# Supporting Information Available



Manuscript Title: **A Nitrogen Containing 3-Alkyl-1,4-benzoquinone and A Gomphilactone Derivative from *Embelia ribes***


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**THERMO SPECTRONIC ~ VISION32 SOFTWARE V1.25**

**Batch Information - scan006**

| | | | |
|---|---|---|---|
| Batch Type | Scan | Operator Name | (None Entered) |
| Instrument ID | 110514 | Aborted | No |

**Results Table - scan006**

Data Mode Absorbance

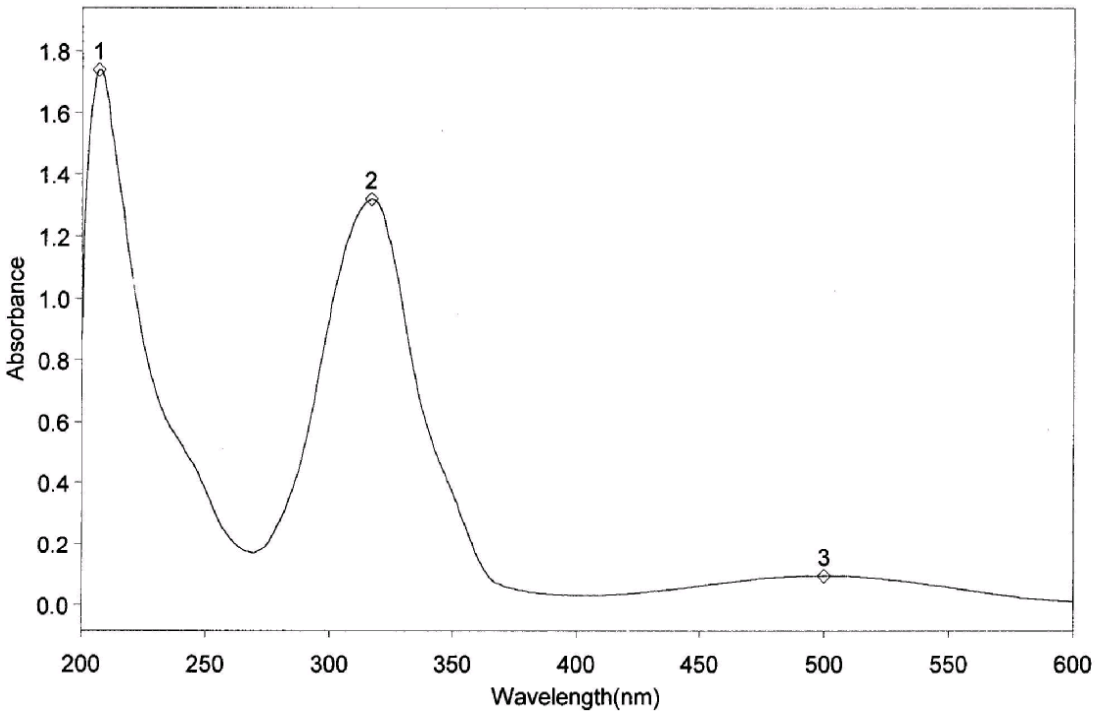
| | A | B | C | D | E |
|---|---|---|---|---|---|
| 1 | **Lpc-12** | | 1 | 2 | 3 |
| 2 | Cycle01 | nm | 207.0 | 317.0 | 500.0 |
| 3 | Manual | A | 1.739 | 1.318 | .094 |

All calculations have been performed to double precision as defined by ANSI/IEEE STD 754-1985 but have been rounded for display purposes.

