

**Effect of Temperature on  $^1\text{H}$  NMR Spectra, Antitrypanosomal Activity, Conformational Analysis and, Molecular Docking of Curine Derivatives from *Berberis brevissima*.**

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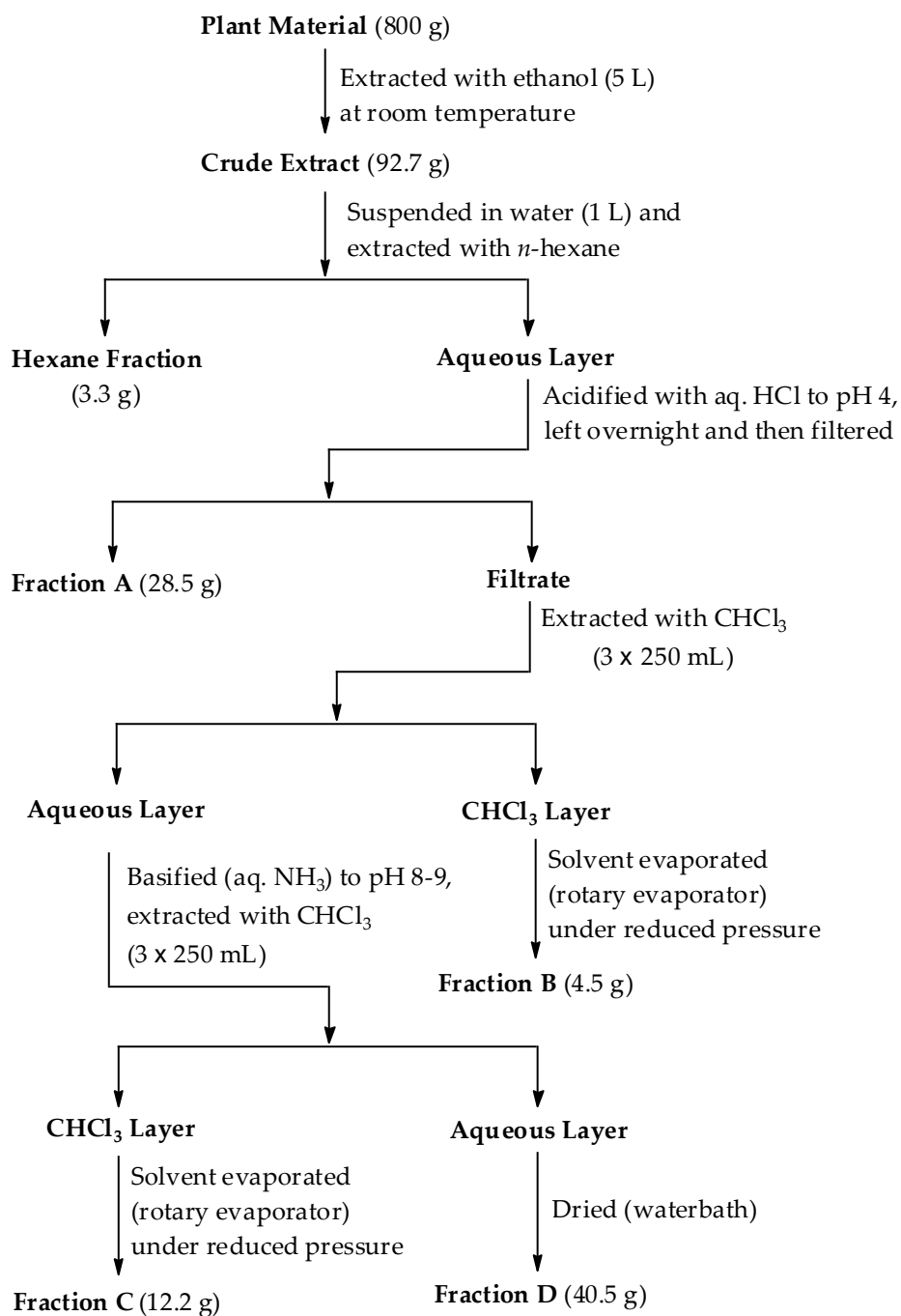
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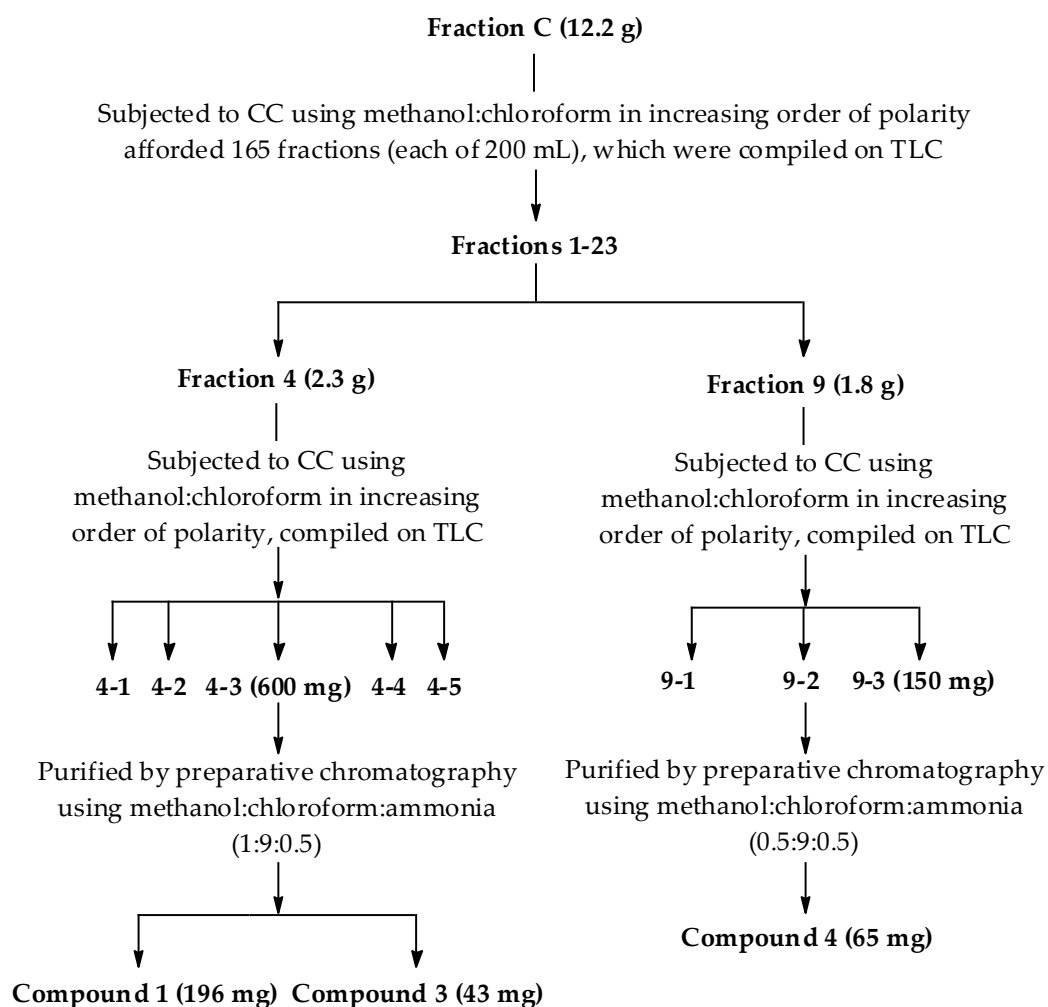
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**Figure S1.** General scheme for the extraction and fractionation of the roots of *Berberis brevissima* Jafri.



