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

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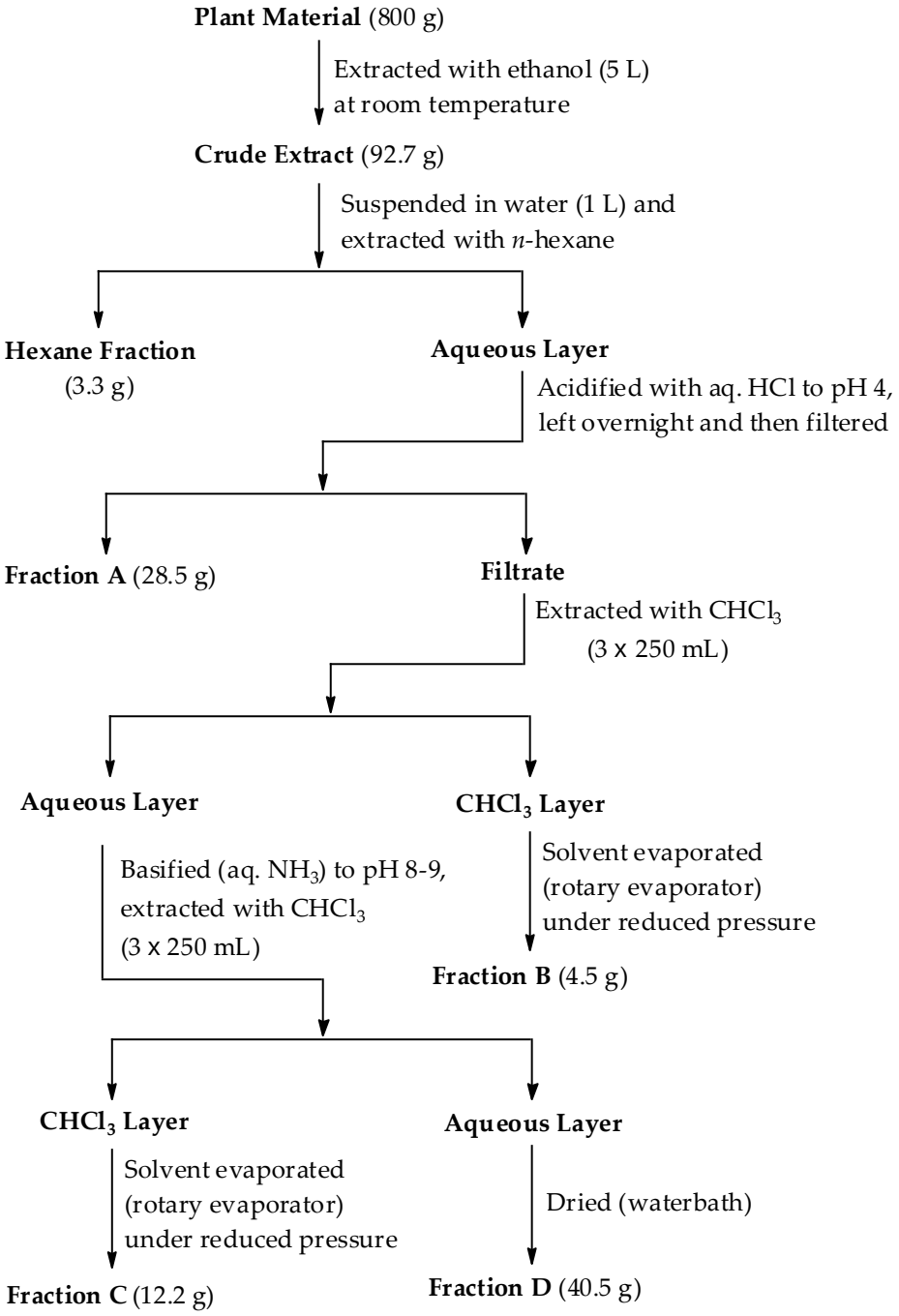


Figure S1. General scheme for the extraction and fractionation of the roots of *Berberis brevissima* Jafri.

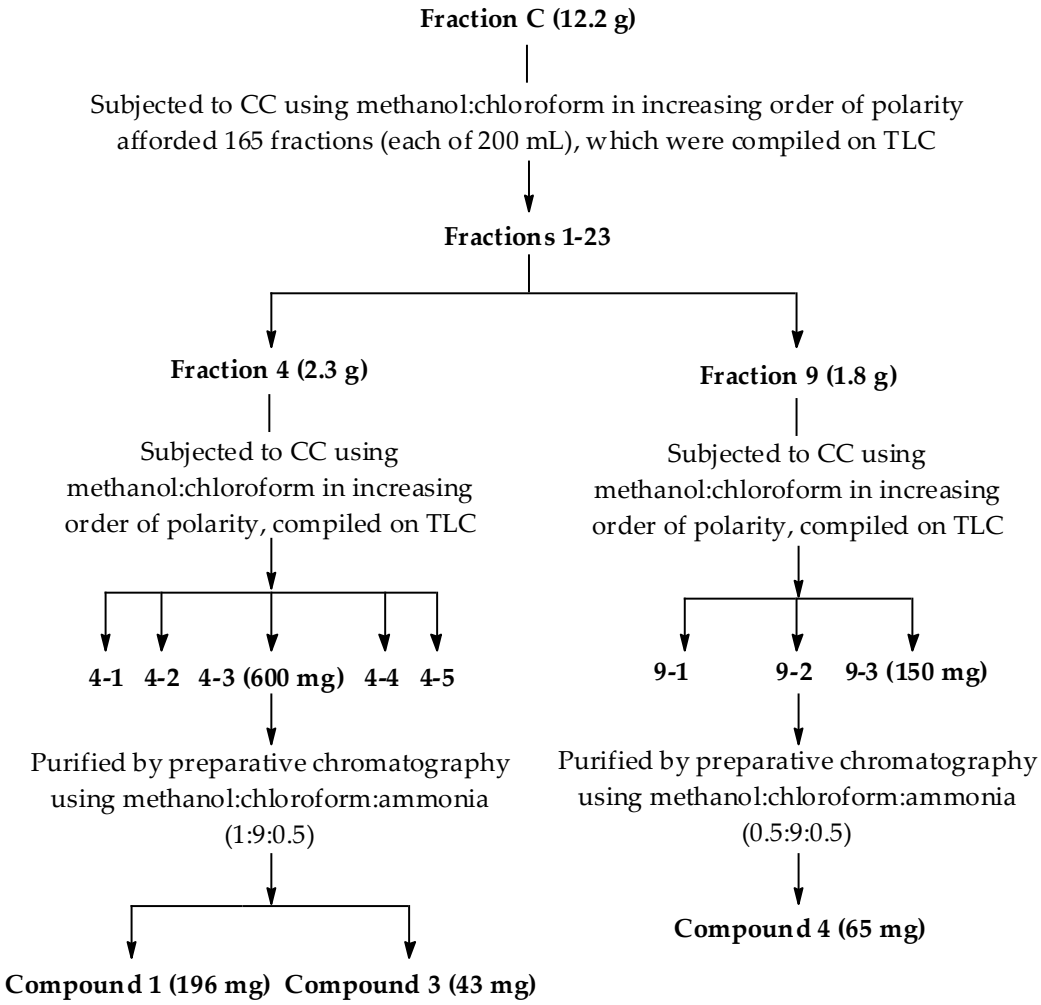


Figure S2. Scheme for the isolation of curine alkaloids from the alkaloid fraction of *Berberis brevissima* roots.

