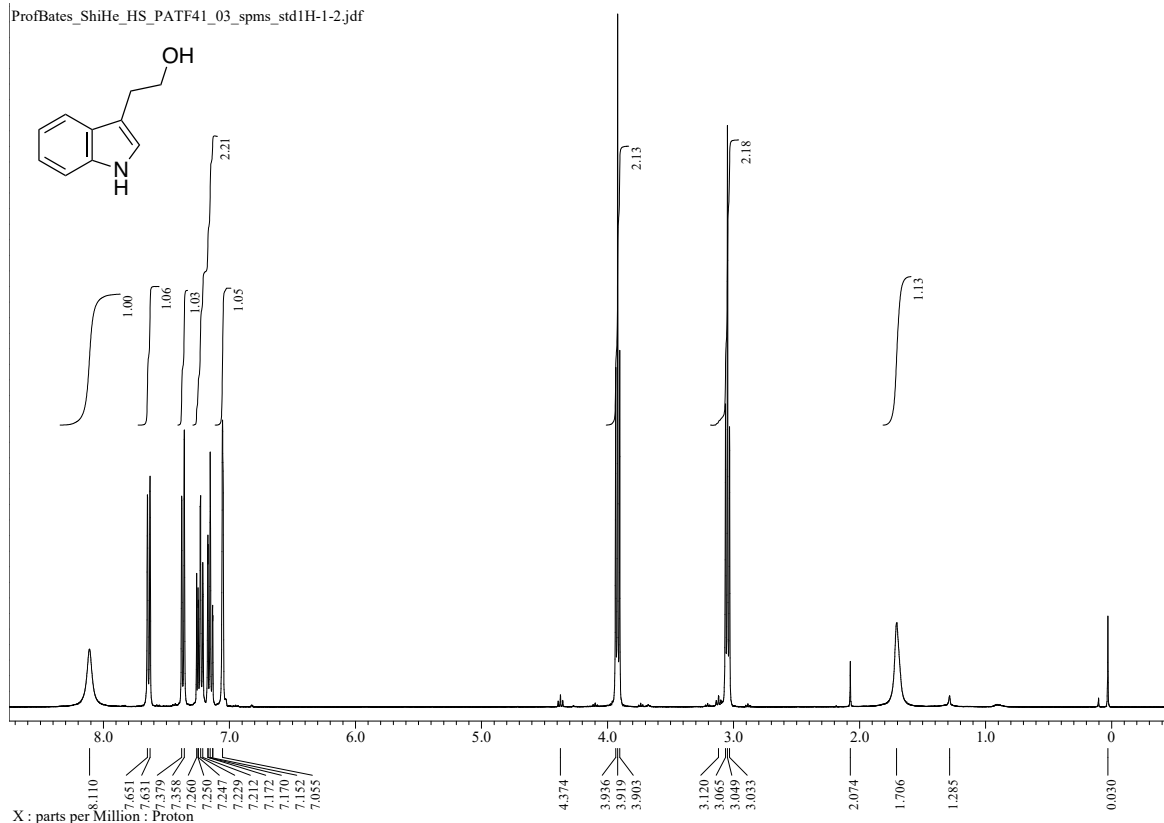


¹³C NMR spectroscopic data

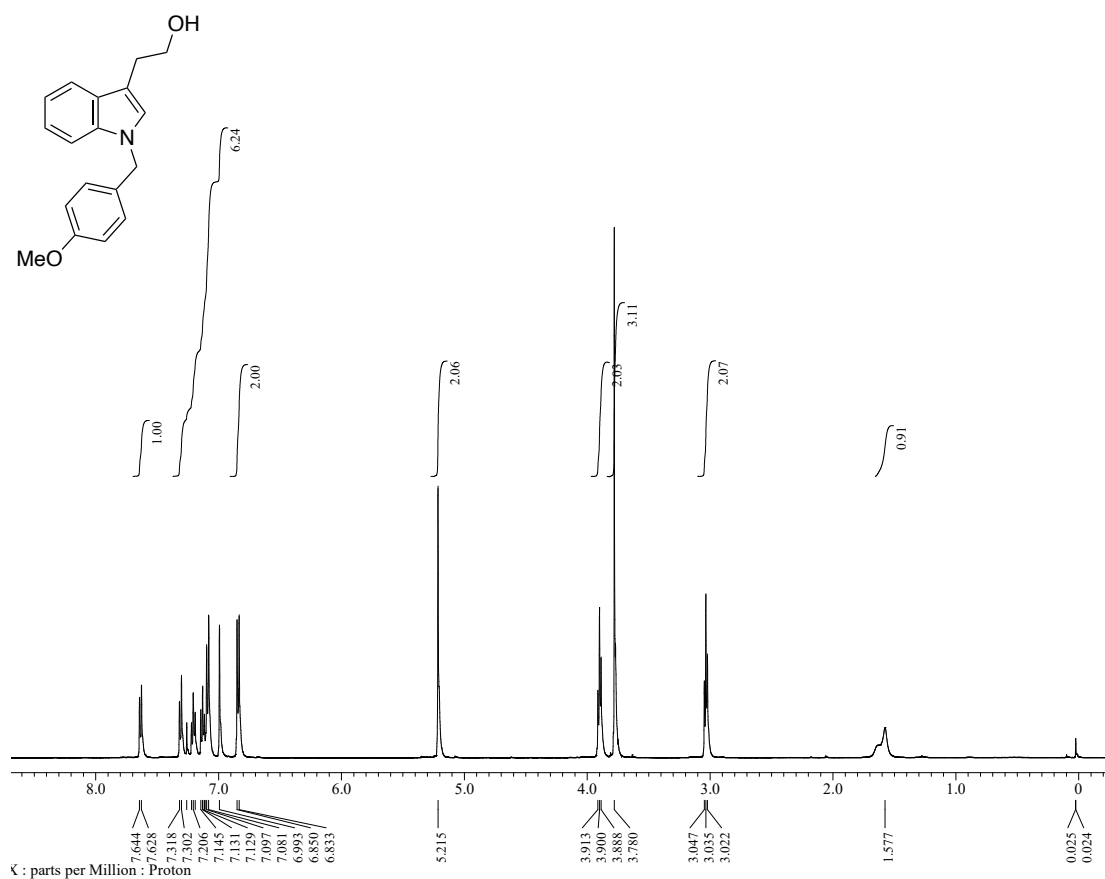
reported data, ¹ (100 MHz, CDCl ₃)	synthetic material, (100 MHz, CDCl ₃)
167.7	167.6
136.4	136.3
136.0	136.0
135.6	135.6
134.3	134.3
130.9	130.9
129.2	129.2
129.0	128.9
127.1	127.1
125.8	125.7
121.6	121.6
119.5	119.4
118.2	118.1
110.9	110.9
108.6	108.5
58.2	58.1
56.4	56.3
52.4	52.4
51.9	51.9
33.6	33.5
21.5	21.4

¹ Z. Yin, T. Liu, J.-X. Fu *J. Asian Nat. Prod. Res.* **2019**, *31*, 257-261. This paper provides the spectra but not the data in numerical form.

