

Chemical Constituents of Two Endemic *Cephalaria* Species

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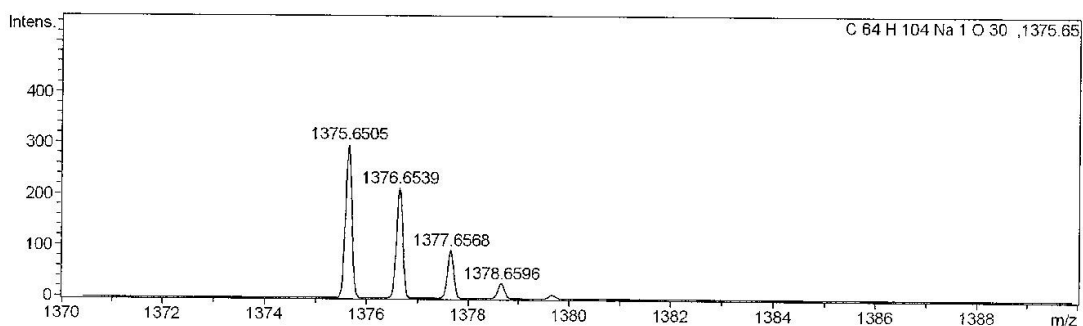
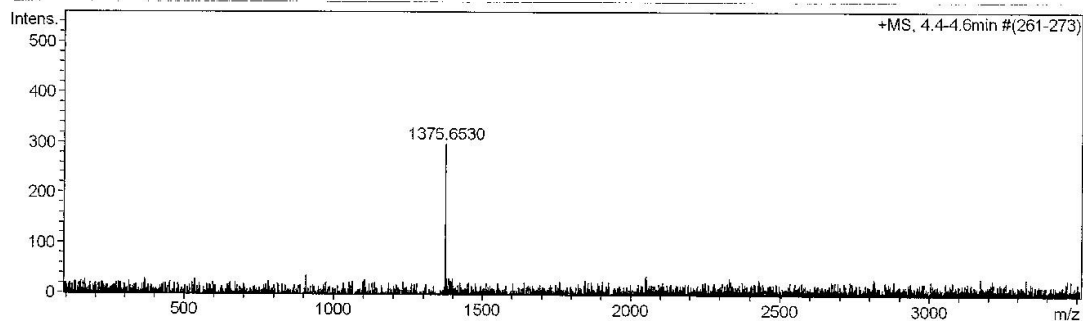
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Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Waste

Generate Molecular Formula Parameter

Formula, min.	C58H104Na1O30				
Formula, max.					
Measured m/z	1375.65	Tolerance	2 ppm	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nitrogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				

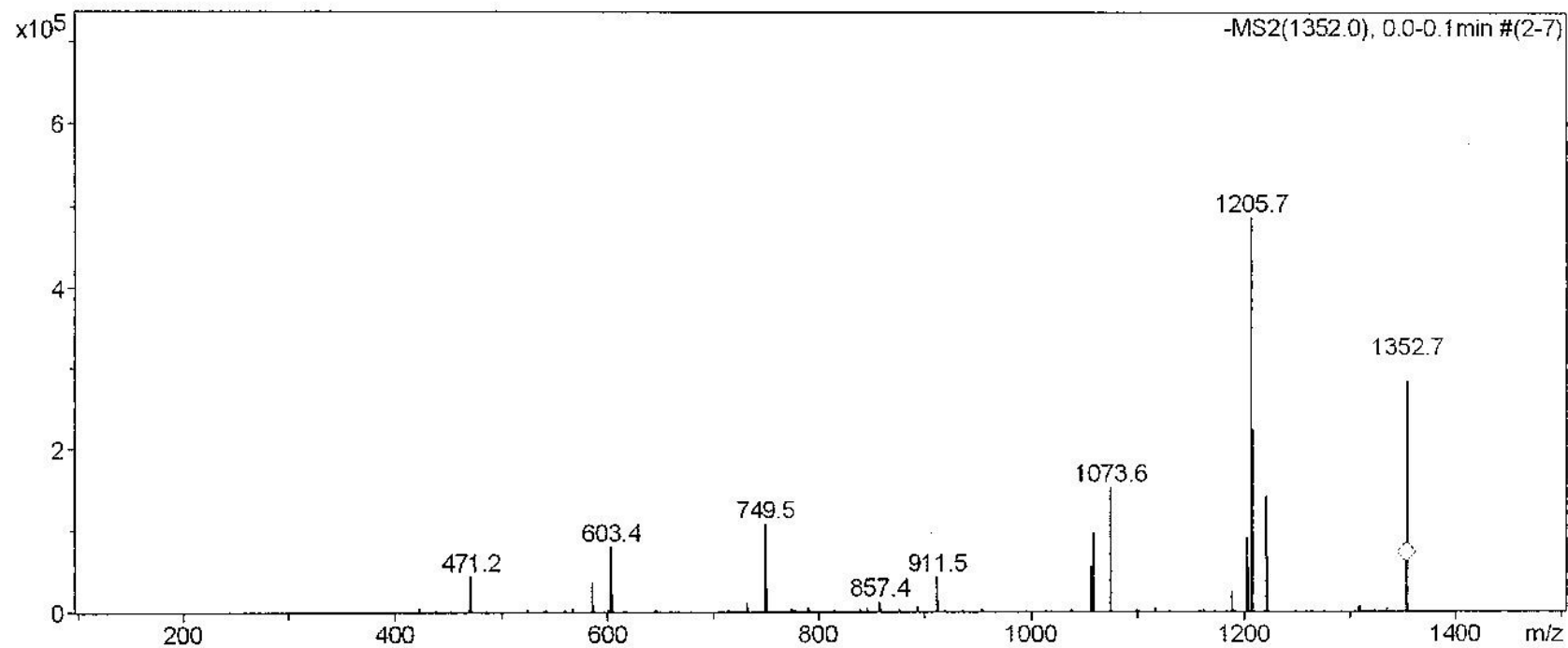


Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 64 H 104 Na 1 O 30	0.049	1375.6505	-1.84	-3.64	-2.53	12.50	ok	even

