

Support Information

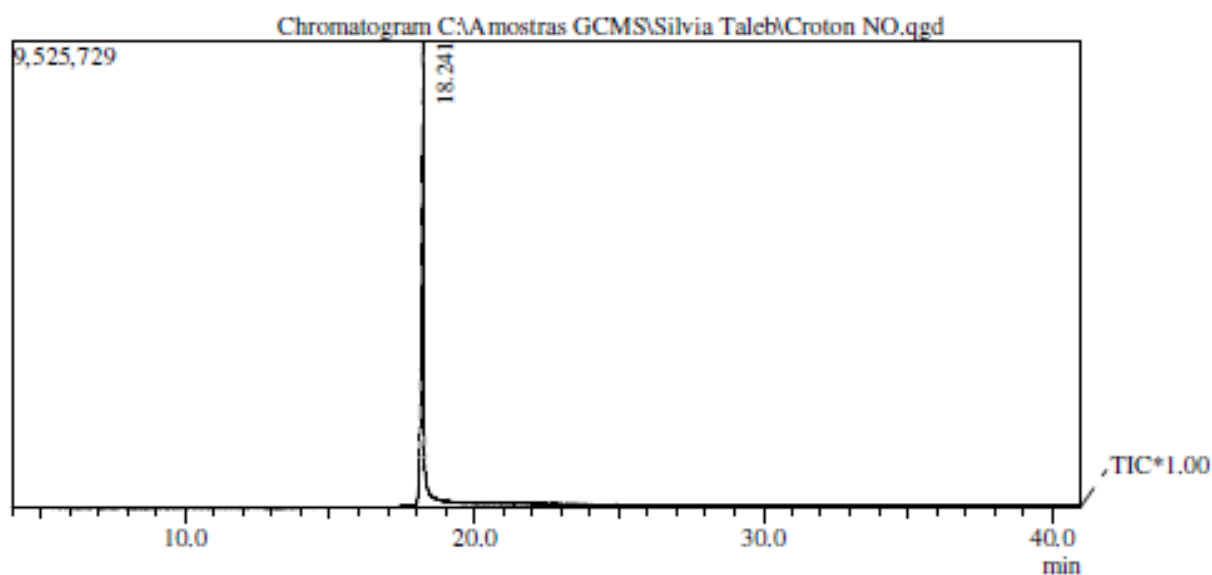
Figure 1. GC chromatogram of compound 1.

Sample Information

Analyzed by : Admin
Analyzed : 29/5/2012 02:04:34
Sample Type : Unknown
Level # : 1

IS Amount : [1]=1.000
Sample Amount : 1.000
Dilution Factor : 1.000
Vial # : 18
Injection Volume : 1.000
Data File : C:\Amostras GCMS\Silvia Taleb\Croton NO.qgd

Method File : C:\Amostras GCMS\Silvia Taleb\Triterpeno DB5.qgm
Org Method File : C:\Amostras GCMS\Silvia Taleb\Triterpeno DB5.qgm
Report File :
Tuning File : C:\GCMSsolution\System\Tune1\24-05-2012.qgt
Modified by : Admin
Modified : 29/5/2012 08:44:24



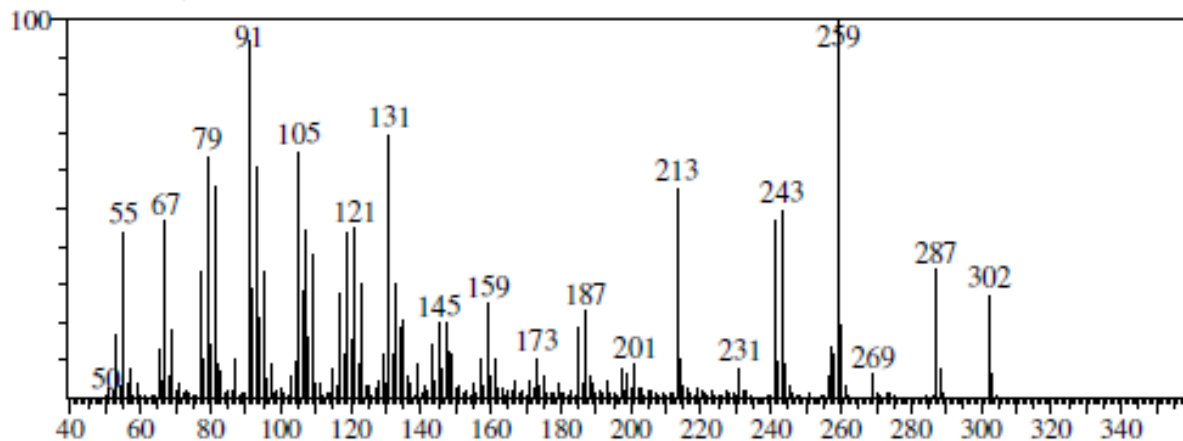
Peak Report TIC					
Peak#	R.Time	Area	Area%	Name	Base m/z
1	18.241	50730346	100.00		259.15
		50730346	100.00		

Figure 2. EI-MS spectrum of compound 1.

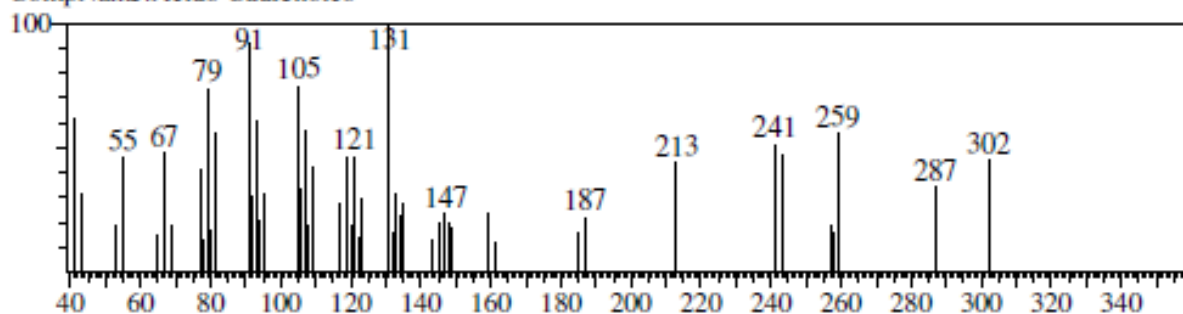
Library

<< Target >>

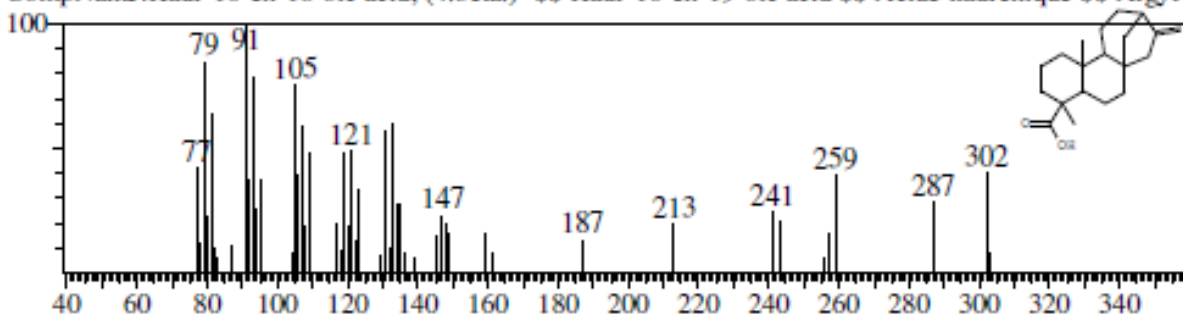
Line#: 1 R.Time: 18.240(Scan#: 2849) MassPeaks: 228
 RawMode: Averaged 18.235-18.245(2848-2850) BasePeak: 259.15(442988)
 BG Mode: Calc. from Peak