**Lpc-12**

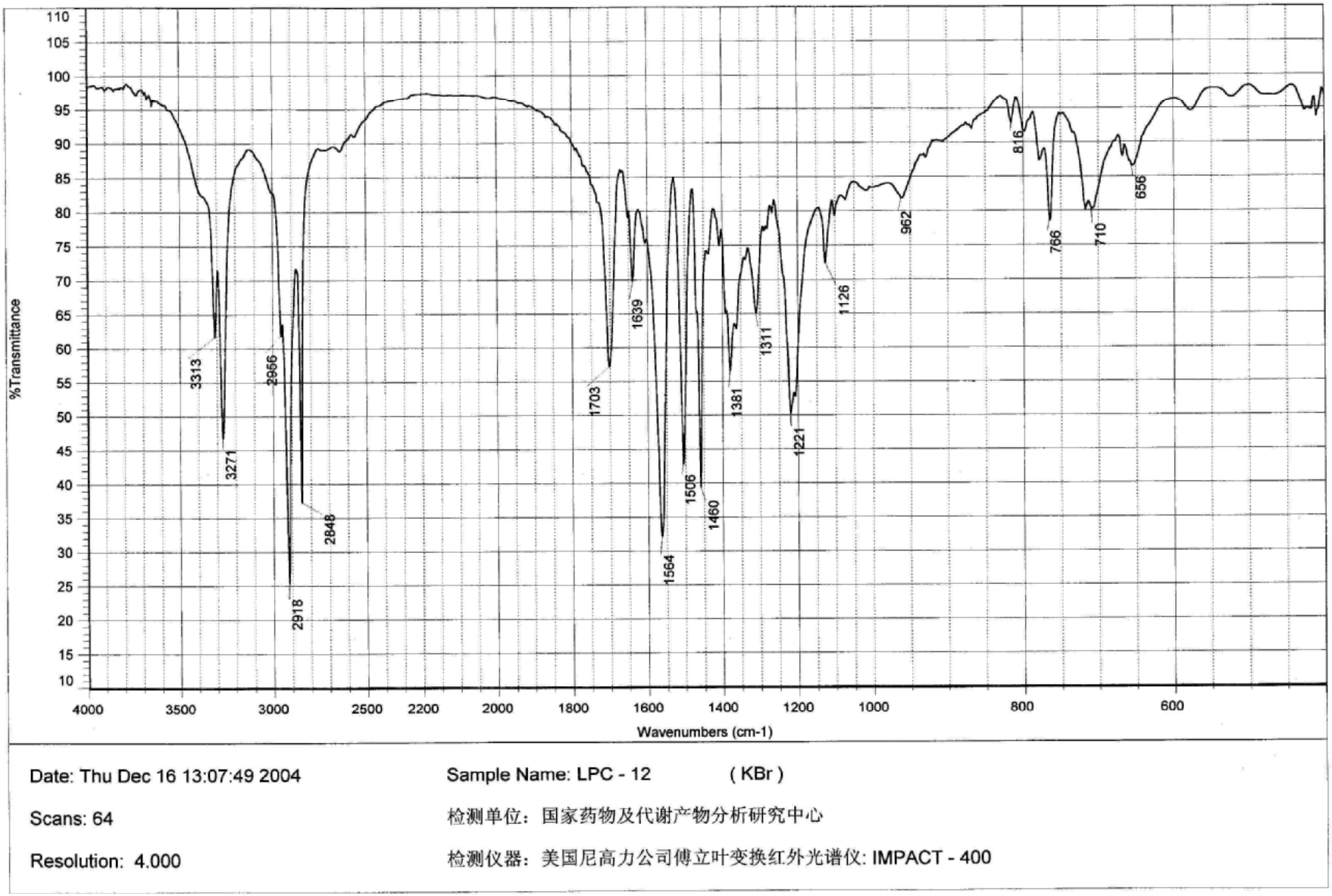
Description 0.615mg/10mlMeOH

**Lpc-12,Cycle01**

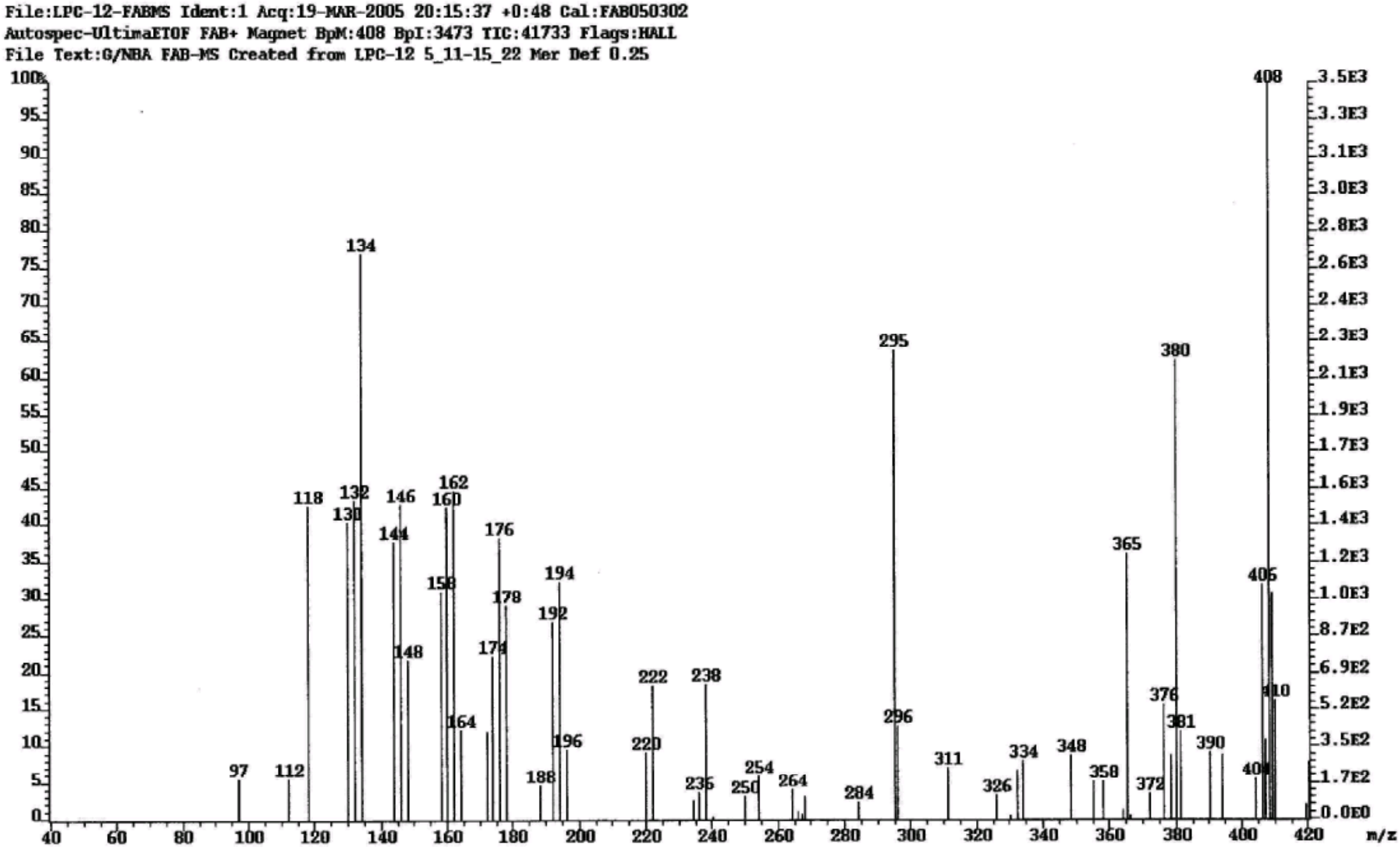





**The UV Spectrum of Compound 1**




**The IR Spectrum of Compound 1**



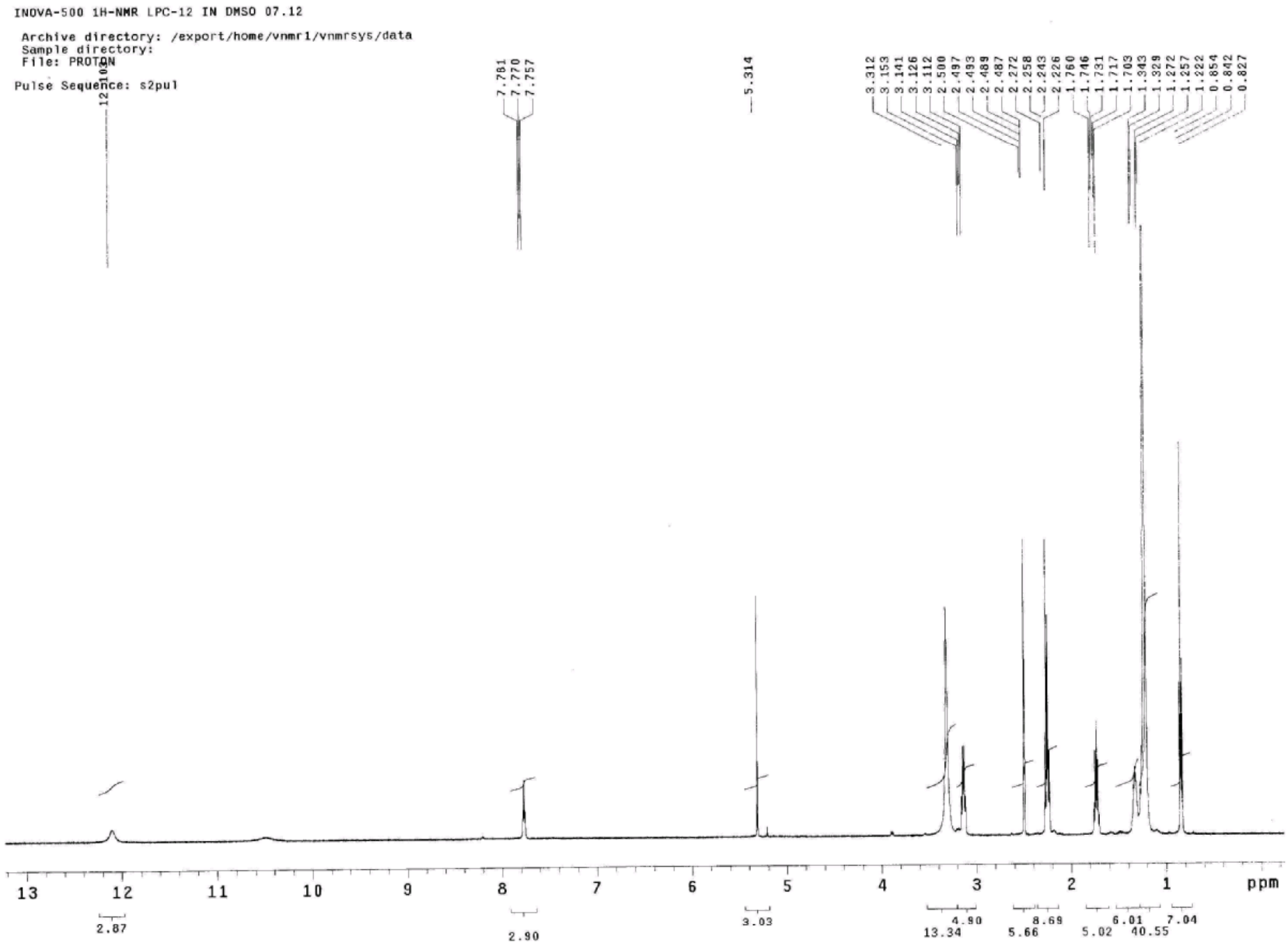

**The FAB Mass Spectrum of Compound 1**

File:LPC-12-HRFAB Ident:1 Acq:12-DEC-2004 01:36:30 +2:37 Cal:LPC-12
Autospec-UltimaETOF FAB+ Voltage BpM:415 BpI:93209 TIC:416071 Flags:NORM
File Text:HRFAB-MS Created from LPC-12 13_19 PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid)
Heteroatom Max: 20 Ion: Both Even and Odd
Limits:

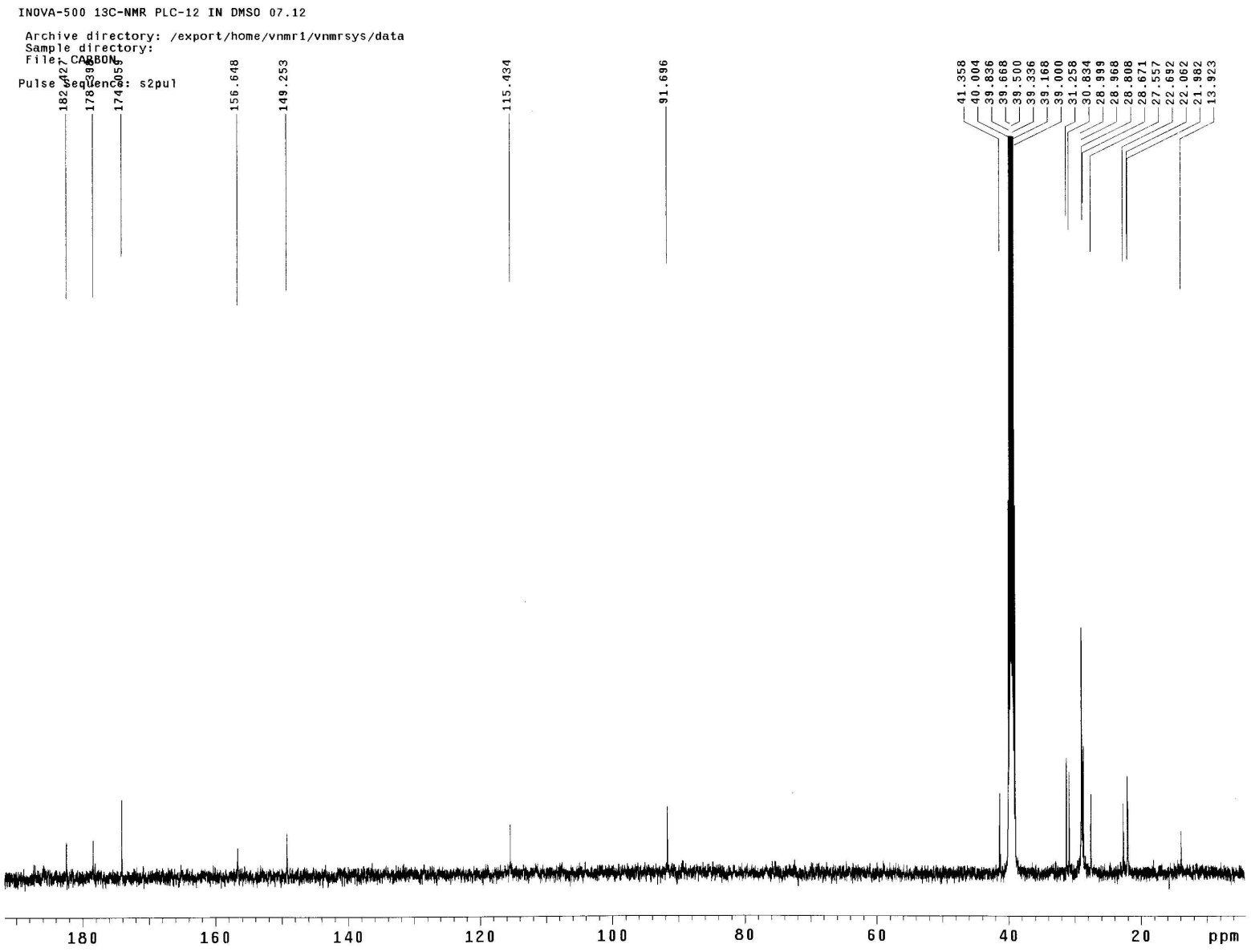
| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 408.264 | 0.0 | | | | | -0.5 | 0 | 0 | 0 | 4 |
| 408.289 | 100.0 | | 10.0 | | | 30.0 | 200 | 400 | 1 | 6 |
| Mass | %RA | Pks | Std | PPM | mDa | Calc. Mass | DBE | C | H | N | O |
| 408.272705 | 89.5 | | | 5.6 | 2.3 | 408.274999 | 5.5 | 23 | 38 | 1 | 5 |