S1: HRESIMS Spectrum of Compound 1 (isacoside)

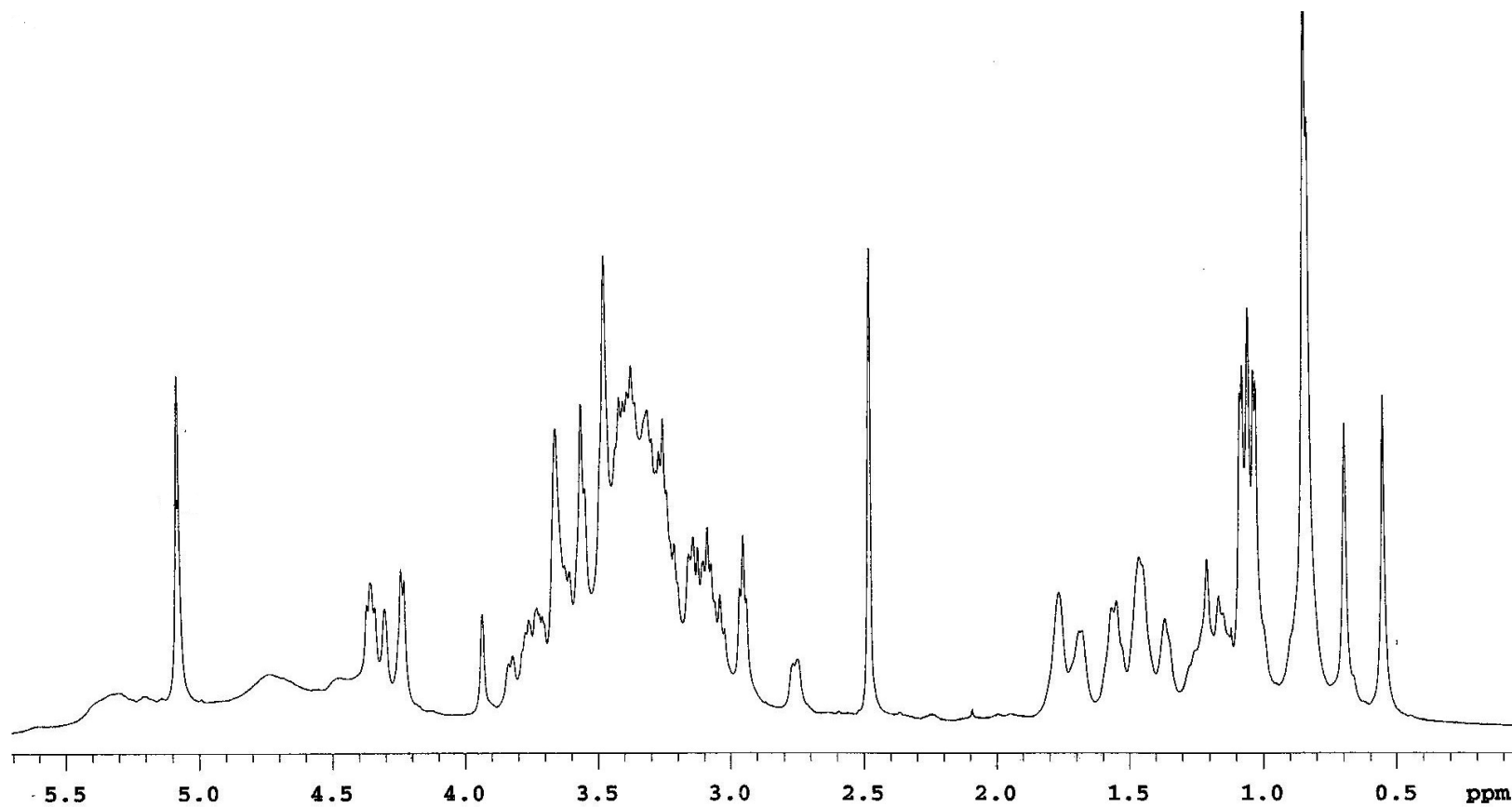
Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	off
Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	1500 m/z
Capillary Exit	-114.1 Volt	Skimmer	-40.0 Volt	Trap Drive	45.8
Accumulation Time	9401 μ s	Averages	5 Spectra	Auto MS/MS	off

