

Supporting Information Available

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

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Batch Information - scan006

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

Results Table - scan006

Data Mode Absorbance

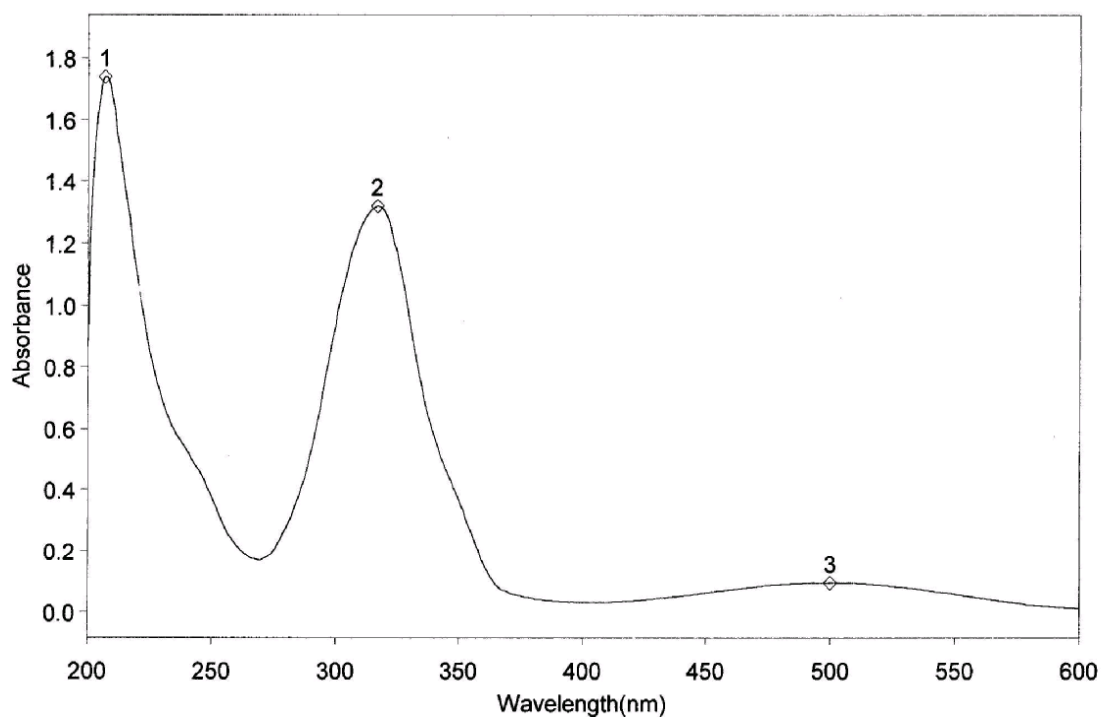
	A	B	C	D	E
1	Lpc-12		1	2	3
2	Cycle01	nm	207.0	317.0	500.0
3	Manual	A	1.739	1.318	.094