Hit#: 1 Entry: 1 Library: MY LIBRARY.lib
 SI: 94 Formula: C₂₀H₃₀O₂ CAS: 6730-83-2 MolWeight: 302 RetIndex: 0
 CompName: Acido Caurenoico



Hit#: 2 Entry: 43171 Library: NIST62.LIB
 SI: 83 Formula: C₂₀H₃₀O₂ CAS: 20316-84-1 MolWeight: 302 RetIndex: 0
 CompName: Kaur-16-en-18-oic acid, (4.beta.)- \$\$ Kaur-16-en-19-oic acid \$\$ Acide kaurenique \$\$ Argyro



Hit#: 3 Entry: 213488 Library: WILEY7.LIB
 SI: 83 Formula: C₂₀H₃₀O₂ CAS: 20316-84-1 MolWeight: 302 RetIndex: 0
 CompName: Kaur-16-en-18-oic acid, (4.beta.)- (CAS) Kaur-16-en-19-oic acid \$\$ Acide kaurenique \$\$ Ar

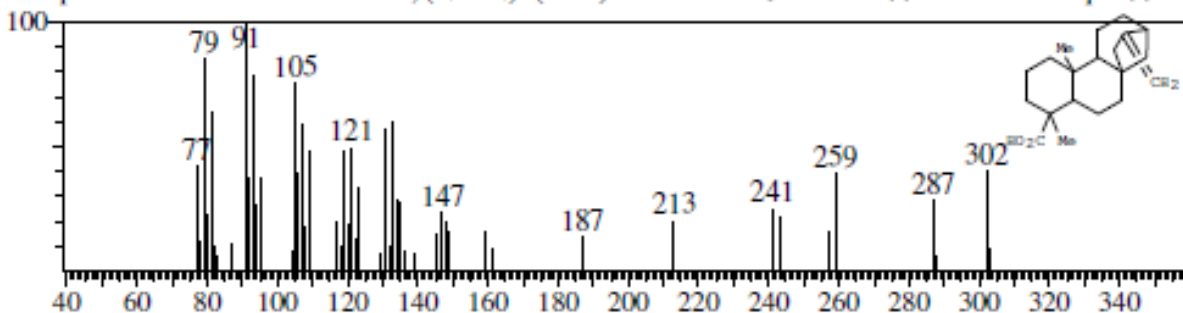


Figure 3. HR-ESI-MS spectrum of compound 1.

Generic Display Report

Faculdade de Ciencias Farmaceuticas de Ribeirao Preto-USP

Analysis Info

Analysis Name D:\Data\SILVIA T\croton_0.d
Method tune_low_Tomaz1200_POS.m
Sample Name croton_0
Comment

Acquisition Date 6/29/2012 4:31:55 PM
Operator BDAL@DE
Instrument micrOTOF-Q II

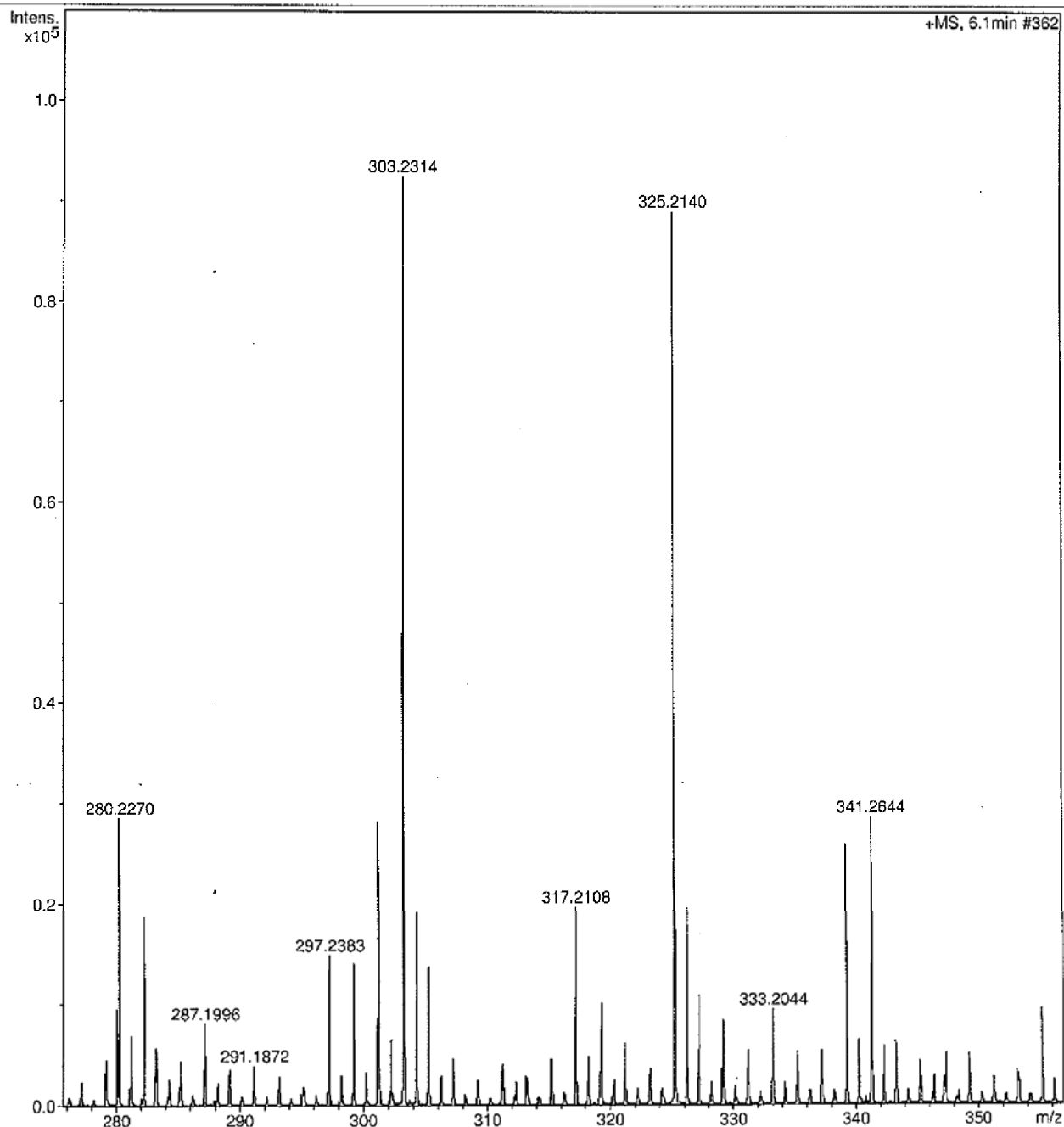


Figure 4. ¹H-NMR spectrum of compound 1.