**Figure S2.** Scheme for the isolation of curine alkaloids from the alkaloid fraction of *Berberis brevissima* roots.

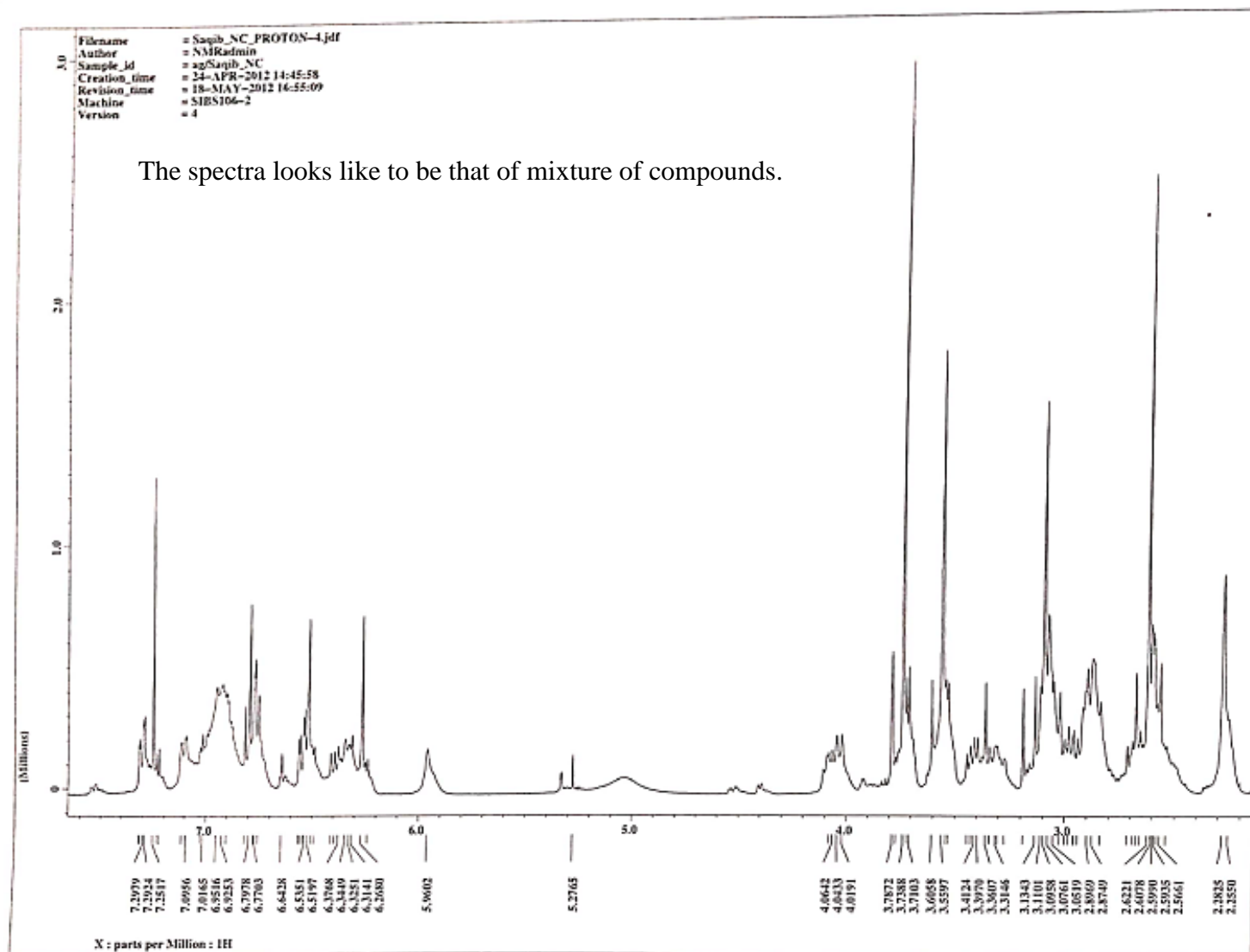


Figure S3.  $^1\text{H}$ -NMR Spectrum of Chondrofoline (**1**) in  $\text{CDCl}_3$  at  $25^\circ\text{C}$

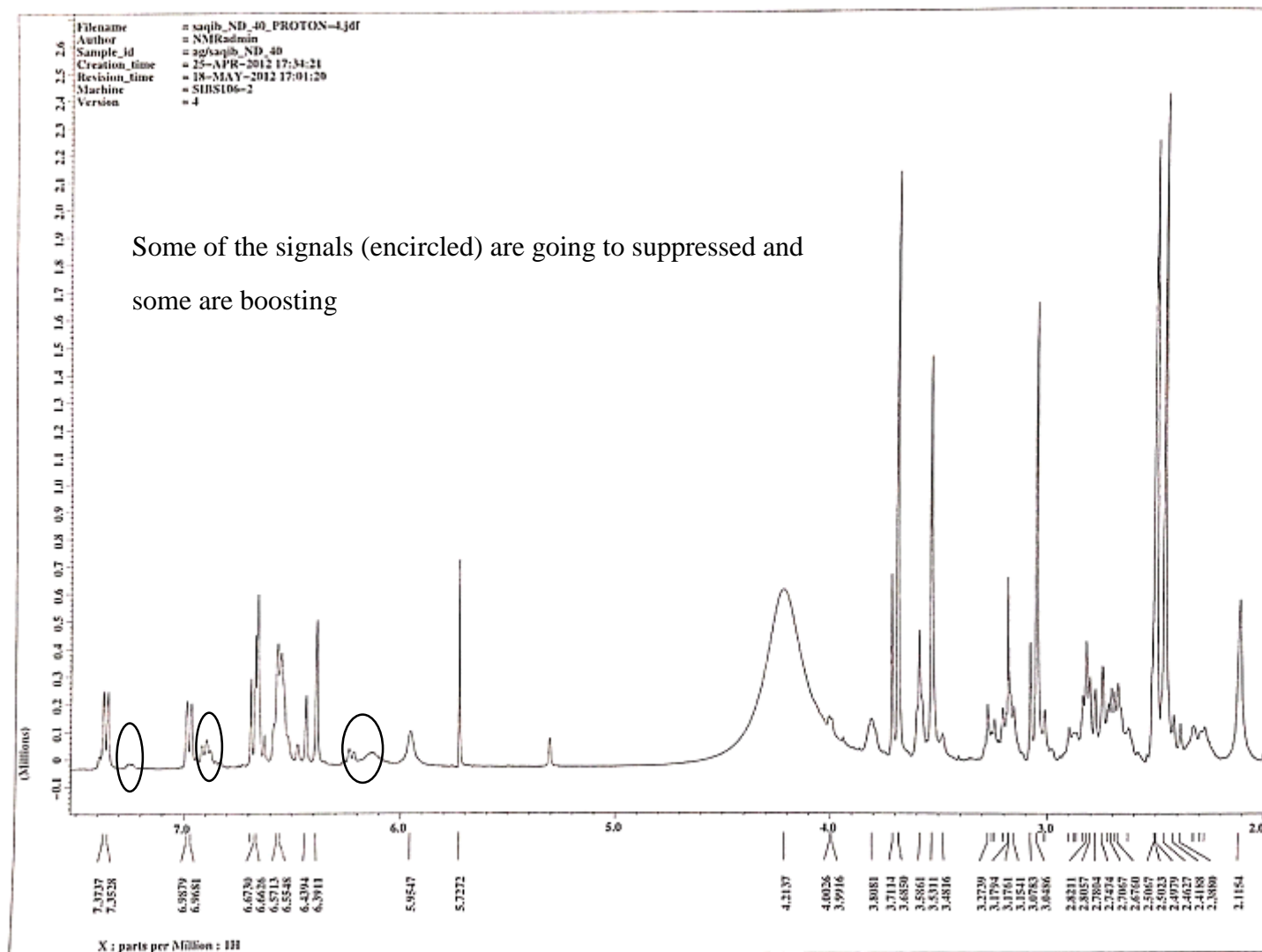
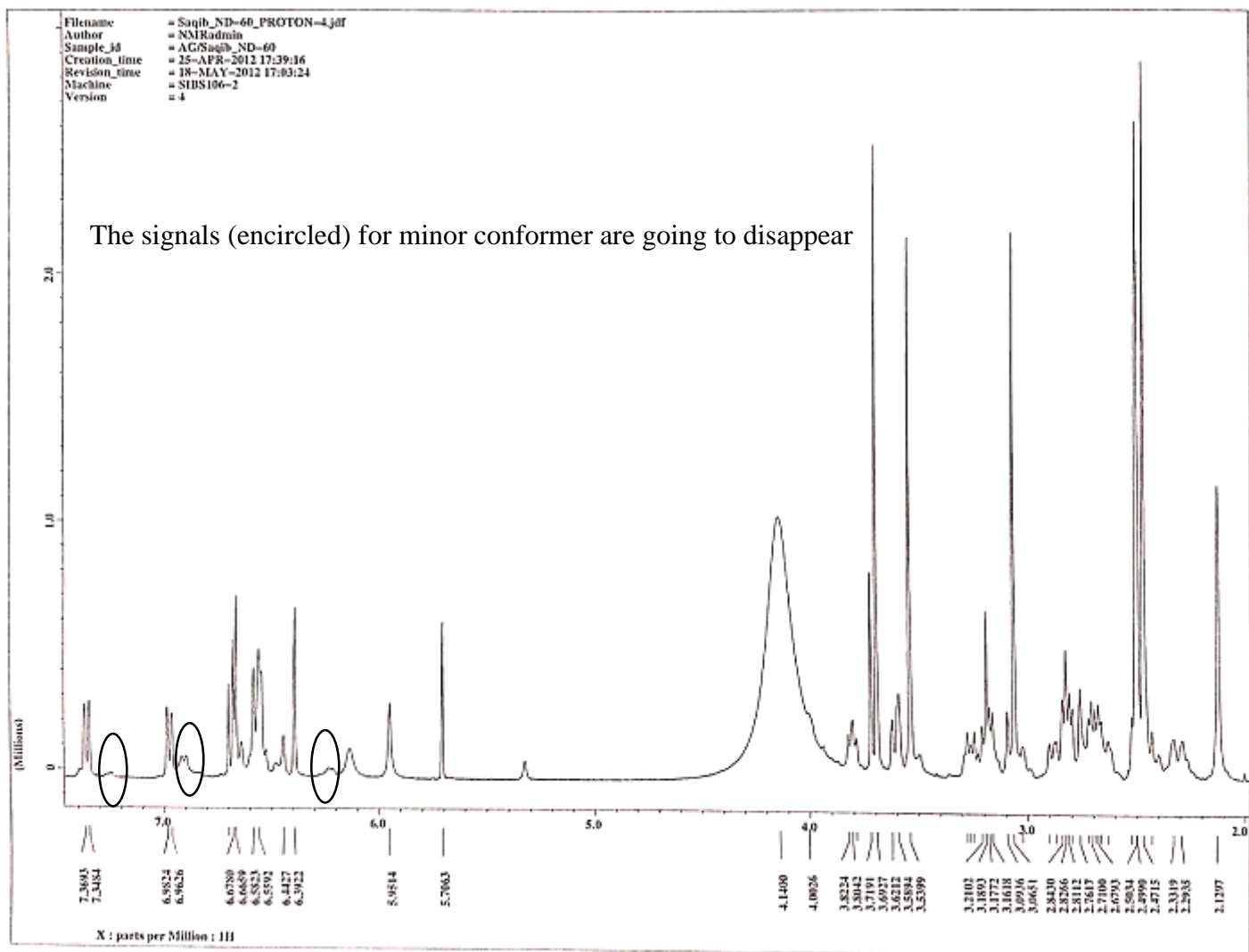
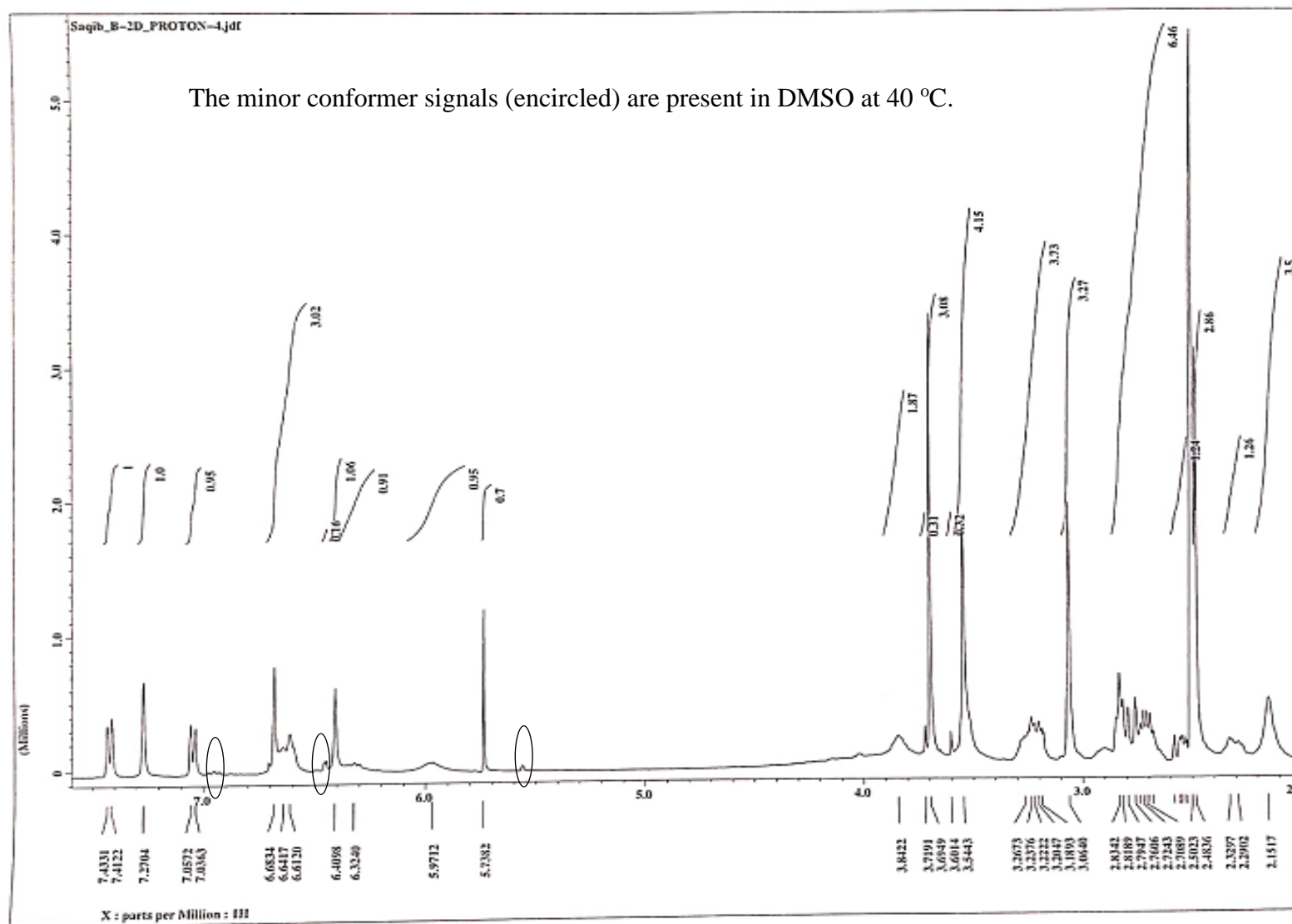