End of listing Calculation: Automatic Sort: Deviation

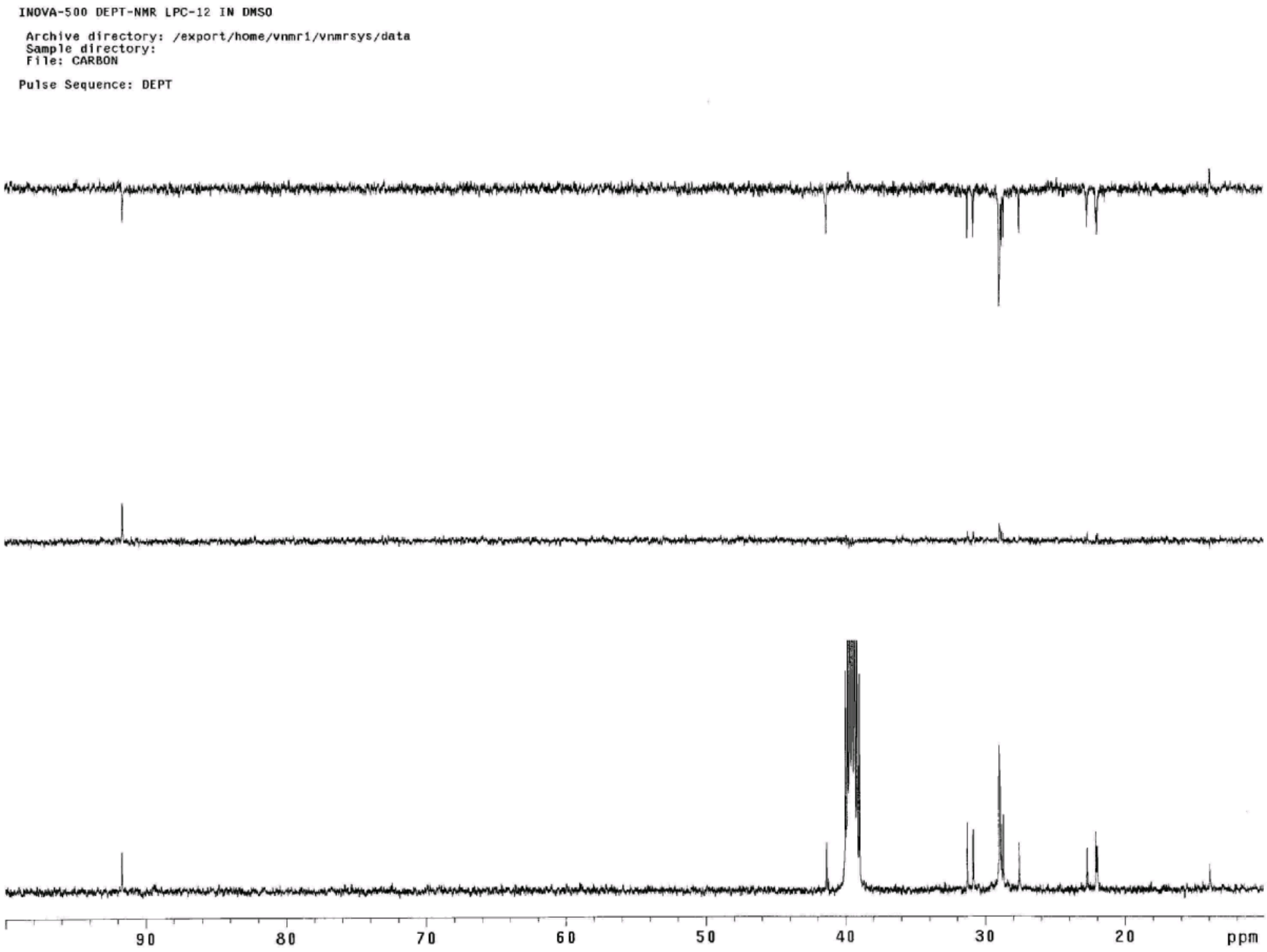
**The HRFAB Mass Spectral Data of Compound 1**




**The $^{1}$H NMR Spectrum of Compound 1**




**The $^{13}$C NMR Spectrum of Compound 1**



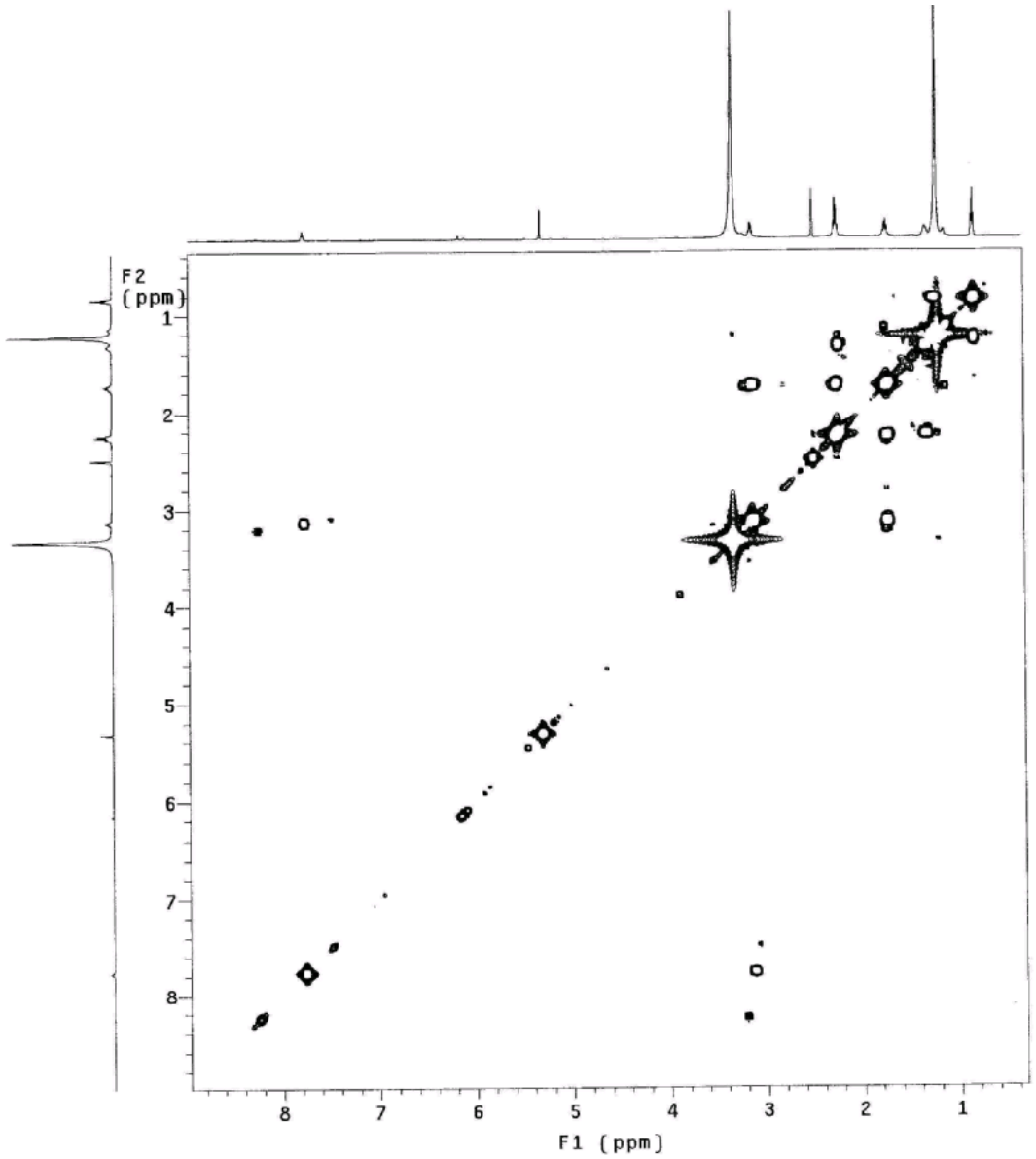

**The DEPT Spectrum of Compound 1**

INOVA-501 gCOSY LPC-12 IN DMSO 04.11.26

File: PROTON

Solvent: DMSO
Temp. 25.0 C / 298.1 K
INOVA-500 "NMR501"

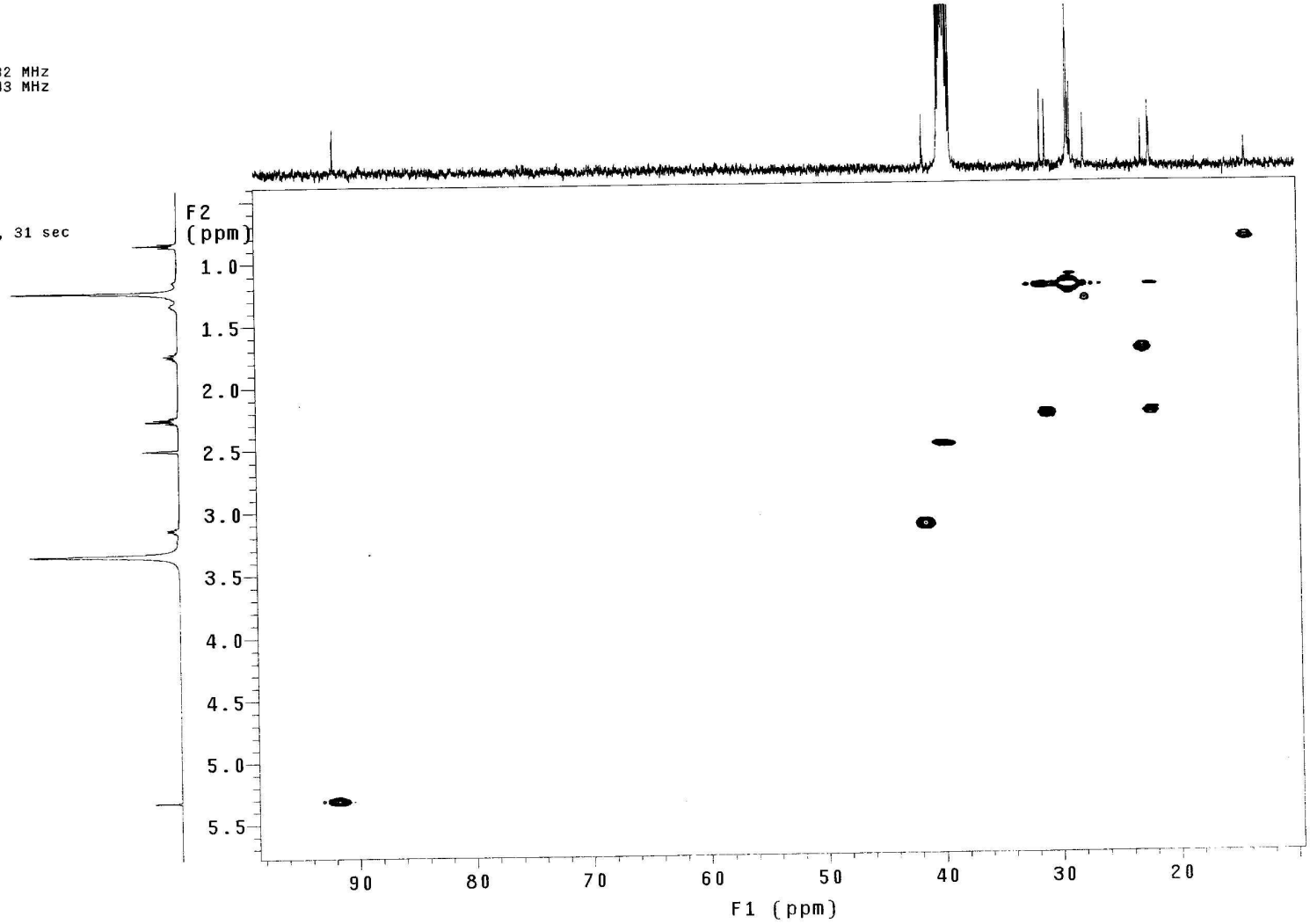
Relax. delay 1.000 sec
Acq. time 0.137 sec
Width 7472.4 Hz
2D Width 7472.4 Hz
2 repetitions
300 increments
OBSERVE H1, 499.7474032 MHz
DATA PROCESSING
Sine bell 0.068 sec
F1 DATA PROCESSING
Sine bell 0.020 sec
FT size 2048 x 2048
Total time 12 min, 0 sec