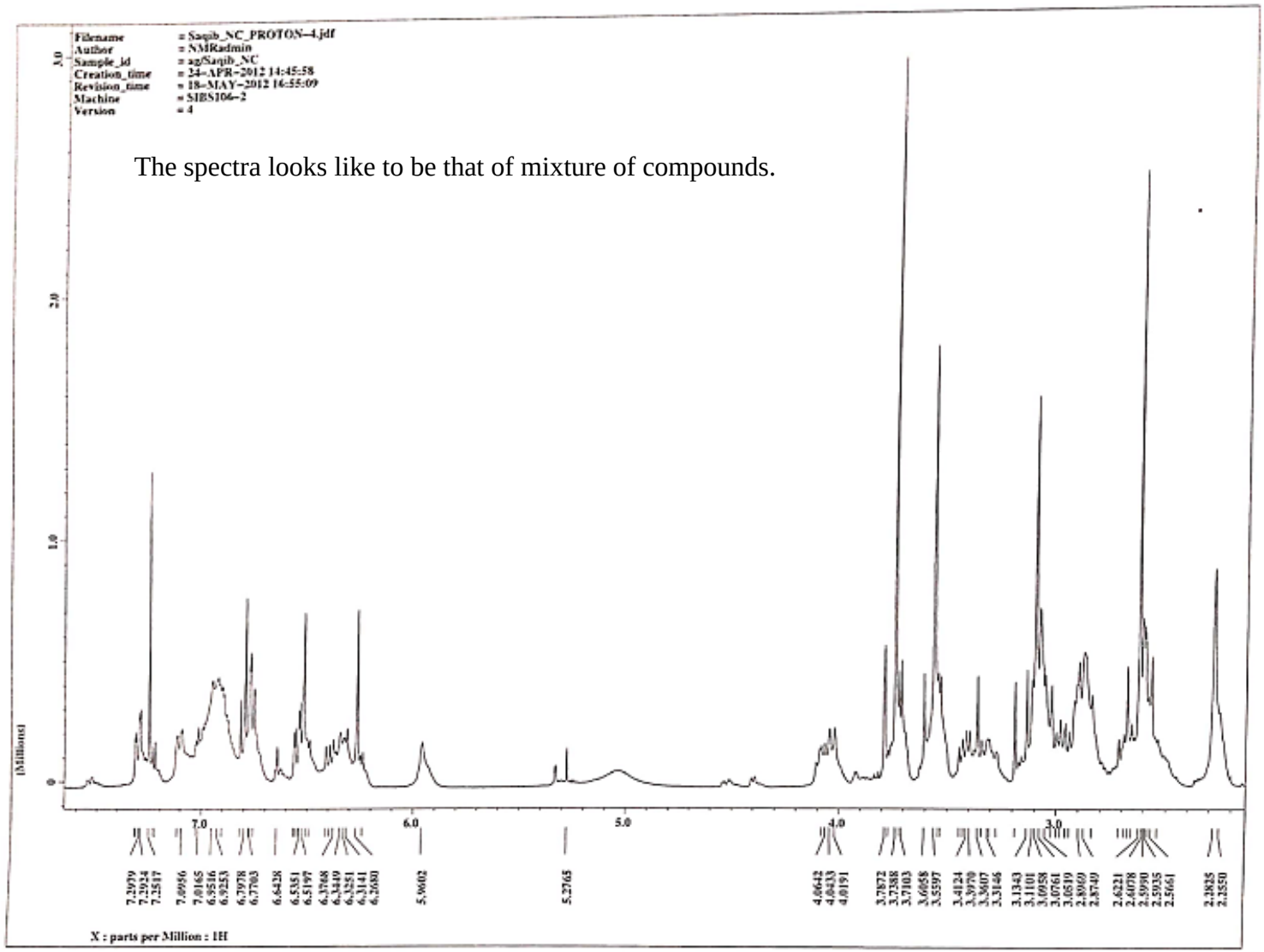


Figure S3. ^{1}H-NMR Spectrum of Chondrofoline (**1**) in $CDCl_3$ at 25 °C

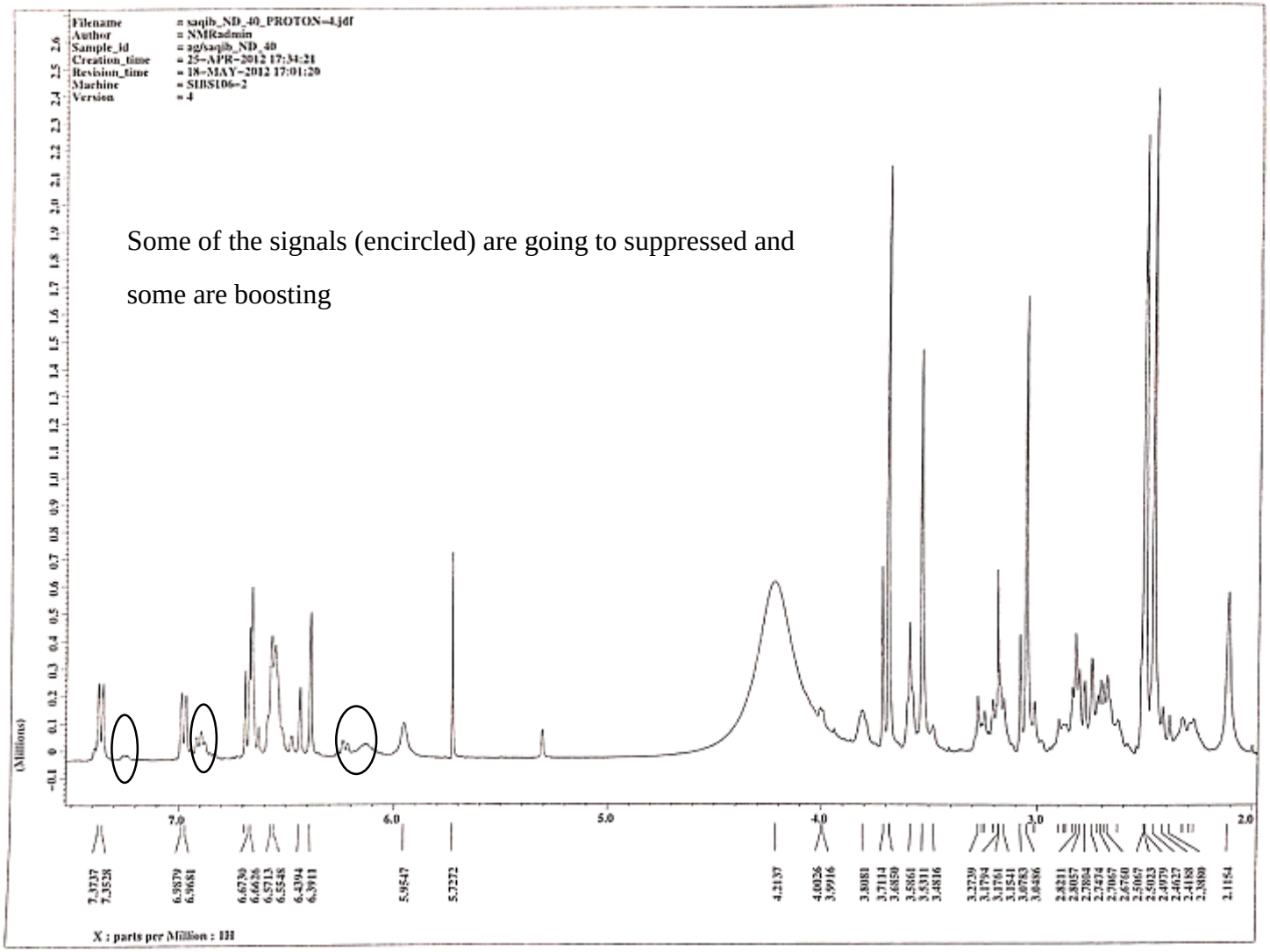


Figure S4. ^{1}H-NMR Spectrum of Chondrofoline (**1**) in DMSO at 40 °C

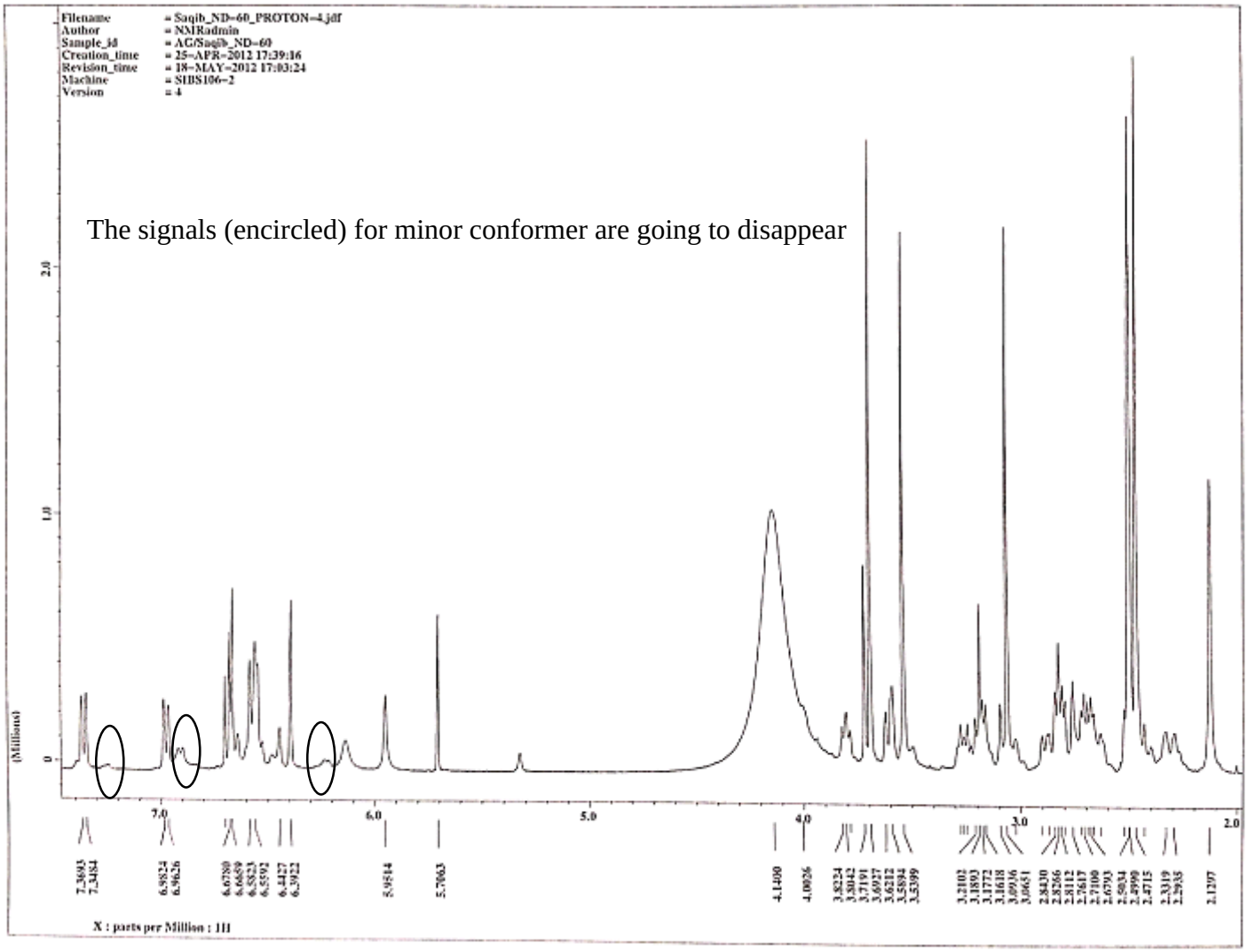


Figure S5. ^{1}H-NMR Spectrum of Chondrofoline (**1**) in DMSO at 60 °C