Figure S4.  $^1\text{H}$ -NMR Spectrum of Chondrofoline (**1**) in DMSO at 40 °C

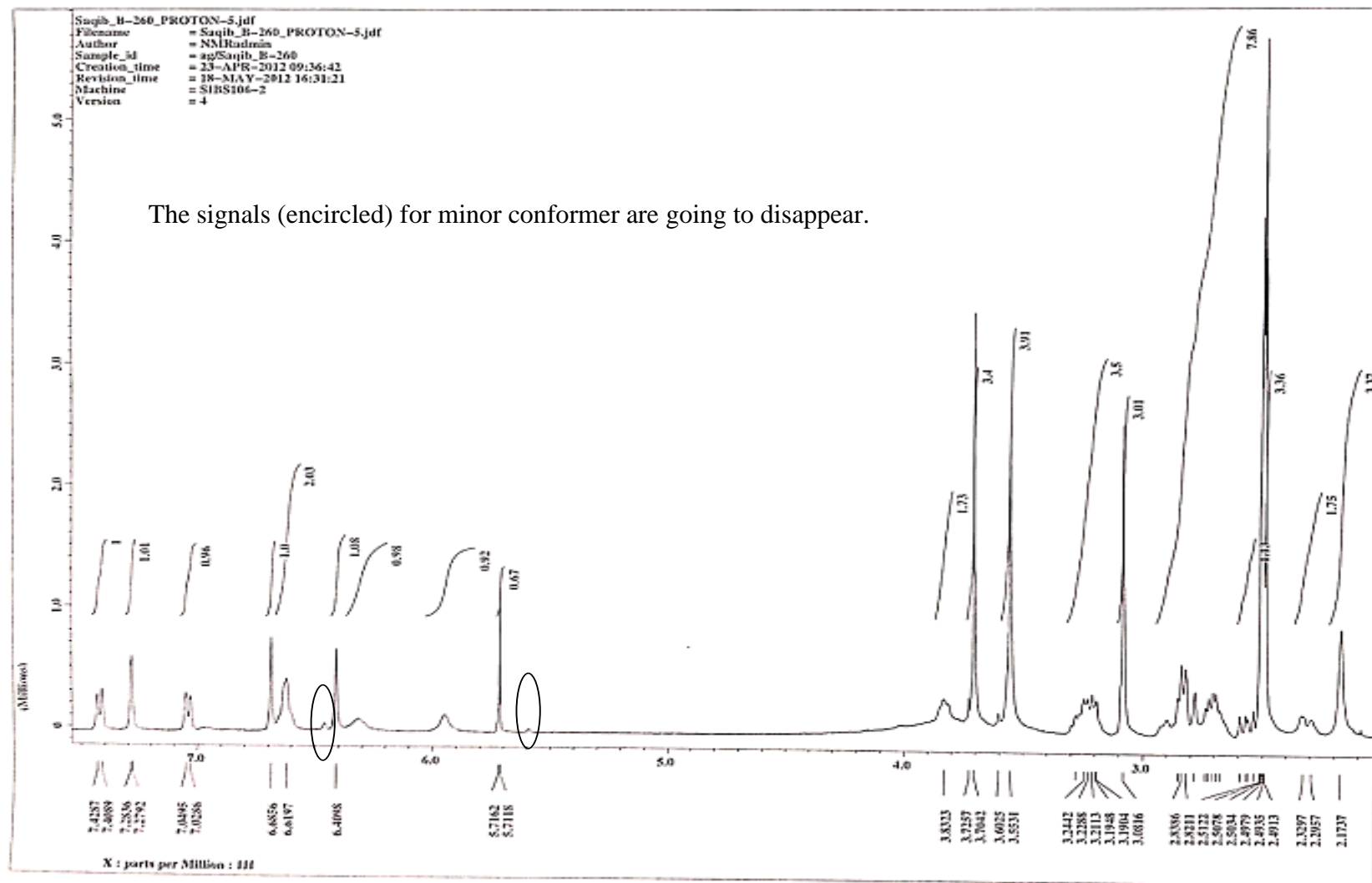


**Figure S5.**  $^1\text{H}$ -NMR Spectrum of Chondrofoline (**1**) in DMSO at 60 °C

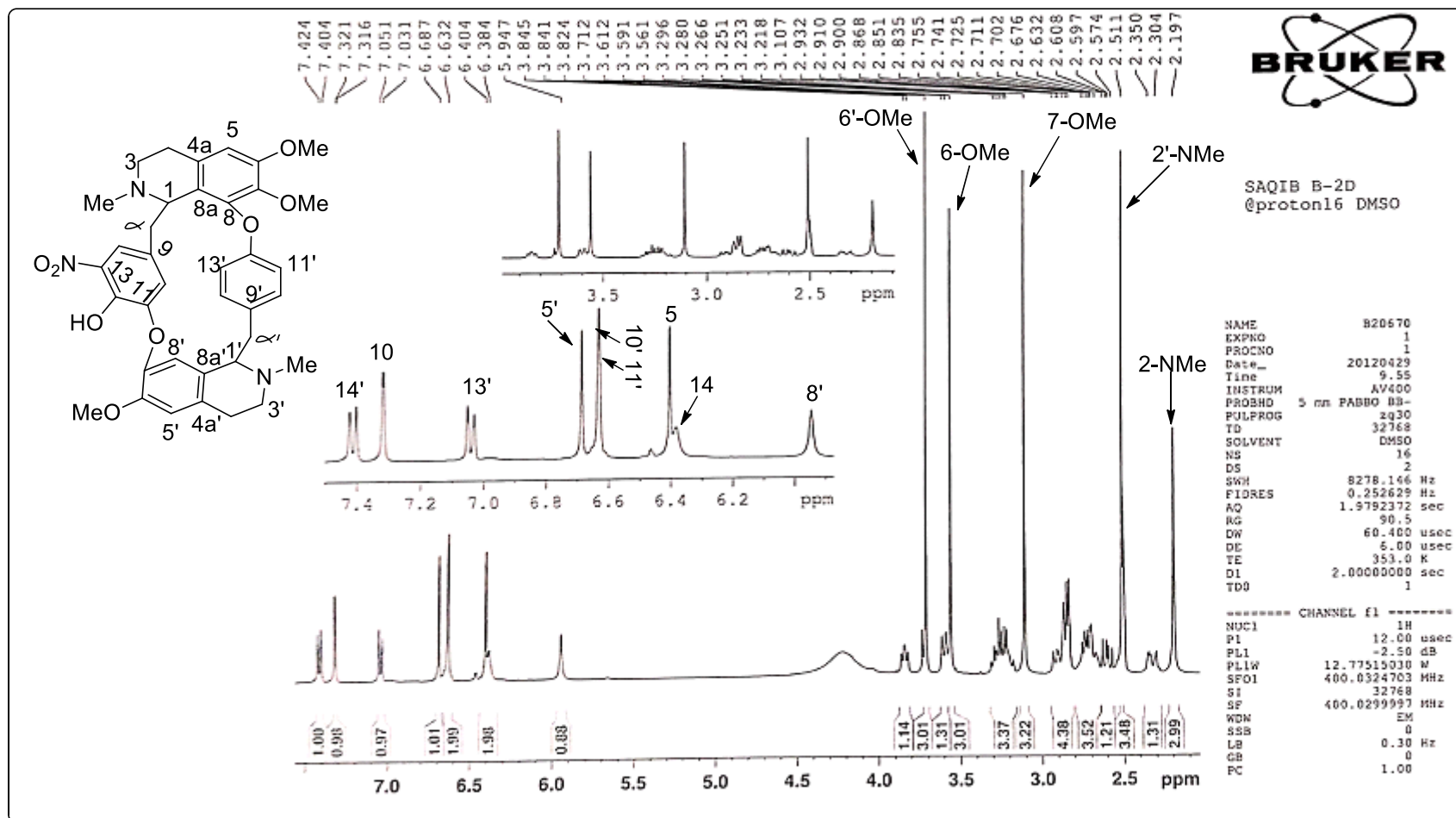




**Figure S7:** The  $^1\text{H}$ -NMR spectrum of 13-nitrochondrofoline (**2**) in DMSO at 40 °C



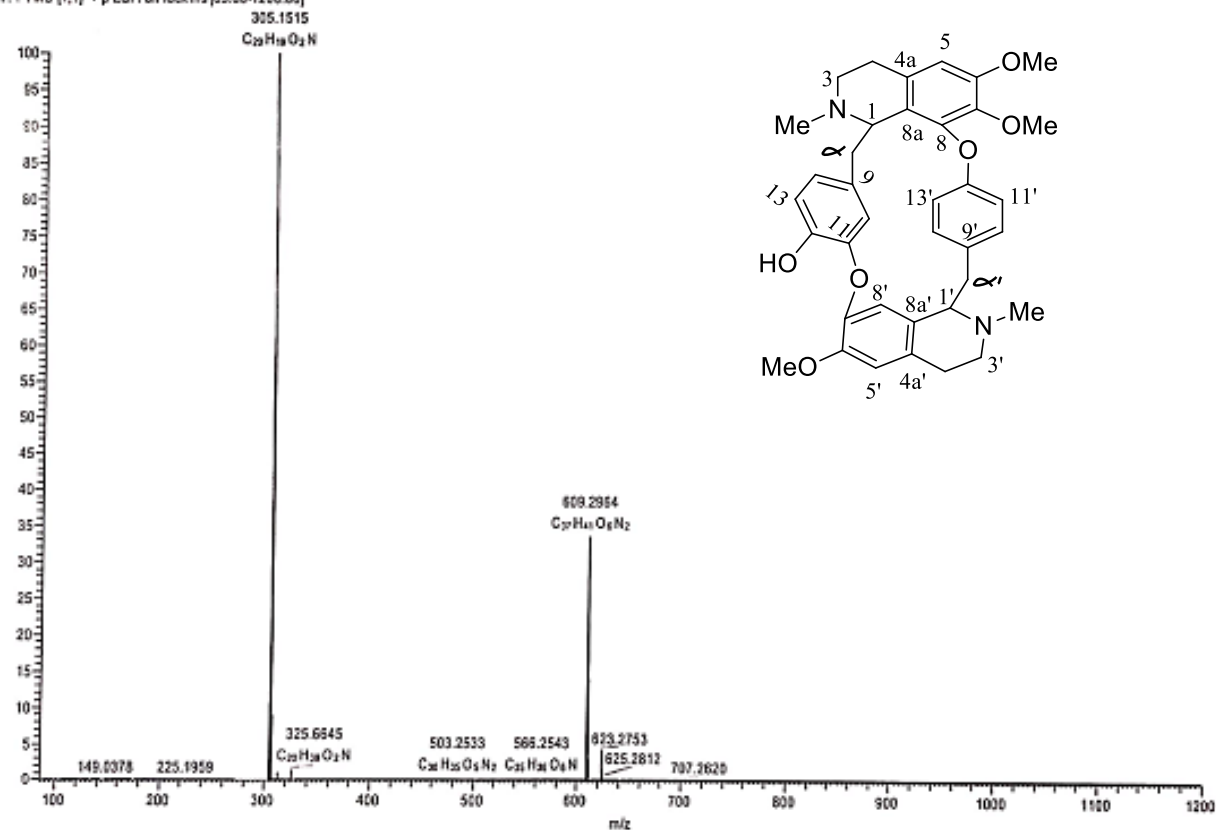
**Figure S8:** The  $^1\text{H}$ -NMR spectrum of 13-nitrochondrofoline (**2**) in DMSO at 60 °C