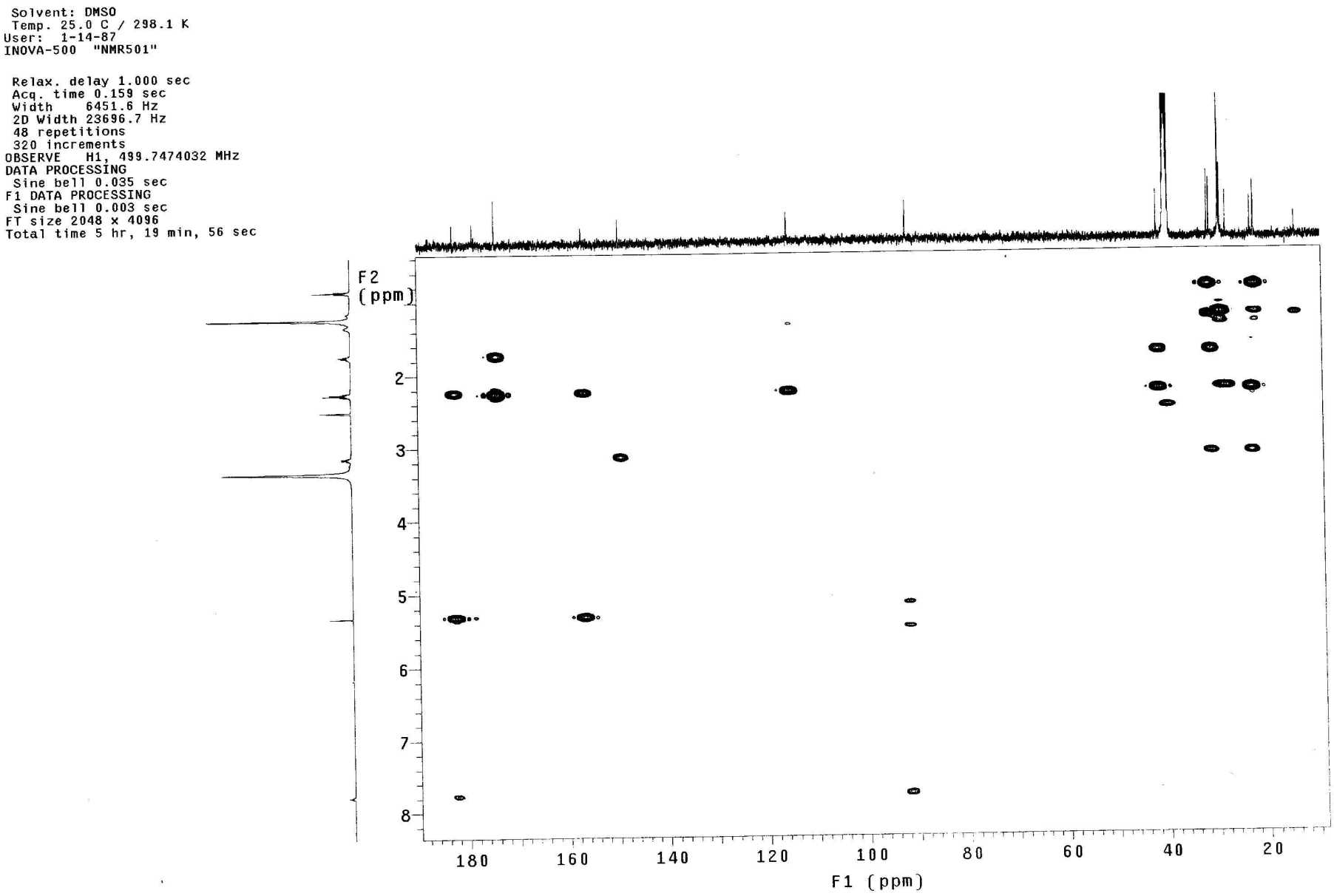

**The $^{1}$H-$^{1}$H gCOSY Spectrum of Compound 1**

Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "NMR501"

Relax. delay 1.000 sec
Acq. time 0.232 sec
Width 4406.3 Hz
2D Width 20865.9 Hz
24 repetitions
256 increments
OBSERVE H1, 499.7474032 MHz
DECOUPLE C13, 125.6725643 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.057 sec
F1 DATA PROCESSING
Sine bell 0.006 sec
FT size 2048 x 4096
Total time 2 hr, 14 min, 31 sec




**The gHSQC Spectrum of Compound 1**




**The gHMBC Spectrum of Compound 1**

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**Batch Information - scan003**

| | | | |
|---|---|---|---|
| Batch Type | Scan | Operator Name | (None Entered) |
| Instrument ID | 110514 | Aborted | No |

**Results Table - scan003**

Data Mode Absorbance

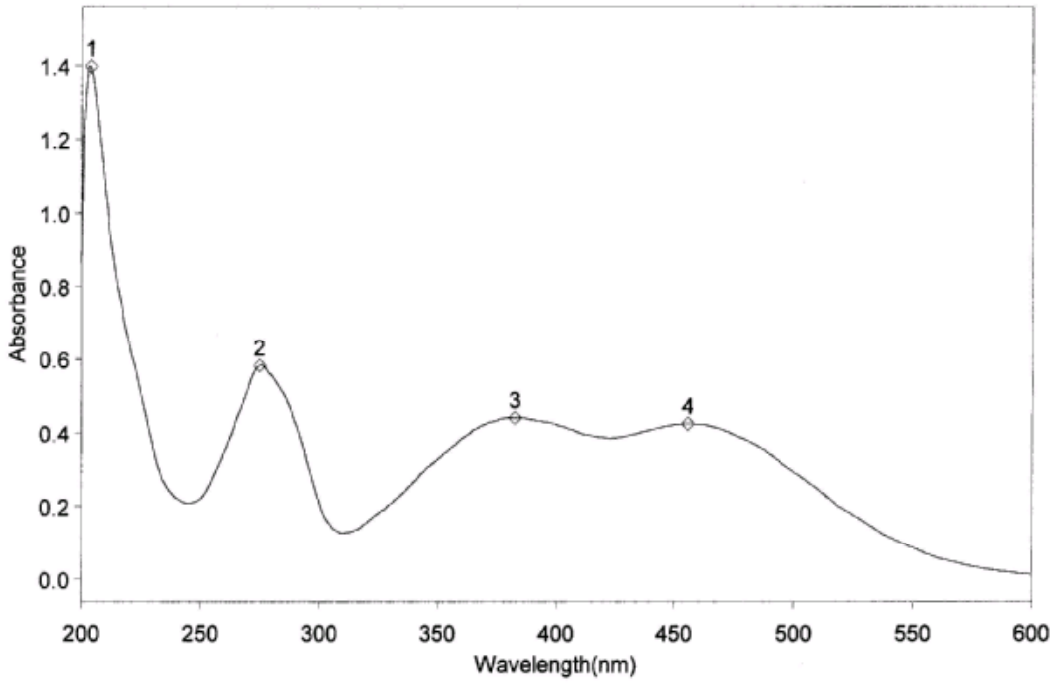
| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| 1 | **Lpc-8** | | **1** | **2** | **3** | **4** |
| 2 | Cycle01 | nm | 204.0 | 275.0 | 383.0 | 456.0 |
| 3 | Manual | A | 1.398 | .584 | .440 | .423 |

All calculations have been performed to double precision as defined by ANSI/IEEE STD 754-1985 but have been rounded for display purposes.