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

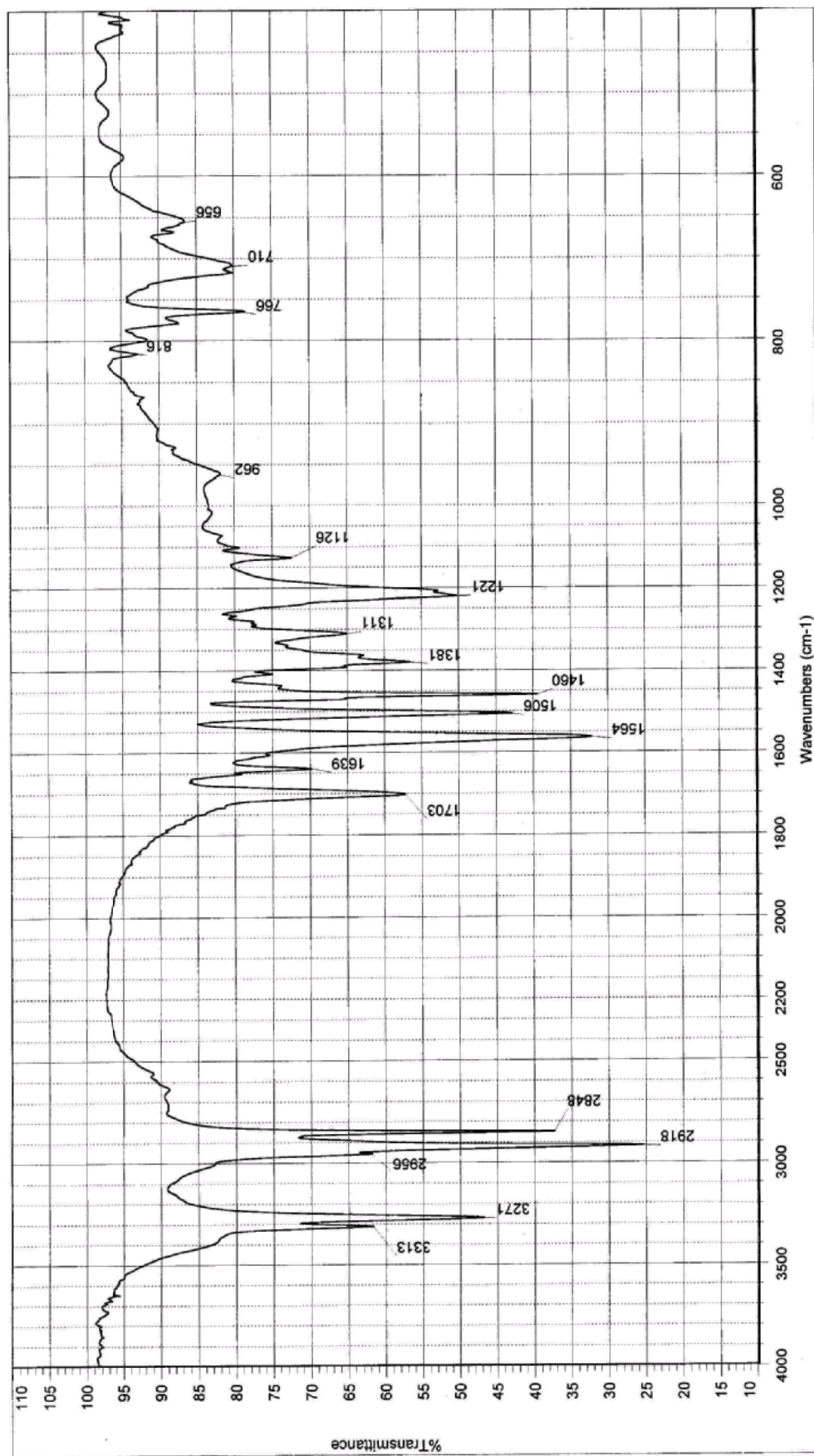
Lpc-12

Description 0.615mg/10mlMeOH

Lpc-12,Cycle01



The UV Spectrum of Compound 1



Date: Thu Dec 16 13:07:49 2004

Sample Name: LPC - 12 (KBr)

Scans: 64

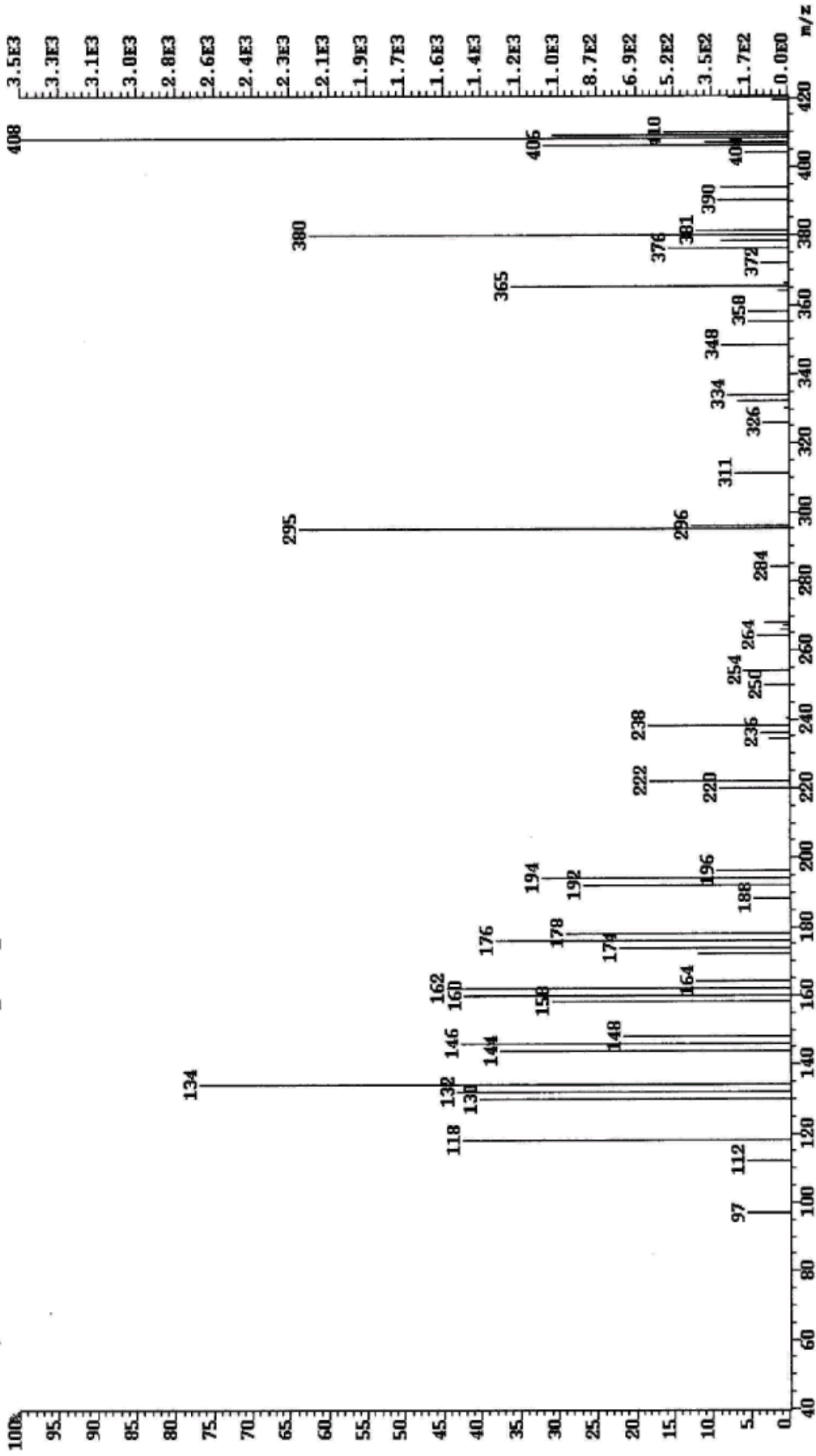
检测单位: 国家药物及代谢产物分析研究中心

Resolution: 4.000

检测仪器: 美国尼高力公司傅立叶变换红外光谱仪: IMPACT - 400

The IR Spectrum of Compound 1

File: LPC-12-FADMS Ident:1 Acq:19-MAR-2005 20:15:37 +0:48 Cal:FAB050302
Autospec-UltimaF10F FAB+ Magnet BpM:408 BpI:3473 TIC:41733 Flags:HALL
File Text:G/NBA FAB-MS Created from LPC-12 5_11-15_22 Mer Def 0.25