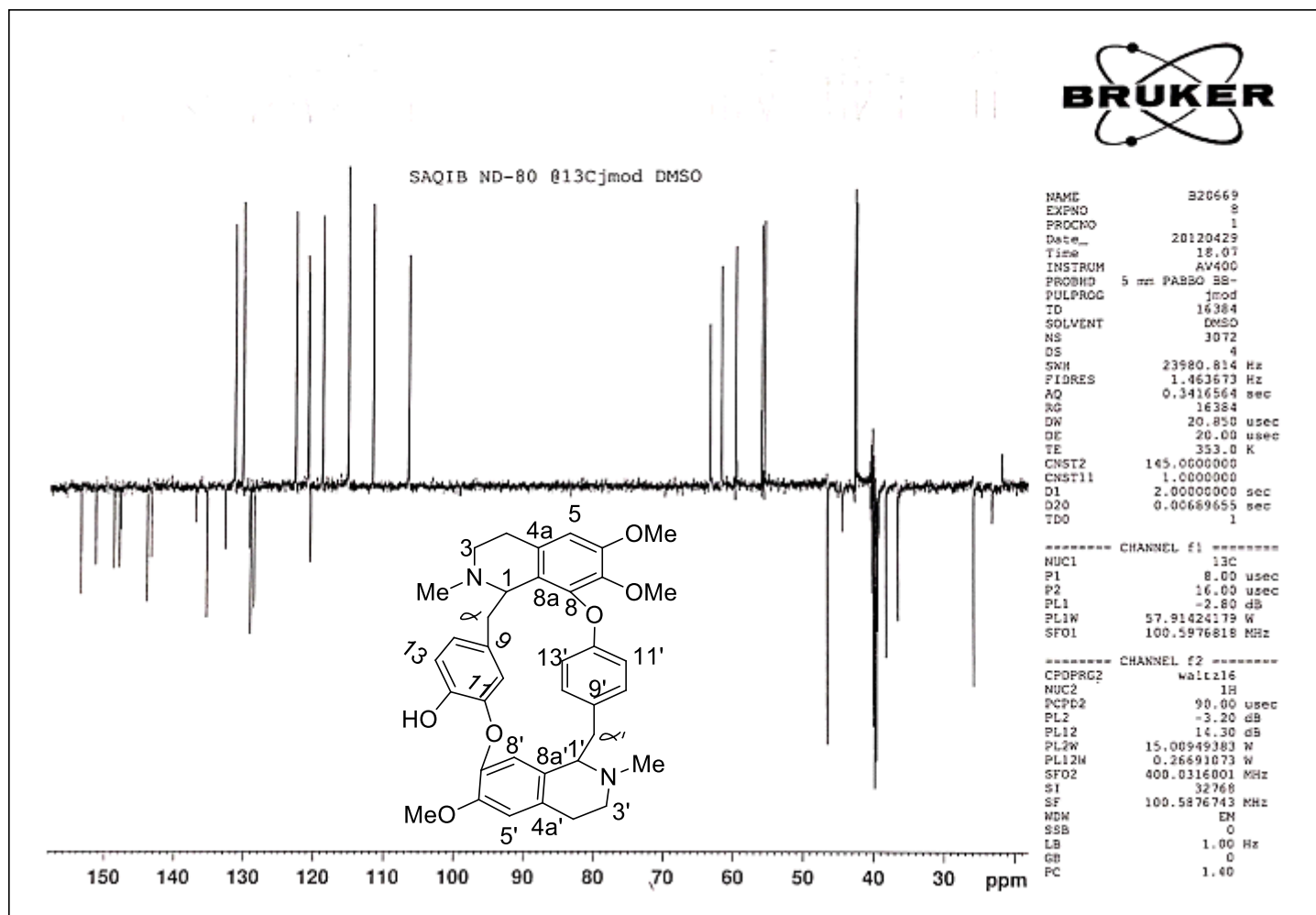


**Figure S9:** The <sup>1</sup>H-NMR spectrum of 13-nitrochondrofoline (**2**) in DMSO at 80 °C

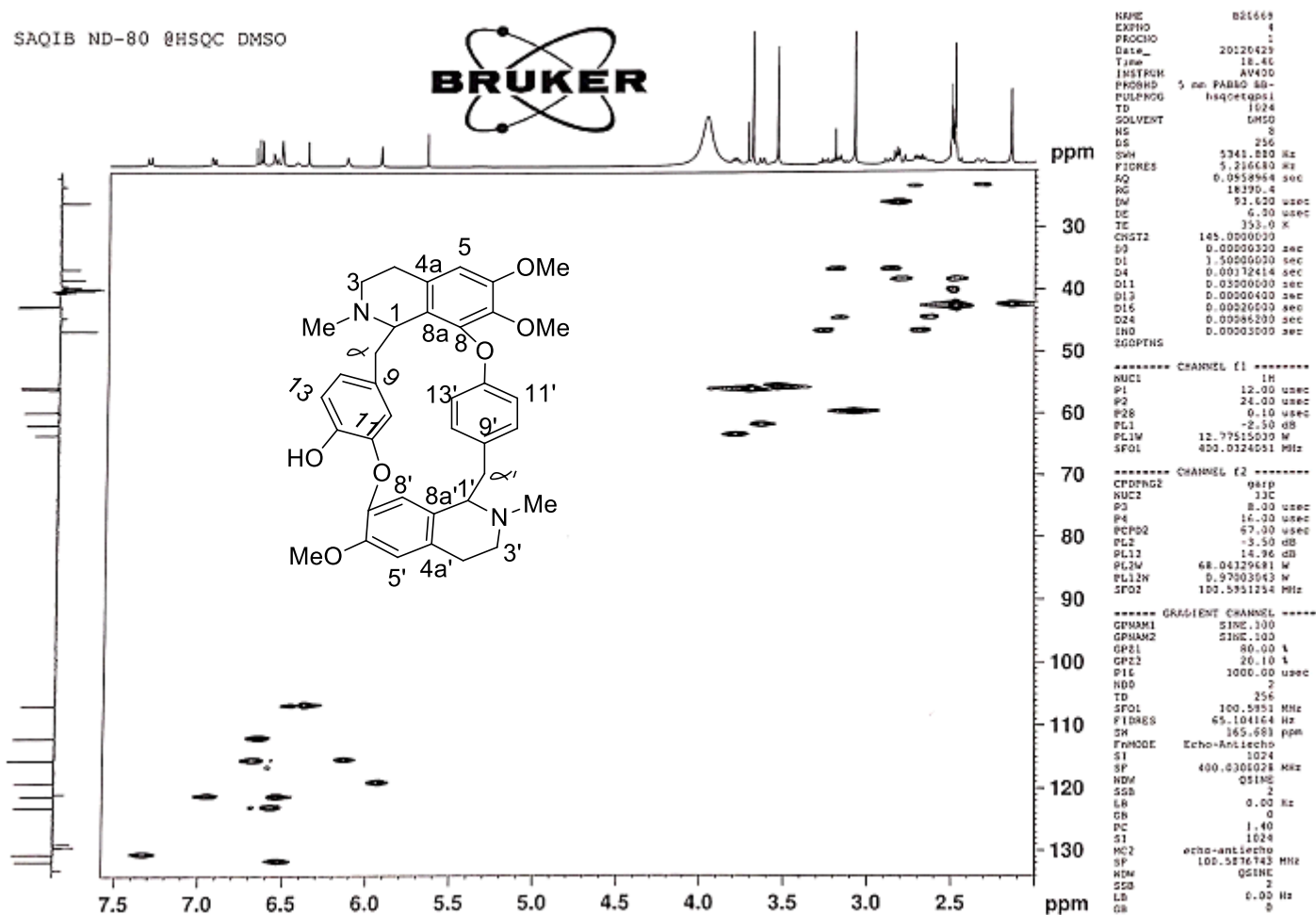
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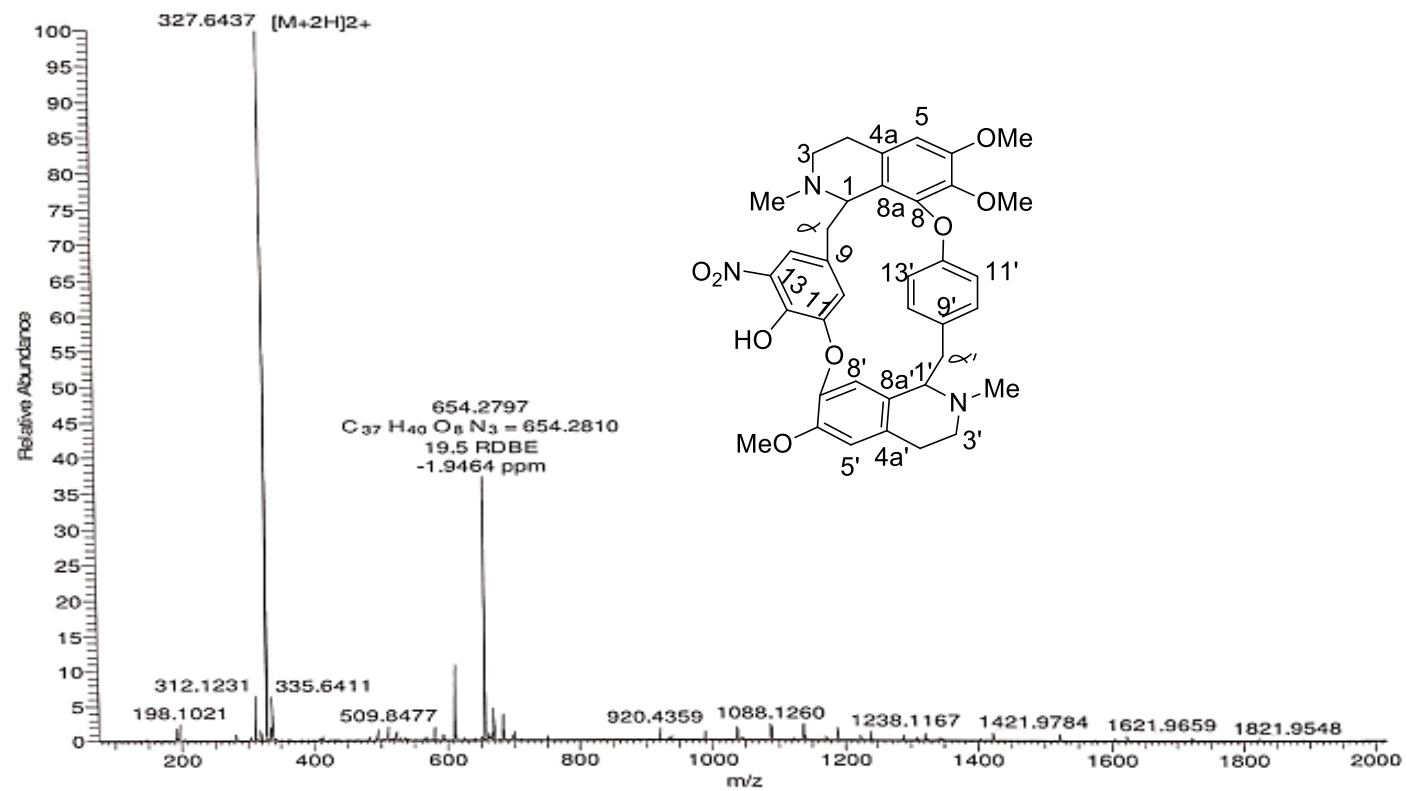
**Figure S10: FTMS, ESIMS Spectrum of Chondrofoline (1)**



**Figure S11:**  $^{13}\text{C}$ -NMR Spectrum of Chondrofoline (1) in DMSO at 80 °C



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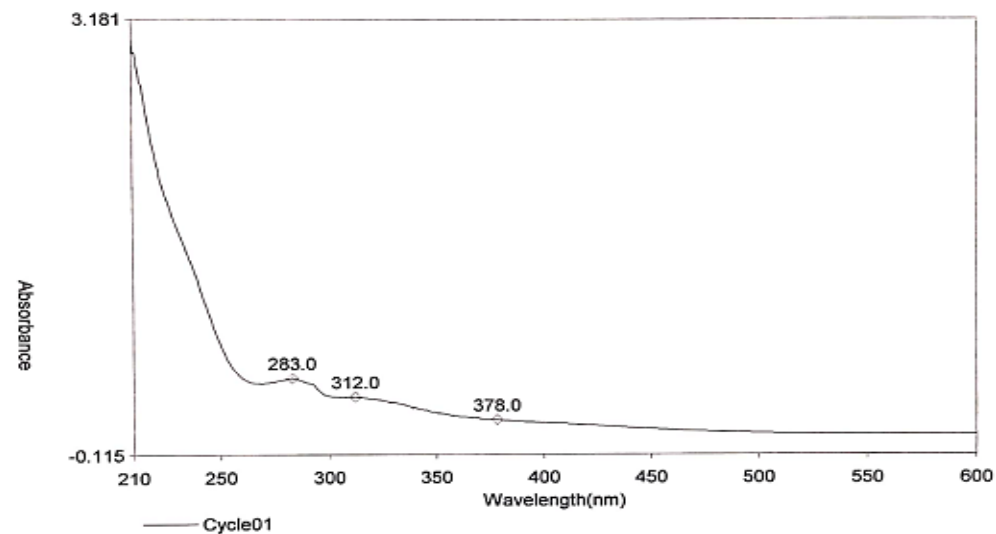


**Figure S13:** FTMS, ESIMS Spectrum of 13-nitrochondrofoline (**2**)

# THERMO SPECTRONIC ~ VISION32 SOFTWARE V1.25

Operator Name Saqib Ali  
 Department SIPBS  
 Organisation University of Strathclyde  
 Information MeOH 0.15mg/10ml  
 Date of Report 01/01/2001  
 Time of Report 00:50:30

## Scan Graph



**Results Table - ND-80 A pt15mg-mL.sre,B-02D A,Cycle01**

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378.00	0.148	Stop Lambda 600.0 nm
		Sort By Wavelength