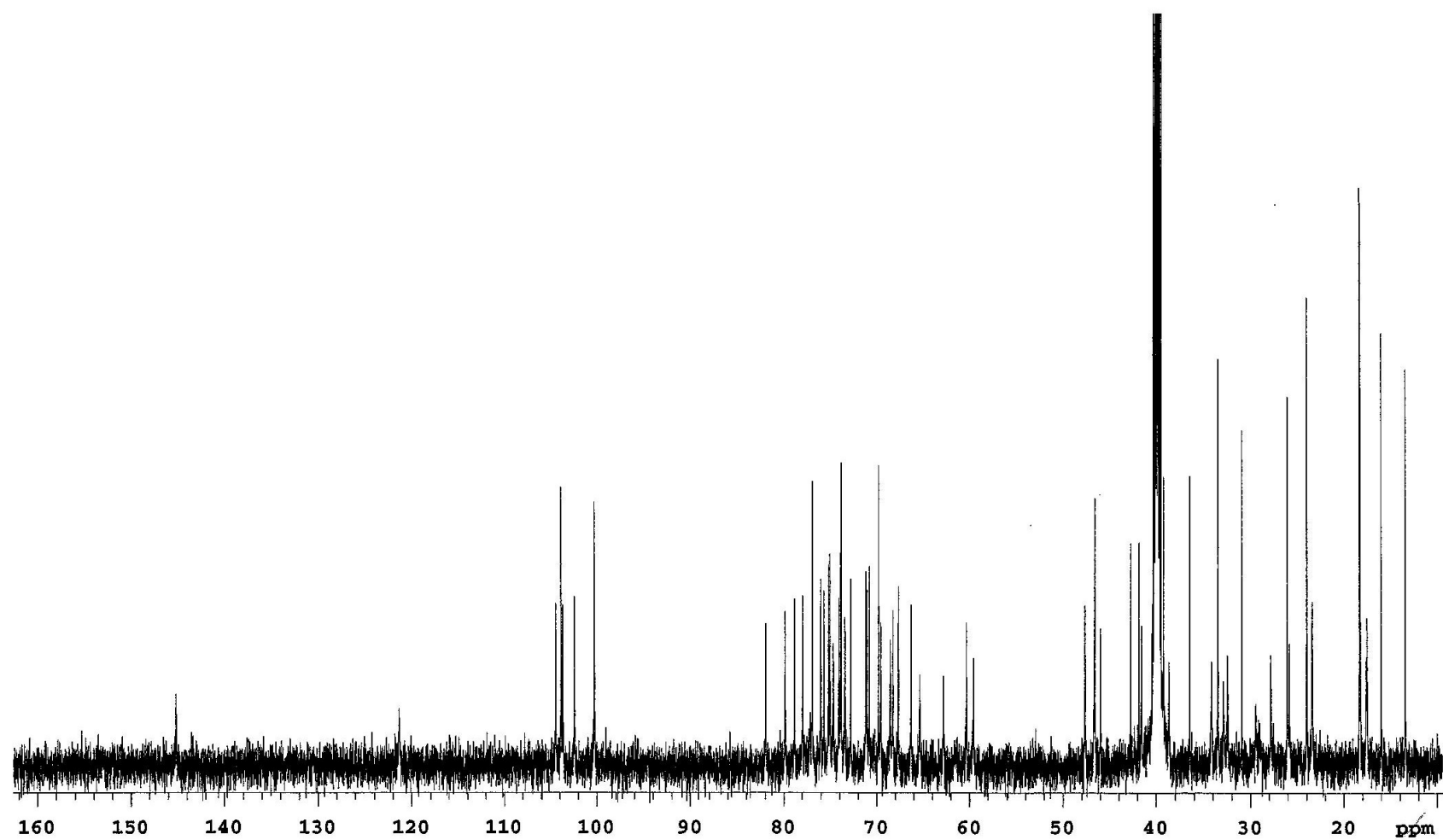


#	RT [min]	Area
n.a.	0.1	n.a.

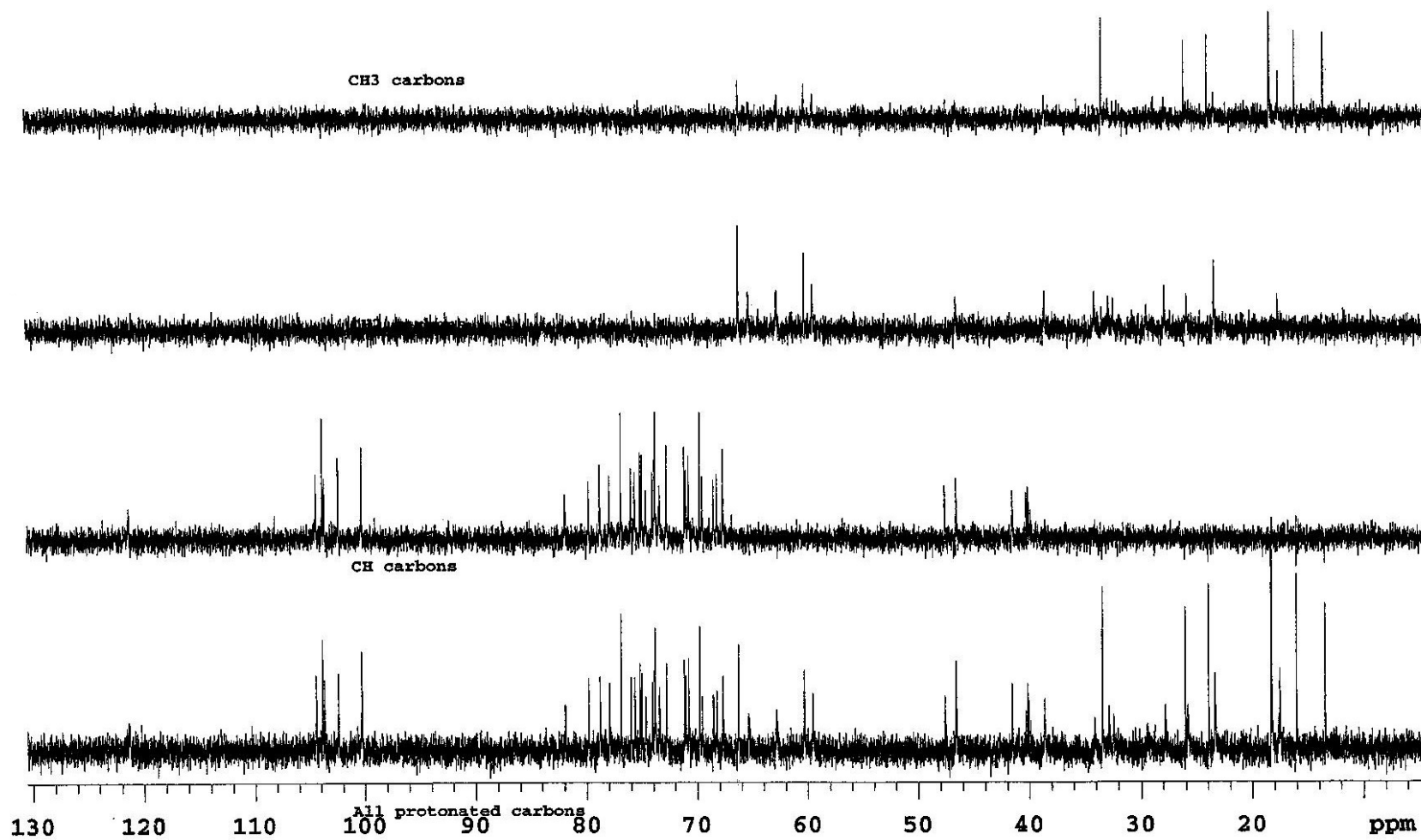
S2: ESIMS Spectrum of Compound **1** (isacoside)