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-UltimateIOTF FAB+ Voltage BpM:415 BpI:93209 TIC:416071 Flags:NORM
 File Text:HRFAB-NS 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

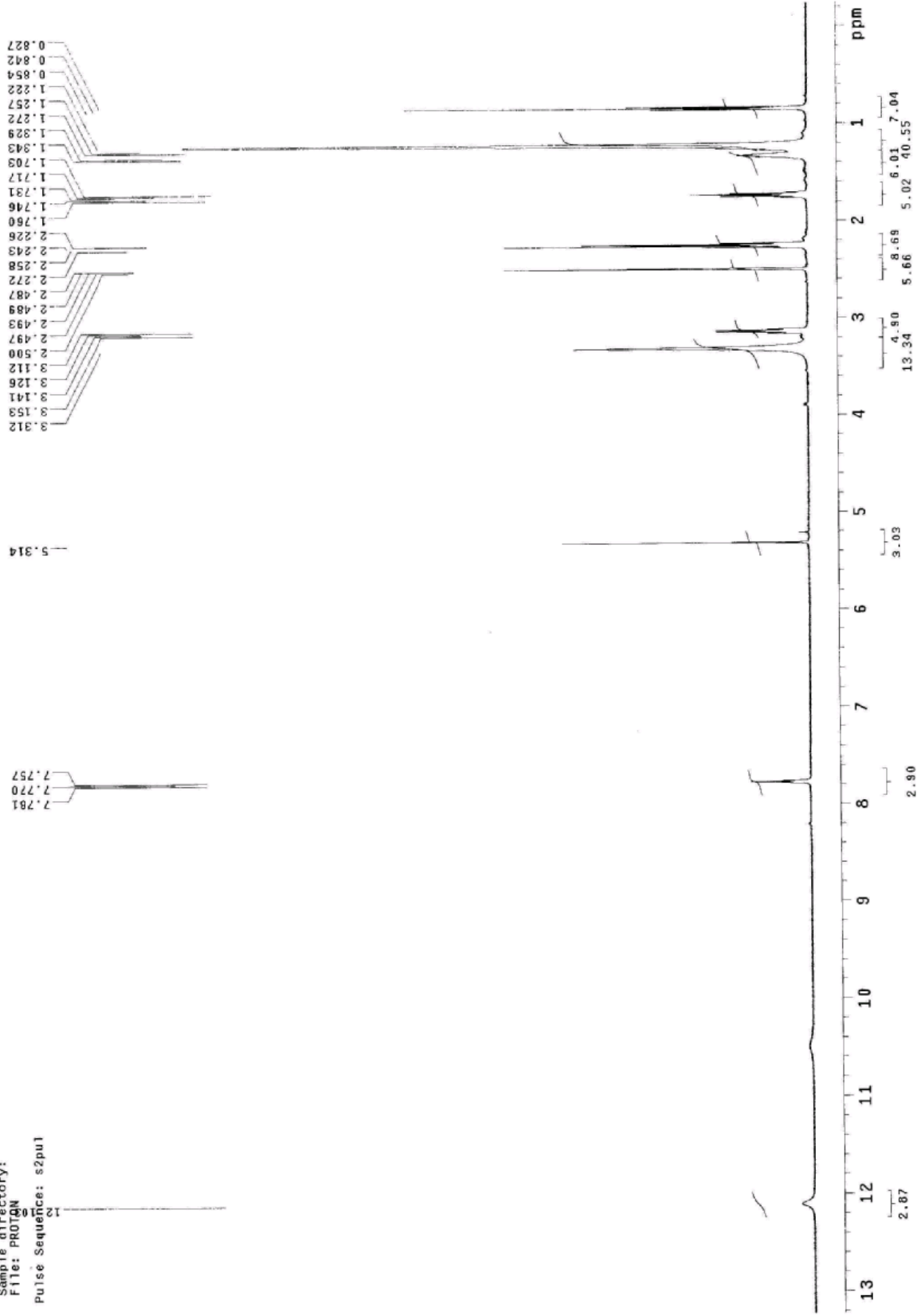
Limits:
 408.264 0.0
 408.289 100.0

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

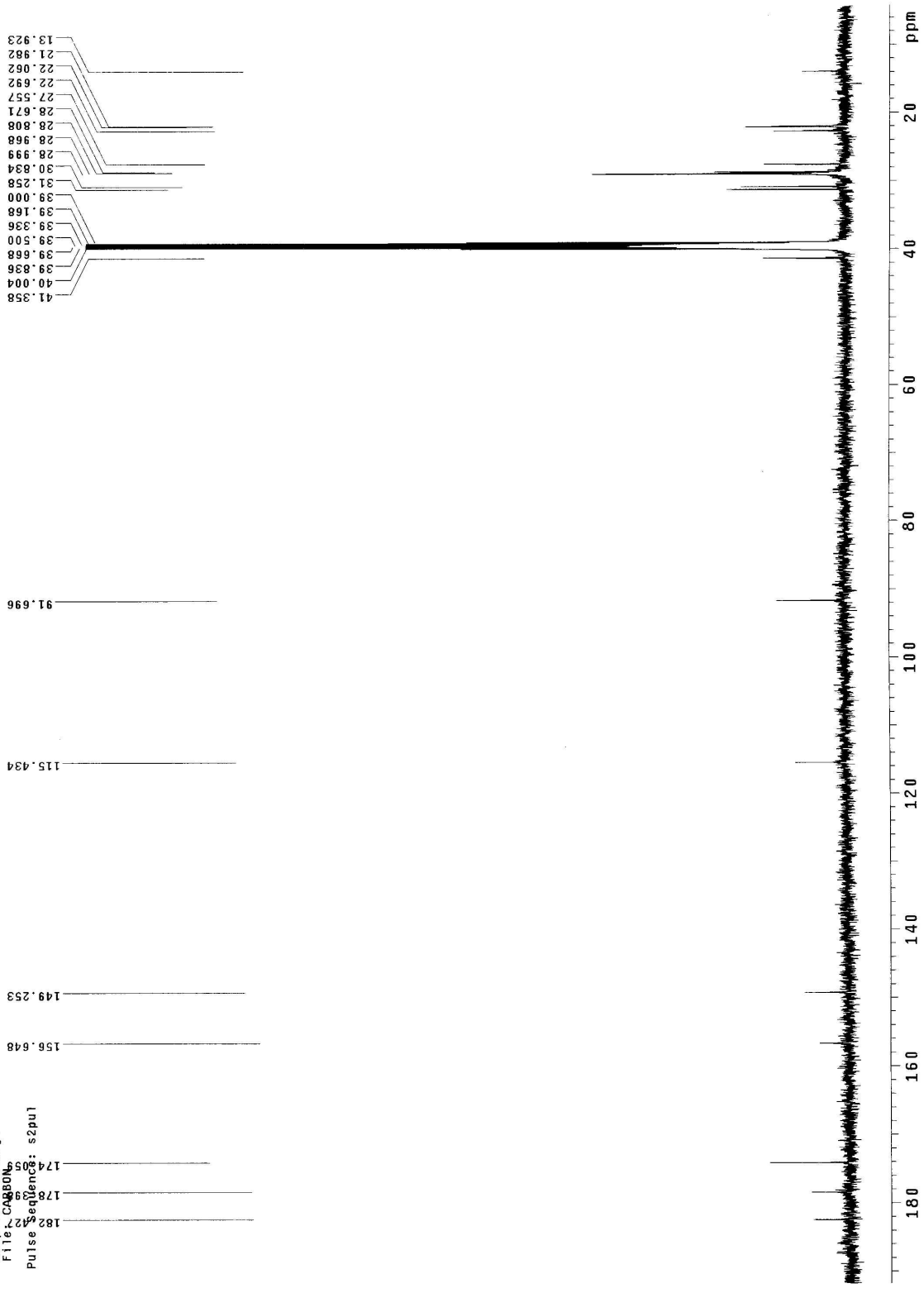
The HRFAB Mass Spectral Data of Compound 1

INOVA-500 1H-NMR LPC-12 IN DMSO 07.12
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory:
 File: PROT01
 Pulse Sequence: s2pu1