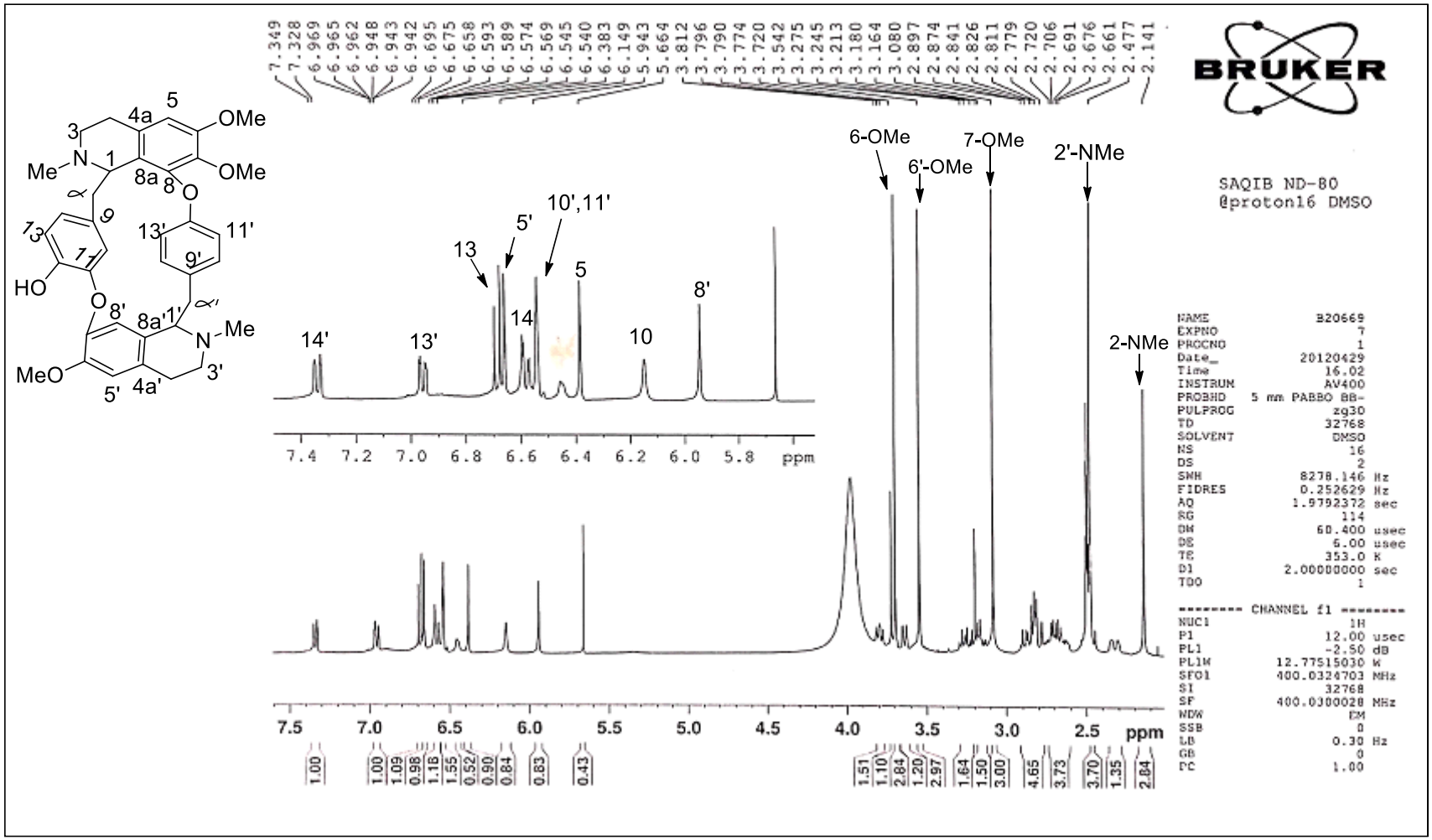


Figure S6: ^{1}H-NMR Spectrum of Chondrofoline (**1**) in DMSO at 80 °C

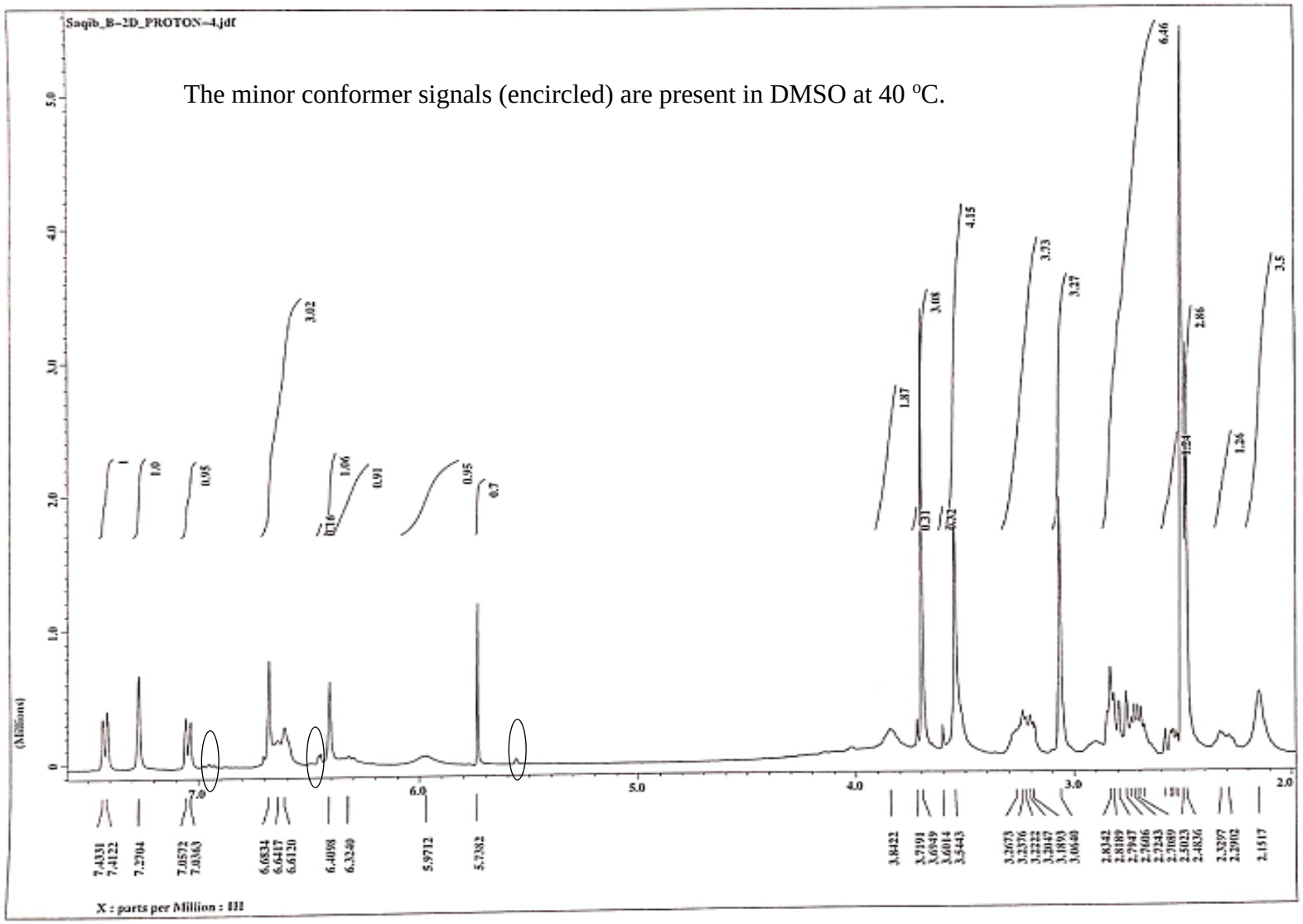


Figure S7: The ^{1}H-NMR spectrum of 13-nitrochondrofoline (**2**) in DMSO at 40 ℃

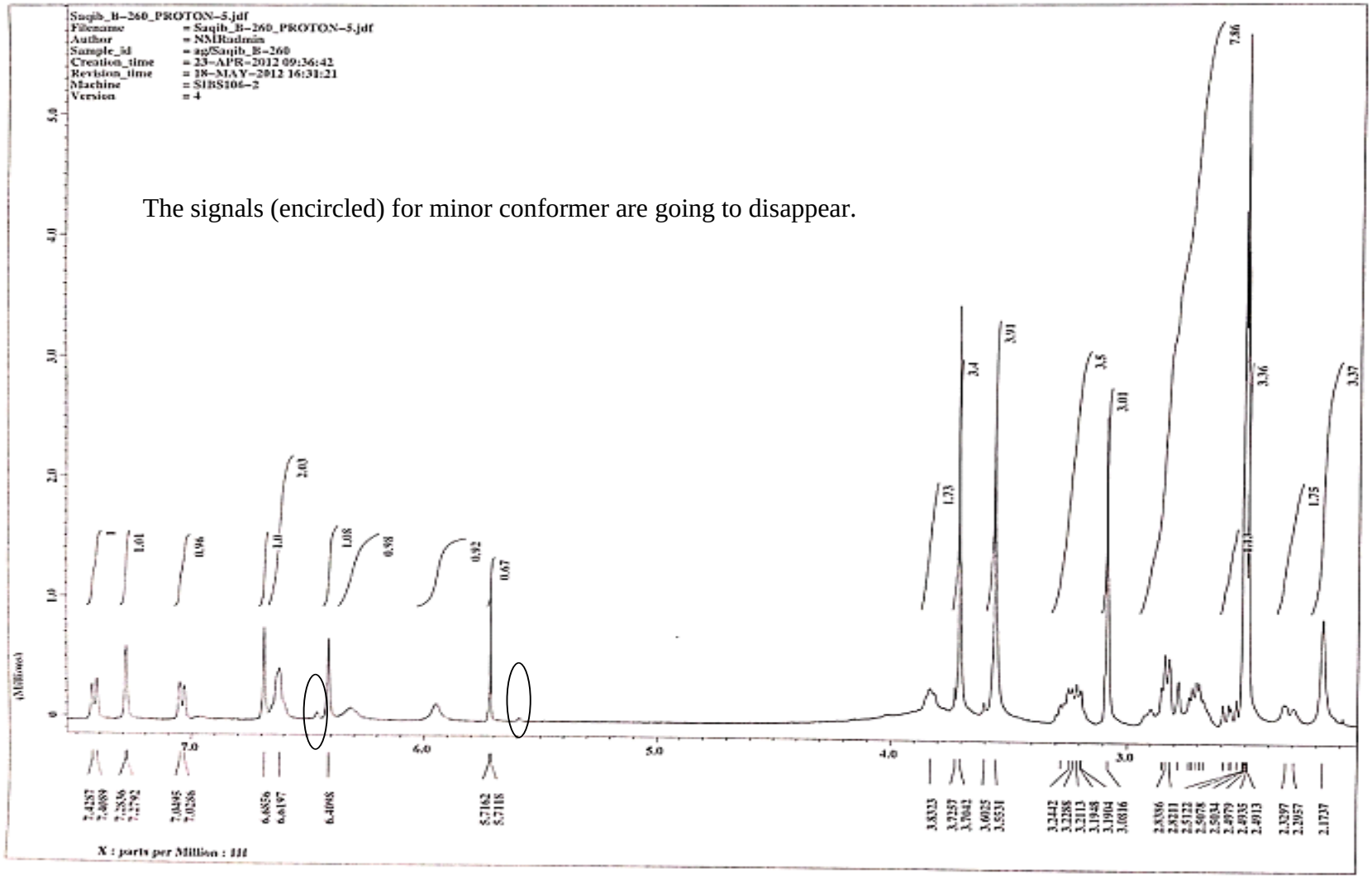


Figure S8: The ^{1}H-NMR spectrum of 13-nitrochondrofoline (**2**) in DMSO at 60 ℃