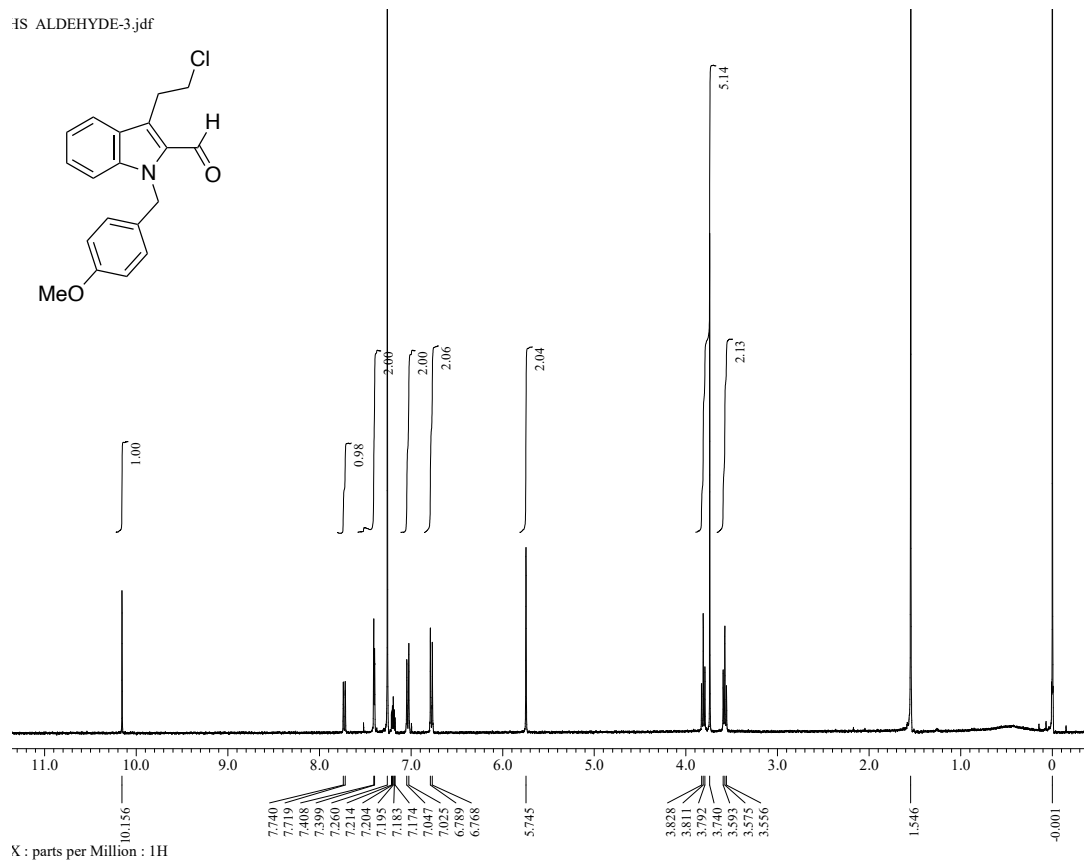
ProfBates_ShiHe_HS_PATF41_03_spms_std1H-1-2.jdf