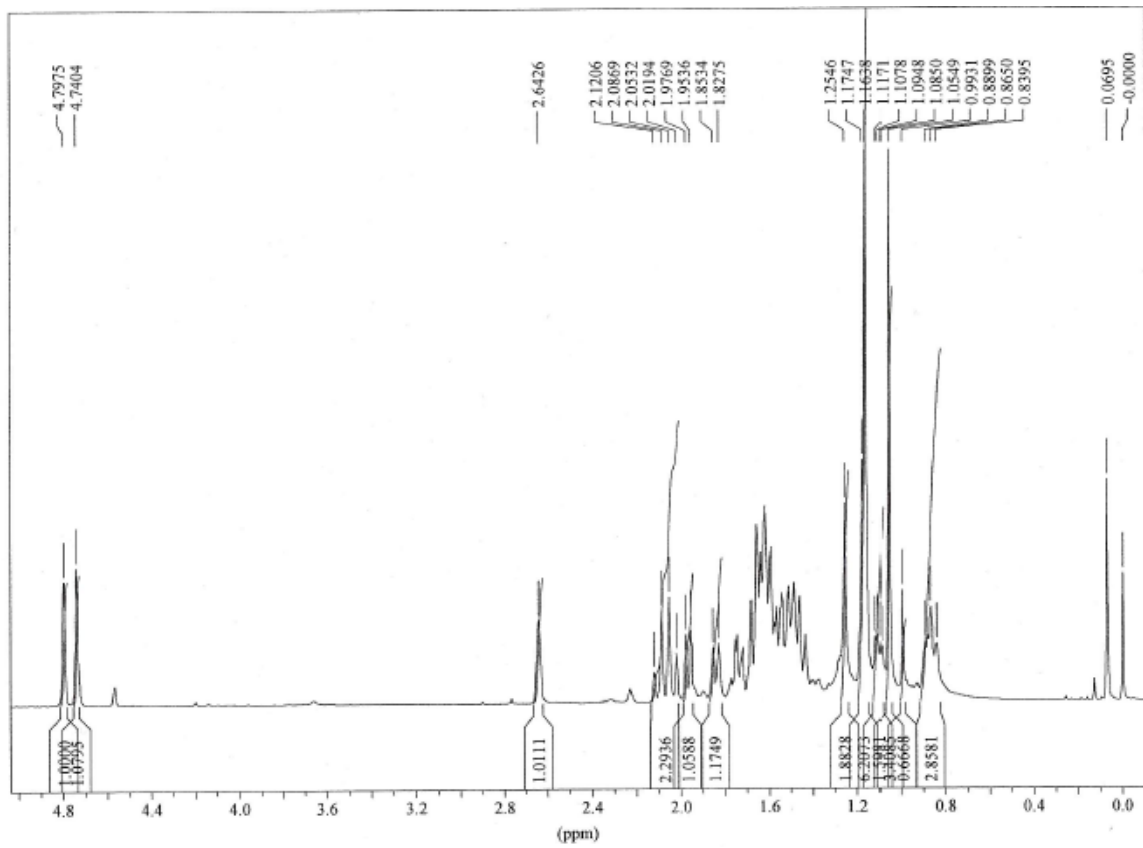


Figure 5. Expansion of ¹H-NMR spectrum of compound 1.