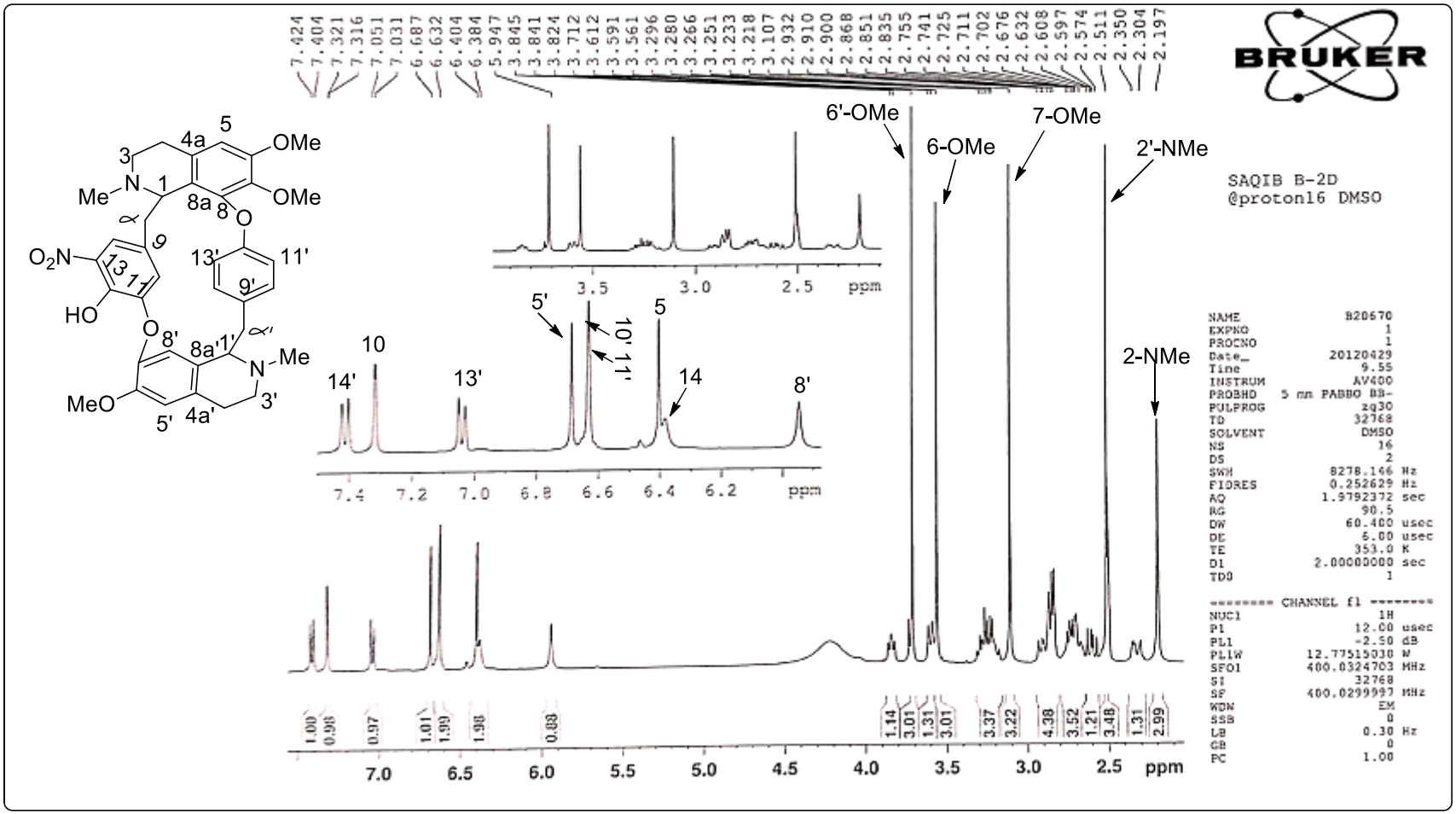


Figure S9: The ^{1}H-NMR spectrum of 13-nitrochondrofoline (**2**) in DMSO at 80 ℃

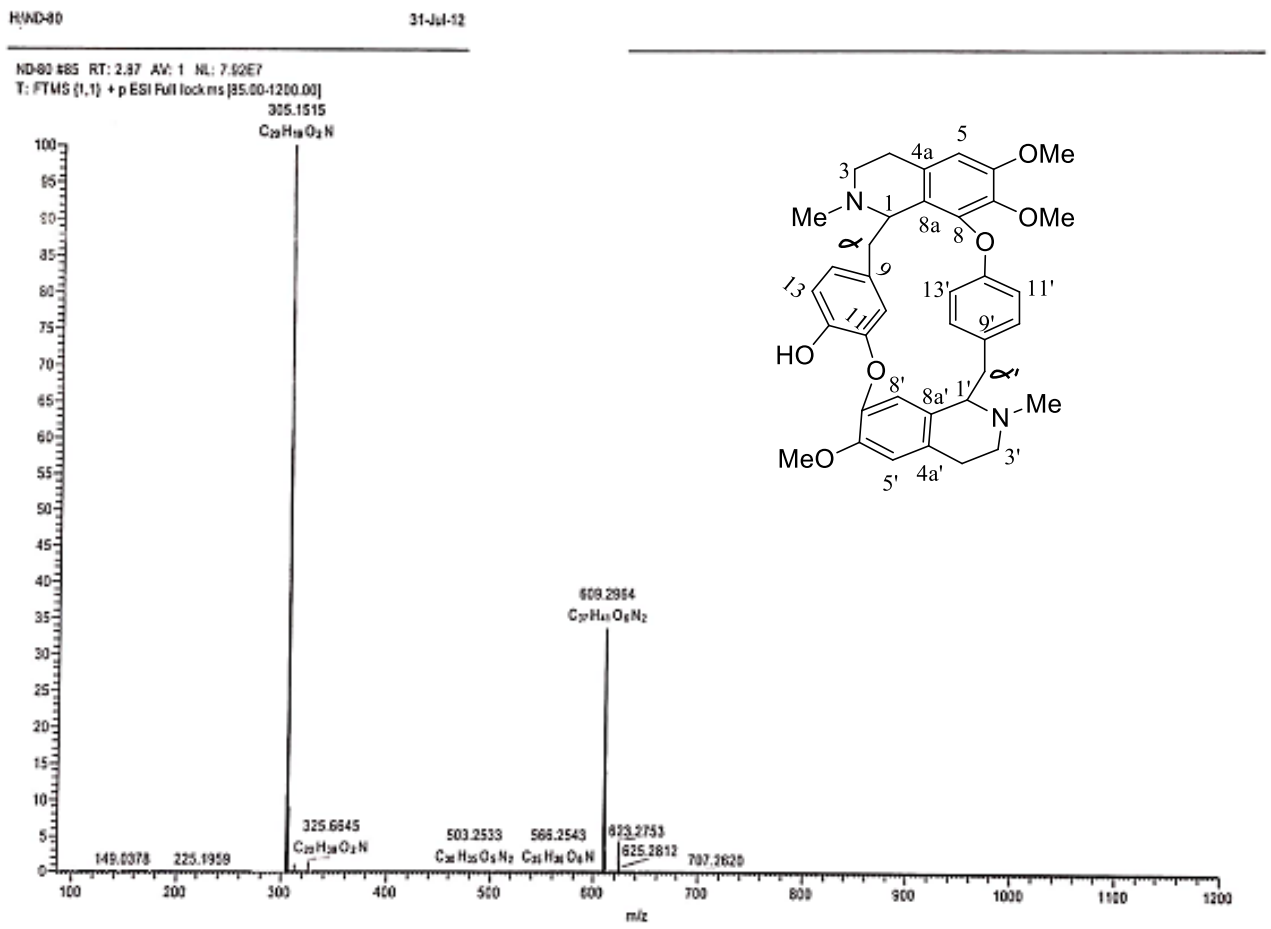


Figure S10: FTMS, ESIMS Spectrum of Chondrofoline (**1**)