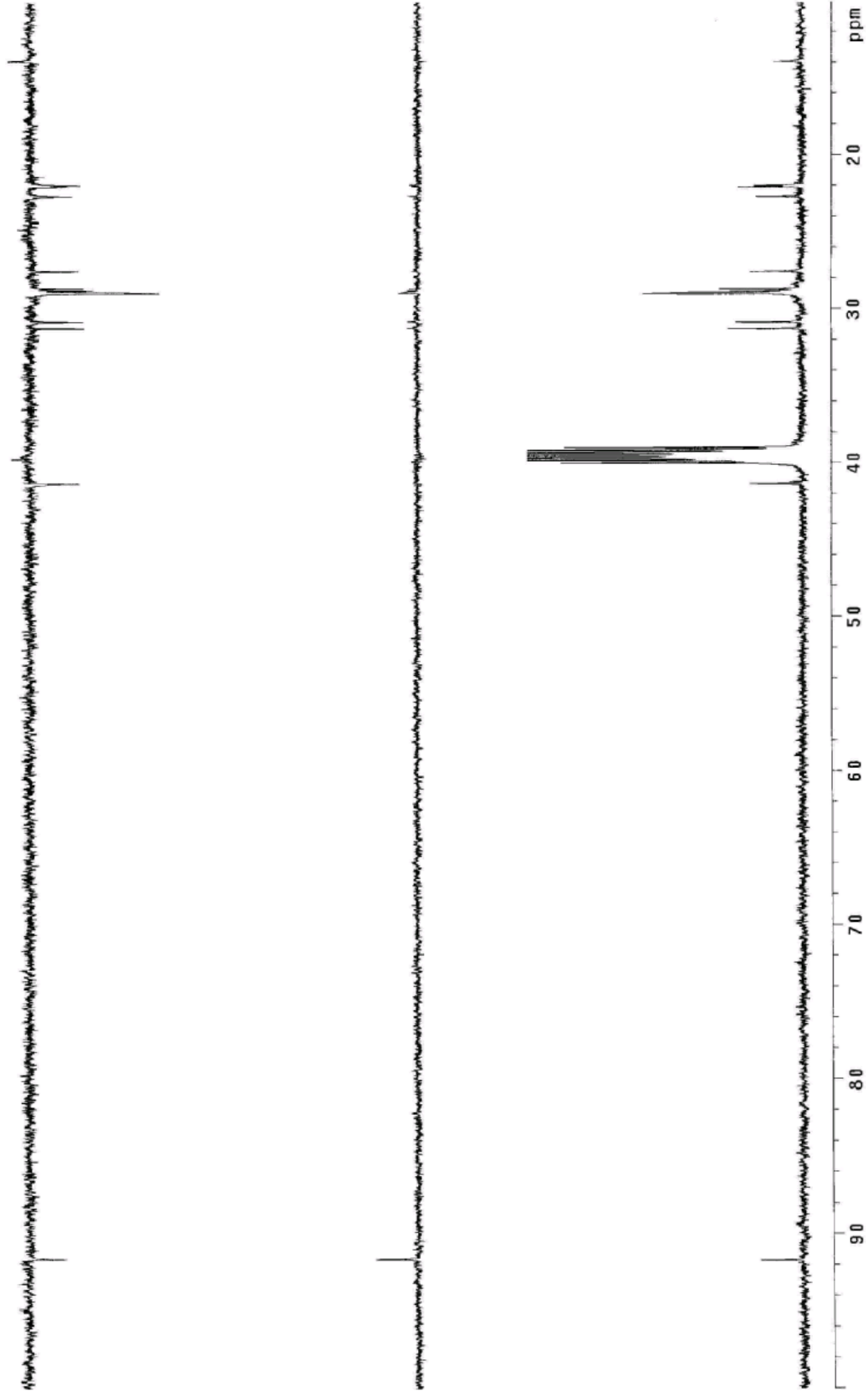
The 1H NMR Spectrum of Compound 1

INDVA-500 13C-NMR PLC-12 IN DMSO 07.12
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: CARBON
Pulse sequence: s2pu1



The ¹³C NMR Spectrum of Compound 1

INOVA-500 DEPT-NMR LPC-12 IN DMSO
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: DEPT



The DEPT Spectrum of Compound 1

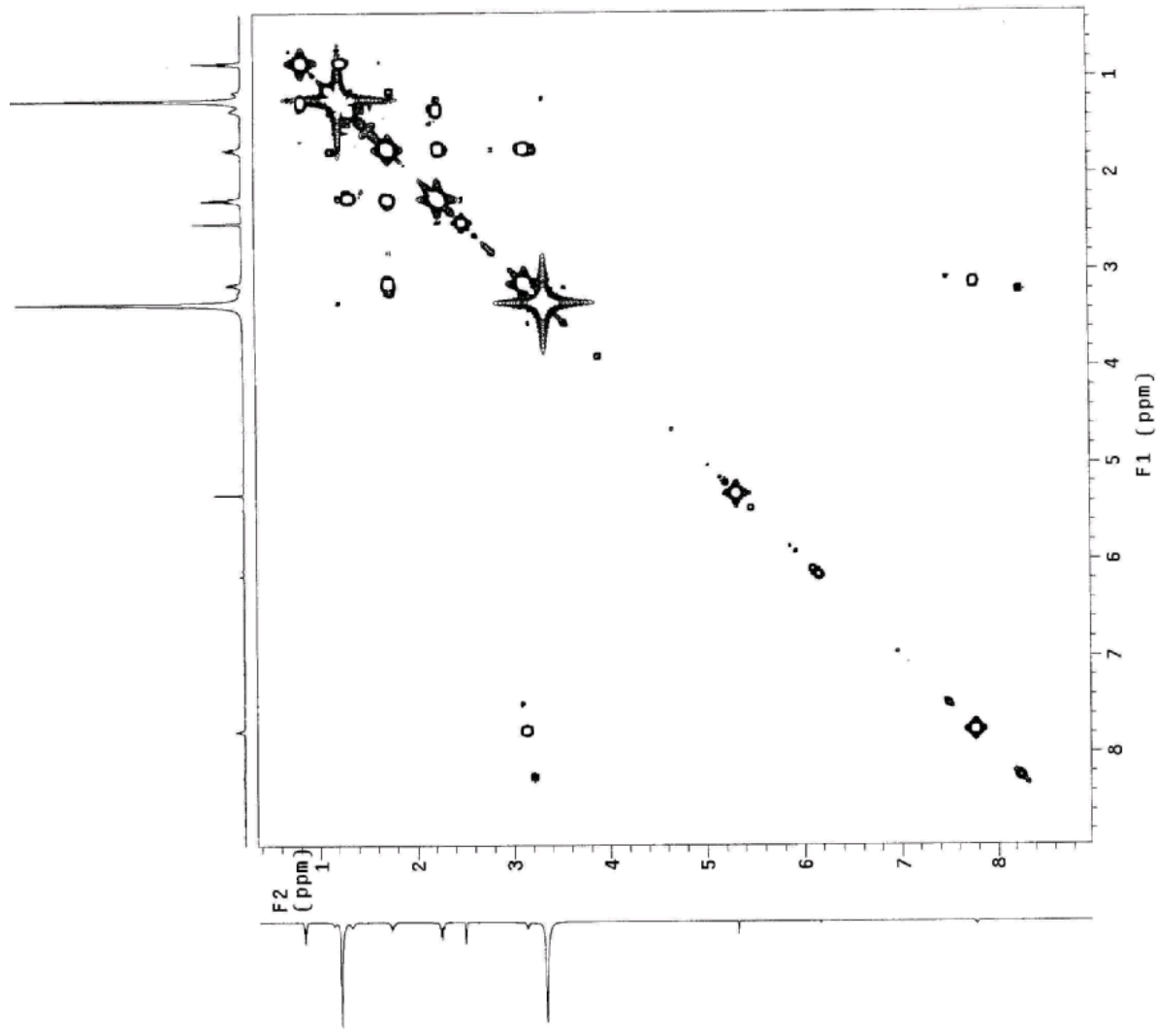
INOVA-501 gCOSY LPC-12 IN DMSO 04.11.26

File: PROTON

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

Relax. delay: 1.000 sec
Acq. time: 0.137 sec
Pulse width: 7.472.4 Hz
20.000 Hz
2 repetitions