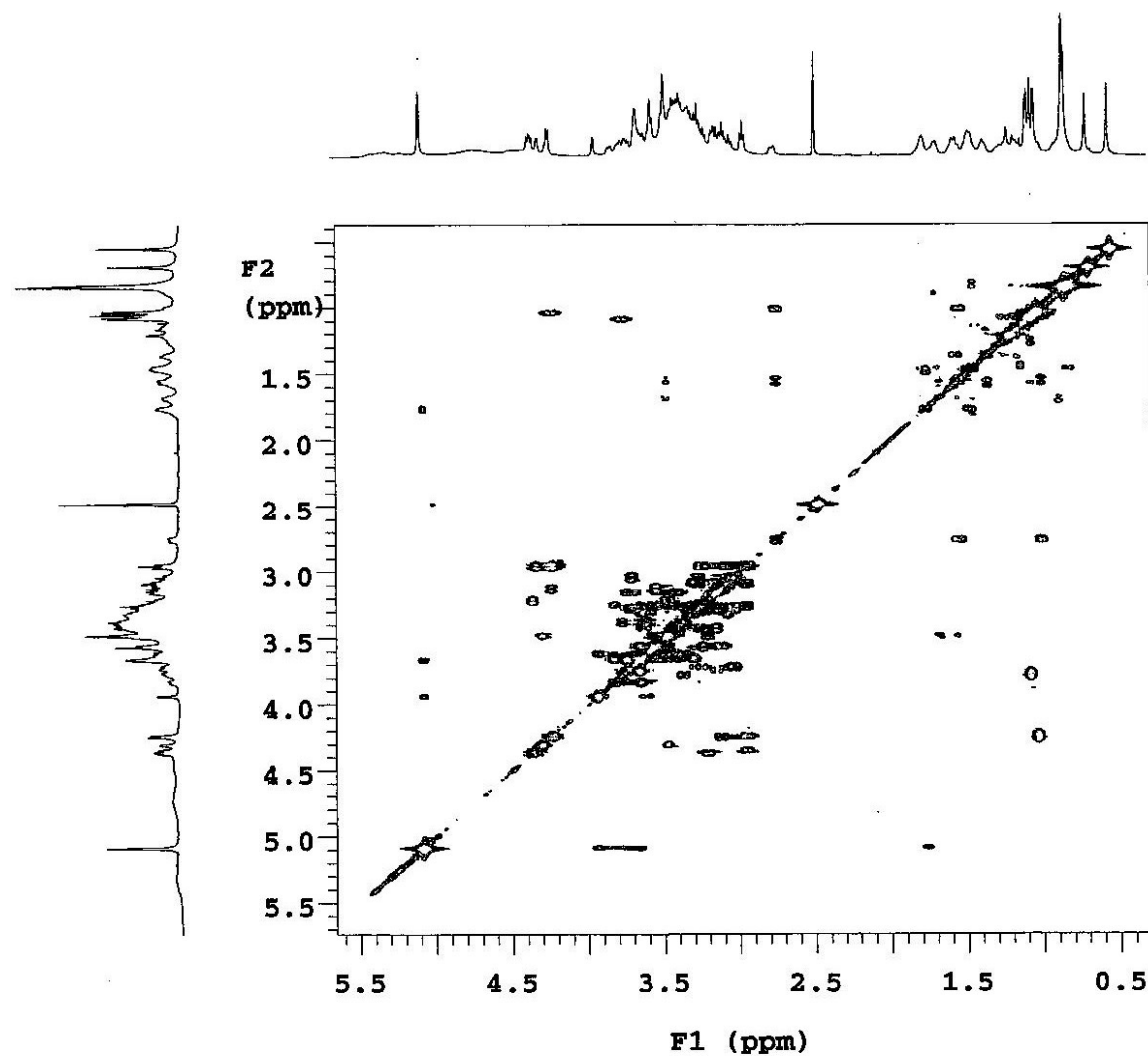
S3: ^1H -NMR Spectrum of Compound **1** (isacoside)