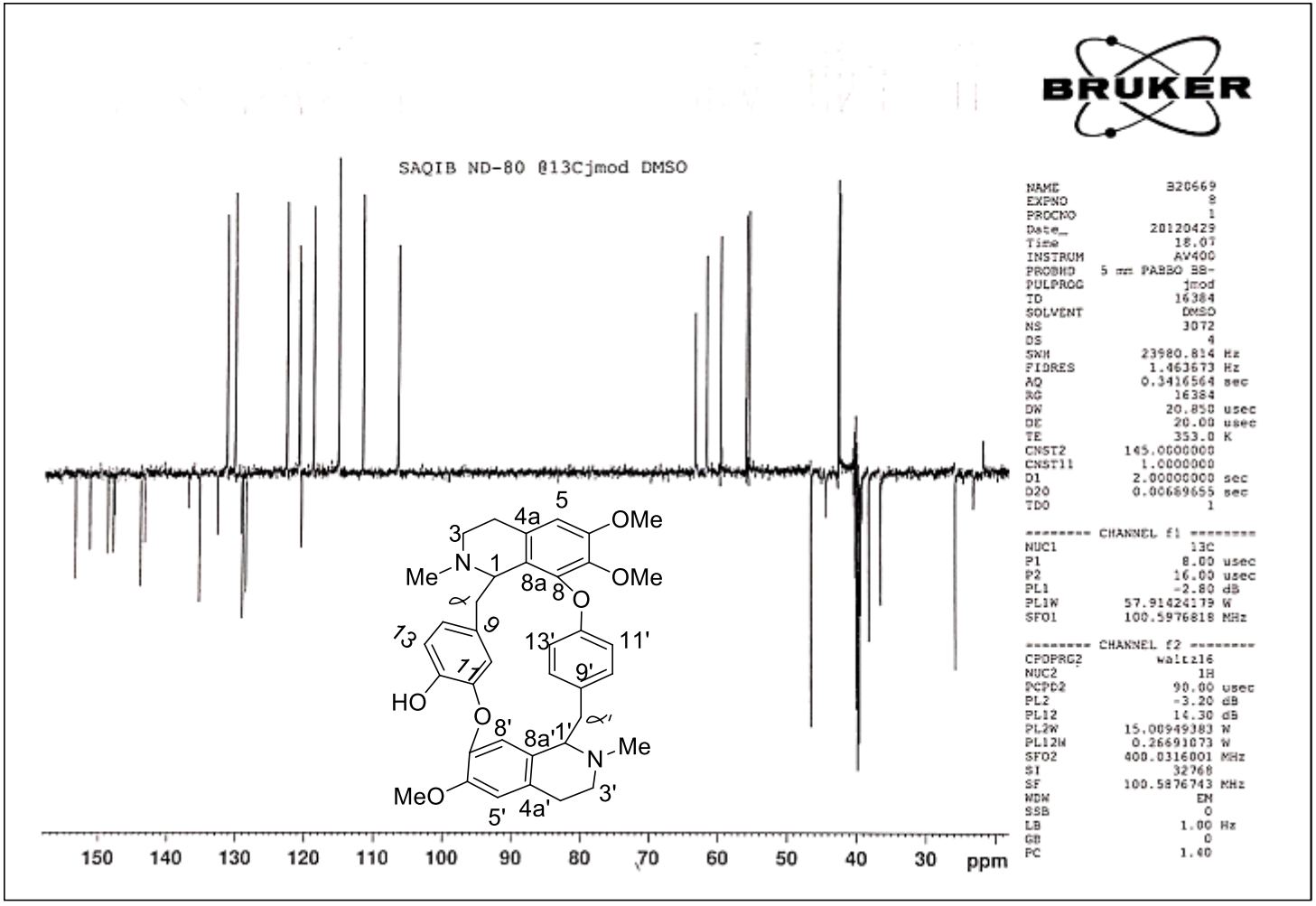


Figure S11: ^{13}C-NMR Spectrum of Chondrofoline (**1**) in DMSO at 80 °C

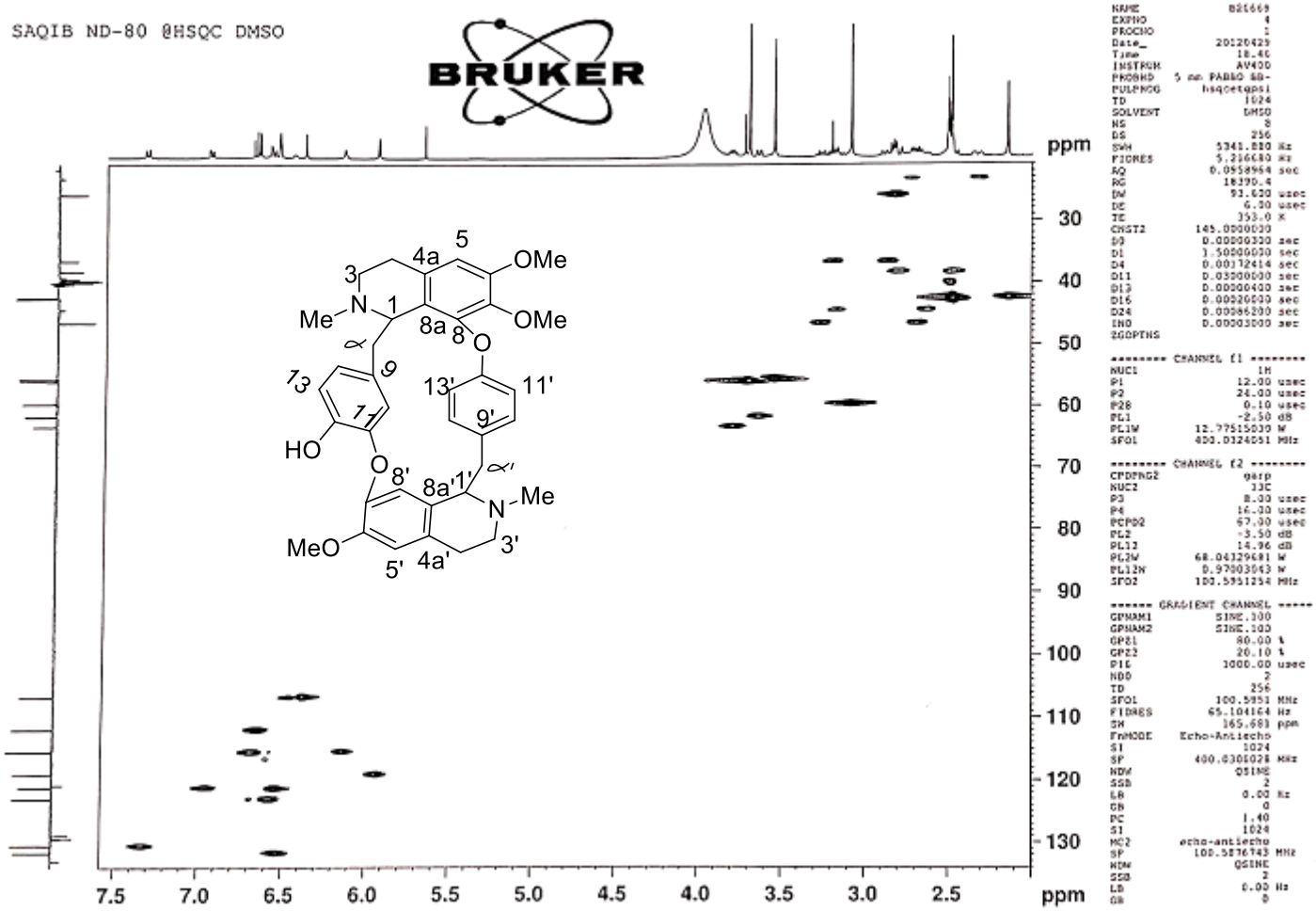


Figure S12: HSQC Spectrum of Chondrofoline (**1**) in DMSO at 80 ℃

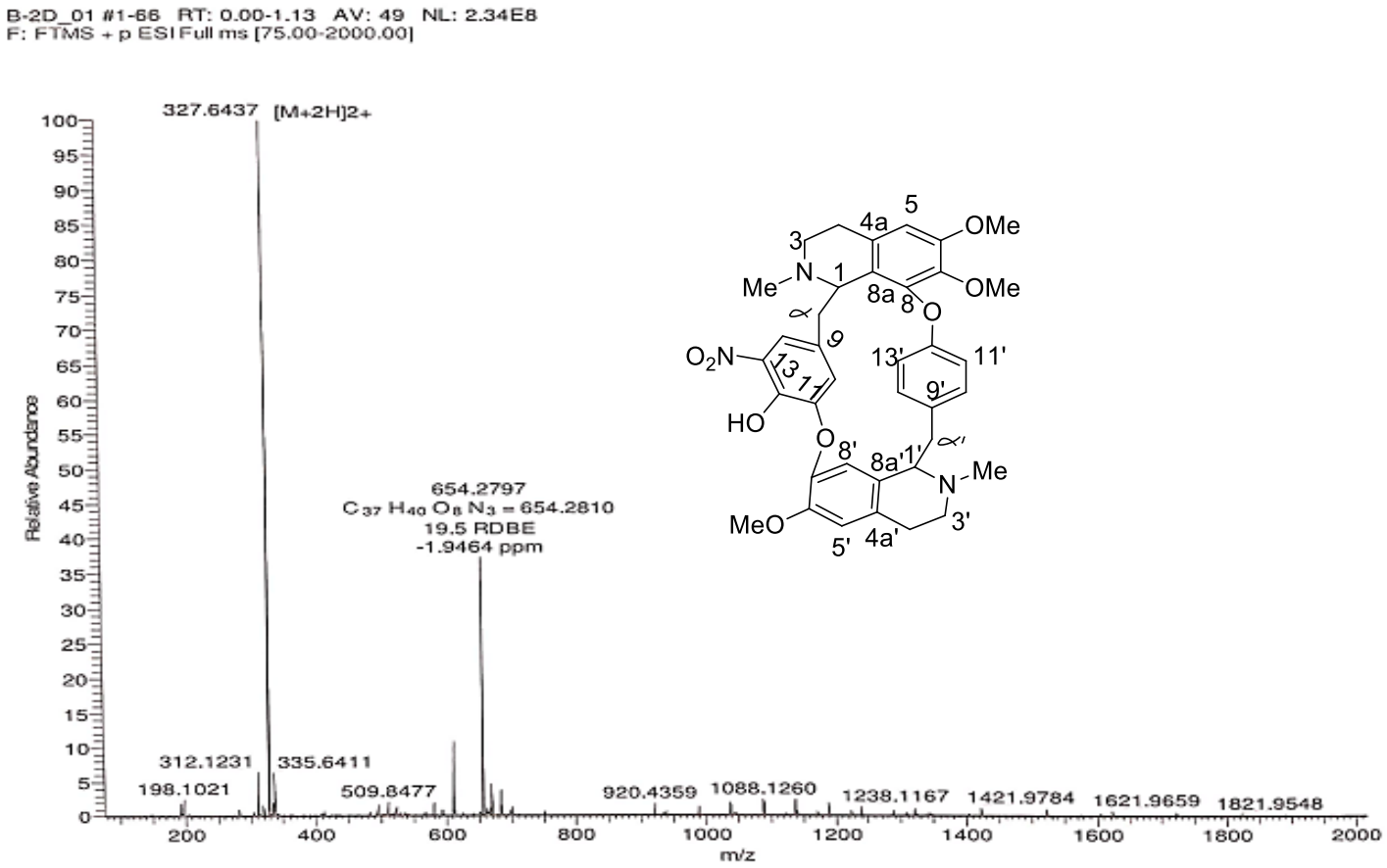
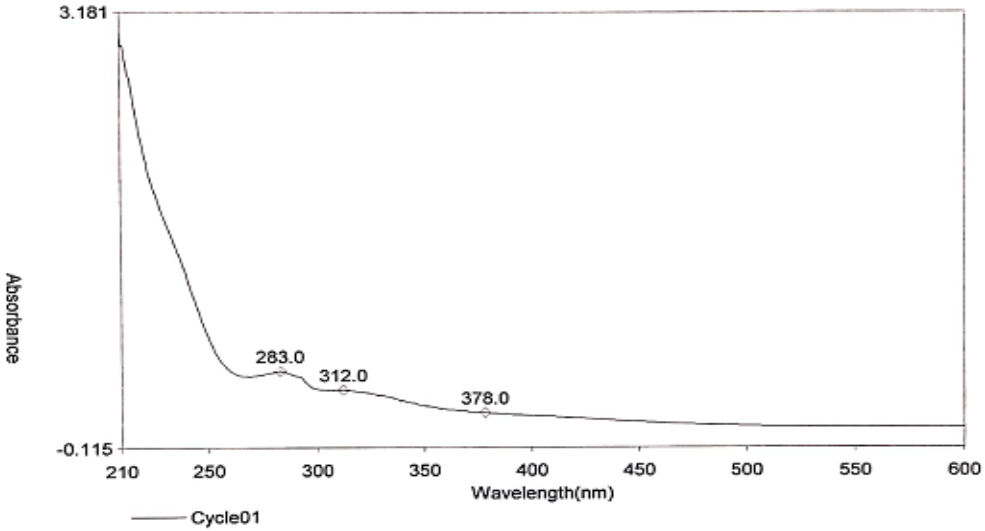


Figure S13: FTMS, ESIMS Spectrum of 13-nitrochondrofoline (**2**)

THERMO SPECTRONIC ~ VISION32 SOFTWARE V1.25

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

Scan Graph



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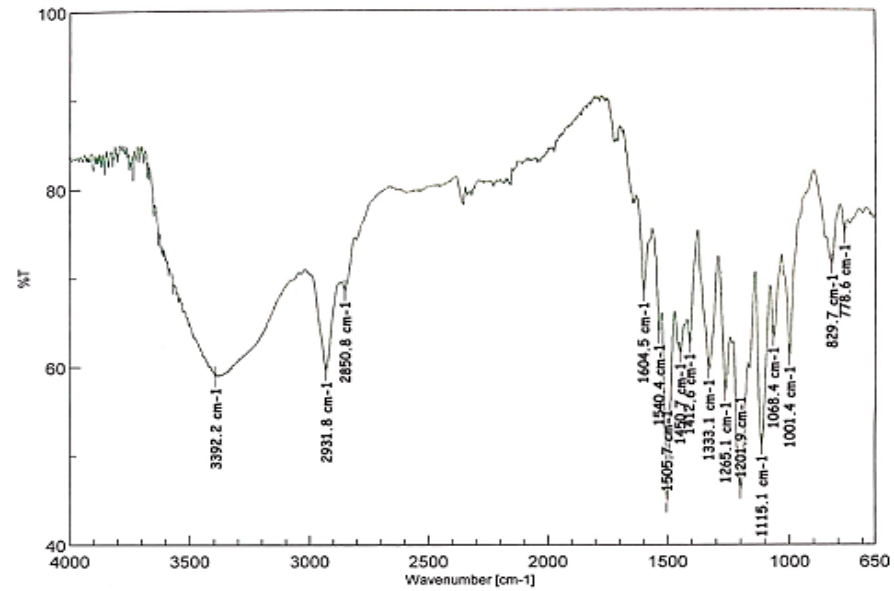
312.00	0.325	Start Lambda 210.0 nm
378.00	0.148	Stop Lambda 600.0 nm
		Sort By Wavelength
Sensitivity	Auto	