**Lpc-8**

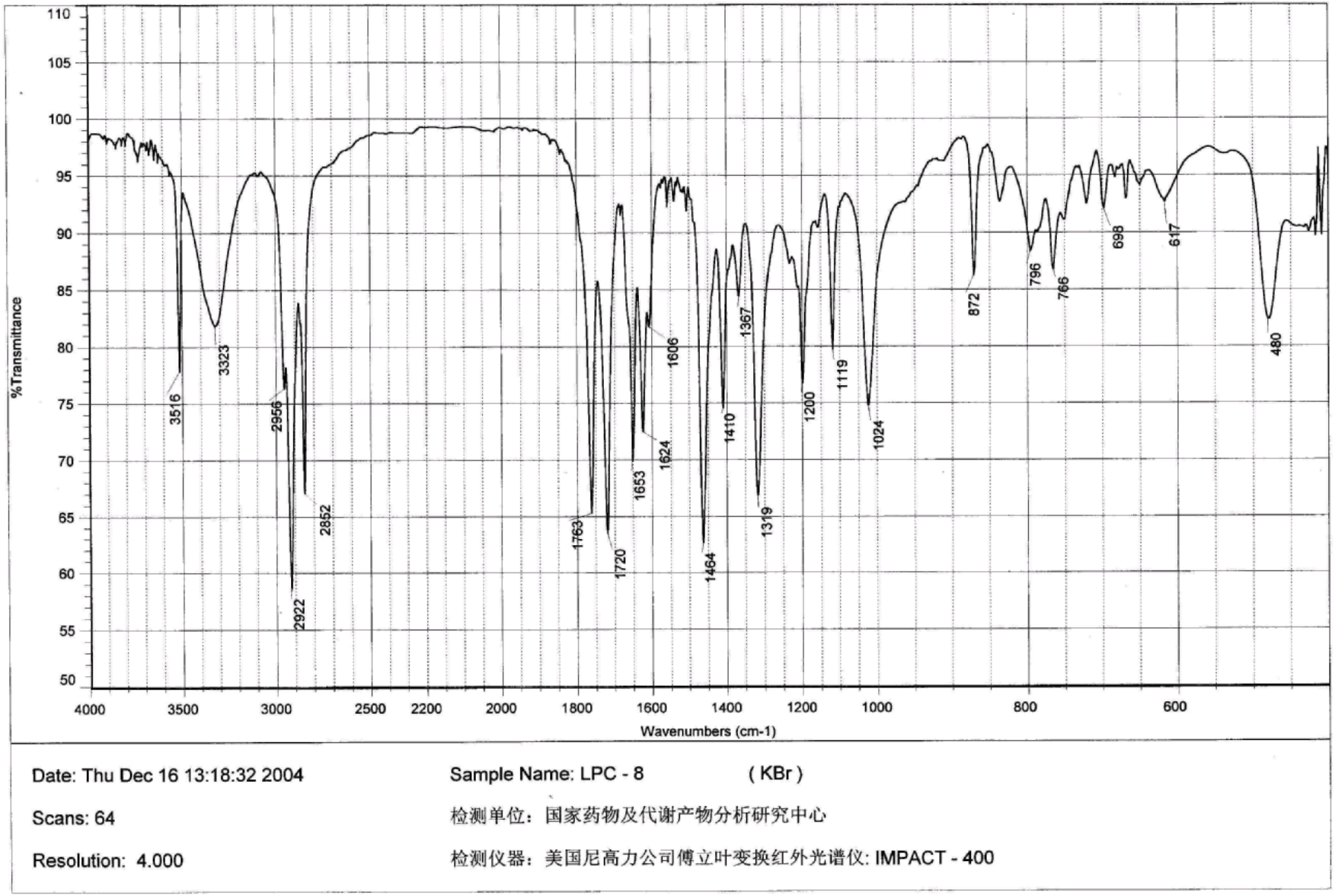
Description 0.284mg/10mlMeOH

**Lpc-8,Cycle01**

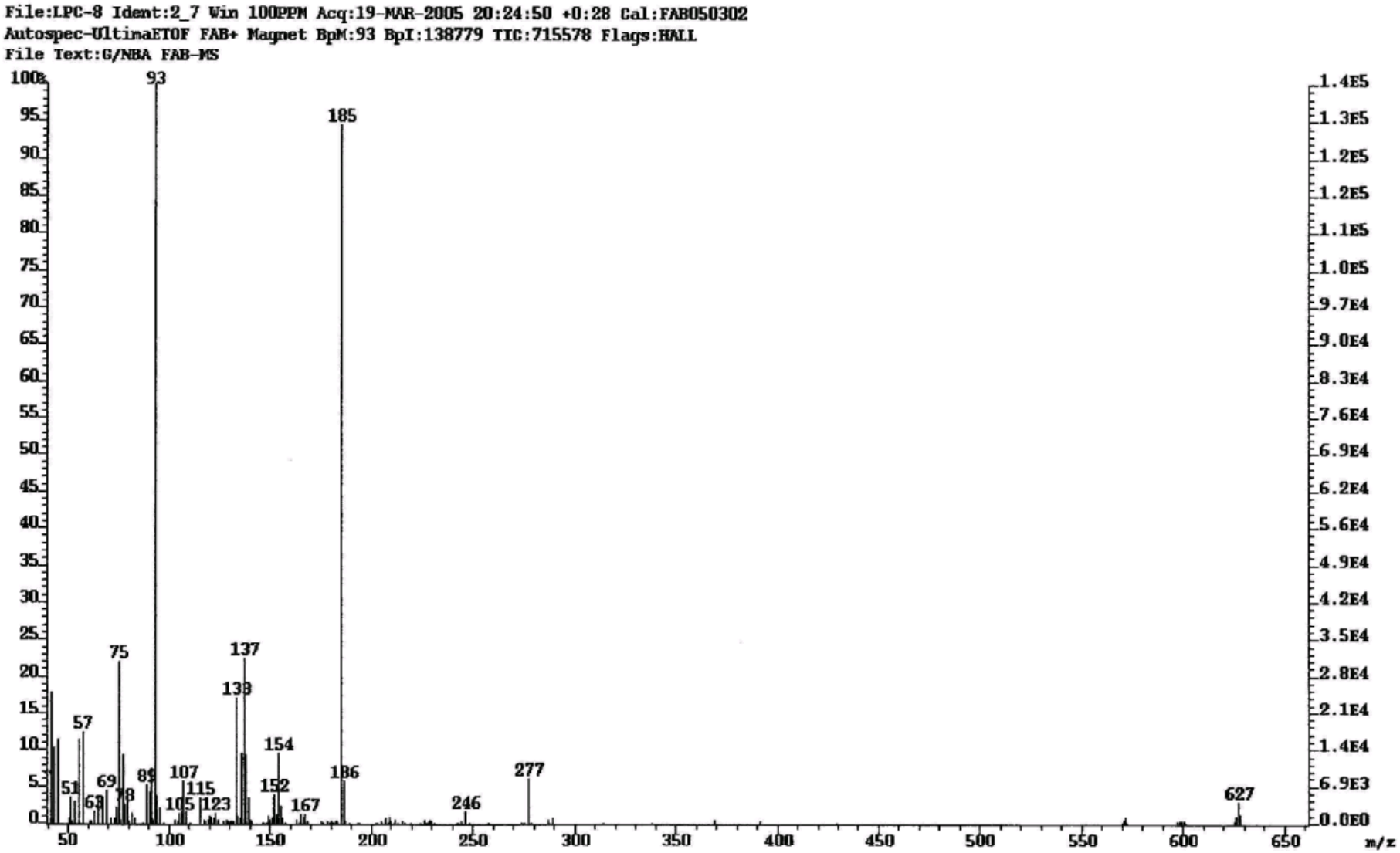





The **UV Spectrum of Compound 2**




The **IR Spectrum of Compound 2**



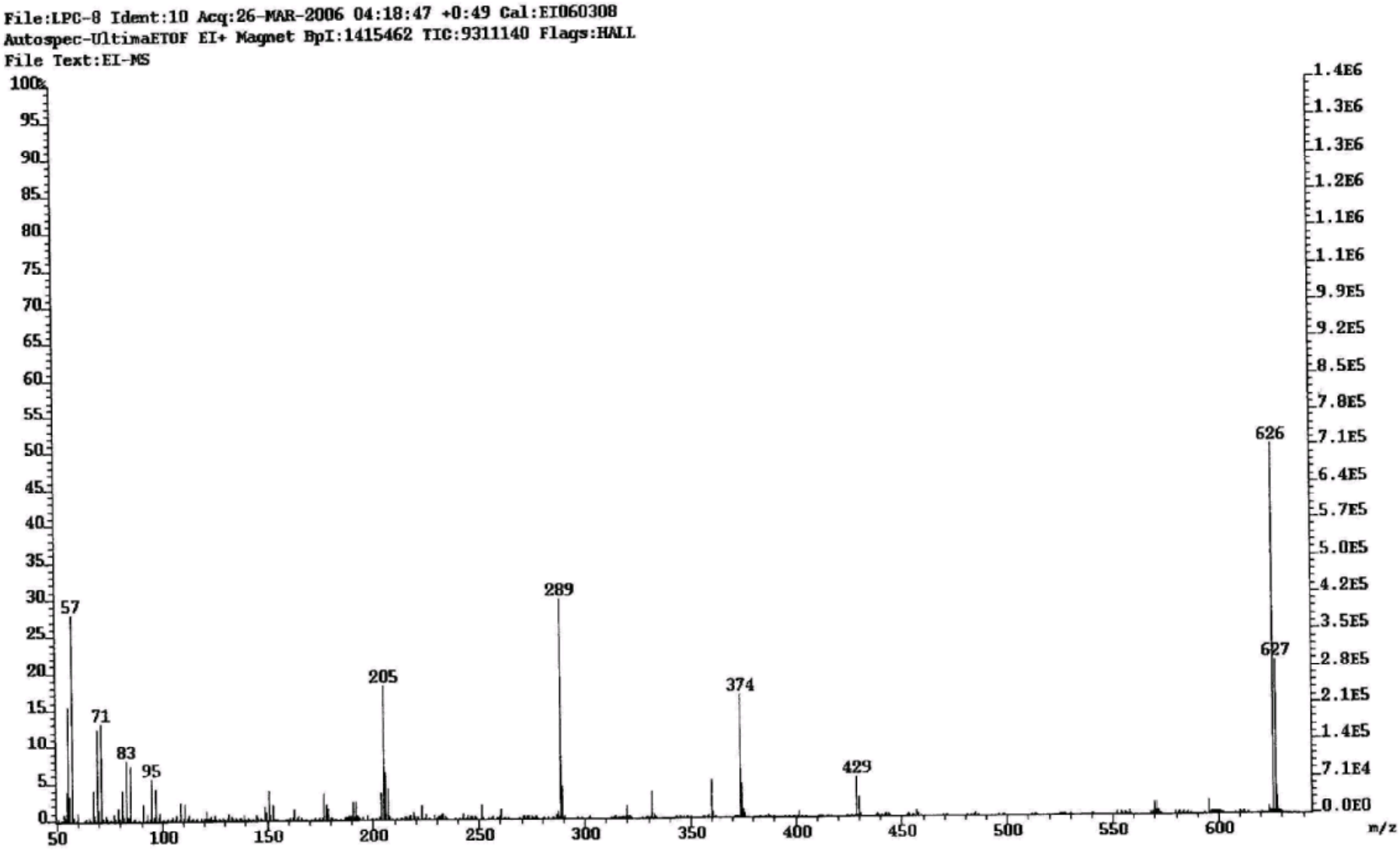

**The FAB Mass Spectrum of Compound 2**

File:LPC-8-HRFAB Ident:1 Acq:12-DEC-2004 01:48:13 +3:50 Cal:LPC-8
Autospec-UltimaETOF FAB+ Voltage BpM:599 BpI:120232 TIC:470540 Flags:NORM
File Text:HRFAB-MS Created from LPC-8 24_30 PKD(7,3,7,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid)
Heteroatom Max: 20 Ion: Both Even and Odd
Limits:

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 627.382 | 0.0 | | | | | -0.5 | 0 | 0 | 5 |
| 627.495 | 100.0 | | 10.0 | | | 30.0 | 200 | 400 | 10 |
| Mass | %RA | Pks | Std | PPM | mDa | Calc. Mass | DBE | C | H | O |
| 627.426514 | 25.7 | | | -0.7 | -0.4 | 627.426080 | 9.5 | 38 | 59 | 7 |

End of listing Calculation: Automatic Sort: Deviation

**The HRFAB Mass Spectral Data of Compound 2**




**The EI Mass Spectrum of Compound 2**

File:LPC-8-1-HR-EI Ident:1 Acq: 6-APR-2006 02:21:12 +1:15 Cal:LPC-8-HR1
Autospec-UltimaETOF EI+ Voltage BpM:598 BpI:208950 TIC:813505 Flags:NORM
File Text:EI-MS Created from LPC-8-HR1 14 SM0(1,11) PKD(11,6,11,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid)
Heteroatom Max: 20 Ion: Both Even and Odd
Limits:

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 626.286 | 0.0 | | | | | -0.5 | 0 | 0 | 0 |
| 626.516 | 100.0 | | | 20.0 | | 30.0 | 200 | 400 | 20 |
| Mass | %RA Pks | Std | PPM | mDa | Calc. Mass | DBE | C | H | O |
| 626.420547 | 32.2 | | -3.7 | -2.3 | 626.418255 | 10.0 | 38 | 58 | 7 |
| | | | 5.7 | 3.6 | 626.424128 | 1.0 | 31 | 62 | 12 |
| | | | -13.0 | -8.2 | 626.412381 | 19.0 | 45 | 54 | 2 |
| | | | 20.7 | 13.0 | 626.433511 | 14.0 | 42 | 58 | 4 |
| | | | -28.0 | -17.5 | 626.402999 | 6.0 | 34 | 58 | 10 |
| | | | 30.1 | 18.8 | 626.439384 | 5.0 | 35 | 62 | 9 |

End of listing Calculation: Automatic Sort: Deviation

**The HREI Mass Spectral Data of Compound 2**

File:LPC-8-4-HREI Ident:1 Acq: 6-APR-2006 04:18:13 +1:39 Cal:LPC-8-HR4
Autospec-UltimaETOF EI+ Voltage BpM:415 BpI:76565 TIC:331086 Flags:NORM
File Text:EI-MS Created from LPC-8-HR4 19 SMO(1,11) PKD(11,6,11,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid)
Heteroatom Max: 20 Ion: Both Even and Odd
Limits:

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 429.096 | 0.0 | | | | | -0.5 | 0 | 0 | 0 |
| 429.310 | 100.0 | | | 20.0 | | 20.0 | 200 | 400 | 20 |
| Mass | %RA | Pks | Std | PPM | mDa | Calc. Mass | DBE | C | H | O |
| 429.188393 | 27.5 | | | 6.8 | 2.9 | 429.191329 | 10.5 | 24 | 29 | 7 |
| | | | | -6.8 | -2.9 | 429.185455 | 19.5 | 31 | 25 | 2 |
| | | | | 20.5 | 8.8 | 429.197202 | 1.5 | 17 | 33 | 12 |
| | | | | -28.7 | -12.3 | 429.176073 | 6.5 | 20 | 29 | 10 |
| | | | | 42.4 | 18.2 | 429.206585 | 14.5 | 28 | 29 | 4 |
| | | | | -42.4 | -18.2 | 429.170199 | 15.5 | 27 | 25 | 5 |

End of listing Calculation: Automatic Sort: Deviation

**The HREI Mass Spectral Data of the Fragment Ion *m/z* 429 of Compound 2**

File:LPC-8-9-HREI Ident:1 Acq: 8-APR-2006 21:09:22 +1:10 Cal:LPC-8-HR374
Autospec-UltimaETOF EI+ Voltage BpM:381 BpI:123917 TIC:275182 Flags:NORM
File Text:EI-MS Created from LPC-8-HR374 13 SMO(1,11) PKD(11,6,11,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid)
Heteroatom Max: 20 Ion: Both Even and Odd

| Limits: | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 374.091 | 0.0 | | | | | -0.5 | 0 | 0 | 0 |
| 374.321 | 100.0 | | | 20.0 | | 20.0 | 200 | 400 | 20 |
| Mass | %RA | Pks | Std | PPM | mDa | Calc. Mass | DBE | C | H | O |
| 374.209396 | 13.8 | | | -0.2 | -0.1 | 374.209324 | 8.0 | 22 | 30 | 5 |
| | | | | -15.9 | -5.9 | 374.203451 | 17.0 | 29 | 26 | |
| | | | | 40.6 | 15.2 | 374.224580 | 12.0 | 26 | 30 | 2 |
| | | | | -41.0 | -15.3 | 374.194068 | 4.0 | 18 | 30 | 8 |

End of listing Calculation: Automatic Sort: Deviation

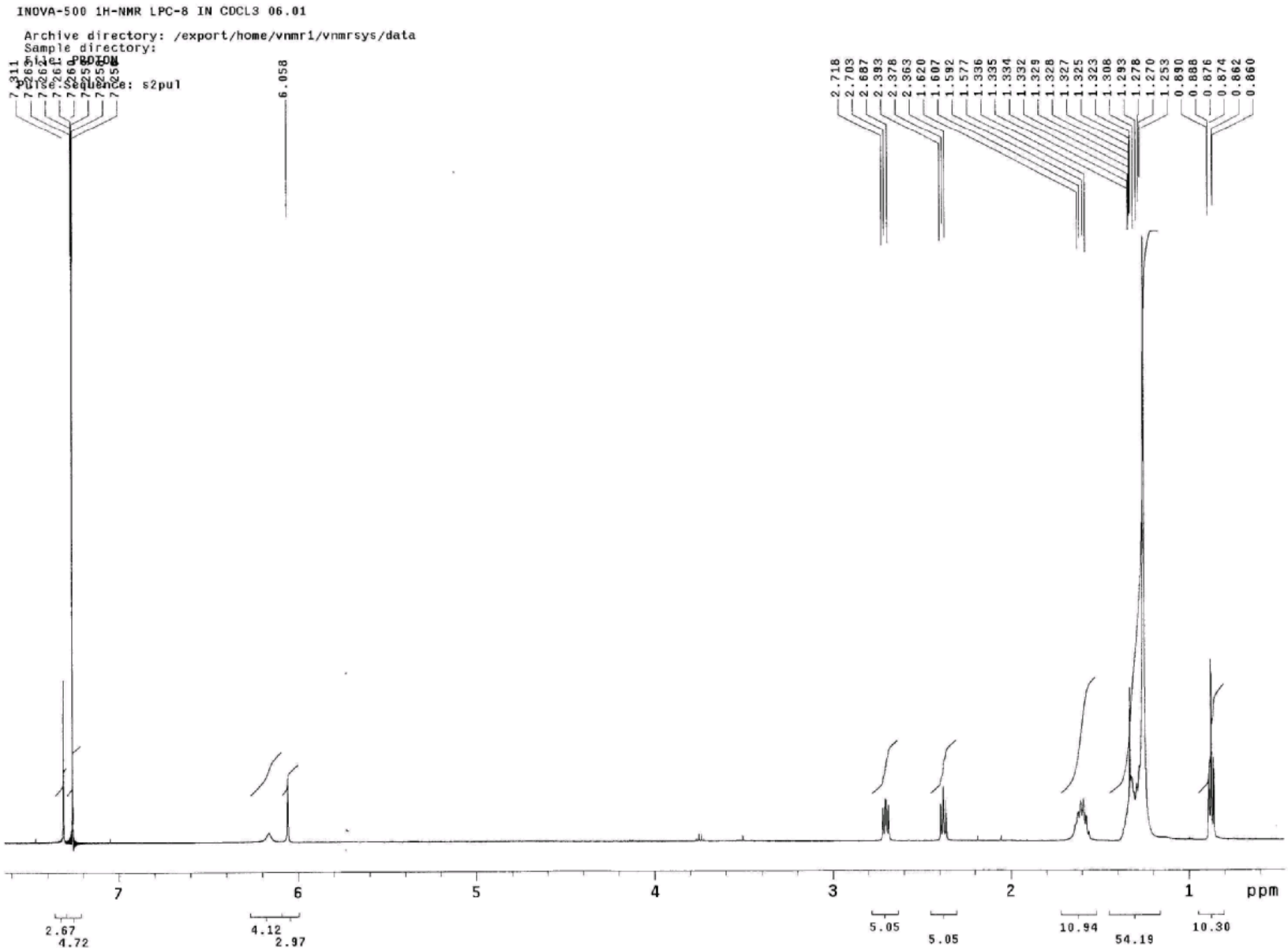
**The HREI Mass Spectral Data of the Fragment Ion *m/z* 374 of Compound 2**

File:LPC-8-6-HREI Ident:1 Acq: 6-APR-2006 04:56:29 +1:28 Cal:LPC-8-HR6
Autospec-UltimaETOF EI+ Voltage BpM:281 BpI:172450 TIC:544577 Flags:NORM
File Text:EI-MS Created from LPC-8-HR6 16 SM0(1,11) PKD(11,6,11,0.50%,0.0,0.00%,F,F) SPEC(Heights,Centroid)
Heteroatom Max: 20 Ion: Both Even and Odd
Limits:

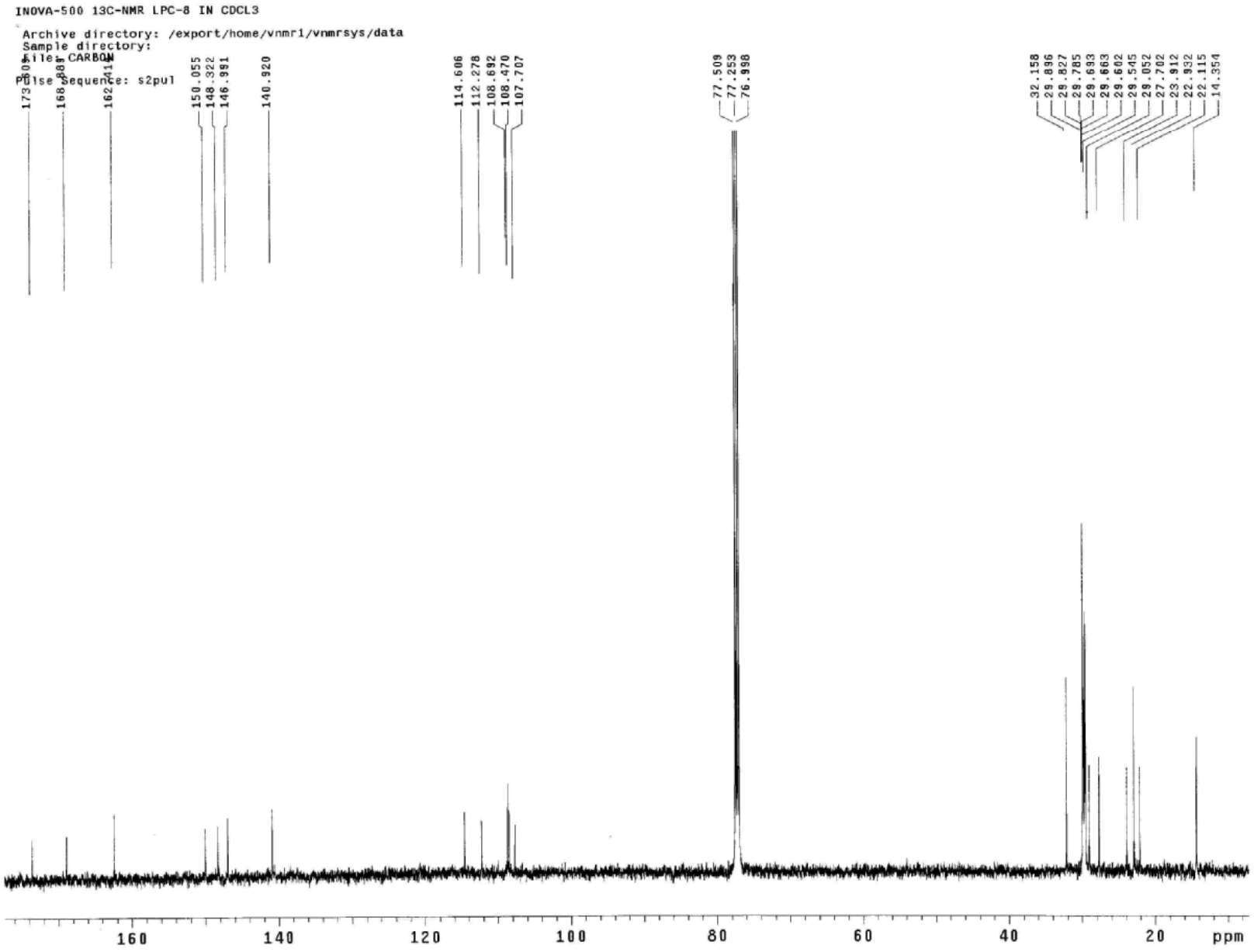
| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 288.990 | 0.0 | | | | | -0.5 | 0 | 0 | 0 |
| 289.103 | 100.0 | | | 20.0 | | 20.0 | 200 | 400 | 20 |
| Mass | %RA Pks | Std | PPM | mDa | Calc. Mass | DBE | C | H | O |
| 289.035408 | 41.4 | | -2.0 | -0.6 | 289.034828 | 10.5 | 14 | 9 | 7 |
| | | | 18.3 | 5.3 | 289.040701 | 1.5 | 7 | 13 | 12 |
| | | | -22.3 | -6.5 | 289.028954 | 19.5 | 21 | 5 | 2 |
| | | | 50.8 | 14.7 | 289.050084 | 14.5 | 18 | 9 | 4 |
| | | | -54.8 | -15.8 | 289.019572 | 6.5 | 10 | 9 | 10 |

End of listing Calculation: Automatic Sort: Deviation

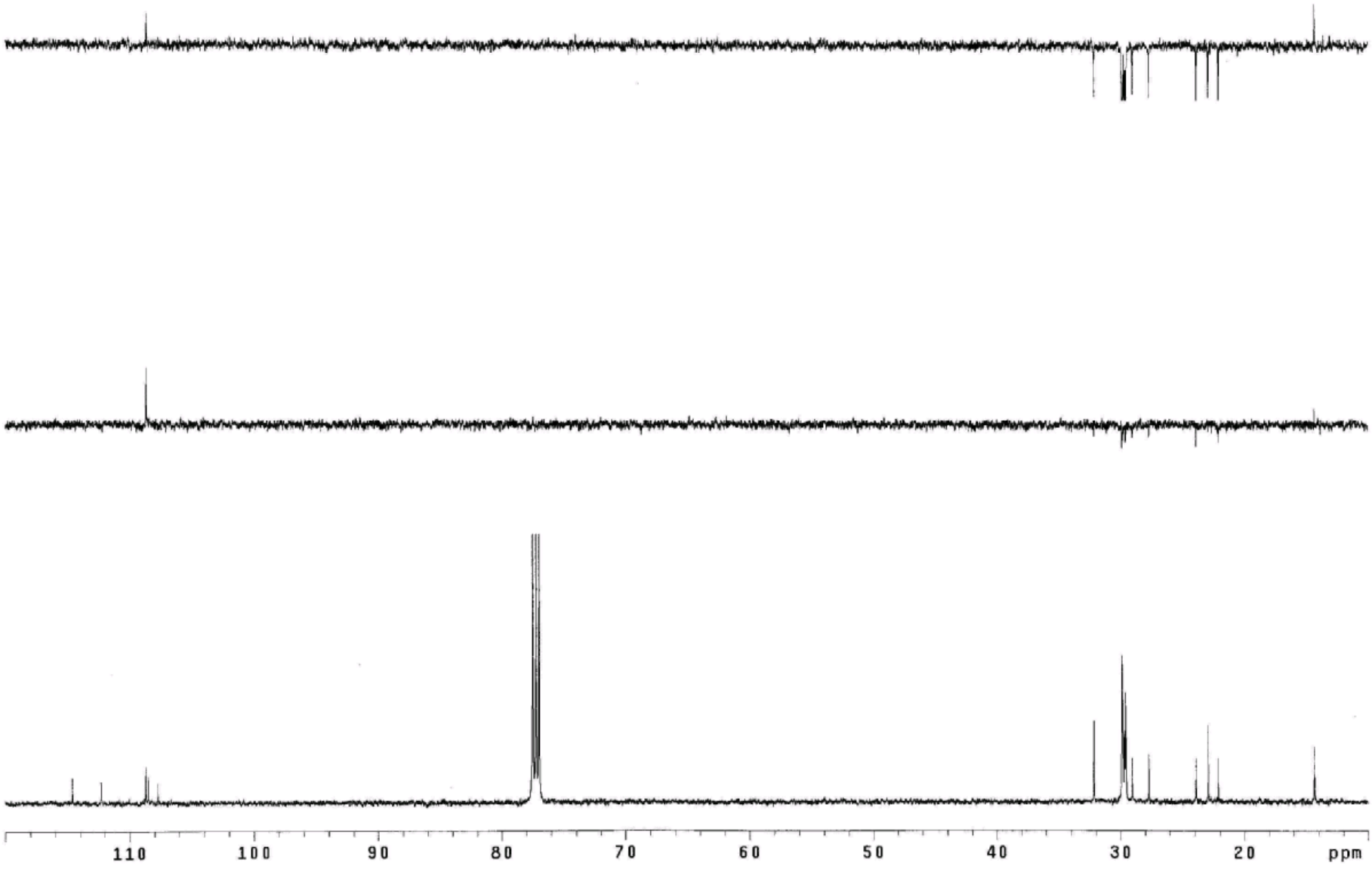
**The HREI Mass Spectral Data of the Fragment Ion *m/z* 289 of Compound 2**