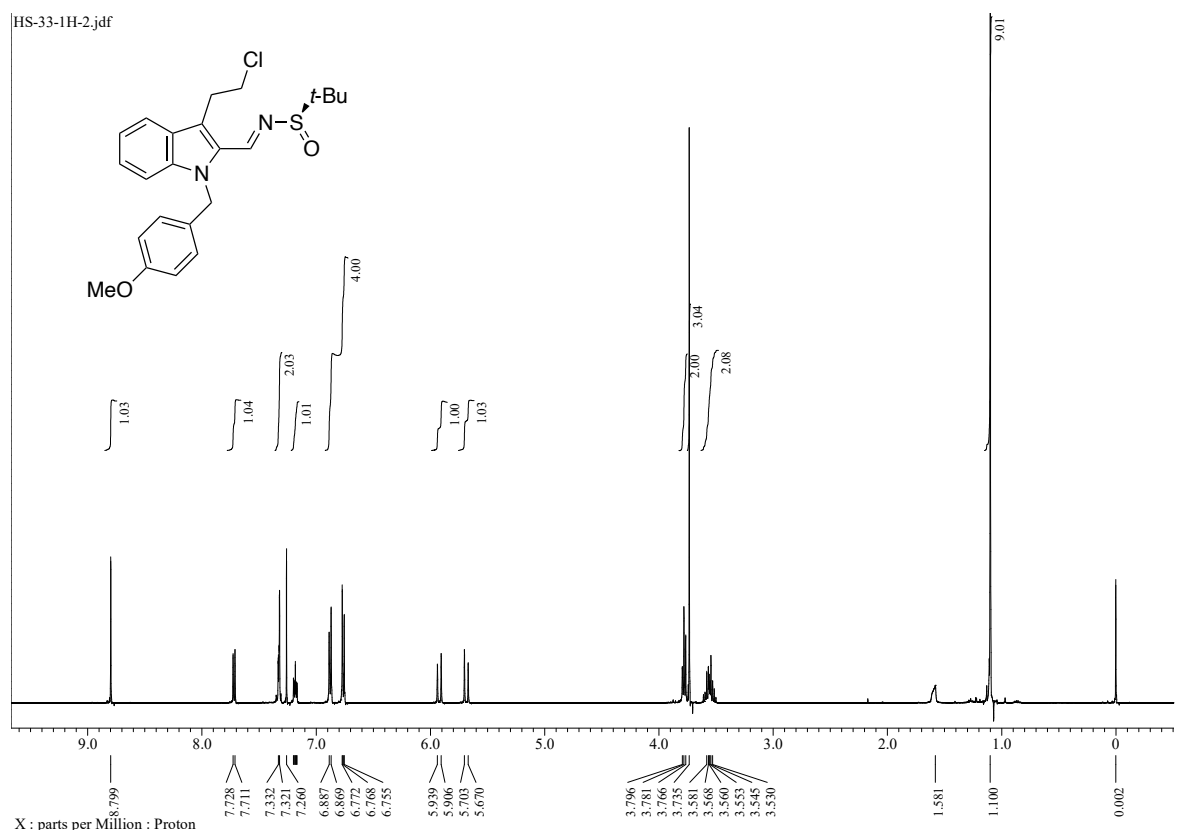
¹H NMR spectrum of alcohol **6**



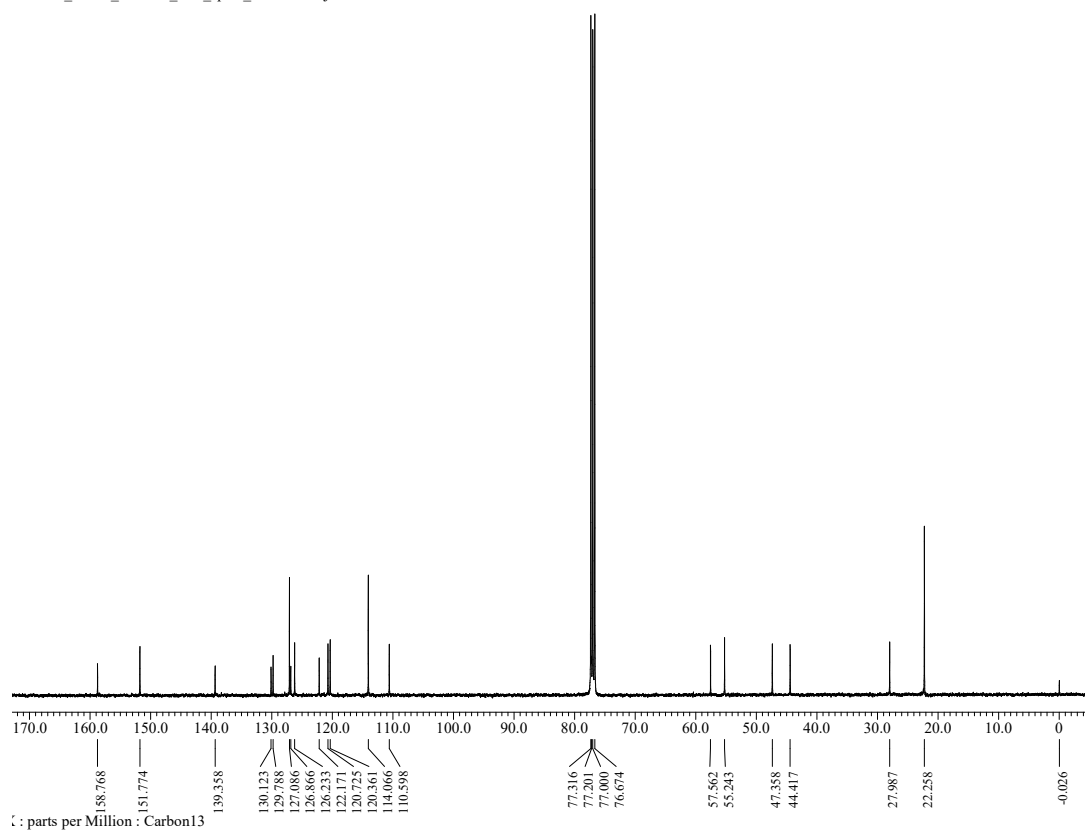
¹H NMR spectrum of alcohol 7



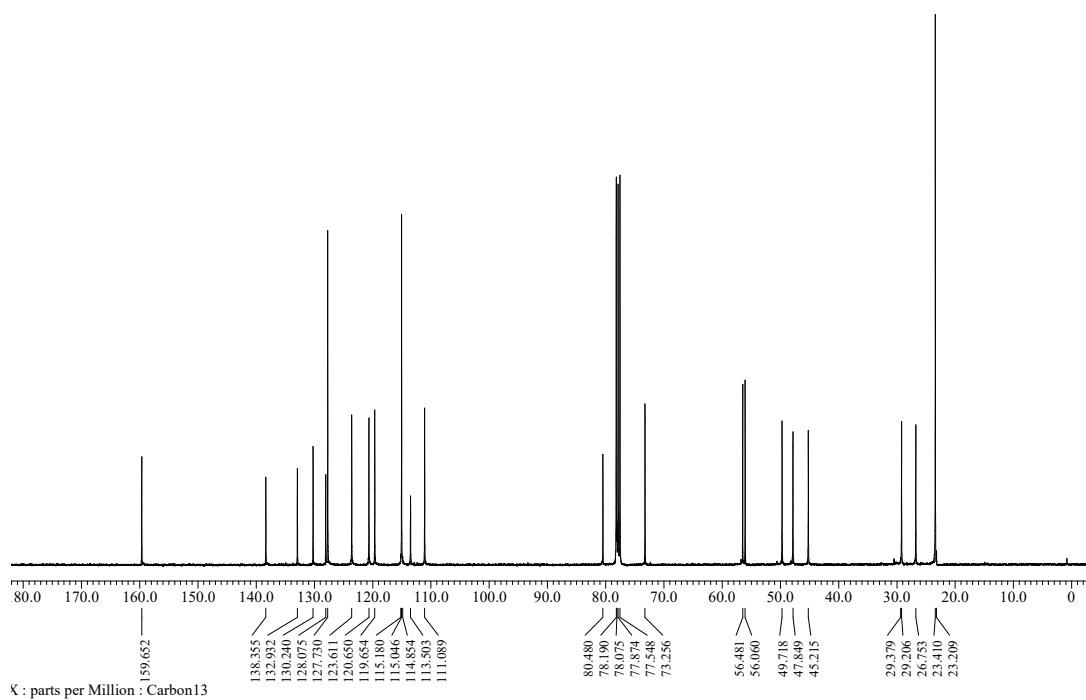
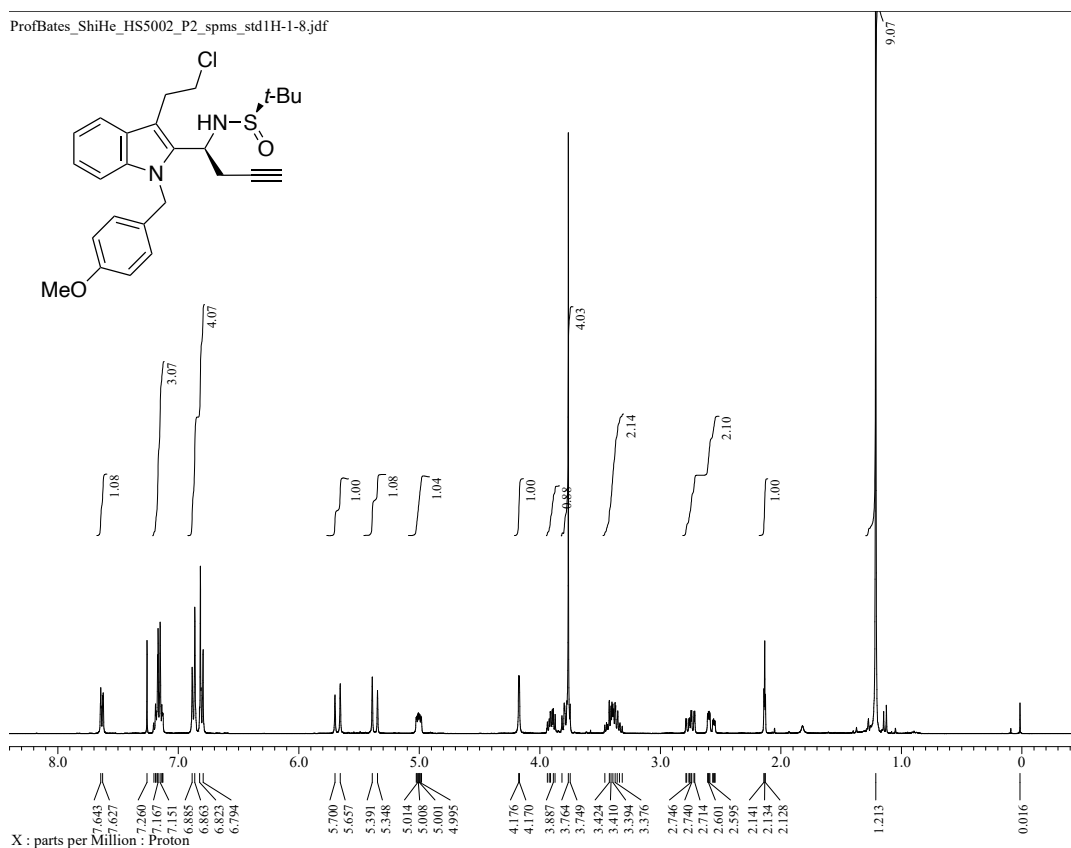
¹H NMR spectrum of aldehyde 8