Sensitivity Auto

Description MeOH 0.15mg/mL

Date Collected 01/01/2001 Time Collected 00:42:48

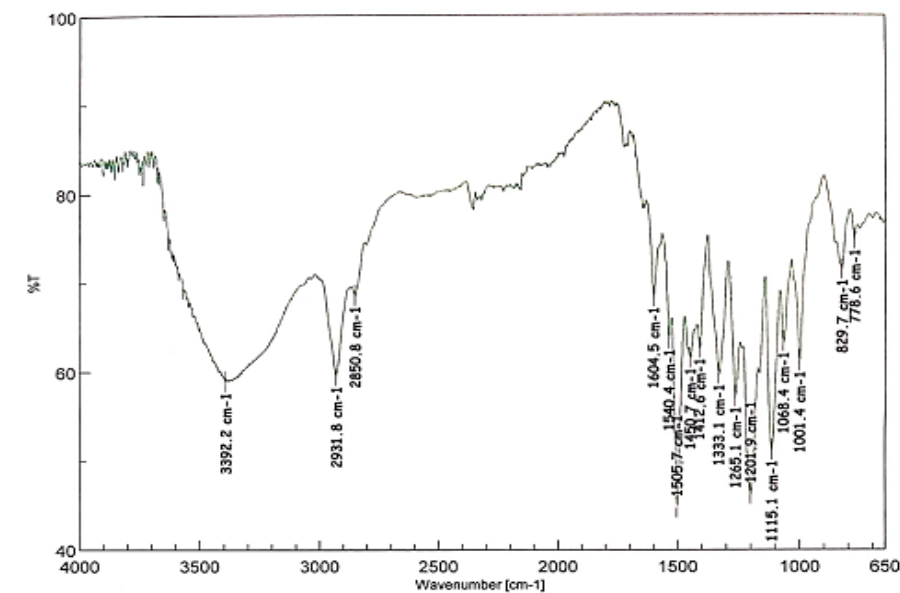
Operator Name Saqib Ali Instrument ID 093302

**Manipulations**

Manipulation 1 Convert to Absorbance

Date Performed 01/01/2001 Time Performed 00:42:49

**Figure S14:** UV-Visible spectra of 13-nitrochondrofoline (2)

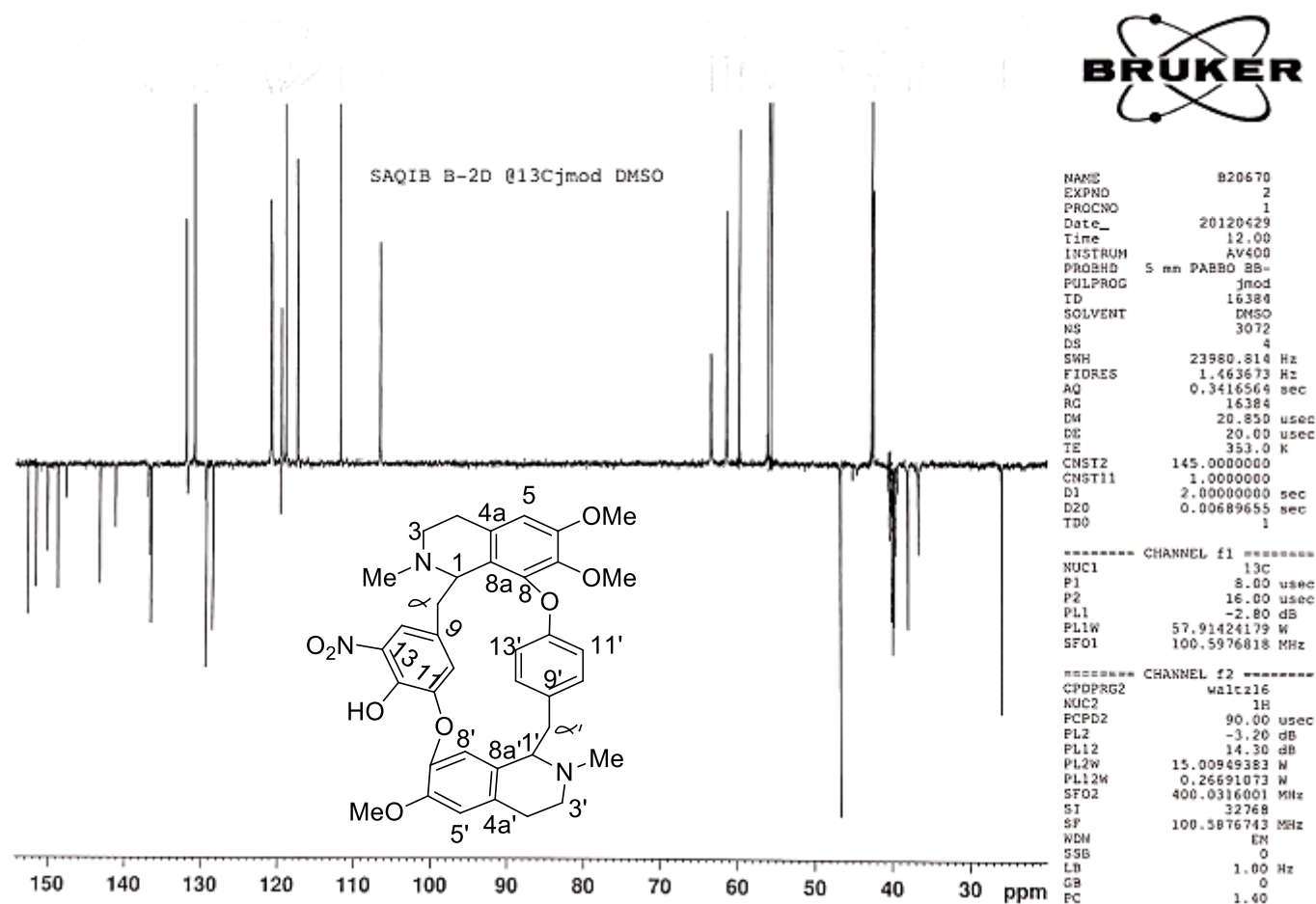


[Comment]  
 Sample Name B-02D  
 Comment ATR  
 User  
 Division  
 Company University of Strathclyde

B-02D ATR CORR

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		Vertical	%T
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Accessory S/N	13871	End	4000.12 cm-1
Light Source	Standard	Data pitch	0.482117 cm-1
Detector	TGS	Data points	6950
Accumulation	50		
Resolution	2 cm-1		
Zero Filling	On		
Apodization	3-Sigma Gaussian		
Gain	Auto (8)		
Aperture	3.5 mm		
Scanning Speed	1 mm/sec		
Filter	Auto (30000 Hz)		