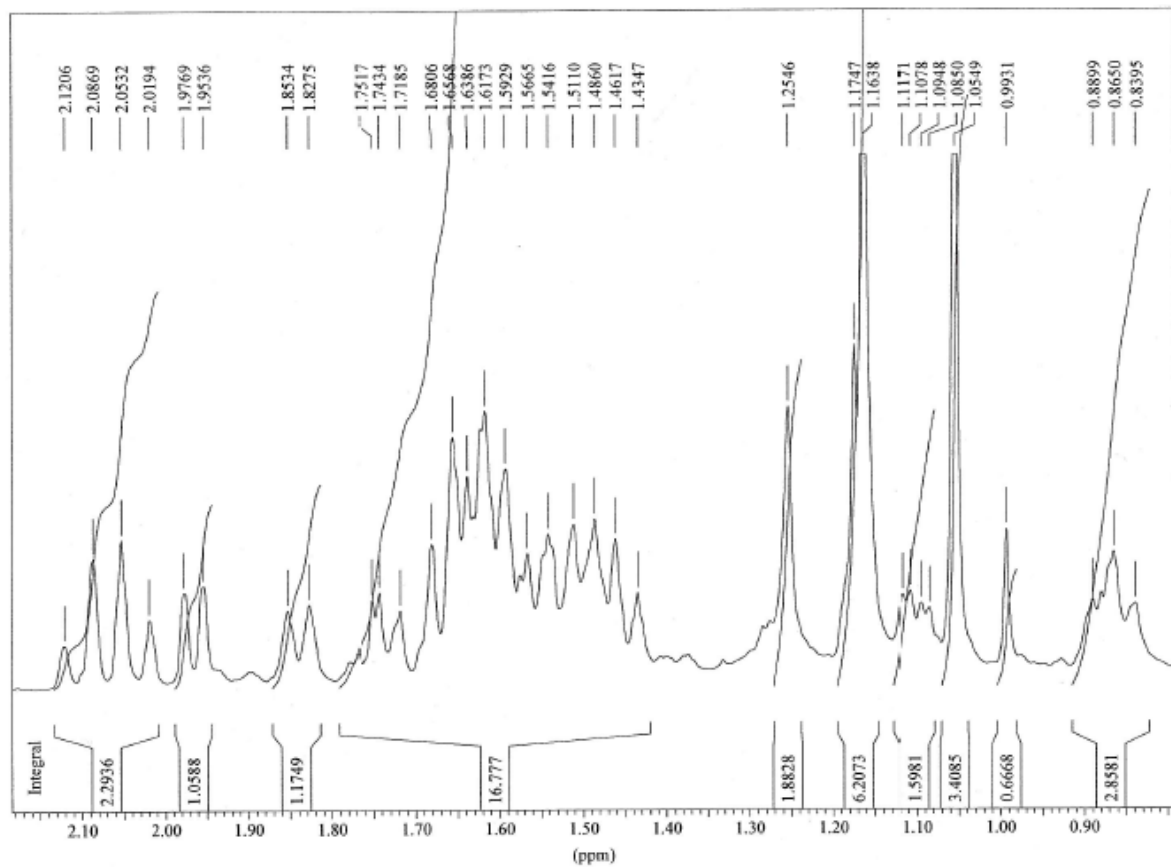


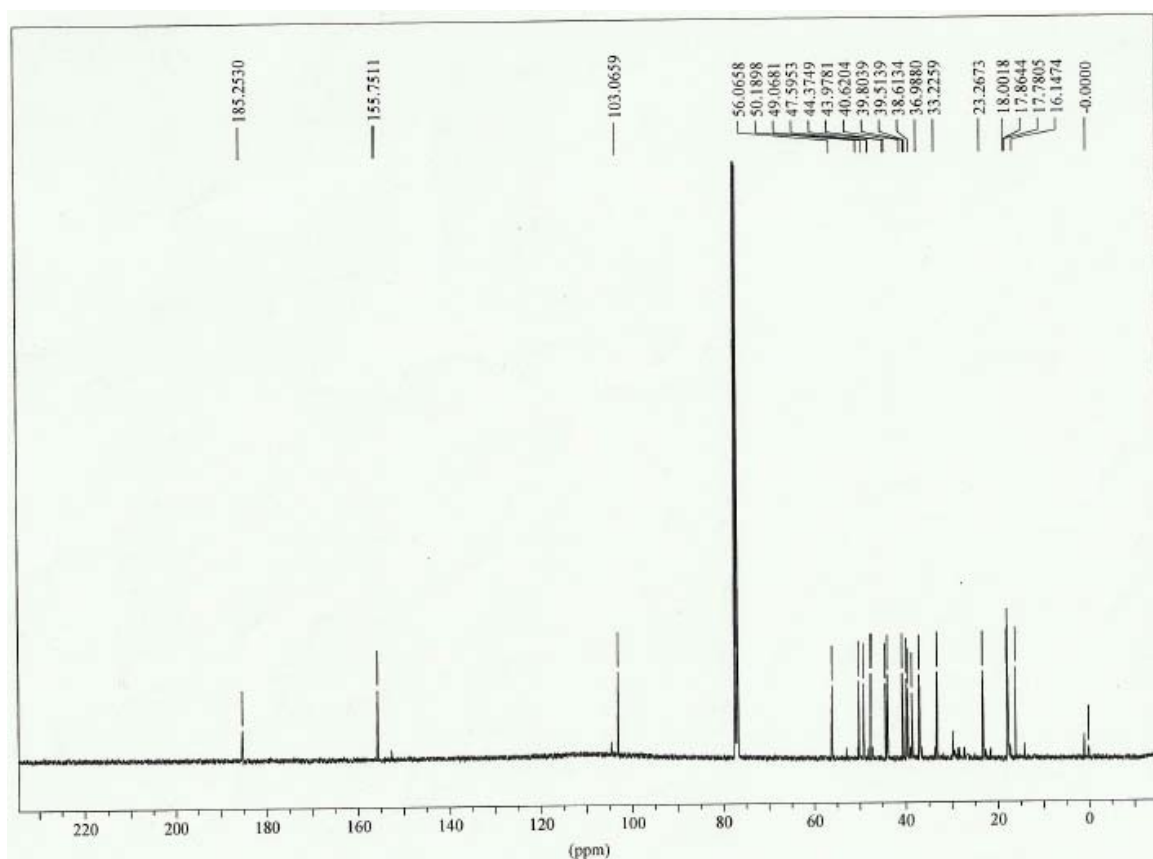
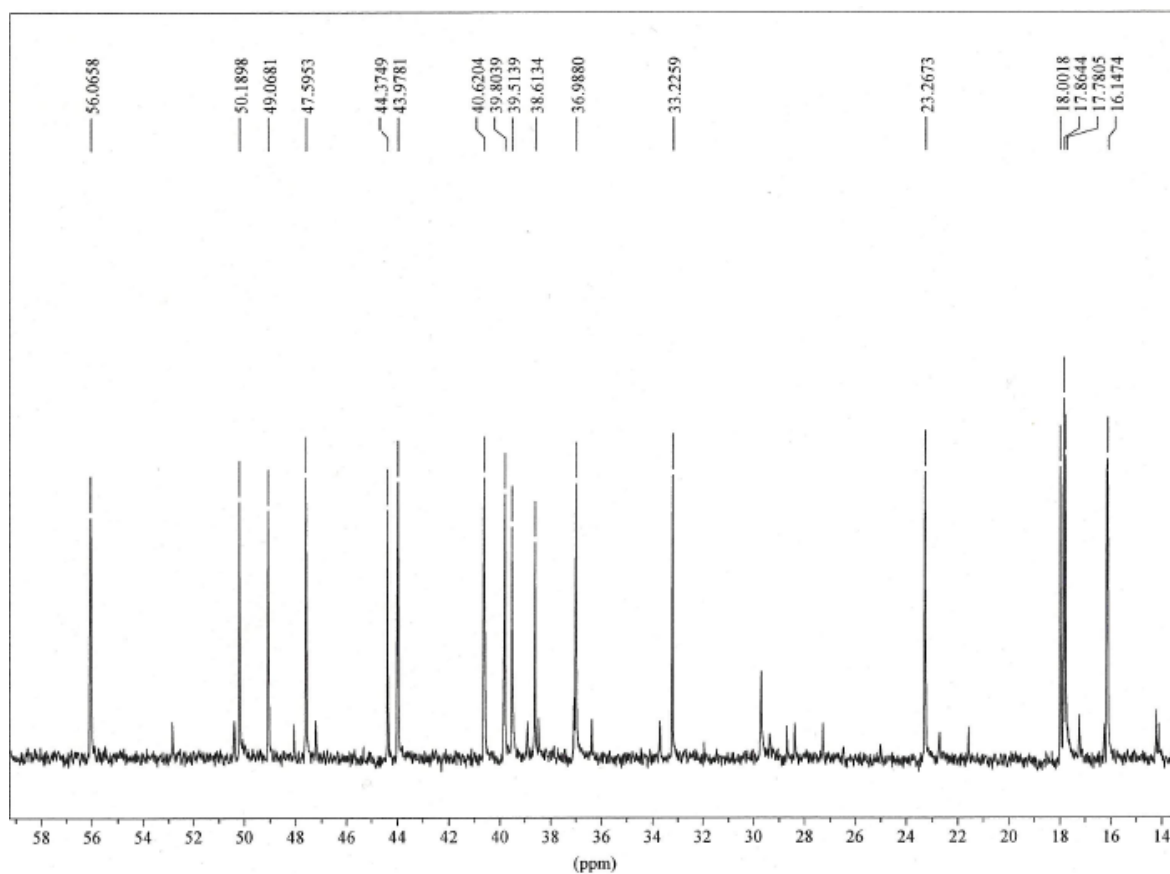
Figure 6. ^{13}C -NMR spectrum of compound 1.Figure 7. Expansion of ^{13}C -NMR spectrum of compound 1.