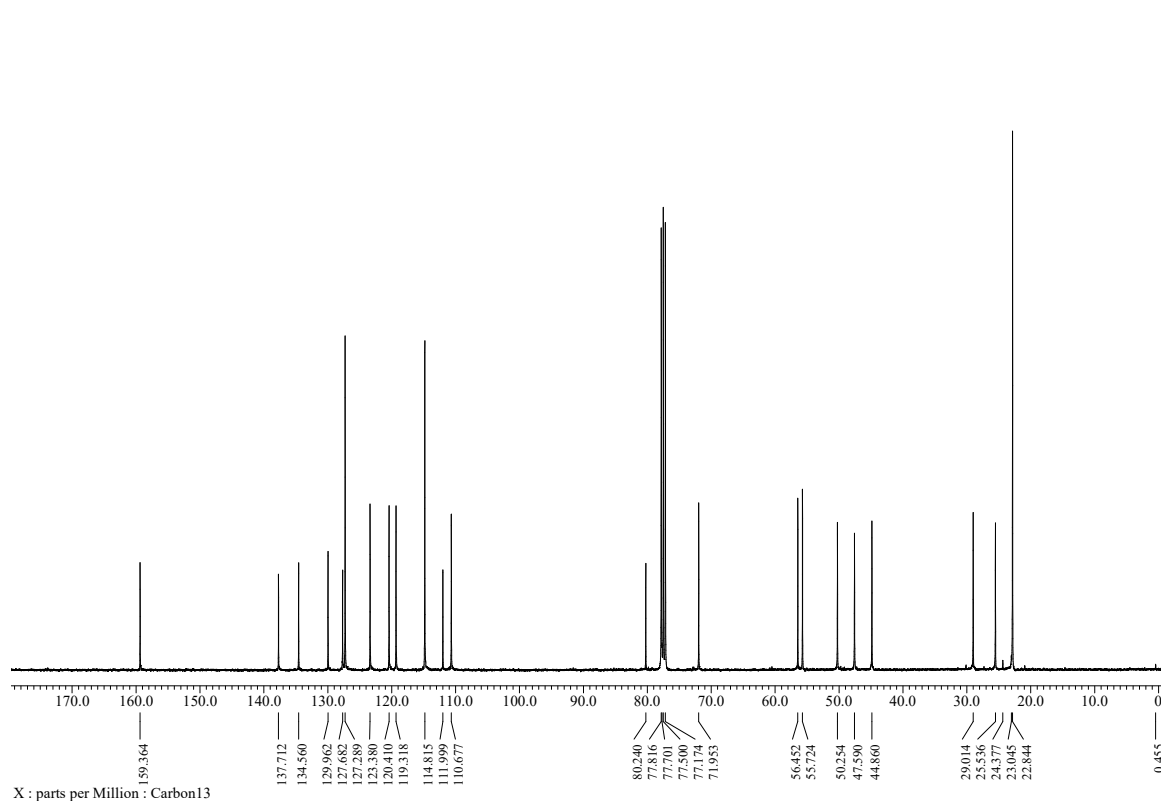
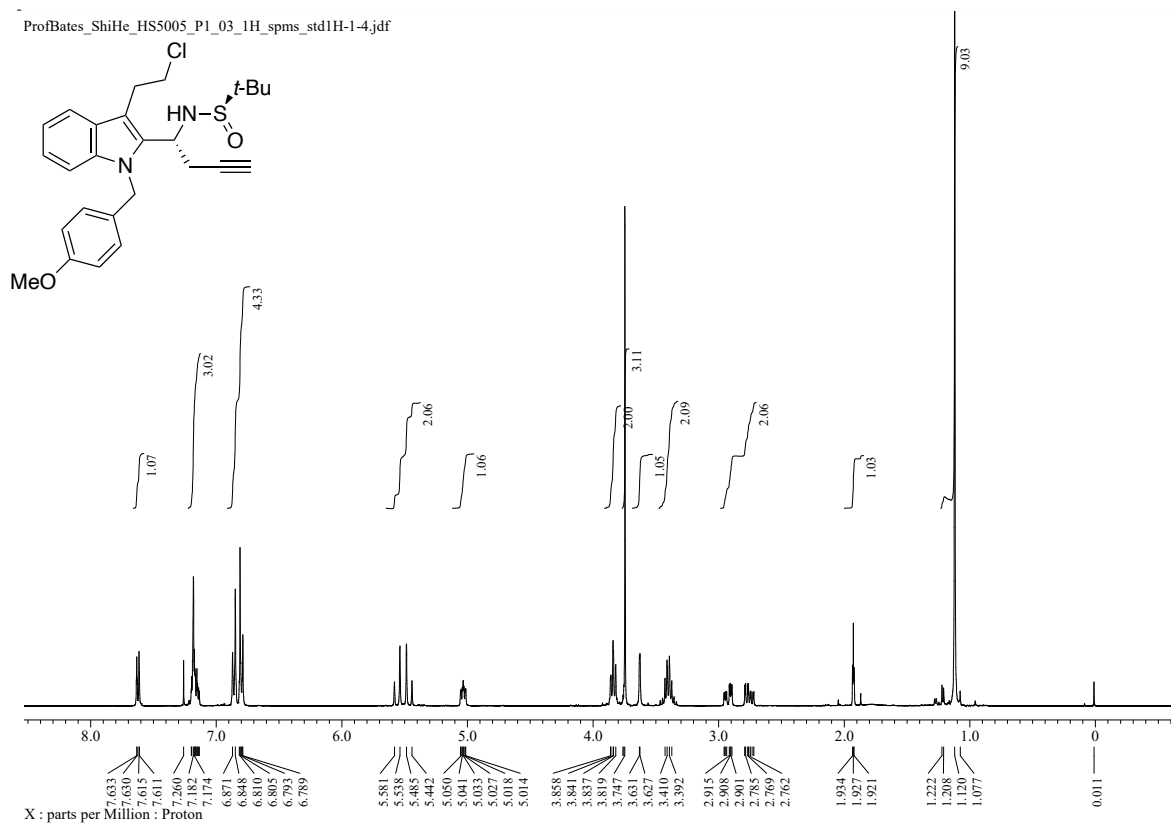
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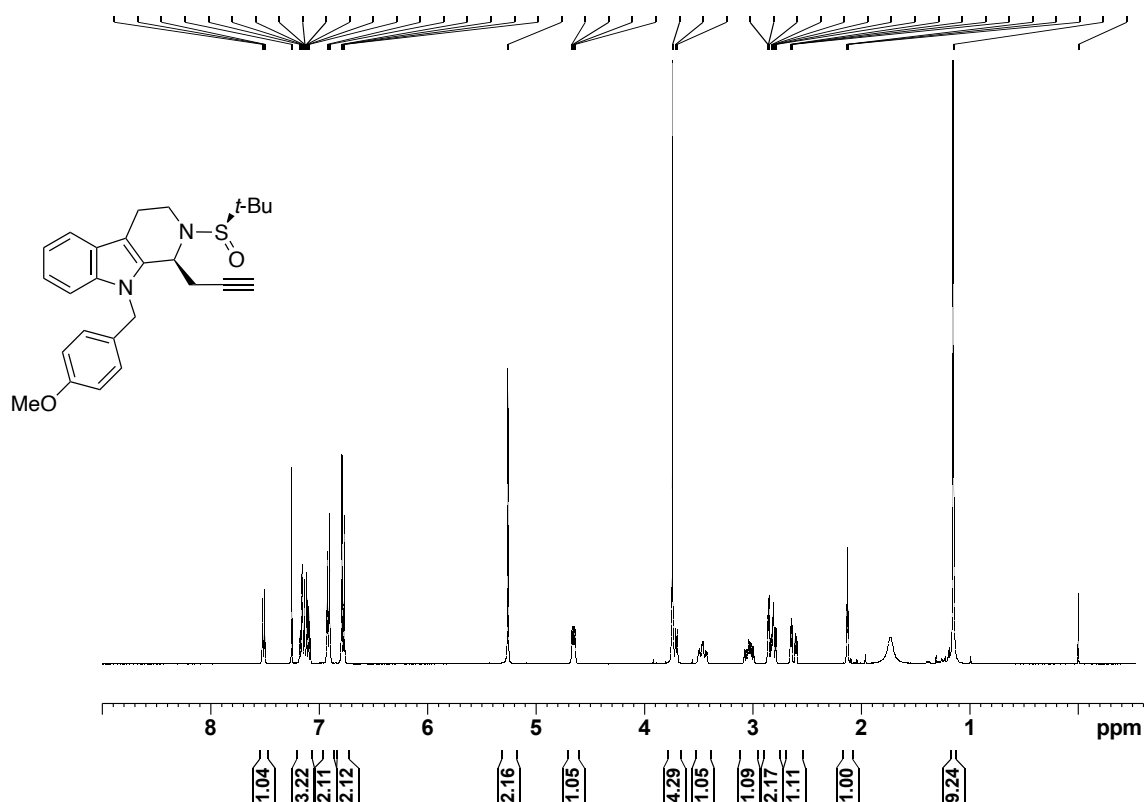
¹H and ¹³C NMR spectra of sulfinyl imine **9**



¹H and ¹³C NMR spectra of alkyne **10**



¹H and ¹³C NMR spectra of the diastereoisomer of alkyne 10



Current Data Parameters
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PROCNO 1

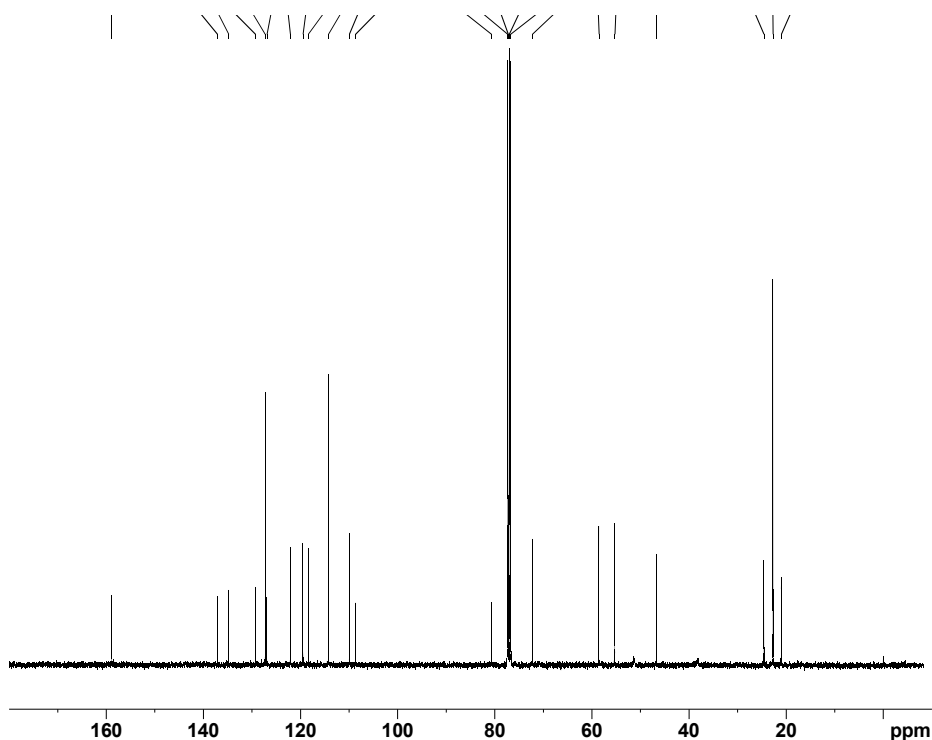
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SOLVENT CDCl3
NS 929
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SWH 23809.523 MHz
FIDRES 0.363304 Hz
AQ 1.3762560 s
RG 812
DW 21.000 u
DE 6.00 u
TE 298.9 K
D1 2.00000000 s
d11 0.03000000 s
DELTA 1.89999998 s
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 u
PL1 -2.00 dB
SFO1 100.6238360 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 u
PL2 -2.00 dB
PL12 15.23 dB
PL13 18.00 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
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13C NMR_400MHz_CDC13