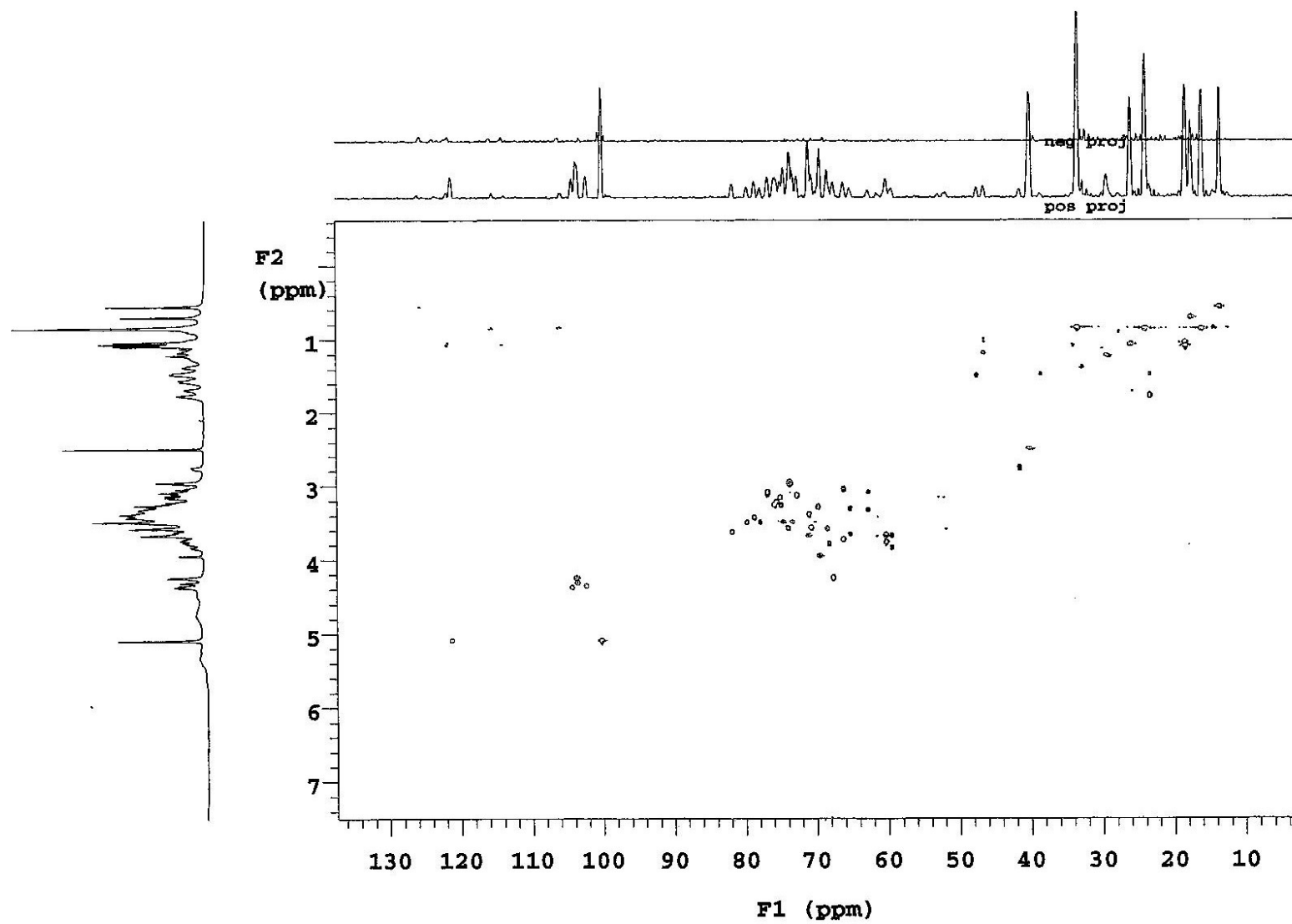
S4: ^{13}C -NMR Spectrum of Compound **1** (isacoside)



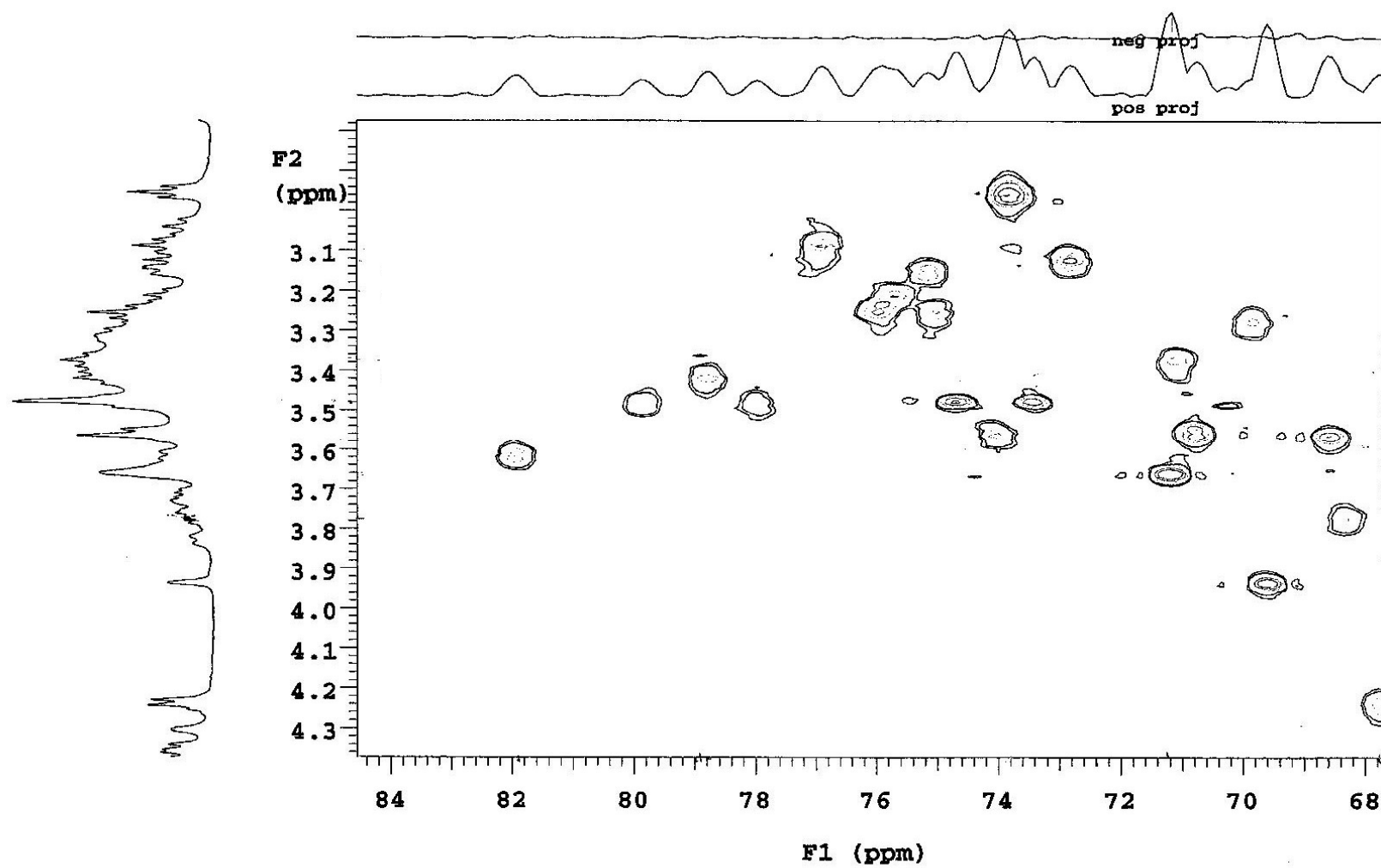
S5: DEPT Spectrum of Compound 1 (isacoside)