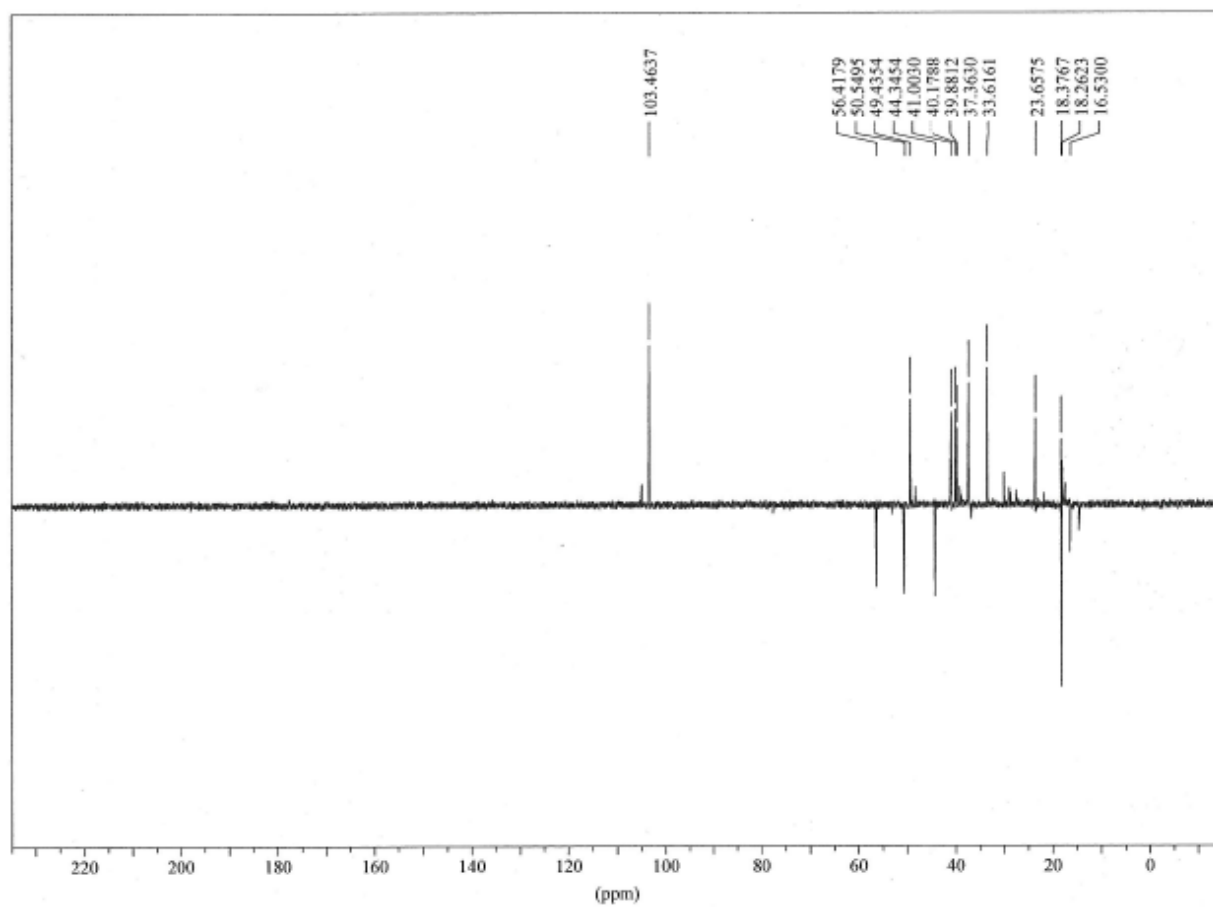
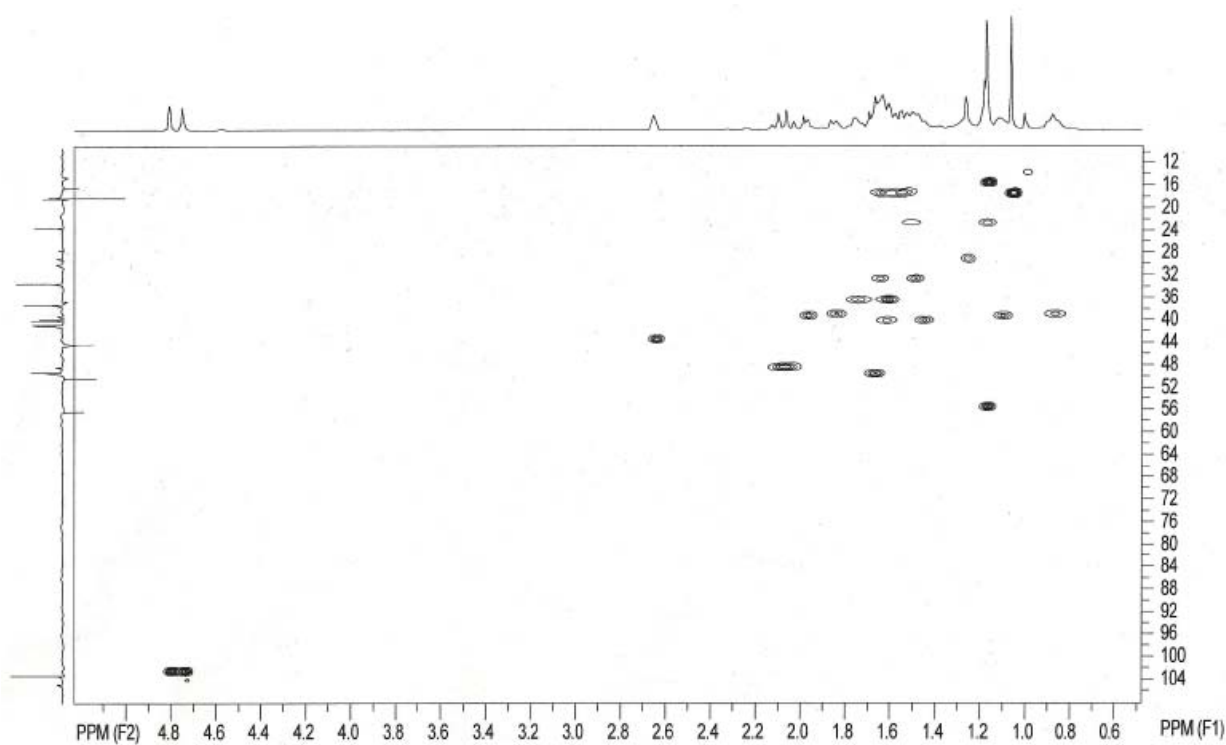
Figure 8. DEPT-135 spectrum of compound 1.**Figure 9.** 2D HMQC spectrum of compound 1.