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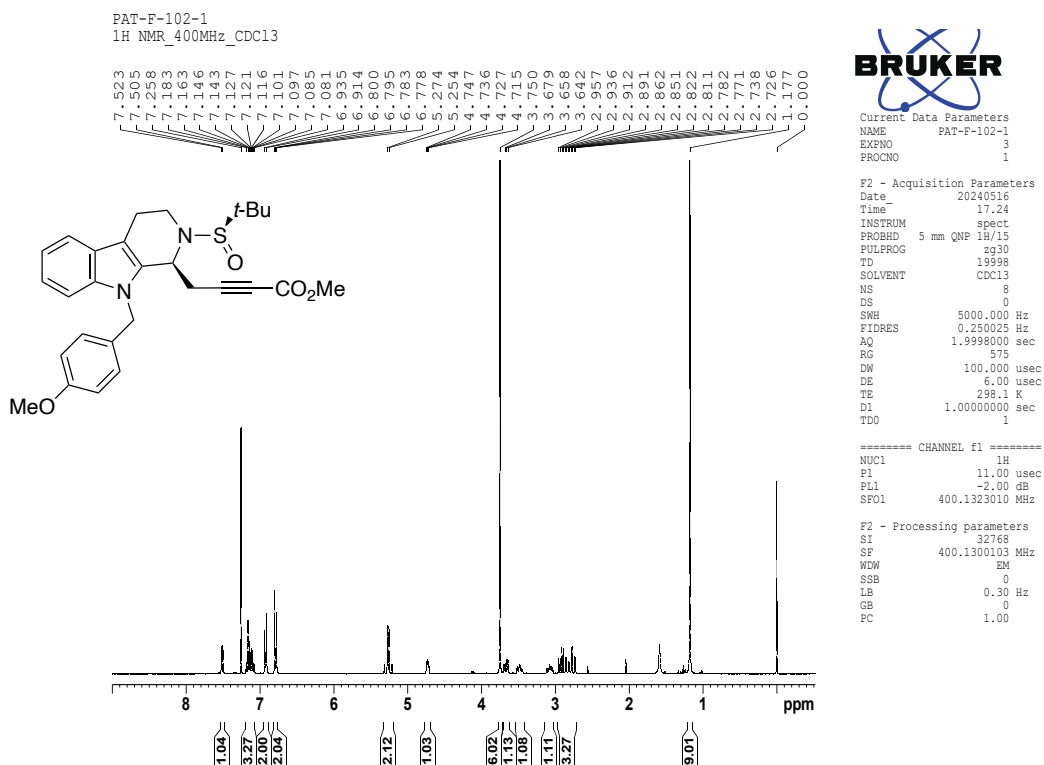
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TD 65536
SOLVENT CDCl3
NS 929
DS 0
SWH 23809.523 MHz
FIDRES 0.363304 Hz
AQ 1.3762560 s
RG 812
DW 21.000 u
DE 6.00 u
TE 298.9 K
D1 2.00000000 s
d11 0.03000000 s
DELTA 1.89999998 s
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===== CHANNEL f1 =====
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P1 10.00 u
PL1 -2.00 dB
SFO1 100.6238360 MHz

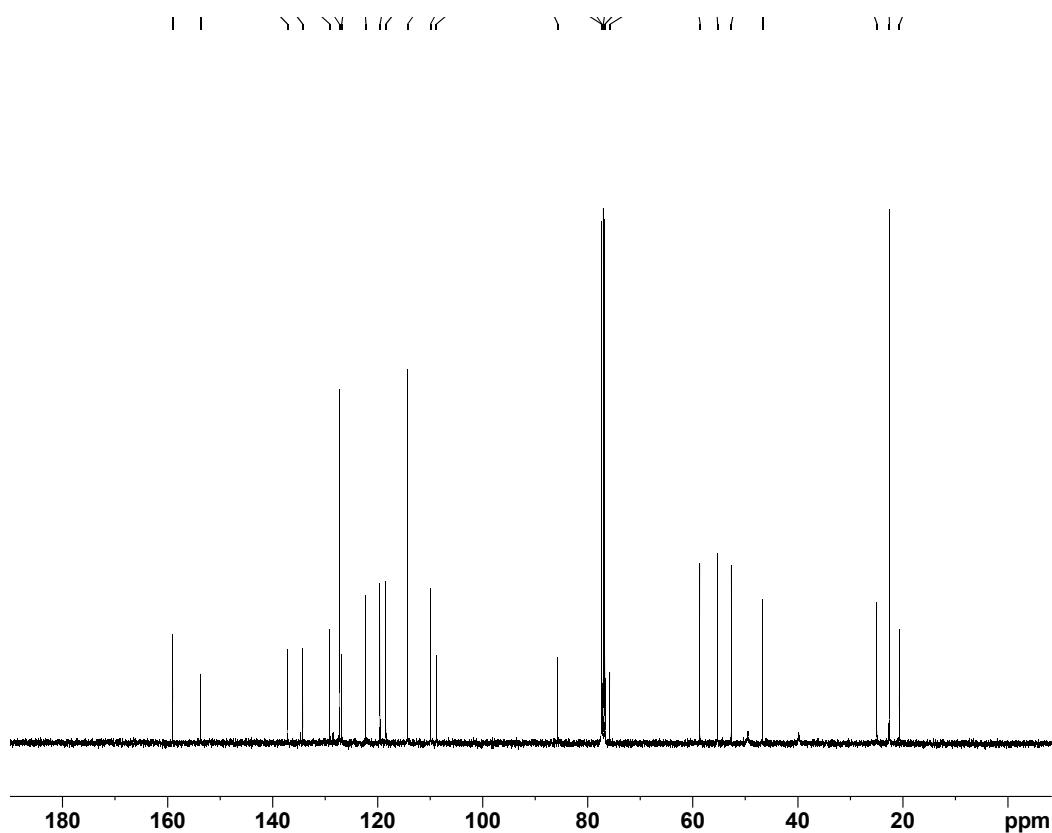
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PL2 -2.00 dB
PL12 15.23 dB
PL13 18.00 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
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SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H and ¹³C NMR spectra of tricycle 11