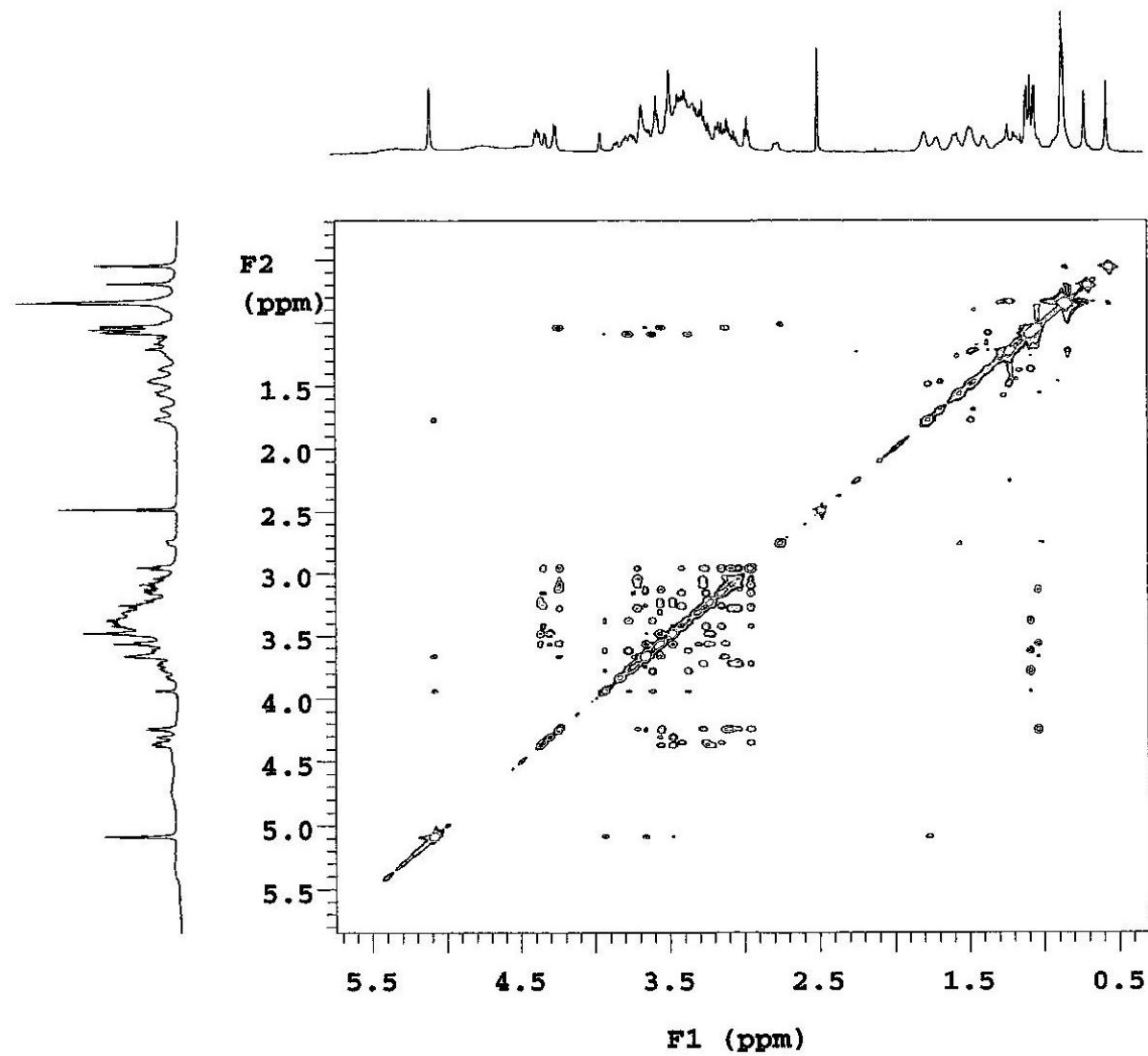
S6: COSY Spectrum of Compound **1** (isacoside)