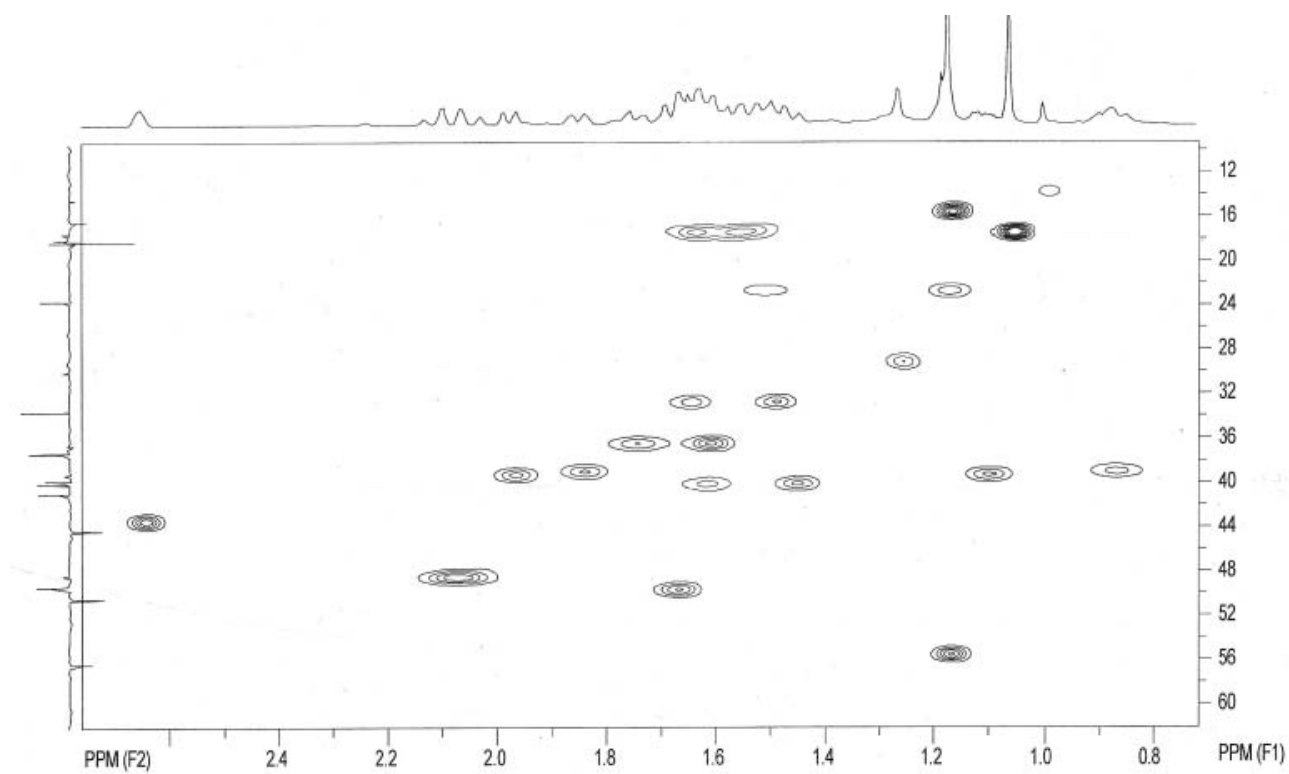
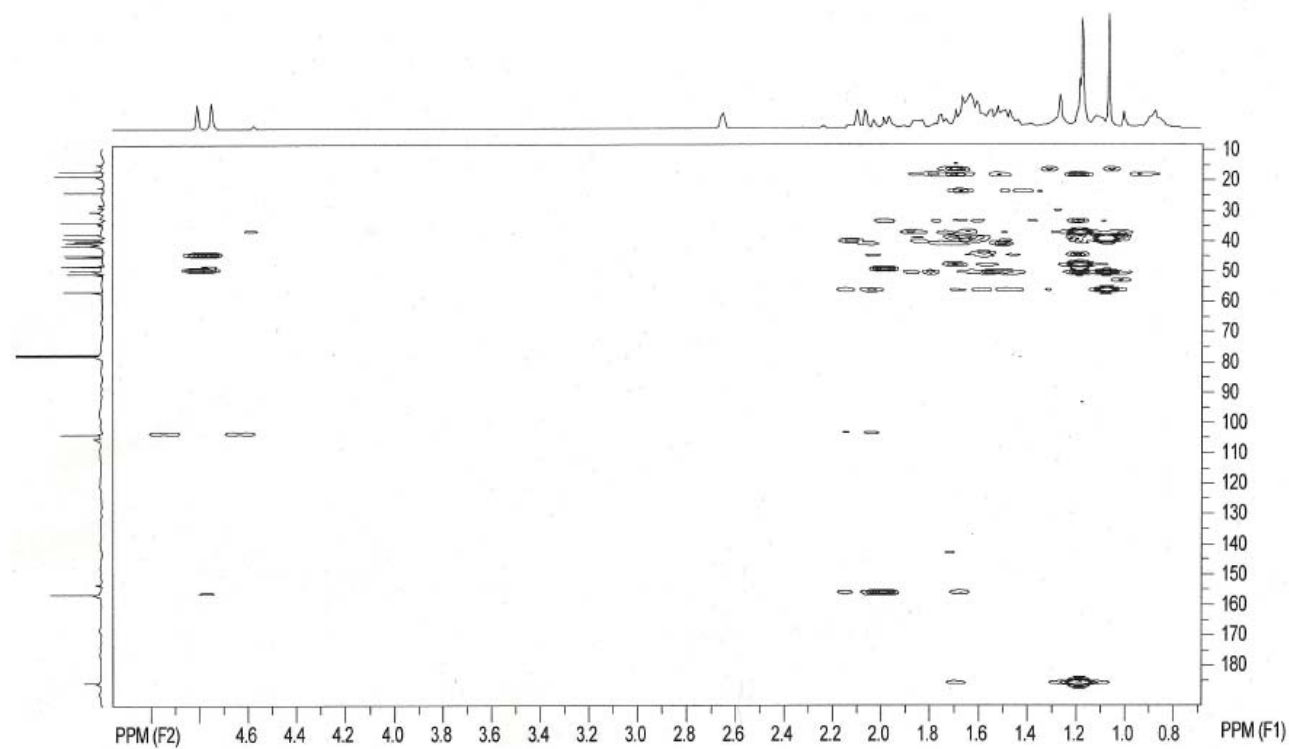
Figure 10. Expansion of 2D HMQC spectrum of compound 1.**Figure 11.** 2D HMBC spectrum of compound 1.

Figure 12. Expansion of 2D HMBC spectrum of compound 1.

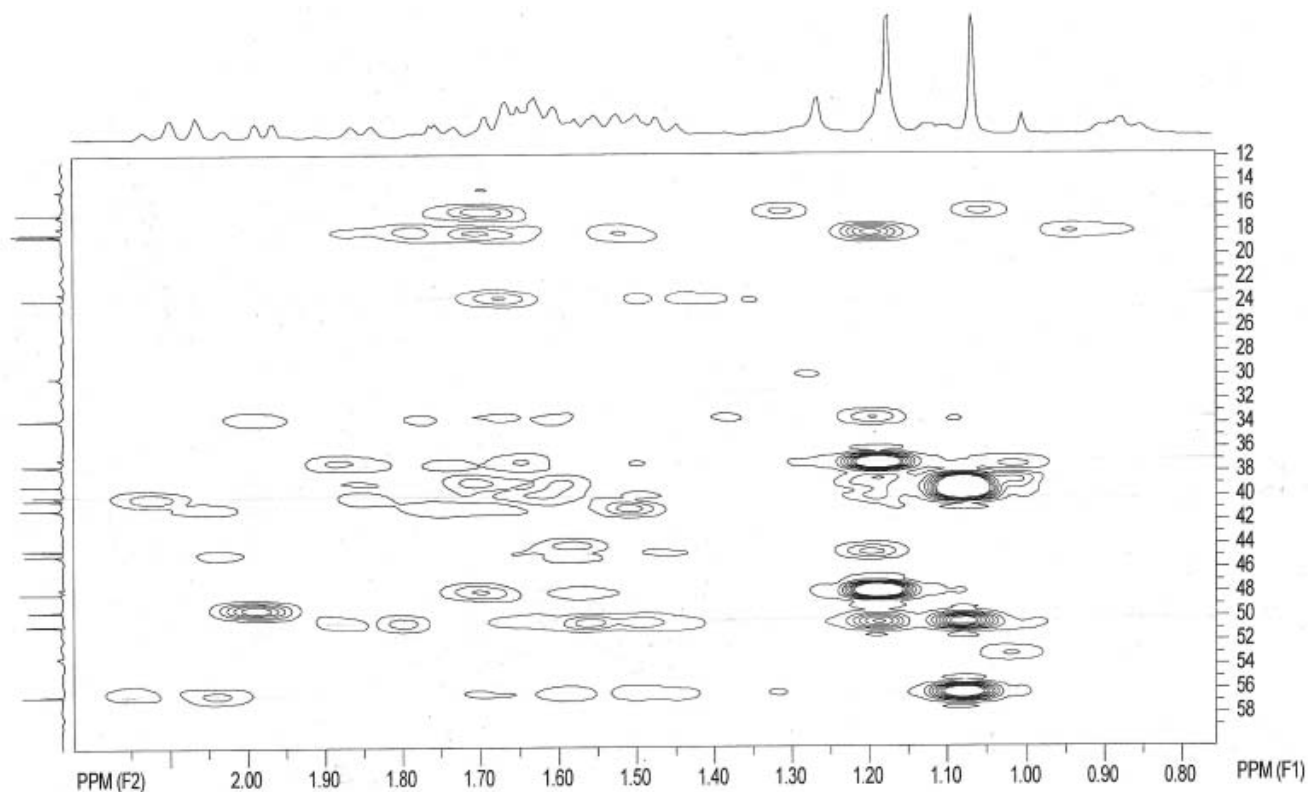


Figure 13. NOEDIFF spectrum of compound 1.