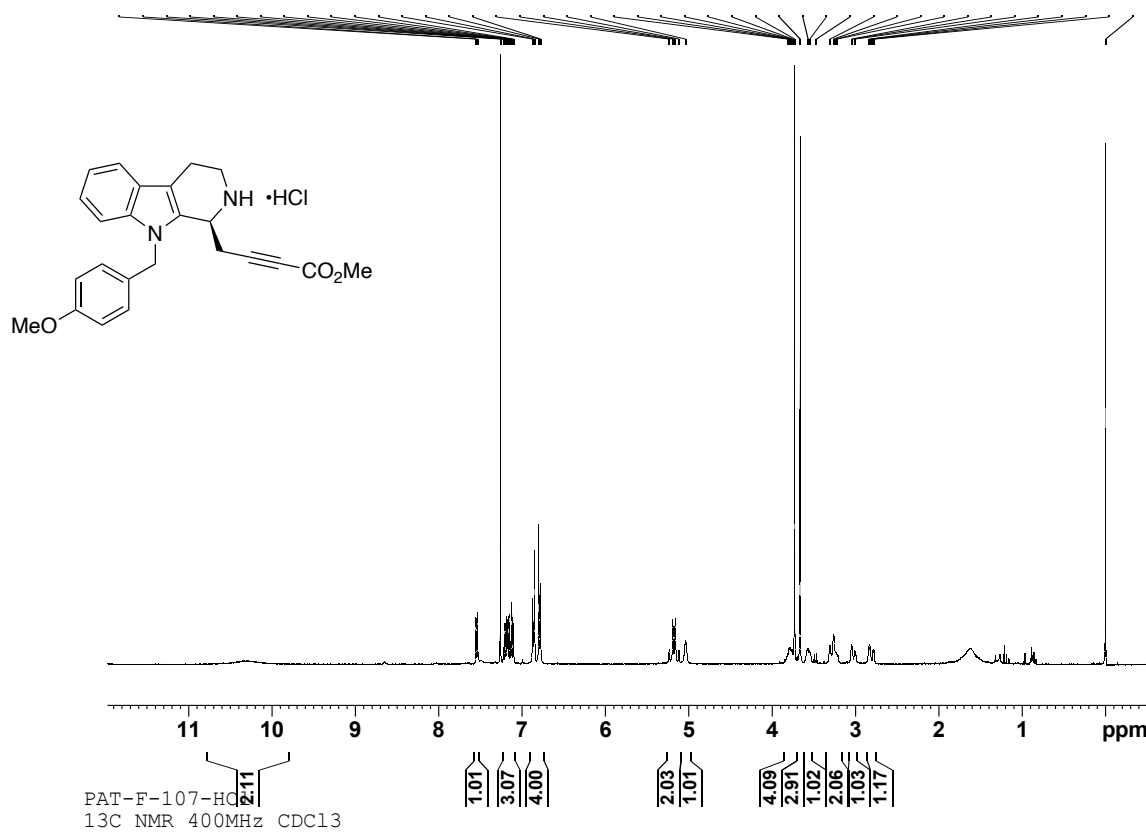


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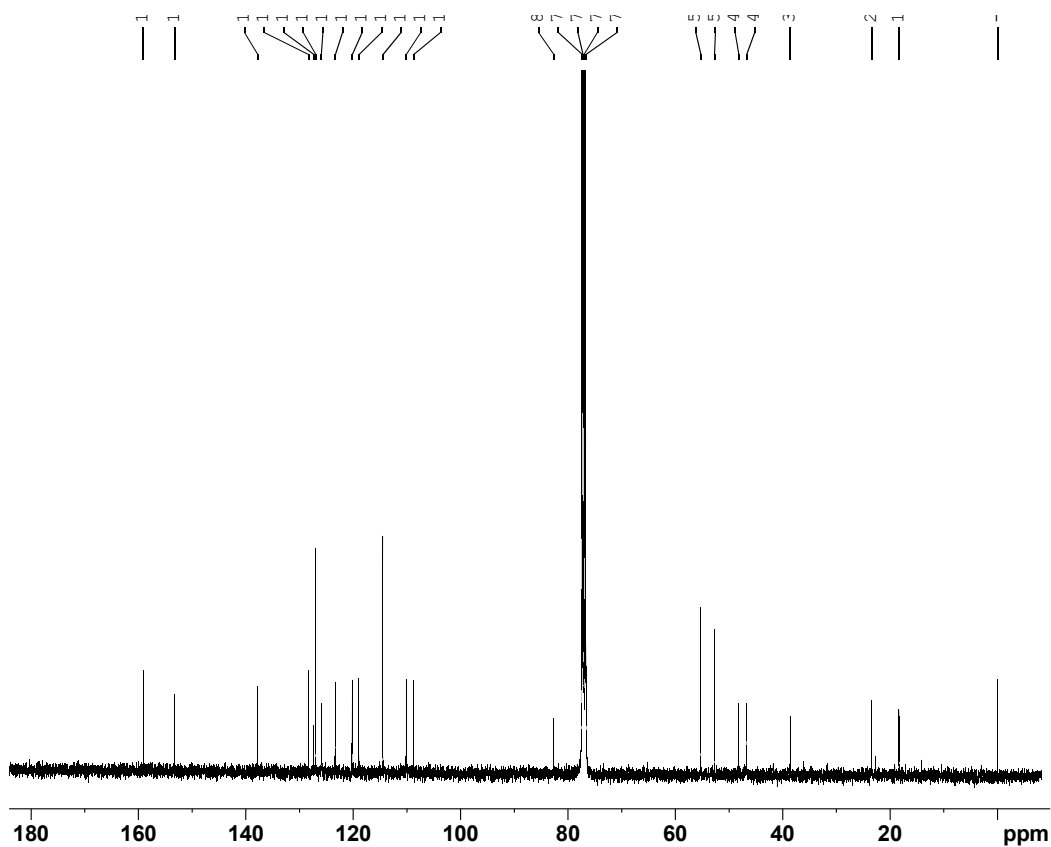