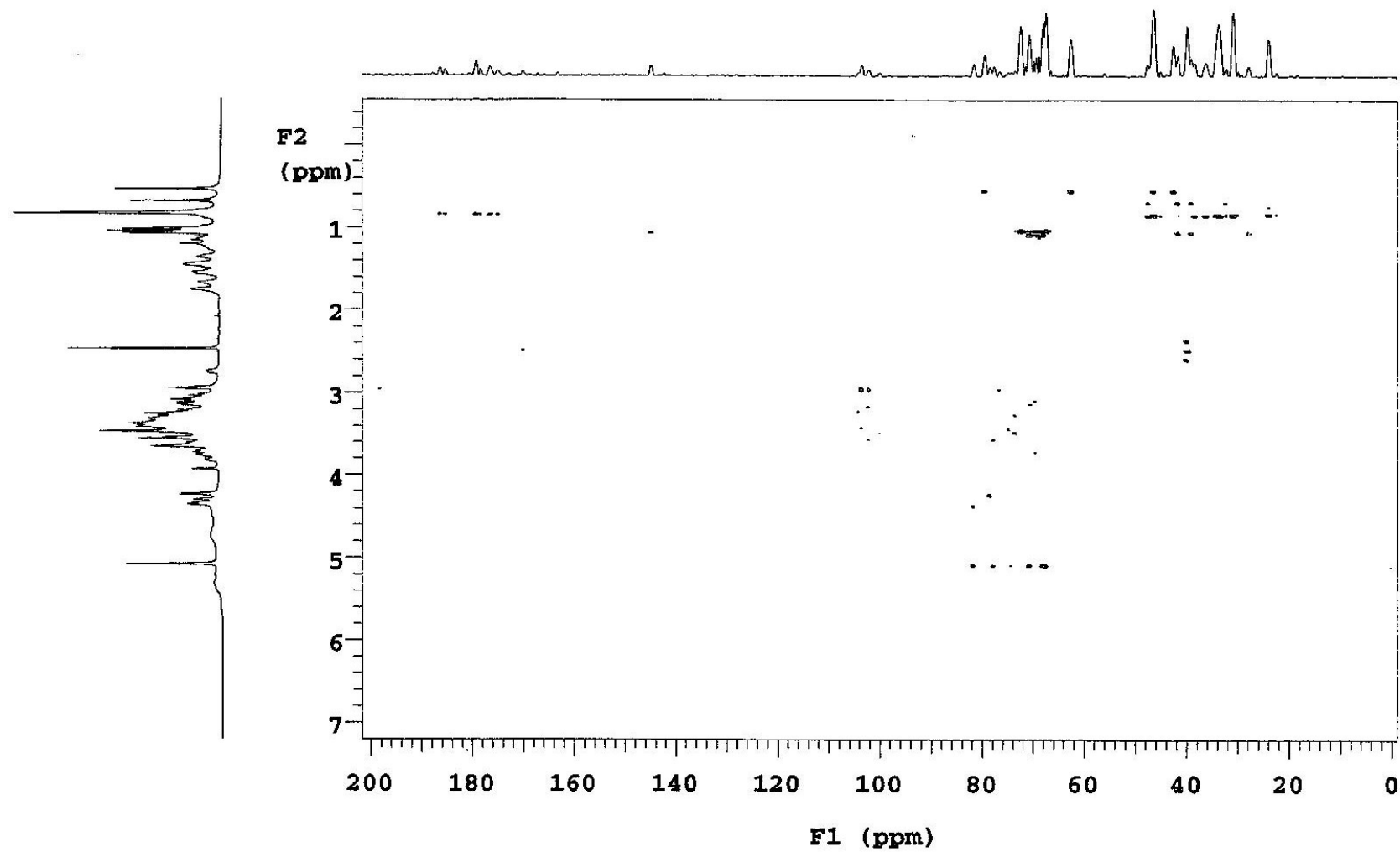
S7: HMQC Spectrum of Compound 1 (isacoside)



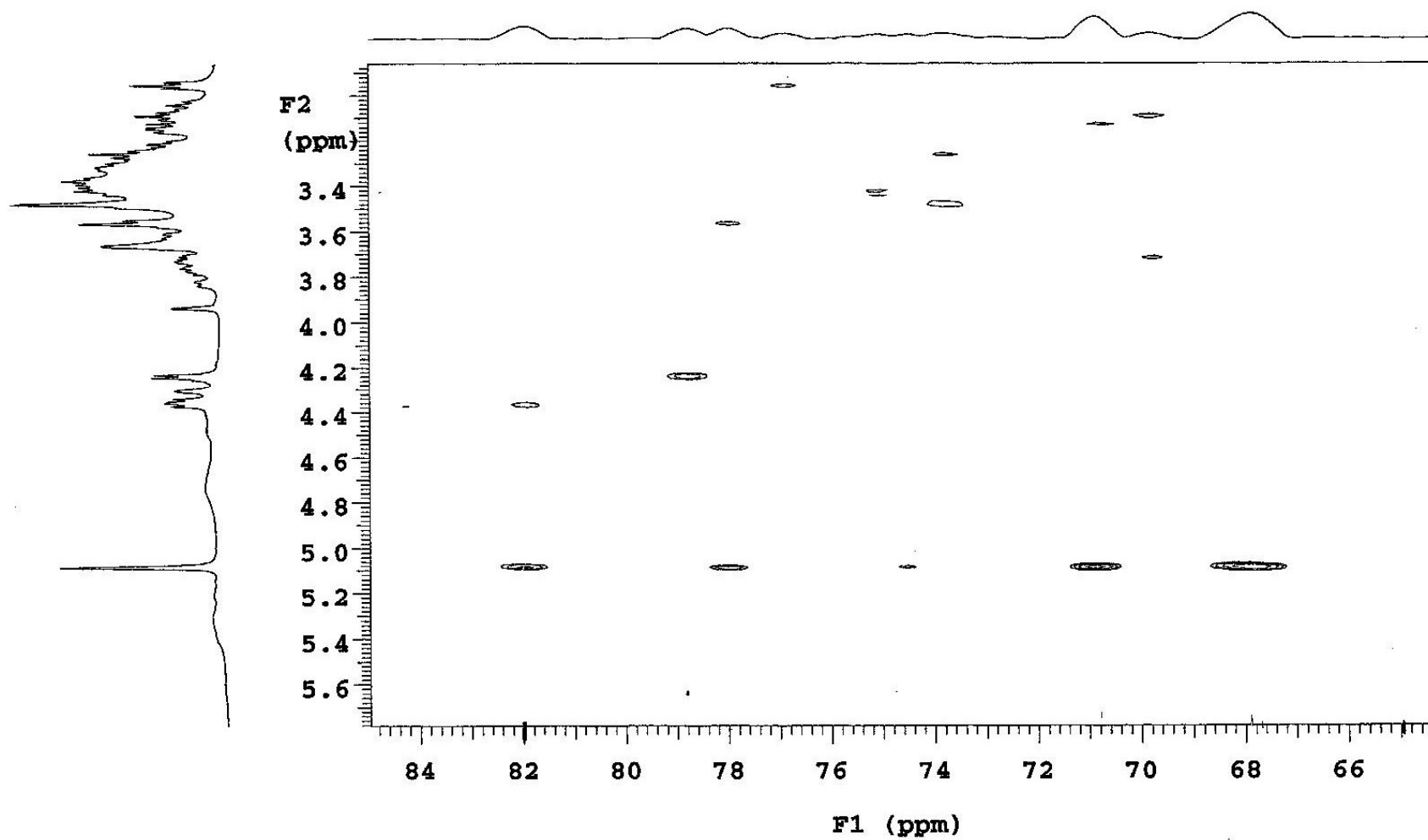
S8: Expansion of the HMQC Spectrum of Compound 1 (isacoside)