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]	
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Comment	ATR
User	
Division	
Company	University of Strathclyde

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Accessory S/N	13871
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Detector	TGS
Accumulation	50
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Zero Filling	On
Apodization	3-Sigma Gaussian
Gain	Auto (8)
Aperture	3.5 mm
Scanning Speed	1 mm/sec
Filter	Auto (30000 Hz)

[Data Information]	
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Data points	6950

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

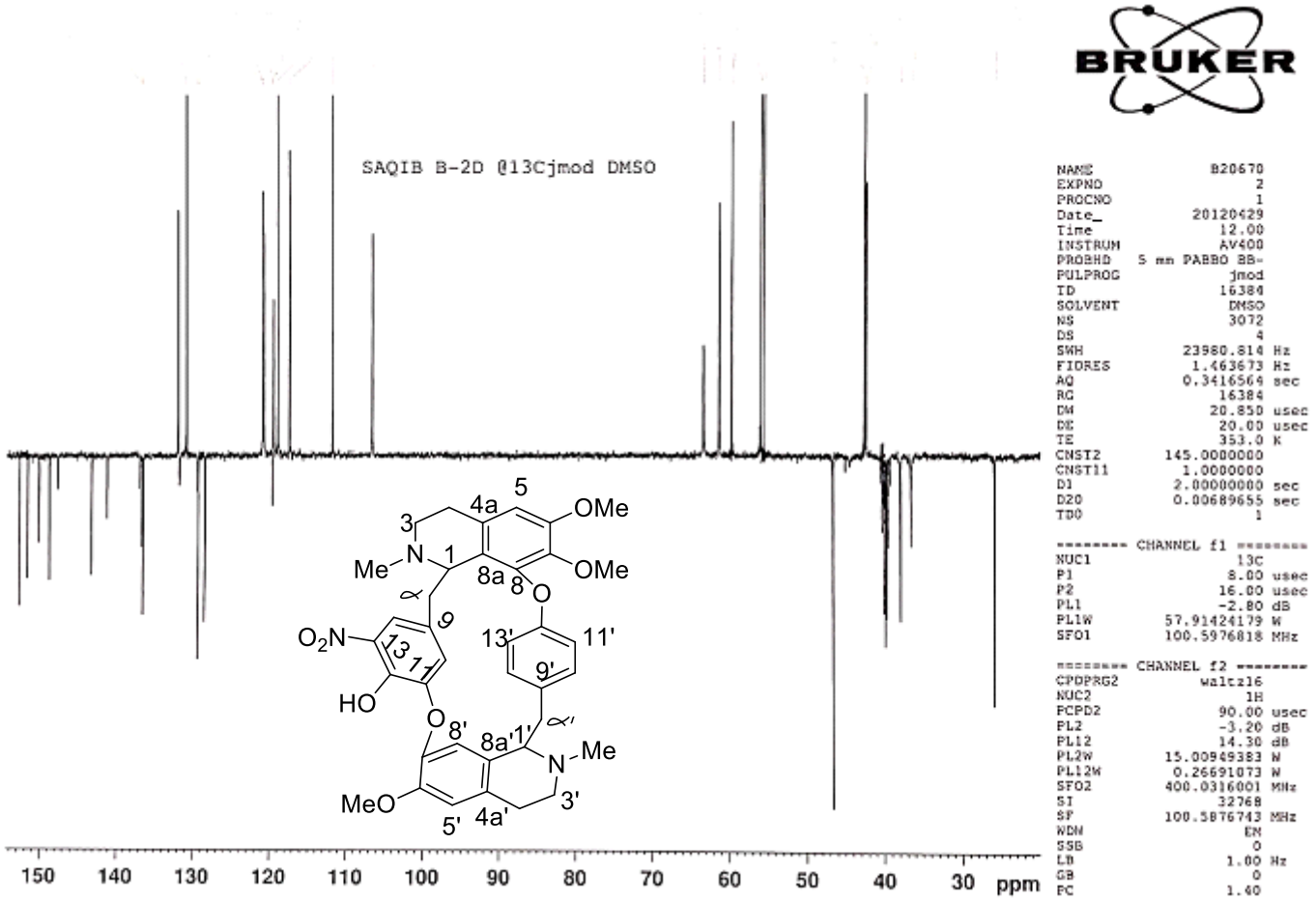

Figure S16: ^{13}C-NMR Spectrum of 13-niteochondrofoline (**2**) in DMSO at 80 ℃

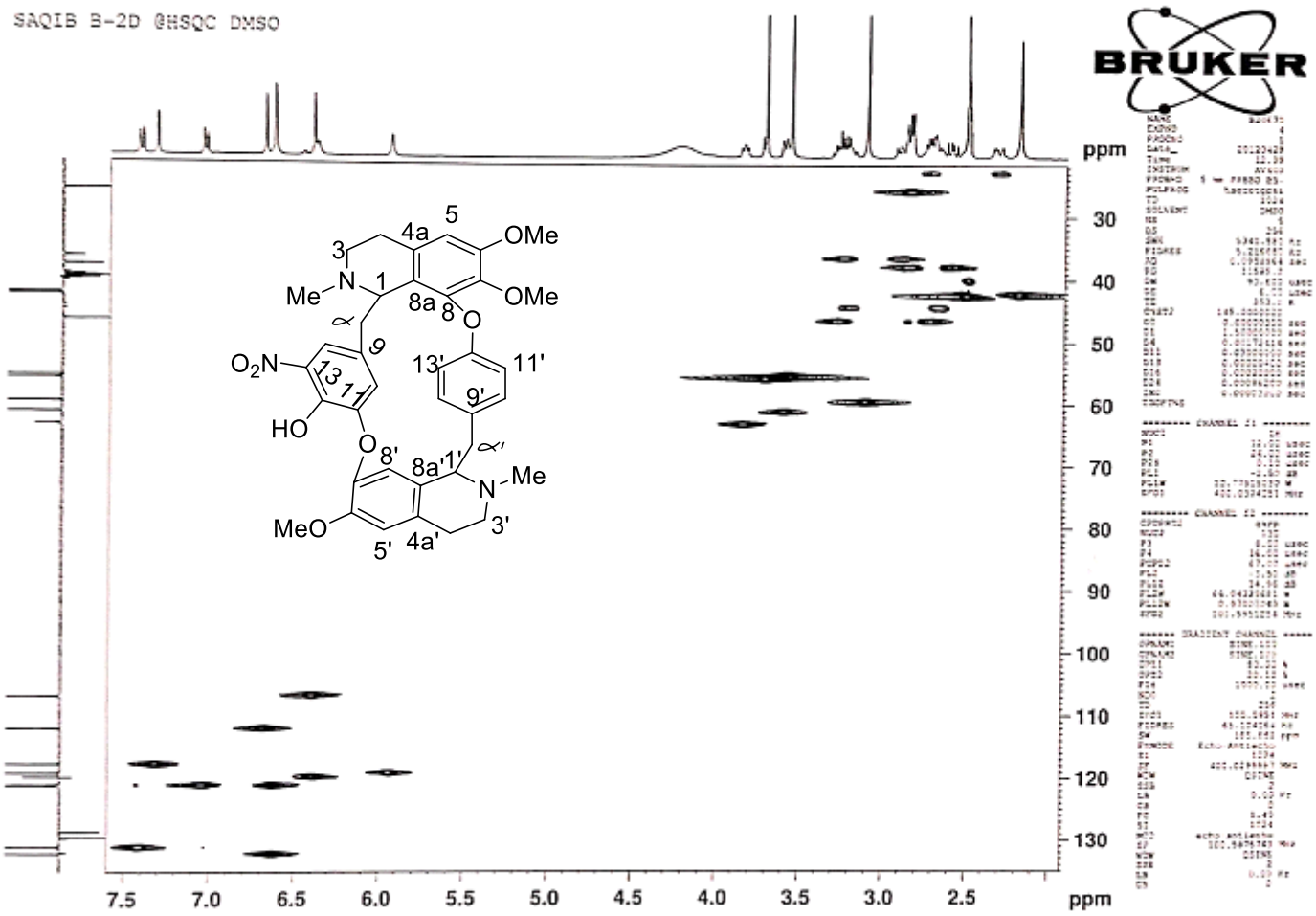

Figure S17: HSQC Spectrum of 13-niteochondrofoline (**2**) in DMSO at 80 ℃

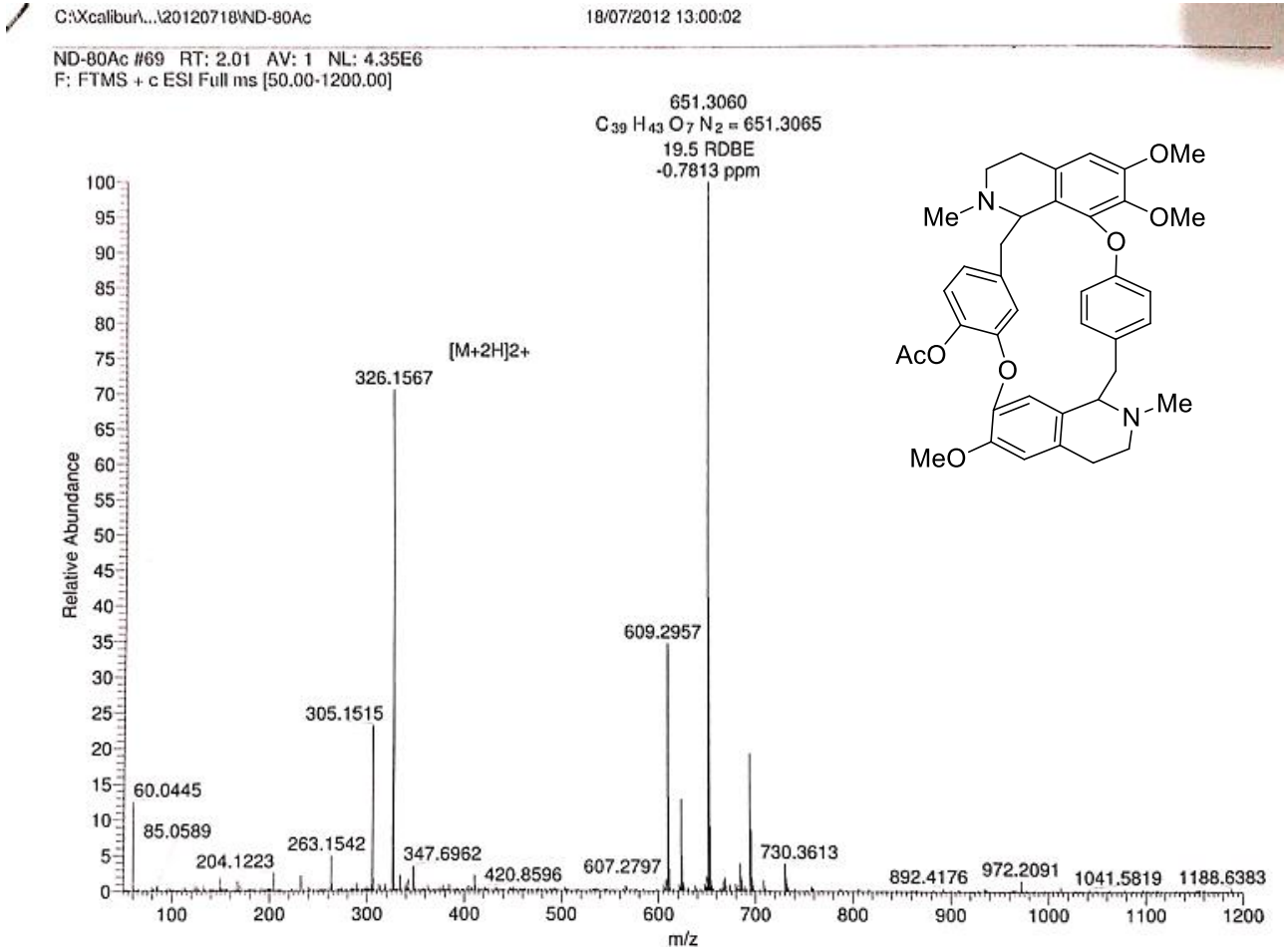

Figure S18: FTMS, ESIMS Spectrum of O-acetylchondrofoline (**3**)

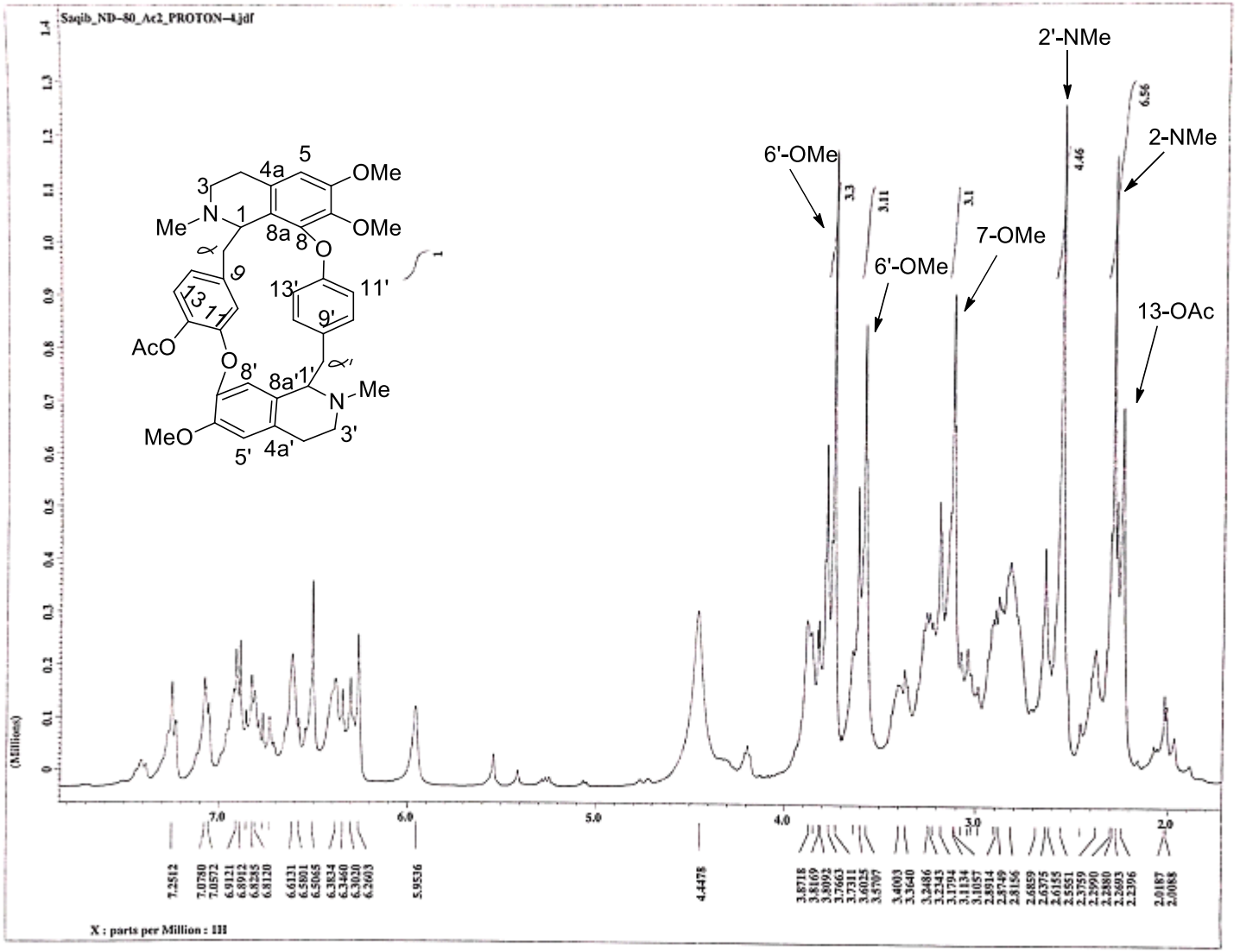

Figure S19: [1]H-NMR Spectrum of O-acetylchondrofoline (**3**)

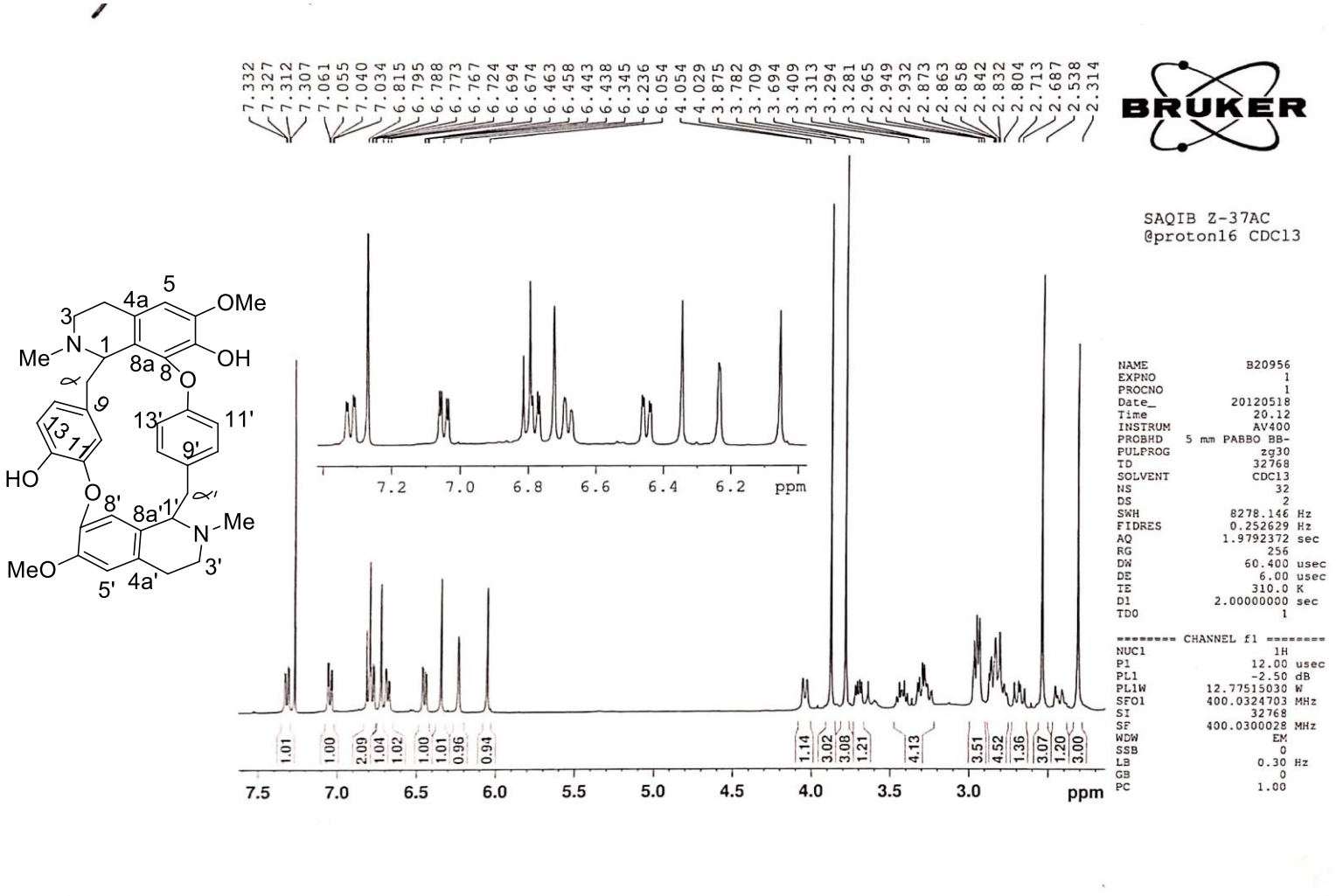

Figure S20: ^{1}H-NMR Spectrum of Curine (**4**)