¹H and ¹³C NMR spectra of alkynyl ester 12

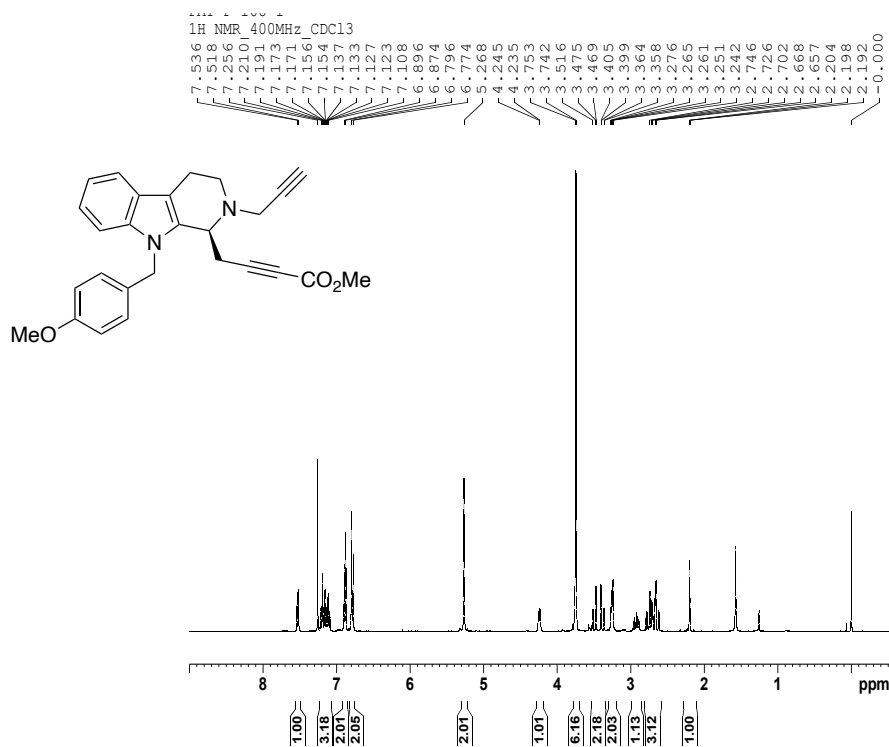
PAT-F-107-HCl
¹H NMR_400MHz_CDCl₃



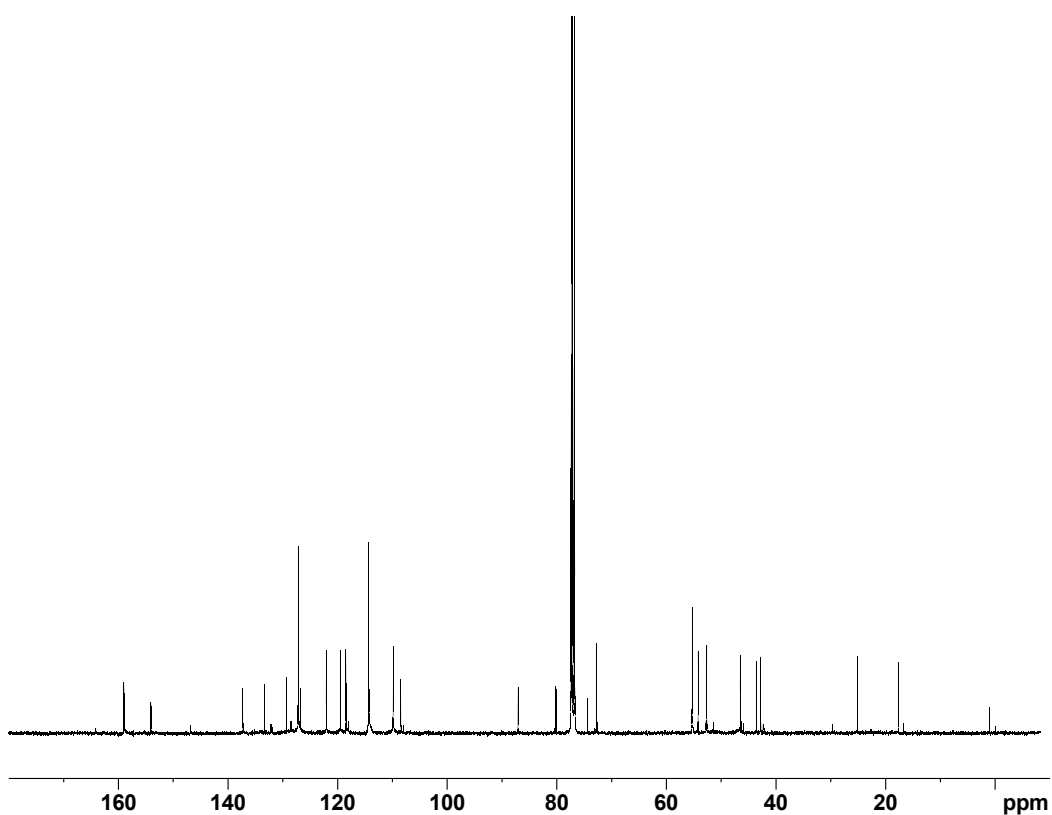
PAT-F-107-HCl
¹³C NMR_400MHz_CDCl₃



¹H and ¹³C NMR spectra of alkynyl ester 13



PAT-F-108
13C NMR_400MHz_CDC13



Current Data Parameters
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PROCNO 1

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PULPROG zg30
TD 19998
SOLVENT CDC13
NS 8
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SWH 5000.000 Hz
FIDRES 0.250025 Hz
AQ 1.9998000 sec
RG 512
DW 100.000 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
SFO1 400.1323010 MHz

F2 - Processing parameters
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SF 400.1300113 MHz
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LB 0.30 Hz
GB 0
PC 1.00



Current Data
NAME
EXPNO
PROCNO

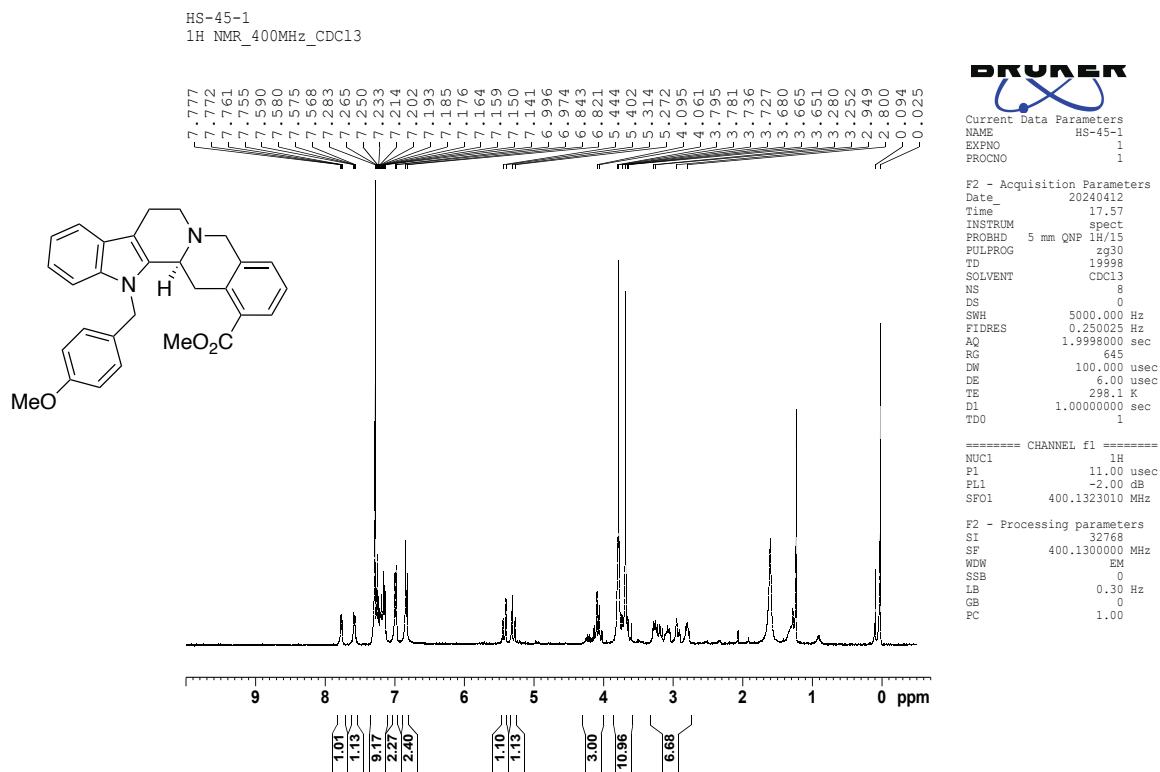
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TD 19998
SOLVENT CDC13
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DS 0
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FIDRES 0.250025 Hz
AQ 1.9998000 sec
RG 512
DW 100.000 usec
DE 6.00 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
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PL1 -2.00 dB
SFO1 400.1323010 MHz

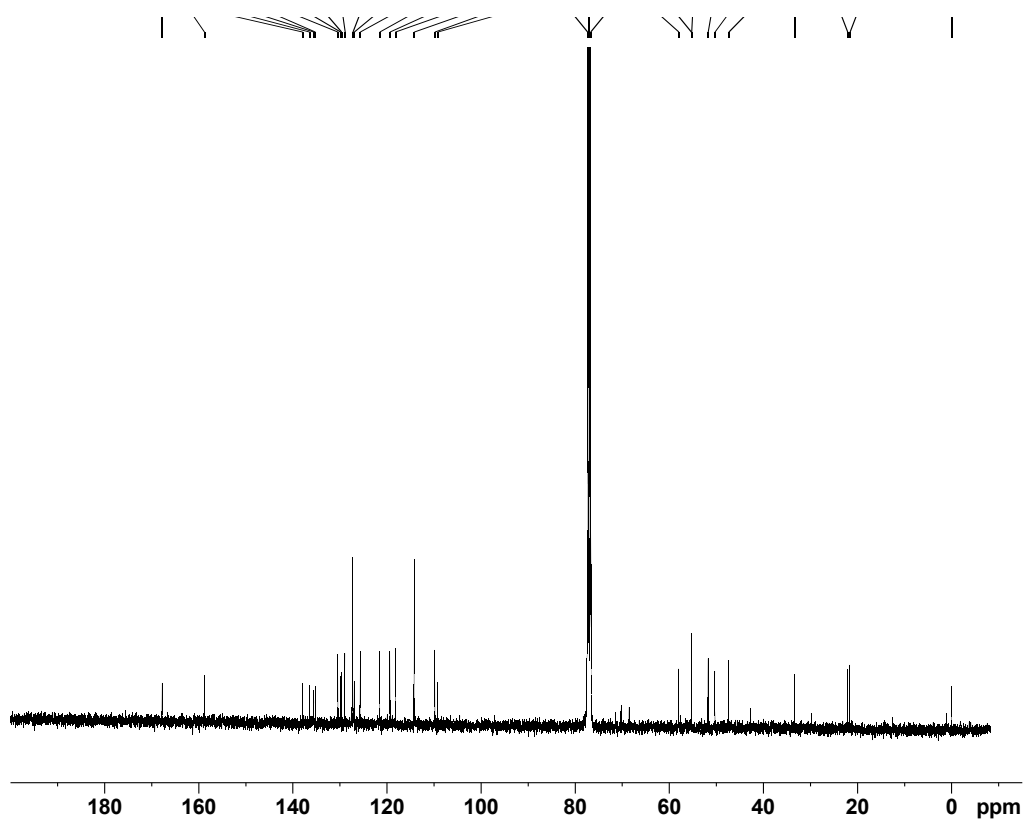
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PCPD2
PL2
PL12
PL13
SFO2 100.6281500 MHz