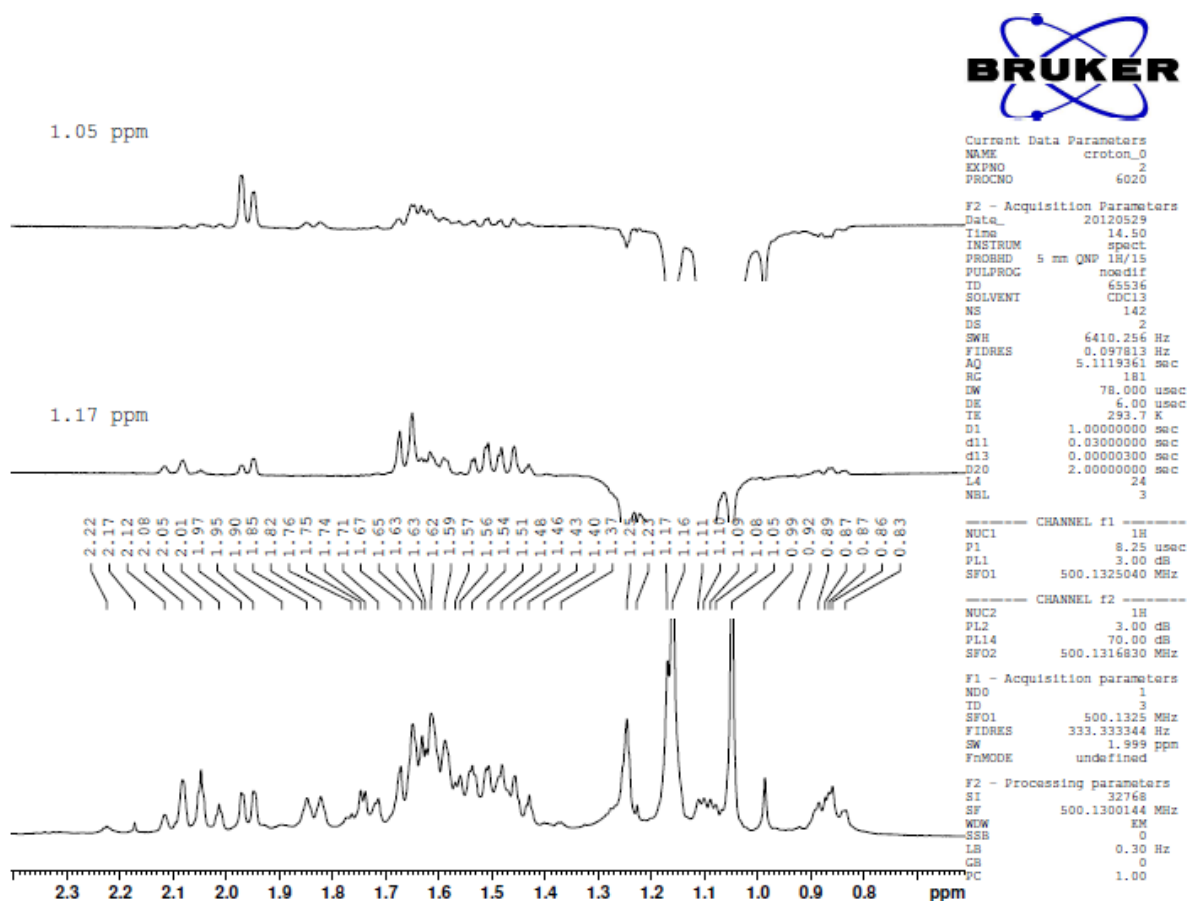


Figure 14. Expansion of NOESY spectrum of compound 1.

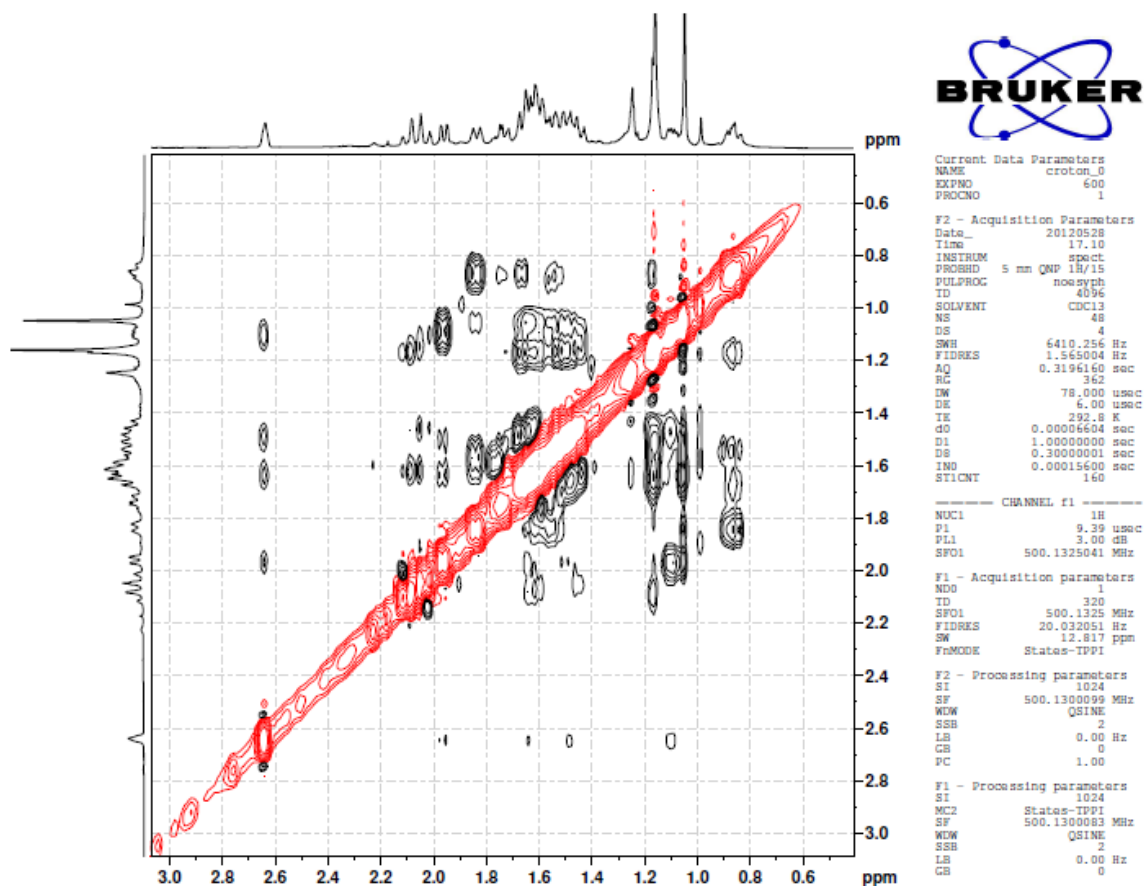


Figure 15. Expansion of NOESY spectrum of compound 1.