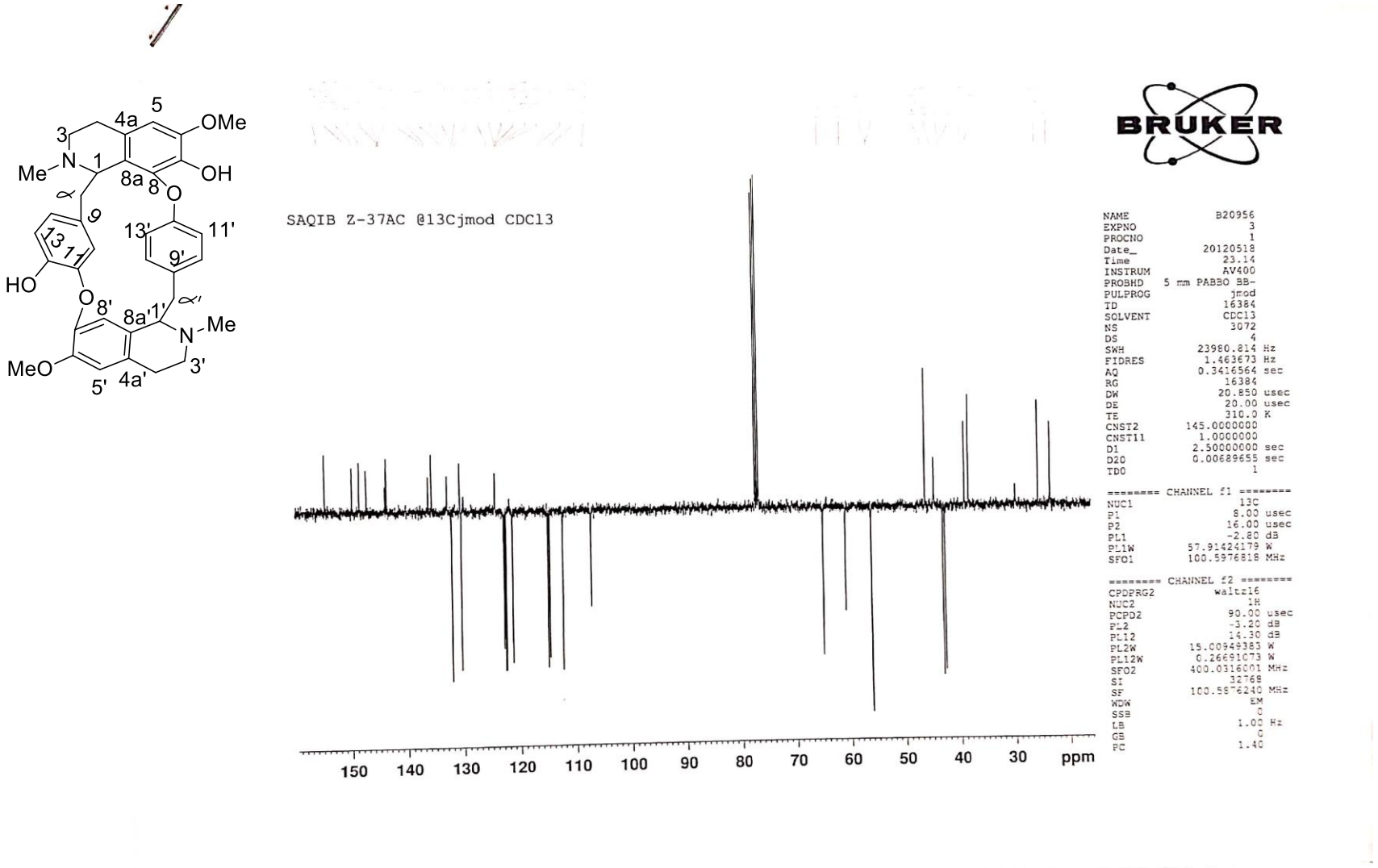

Figure S21: ^{13}C-NMR Spectrum of Curine (**4**)

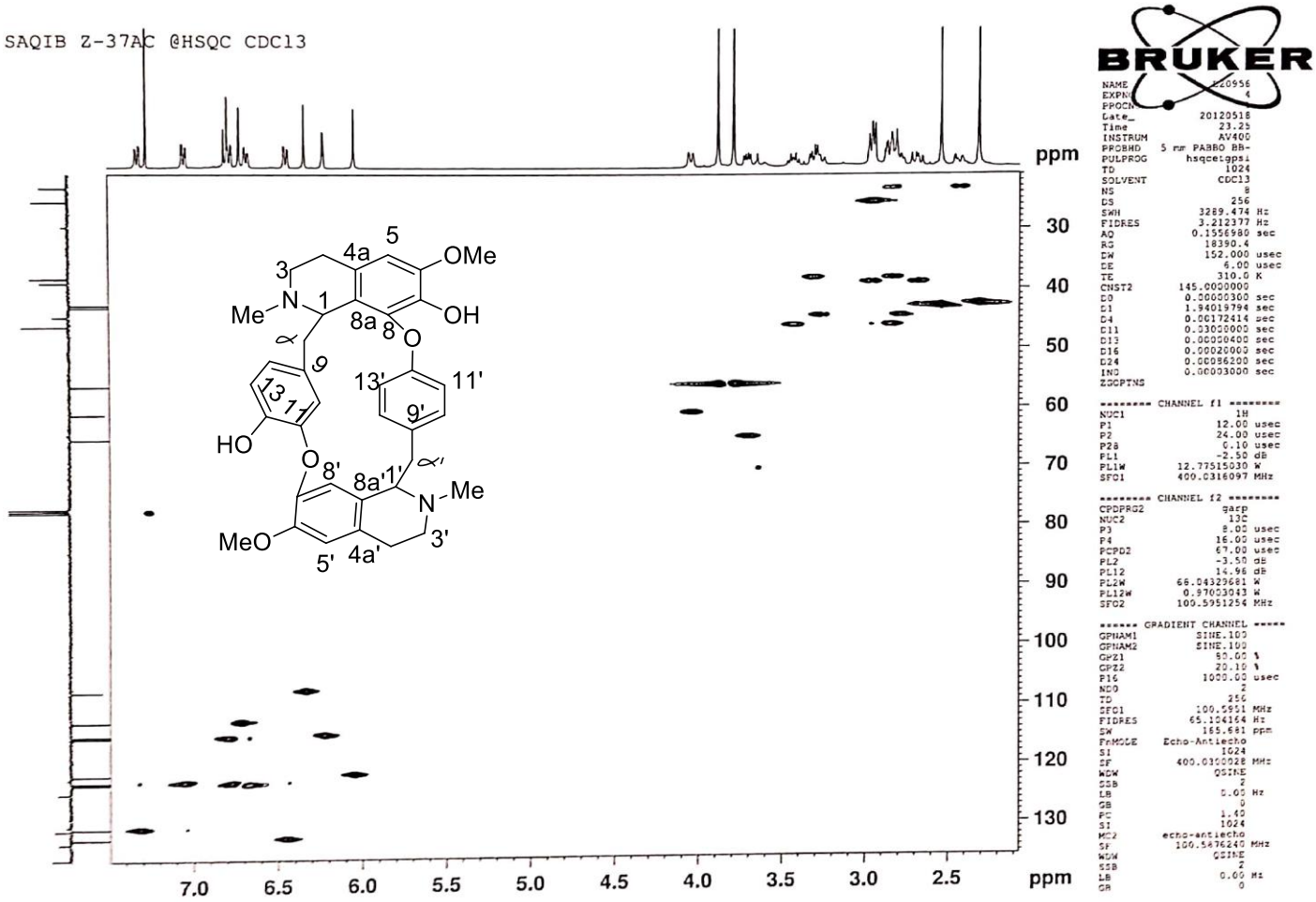

Figure S22: HSQC Spectrum of Curine (**4**)

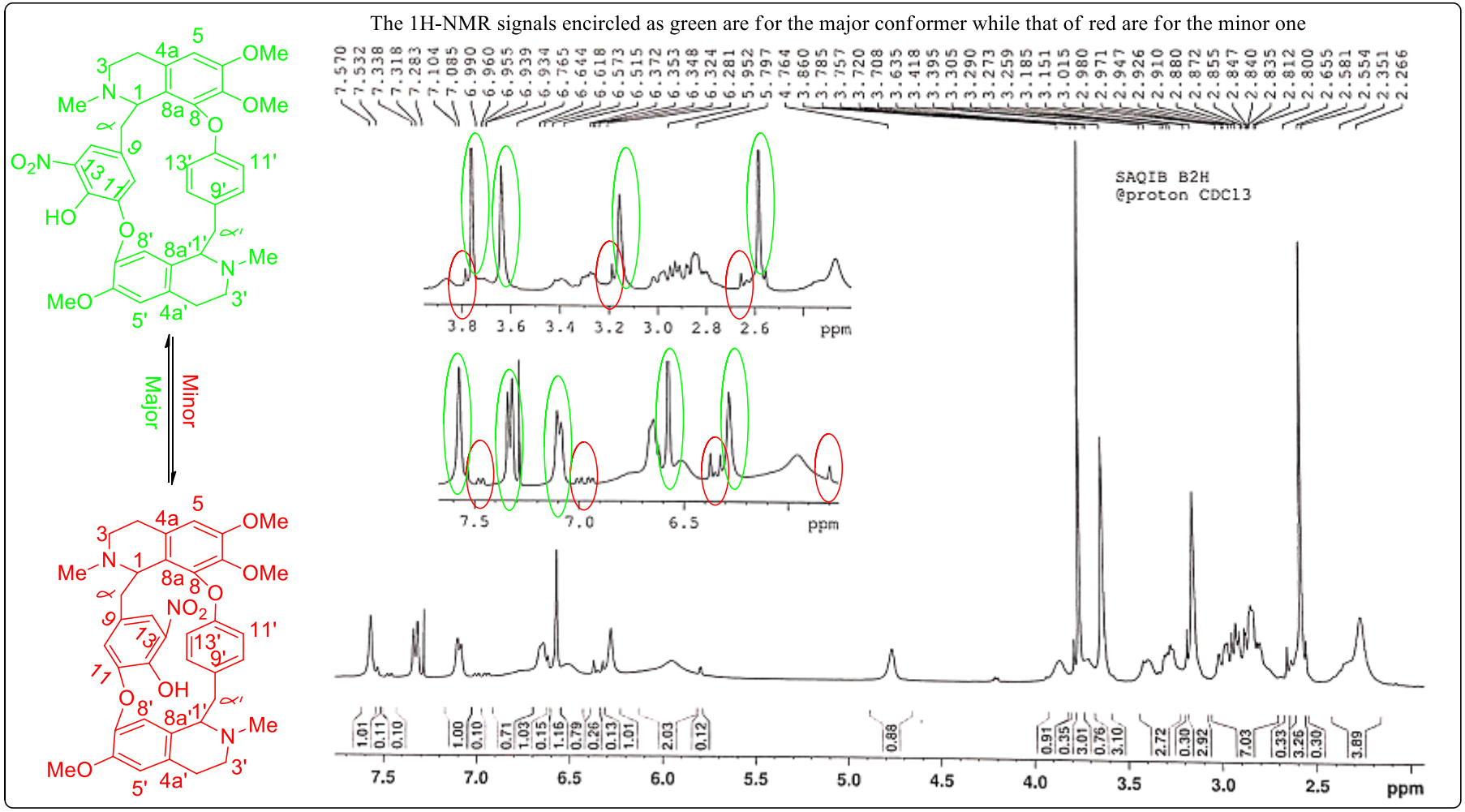

Figure S23: The ^{1}H-NMR spectrum of 13-nitrochondrofoline (**2**) in $CHCl_3$ at 25 °C showing two conformers one major while other minor