F2 - Processing parameters
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SF 100.6281500 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^1H and ^{13}C NMR spectra of diyne 14

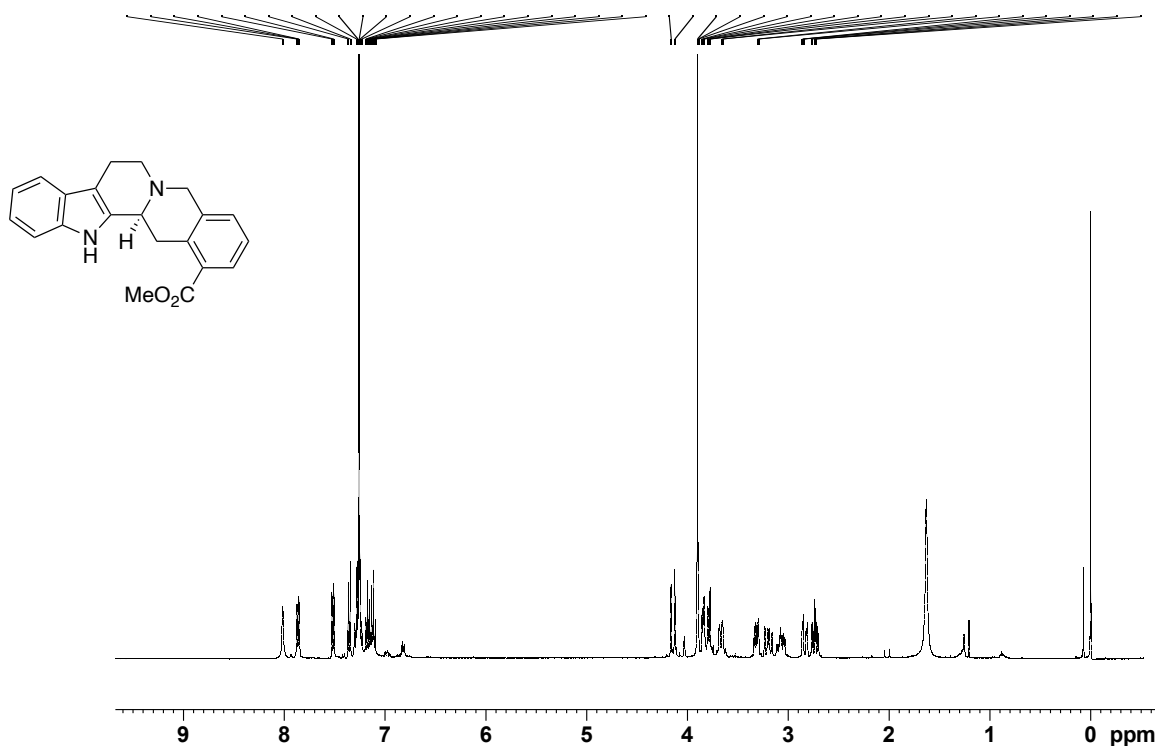


HS-45-1
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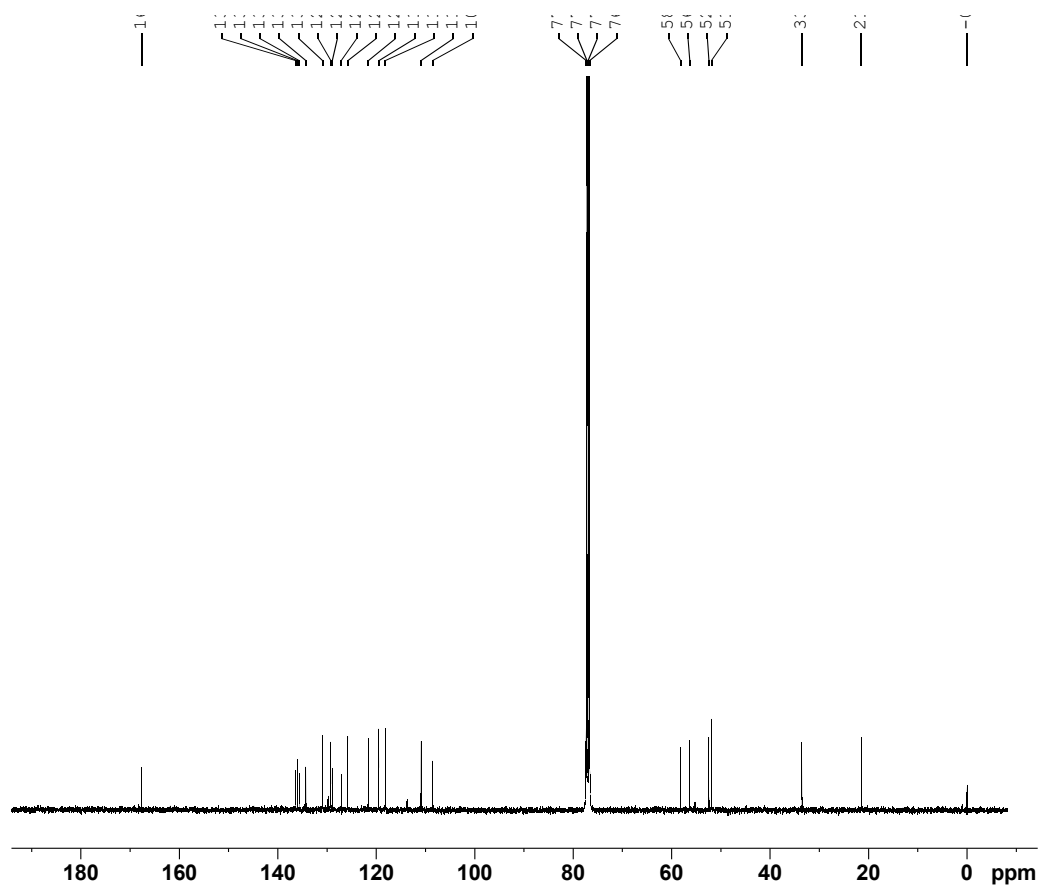


¹H and ¹³C NMR spectra of pentacycle **15**

PAT-F-110-1
¹H NMR_400MHz_CDCl₃



PAT-F-110-1
¹³C NMR_400MHz_CDCl₃



¹H and ¹³C NMR spectra of dihydrogambirtannine 1



Current Data
 NAME
 EXPNO
 PROCNO

F2 - Acquisition
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 Time_
 INSTRUM
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 PULPROG
 TD
 SOLVENT
 NS
 DS
 SWH
 FIDRES
 AQ
 RG
 DW
 DE
 TE
 D1
 TD0

===== CHA
 NUC1
 P1
 PL1
 SFO1

F2 - Process
 SI
 SF
 WDW
 SSB
 LB
 GB
 PC



Current Data Para
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 EXPNO
 PROCNO

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 Time_
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 TD
 SOLVENT
 NS
 DS
 SWH 238
 FIDRES 0.0
 AQ 1.3
 RG
 DW
 DE
 TE
 D1 2.00
 d11 0.03
 DELTA 1.89
 TD0

===== CHANNEL
 NUC1
 P1
 PL1
 SFO1 100.6

===== CHANNEL
 CPDPRG[2]
 NUC2
 PCPD2
 PL2
 PL12
 PL13
 SFO2 400.1

F2 - Processing p
 SI
 SF 100.6
 WDW
 SSB
 LB
 GB
 PC