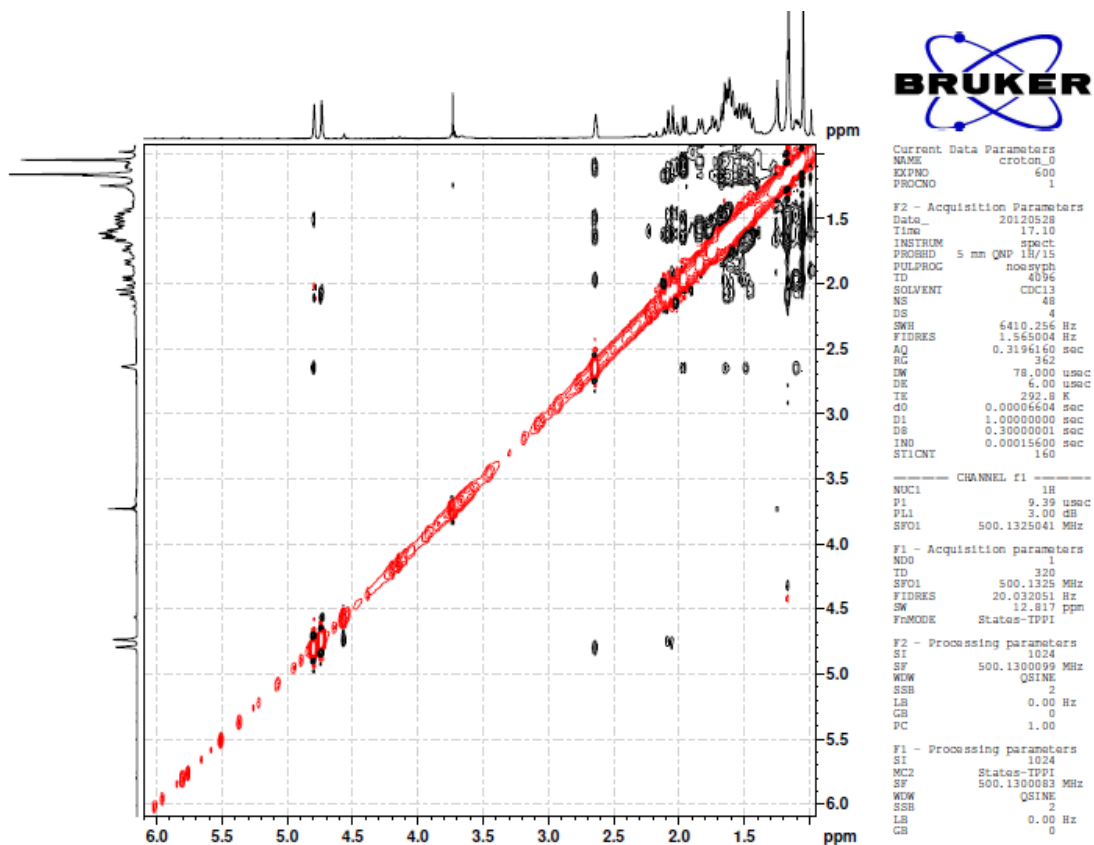


Figure 16. NOESY spectrum of compound 1.

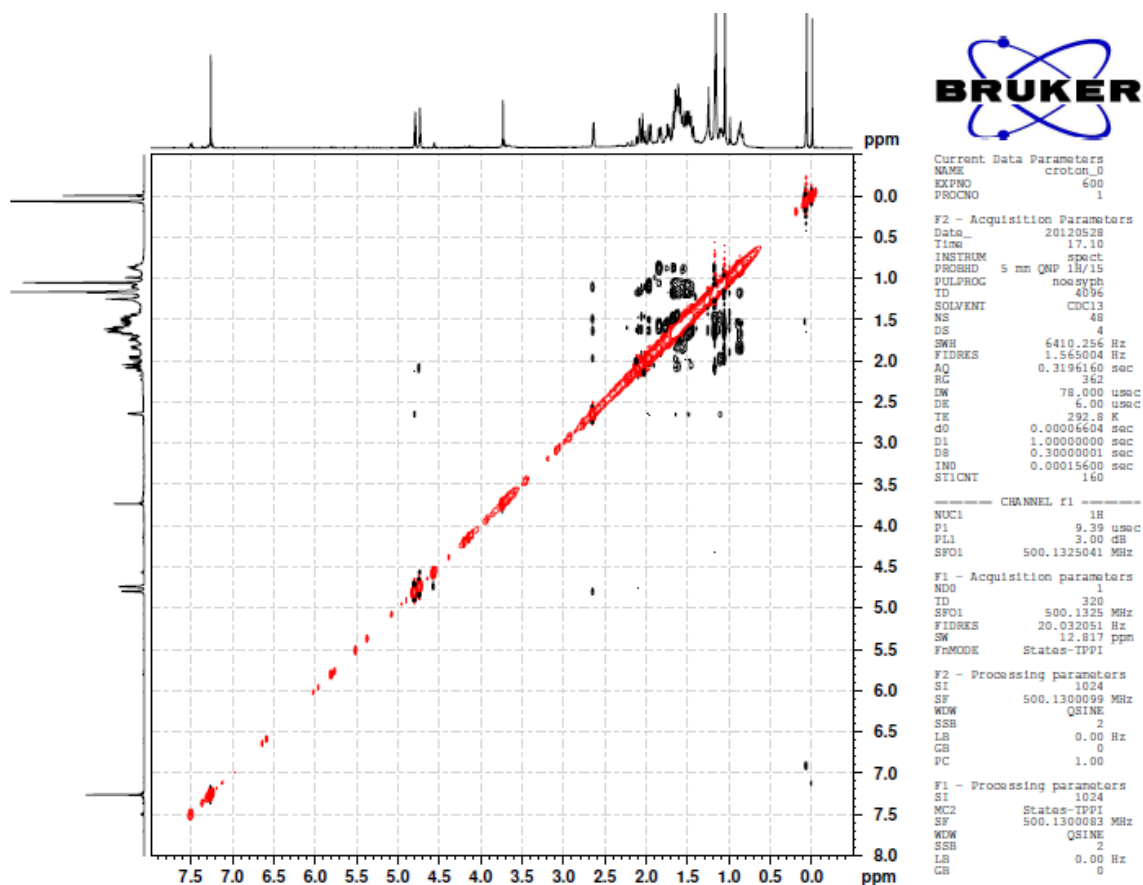


Figure 17. Rows of two-dimensional NOESY spectra of compound 1.