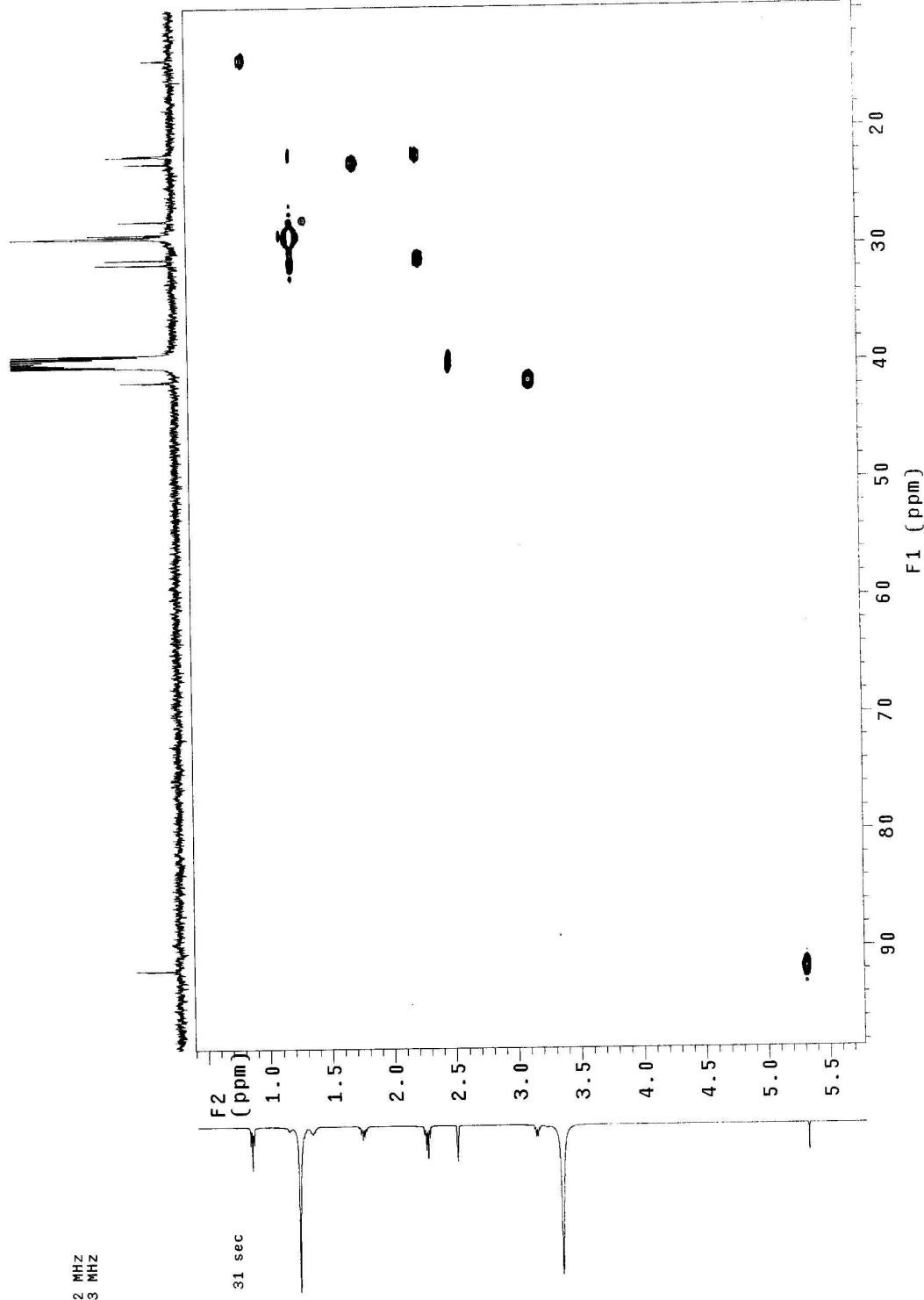
300 increments
OBSERVE: H1, 499.7474032 MHZ
DATA PROCESSING
Sine bell: 0.068 sec
F1 DATA PROCESSING
Sine bell: 0.020 sec
FT size: 2048 x 2048
Total time: 12 min, 0 sec