**Figure S15:** FT-IR spectra of 13-nitrochondrofoline (2)



**Figure S16:**  $^{13}\text{C}$ -NMR Spectrum of 13-niteochondrofoline (2) in DMSO at 80 °C



C:\Xcalibur\...120120718\ND-80Ac

18/07/2012 13:00:02

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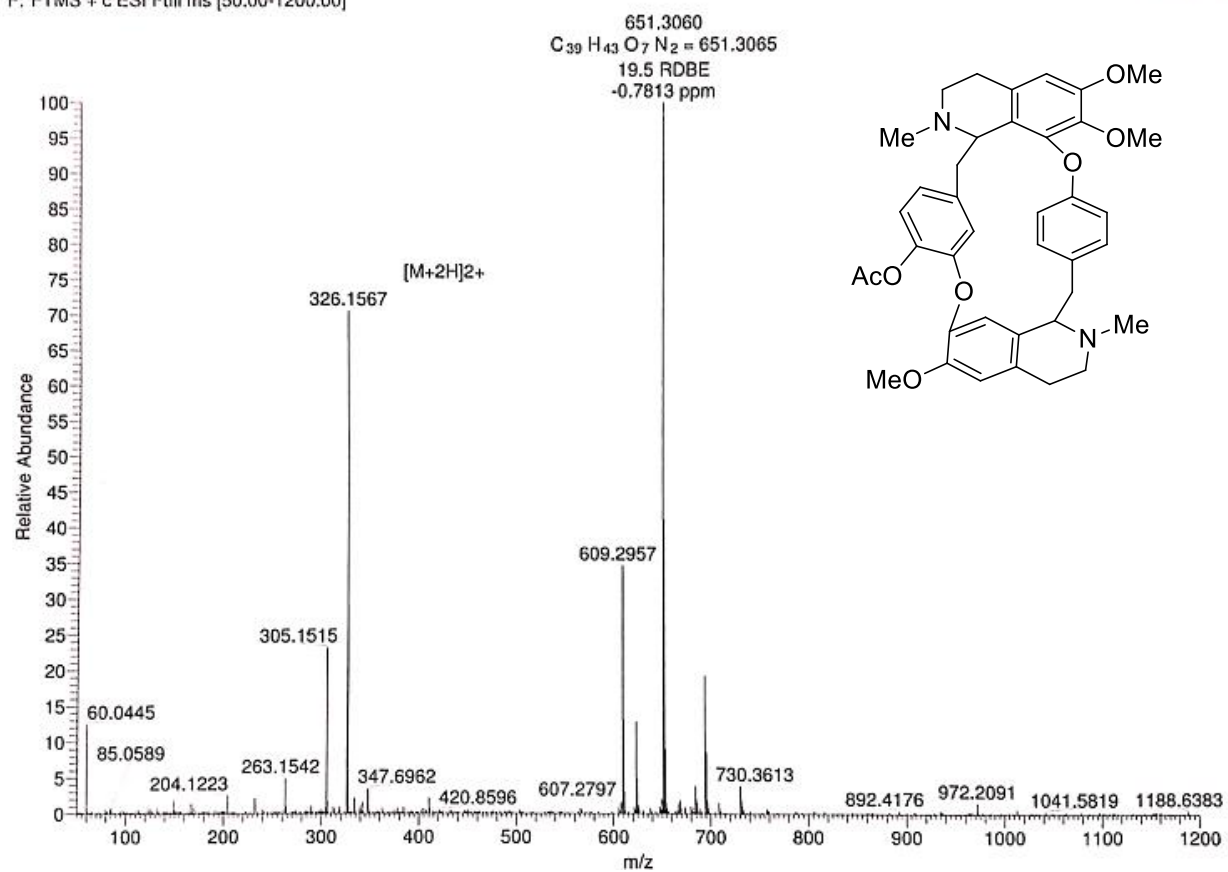
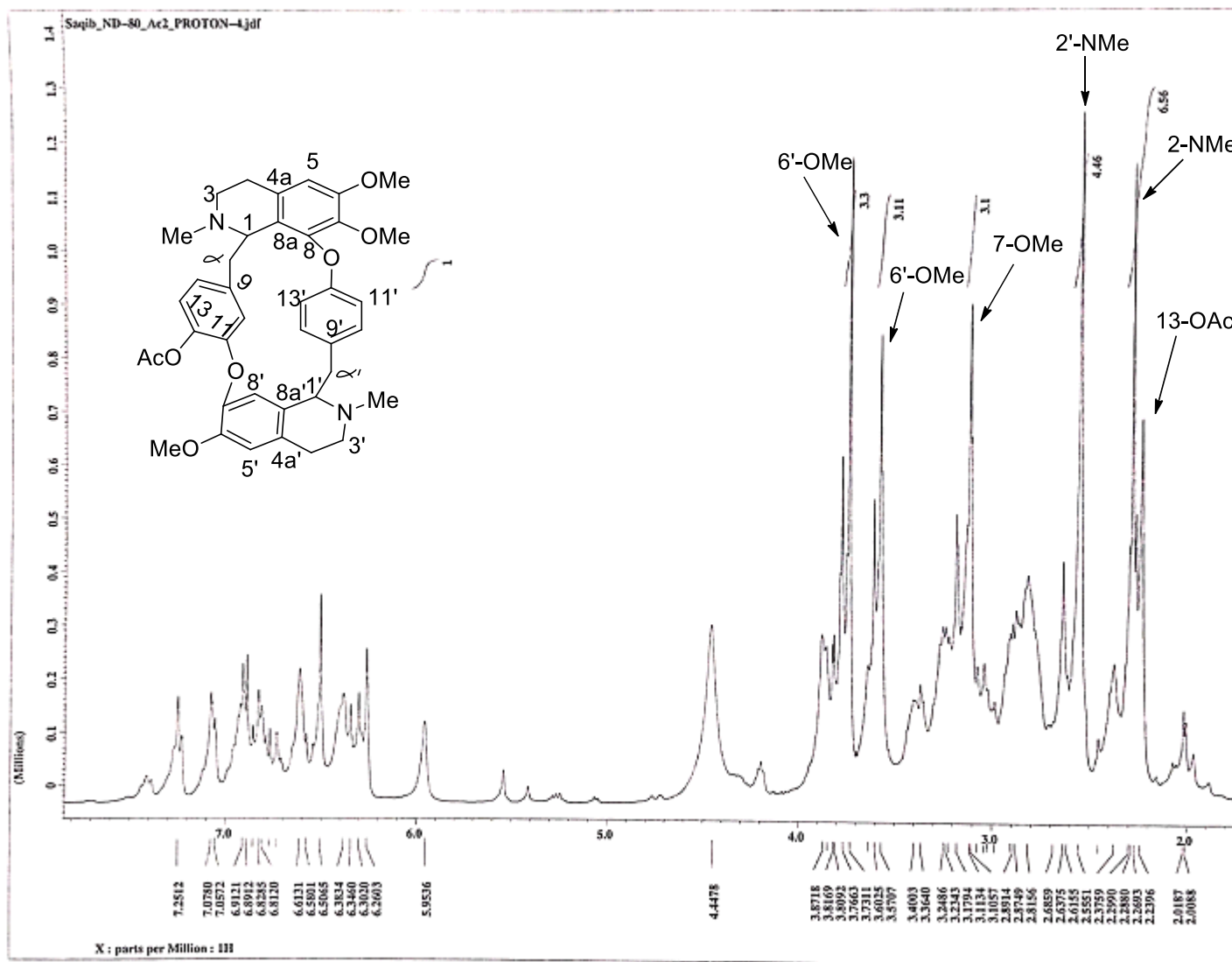
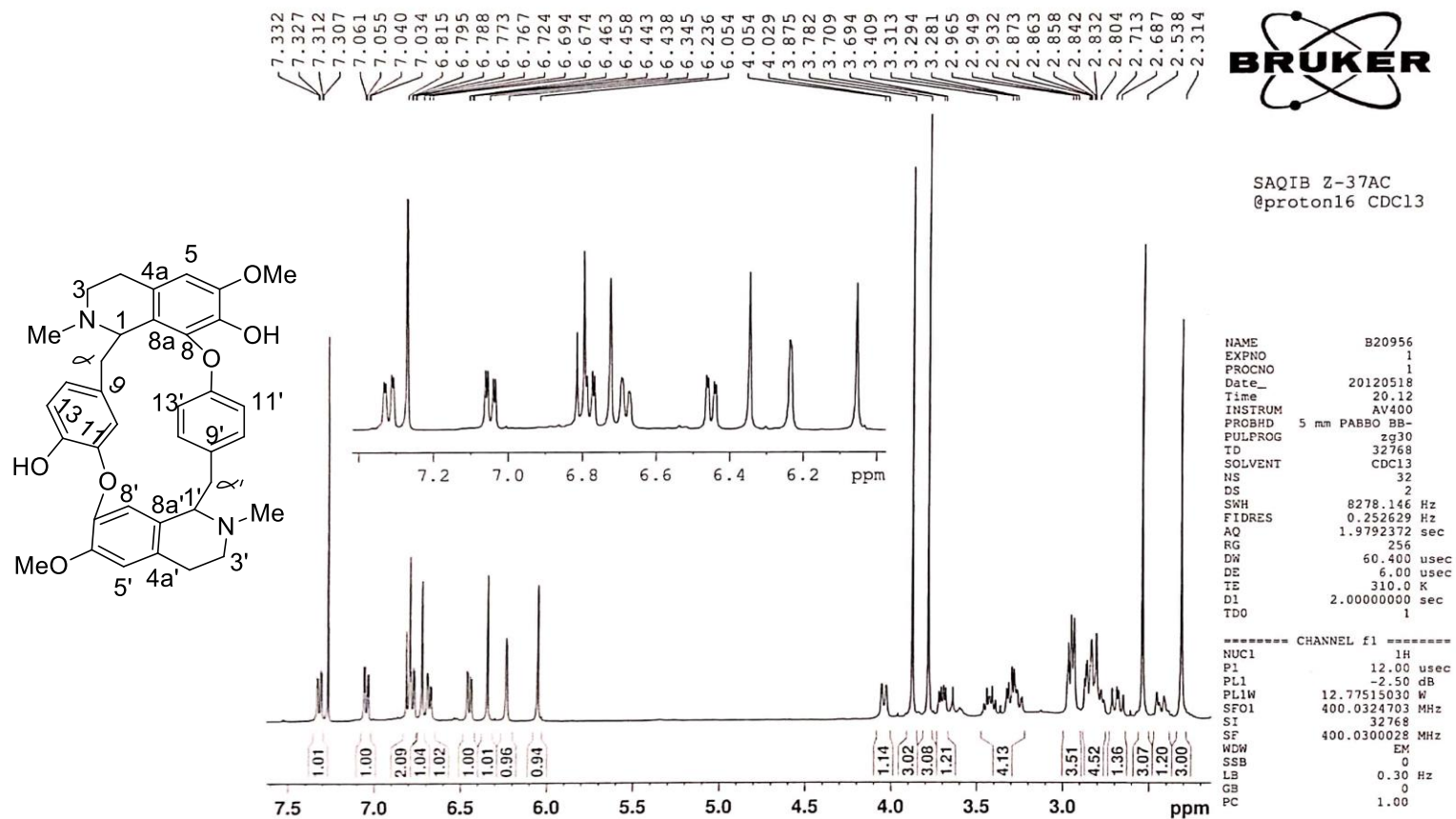


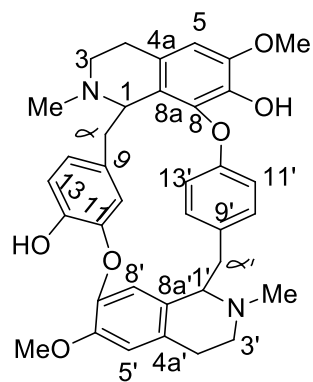
Figure S18: FTMS, ESIMS Spectrum of O-acetylchondrofoline (3)



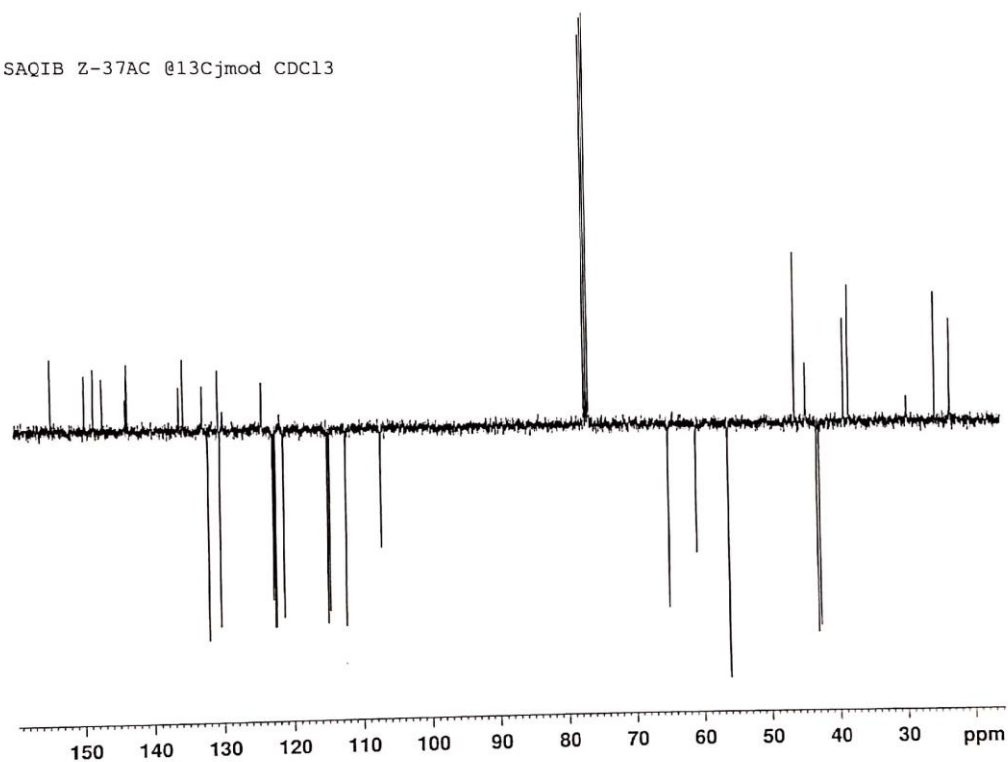
**Figure S19:**  $^1\text{H}$ -NMR Spectrum of O-acetylchondrofoline (3)