**The $^{1}$H NMR Spectrum of Compound 2**




**The $^{13}$C NMR Spectrum of Compound 2**



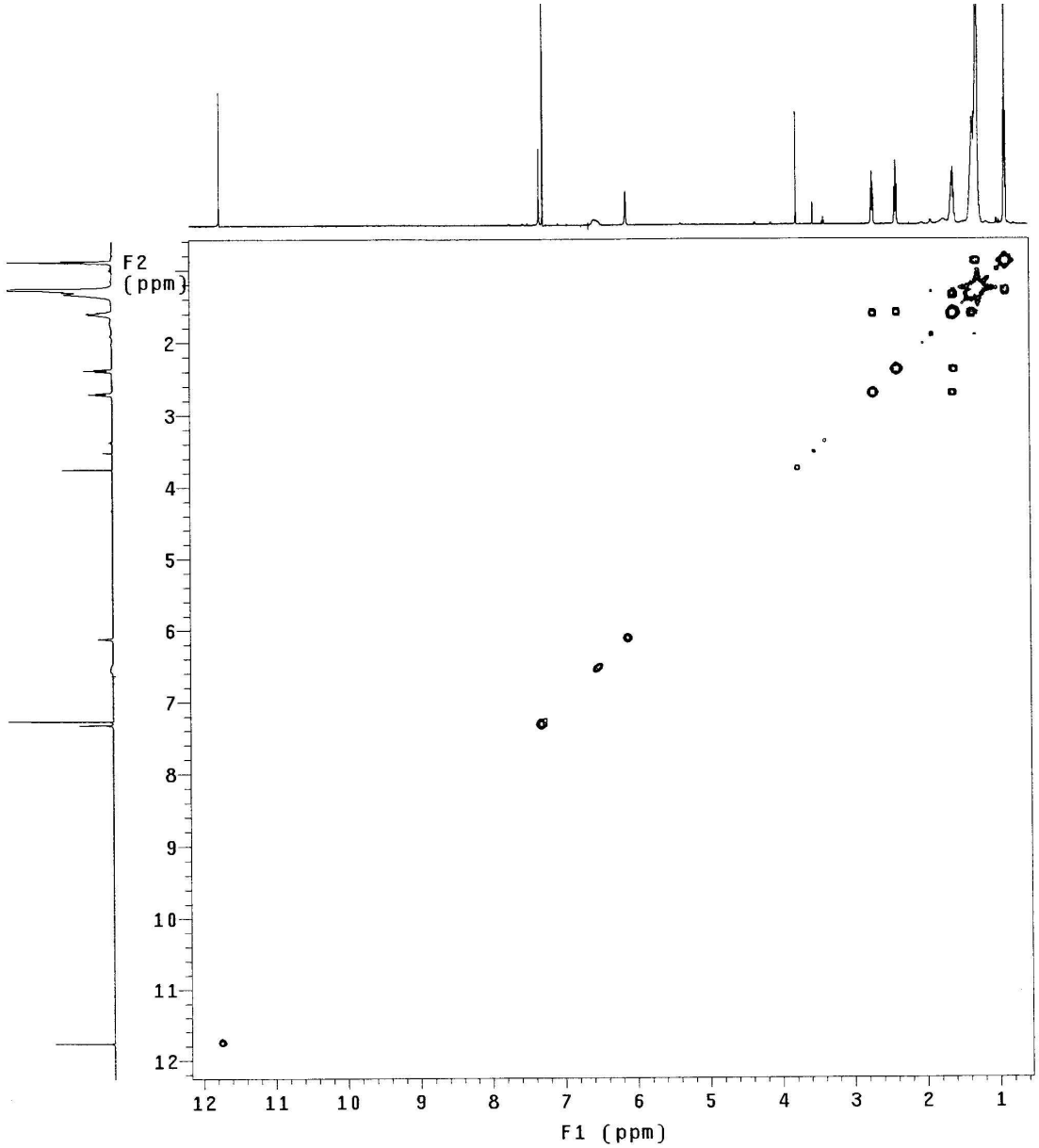

**The DEPT Spectrum of Compound 2**

INOVA-501 gCOSY LPC-8 IN CDCL3 04.11.25

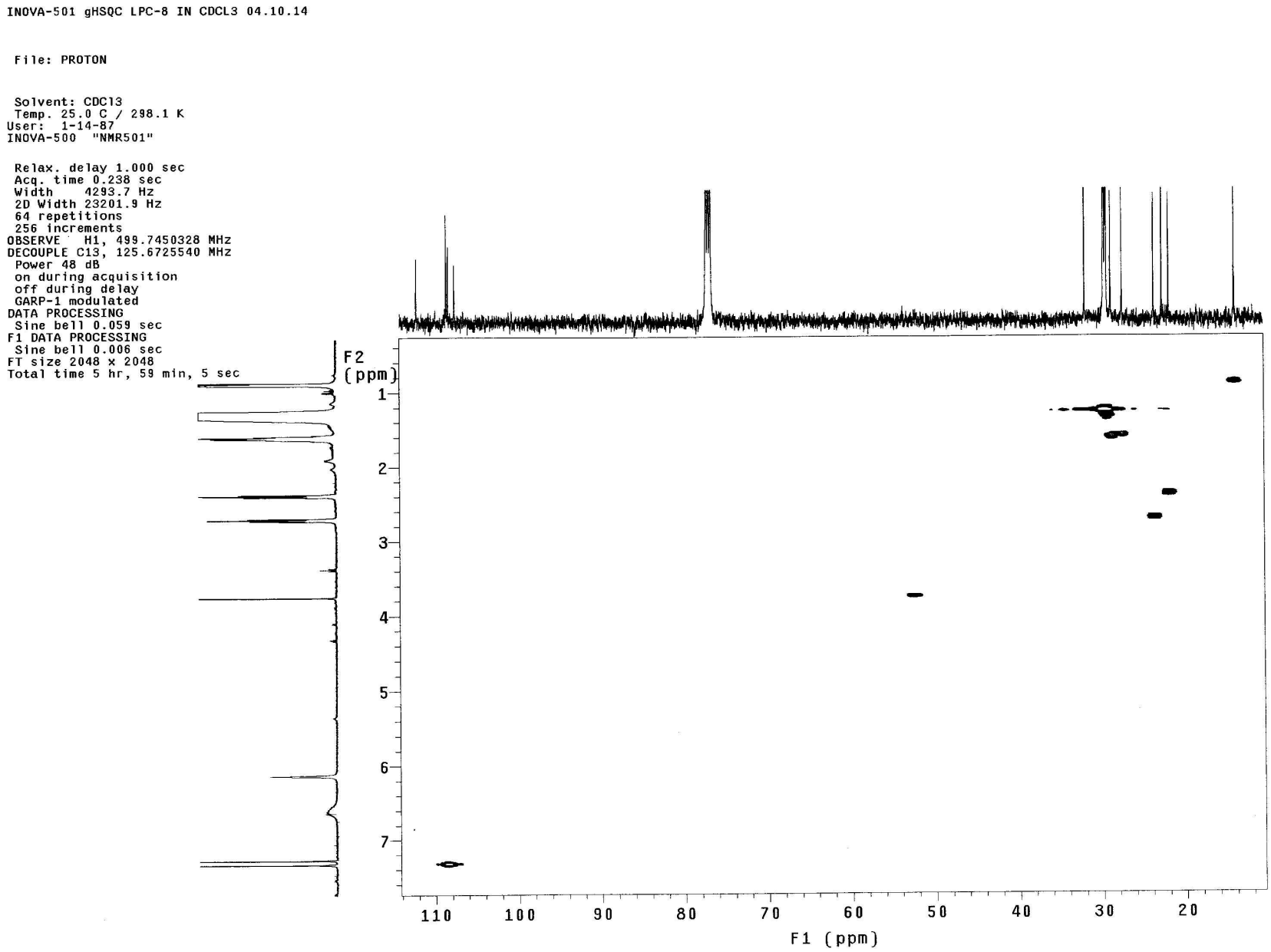
File: PROTON

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 "NMR501"

Relax. delay 1.000 sec
Acq. time 0.138 sec
Width 7435.6 Hz
2D Width 7435.6 Hz
2 repetitions
300 increments
OBSERVE H1, 499.7450326 MHz
DATA PROCESSING
Sine bell 0.068 sec
F1 DATA PROCESSING
Sine bell 0.020 sec
FT size 2048 x 2048
Total time 12 min, 0 sec




**The $^{1}$H-$^{1}$H gCOSY Spectrum of Compound 2**

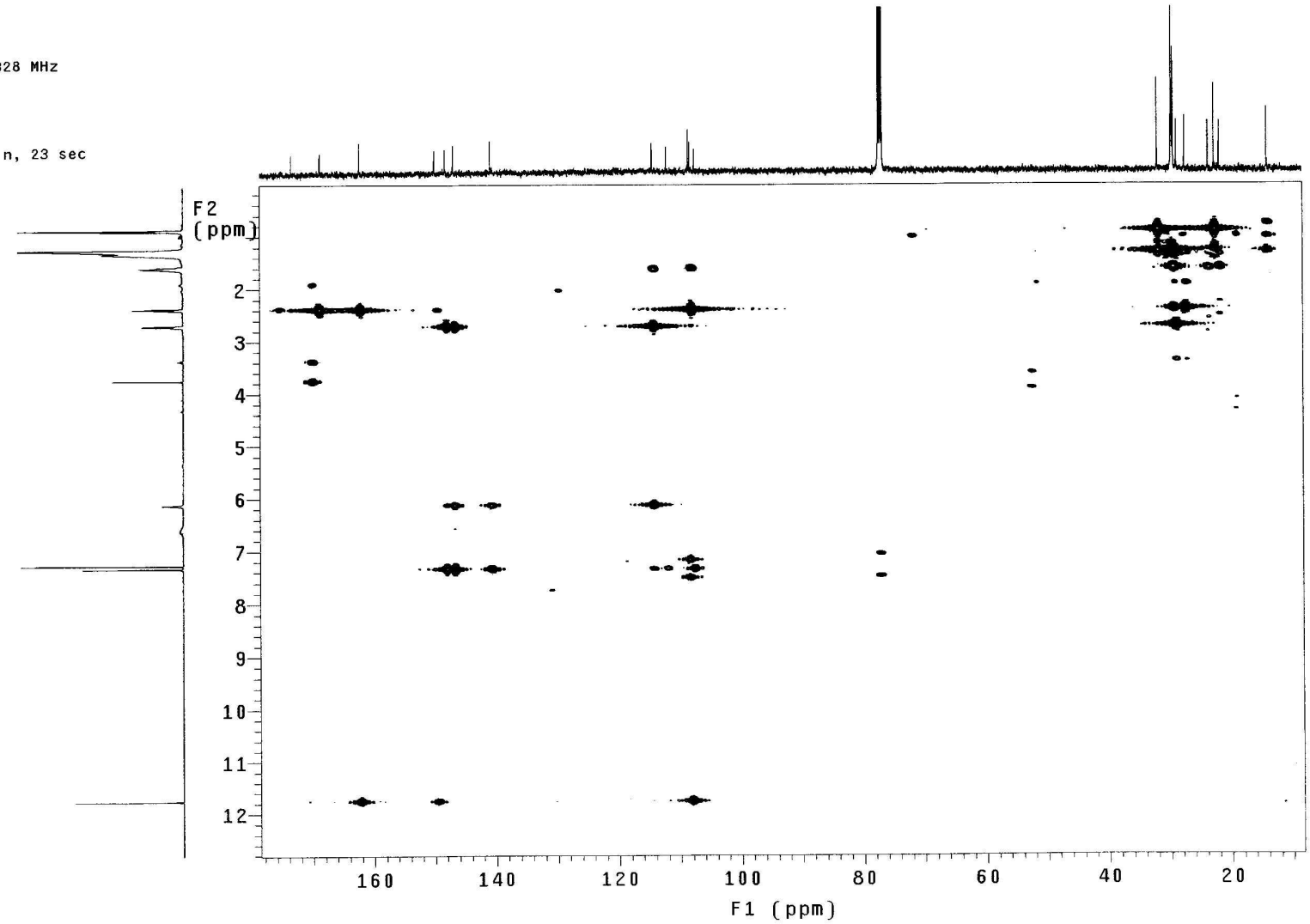



**The gHSQC Spectrum of Compound 2**

File: PROTON

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "NMR501"

Relax. delay 1.000 sec
Acq. time 0.157 sec
Width 6524.8 Hz
2D Width 23201.9 Hz
96 repetitions
320 increments
OBSERVE H1, 499.7450328 MHz
DATA PROCESSING
Sine bell 0.036 sec
F1 DATA PROCESSING
Sine bell 0.007 sec
FT size 2048 x 4096
Total time 10 hr, 38 min, 23 sec




**The gHMBC Spectrum of Compound 2**