The ¹H-¹H gCOSY Spectrum of Compound 1

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

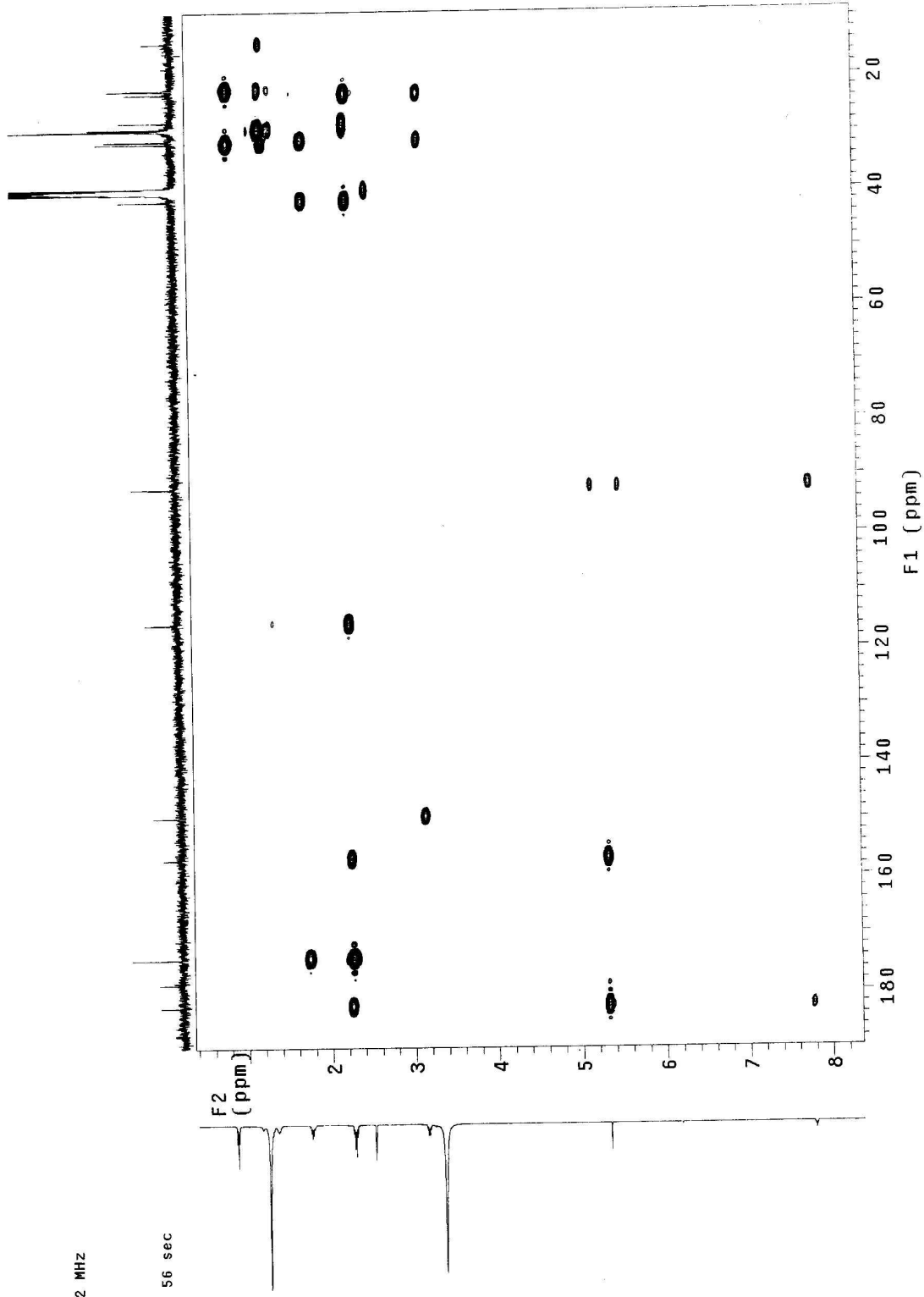
Relax. delay 1.000 sec
Acq. time 0.232 sec
Width 4406.3 Hz
2D Width 20865.9 Hz
24 repetitions
256 increments
OBSERVE H1, 499.7474032 MHz
DECOUPLE C13, 125.6725643 MHz
Power 48 dB
off during acquisition
off during delay
GARP -1 modulated
DATA PROCESSING
Sine bell 0.057 sec
F1 DATA PROCESSING
Sine bell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



The gHSQC Spectrum of Compound 1

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

Relax. delay 1.000 sec
Acq. time 0.159 sec
Width 6451.6 Hz
2D Width 23696.7 Hz
48 repetitions
320 increments
OBSERVE H1, 499.7474032 MHz
DATA PROCESSING
Sine bell 0.035 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 4096
Total time 5 hr, 19 min, 56 sec