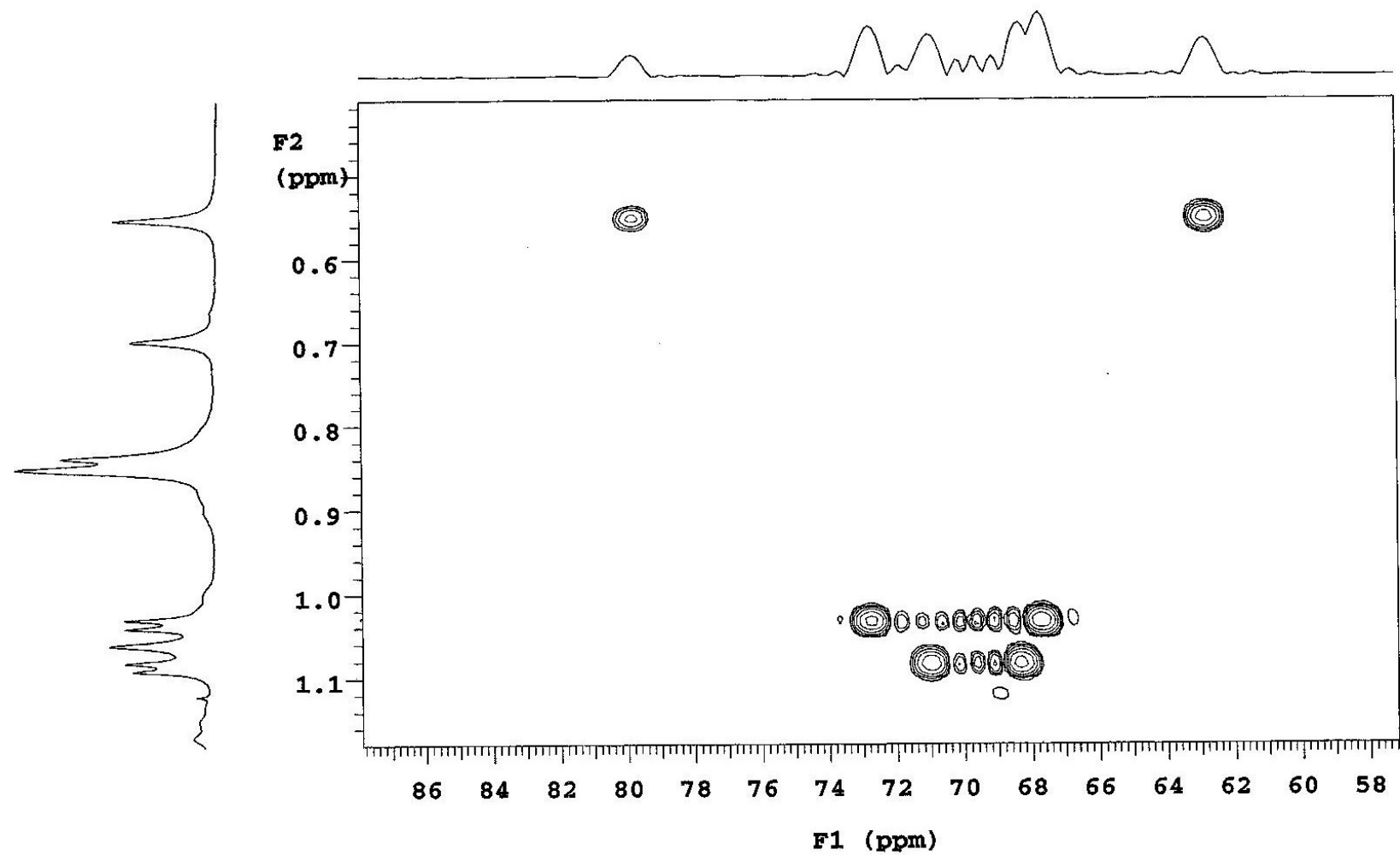
S9: TOCSY Spectrum of Compound 1 (isacoside)



S10: HMBC Spectrum of Compound **1** (isacoside)



S11: Expansion of the HMBC Spectrum of Compound 1 (isacoside)



S12: Expansion of the HMBC Spectrum of Compound 1 (isacoside)