**Figure S20:**  $^1\text{H}$ -NMR Spectrum of Curine (**4**)



SAQIB Z-37AC @13Cjmod CDCl<sub>3</sub>



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PROCNO         1
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Time           23.14
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PULPROG        jmod
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DS             4
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FIDRES         1.463673 Hz
AQ            0.3416564 sec
RG            16384
DW            20.850 usec
DE            20.00 usec
TE            310.0 K
CNST2         145.0000000
CNST11        1.0000000
D1            2.50000000 sec
D2O           0.00689655 sec
TD0           1

===== CHANNEL f1 =====
NUC1           13C
P1             8.00 usec
P2            16.00 usec
PL1           -2.00 dB
PL1W          57.91424179 W
SFO1          100.626115 MHz

===== CHANNEL f2 =====
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NUC2           1H
PCPD2         90.00 usec
P2            -3.20 dB
PL12          14.30 dB
PL2W          15.00949383 W
PL12W         0.26691073 W
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SI            32768
SF            100.626115 MHz
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LB            1.00 Hz
GB            0
PC            1.40
  
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Figure S21: <sup>13</sup>C-NMR Spectrum of Curine (4)

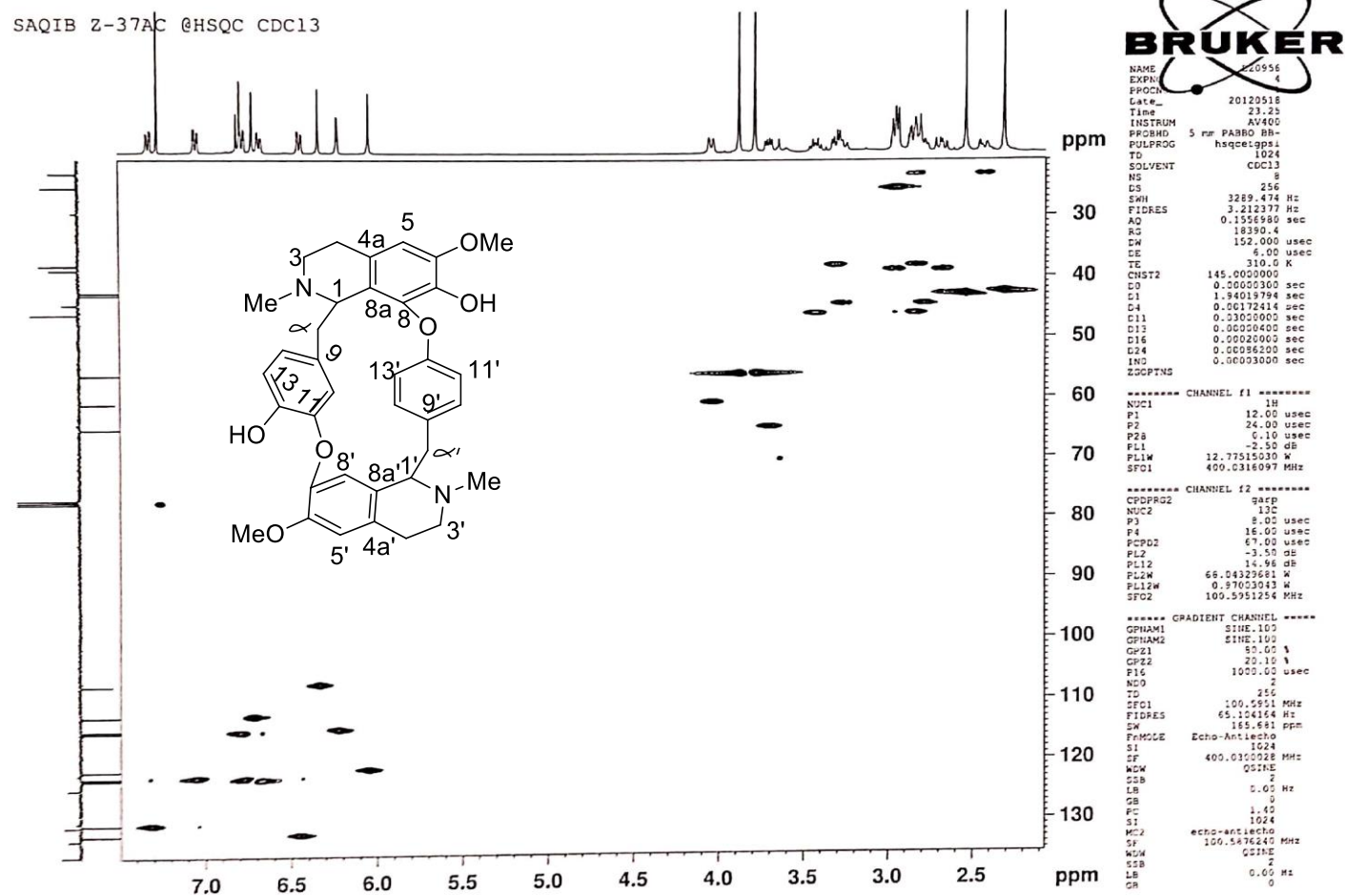
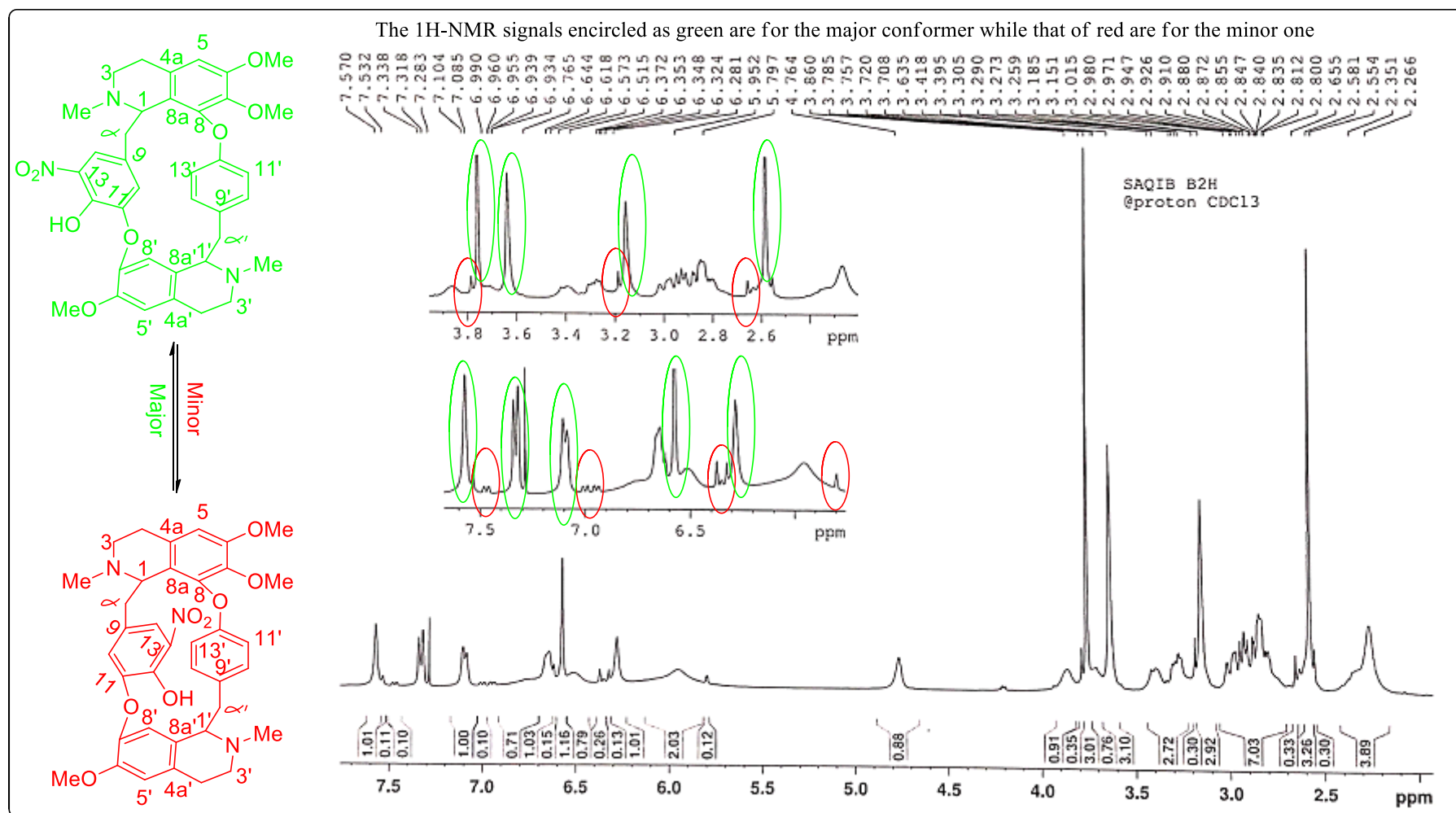


Figure S22: HSQC Spectrum of Curine (4)



**Figure S23:** The  $^1\text{H}$ -NMR spectrum of 13-nitrochondrofoline (2) in  $\text{CHCl}_3$  at 25 °C showing two conformers one major while other minor