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

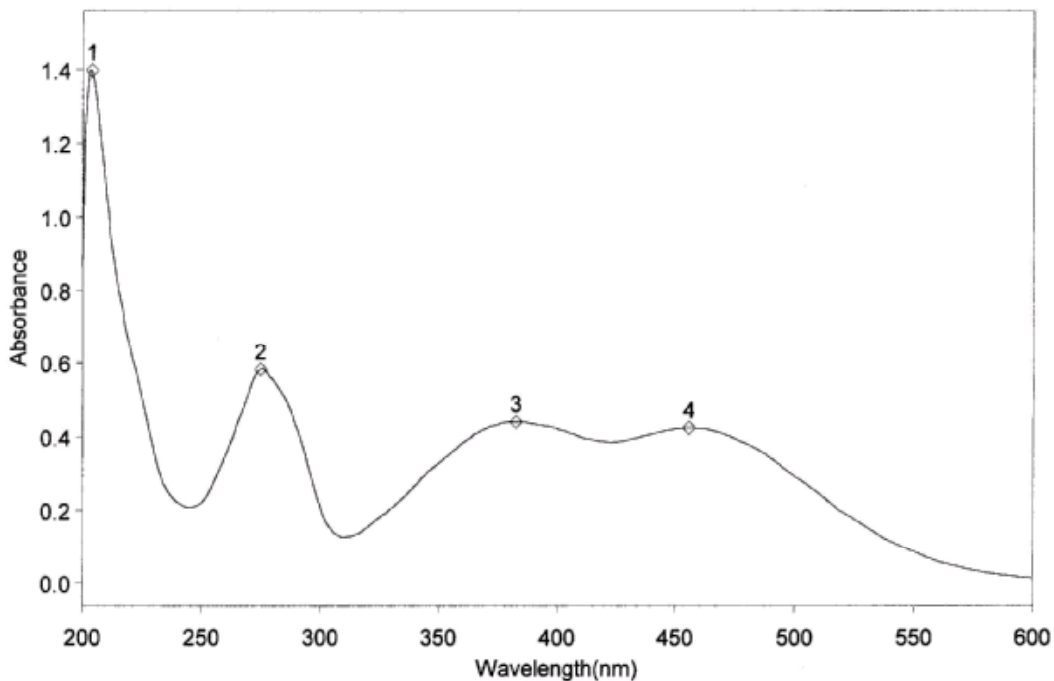
	A	B	C	D	E	F
1	Lpc-8		1	2	3	4
2	Cycle01	nm	204.0	275.0	383.0	456.0
3	Manual	A	1.398	.584	.440	.423

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

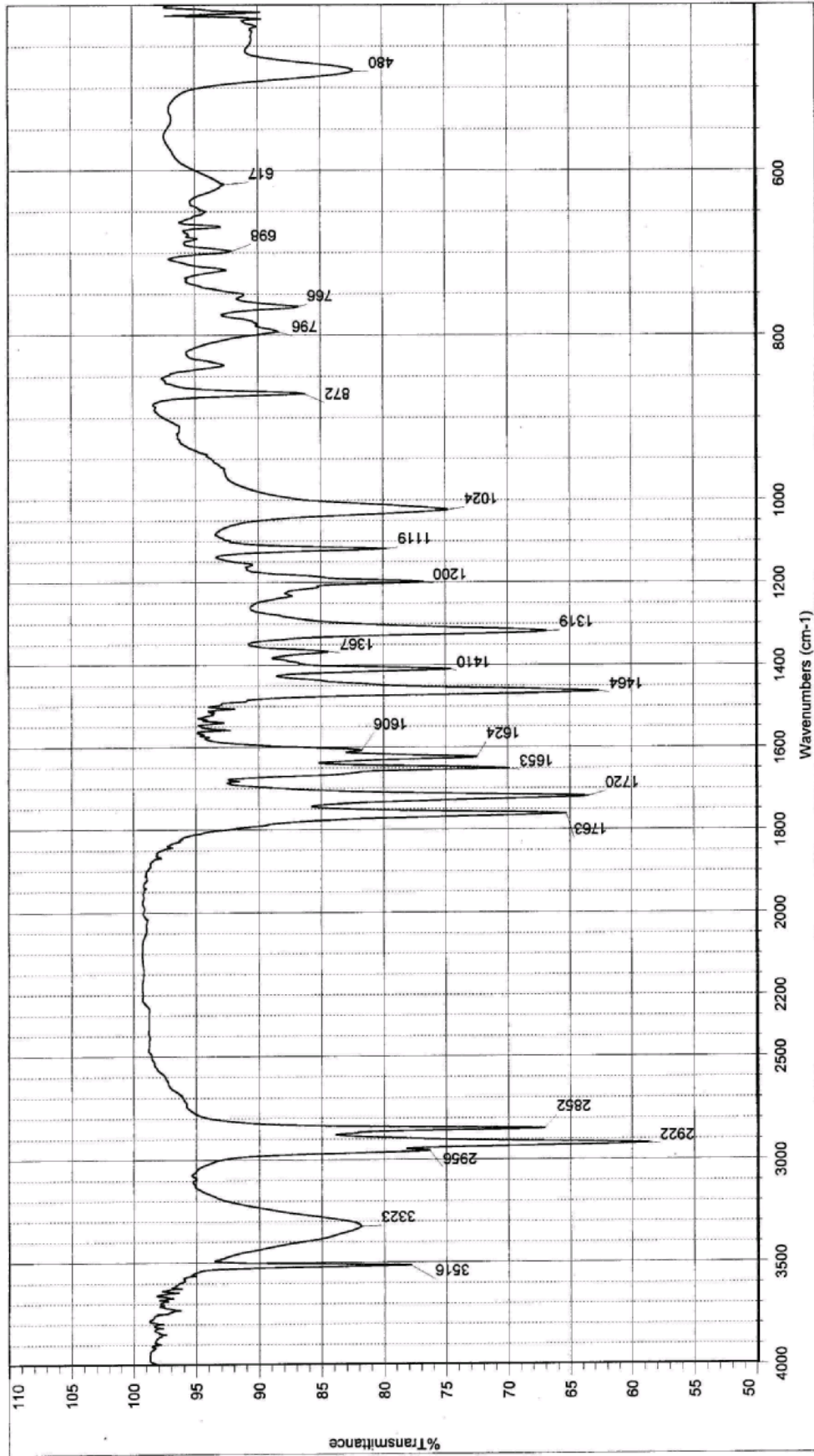
Lpc-8

Description 0.284mg/10mlMeOH

Lpc-8,Cycle01



The UV Spectrum of Compound 2



Date: Thu Dec 16 13:18:32 2004

Scans: 64

Resolution: 4.000

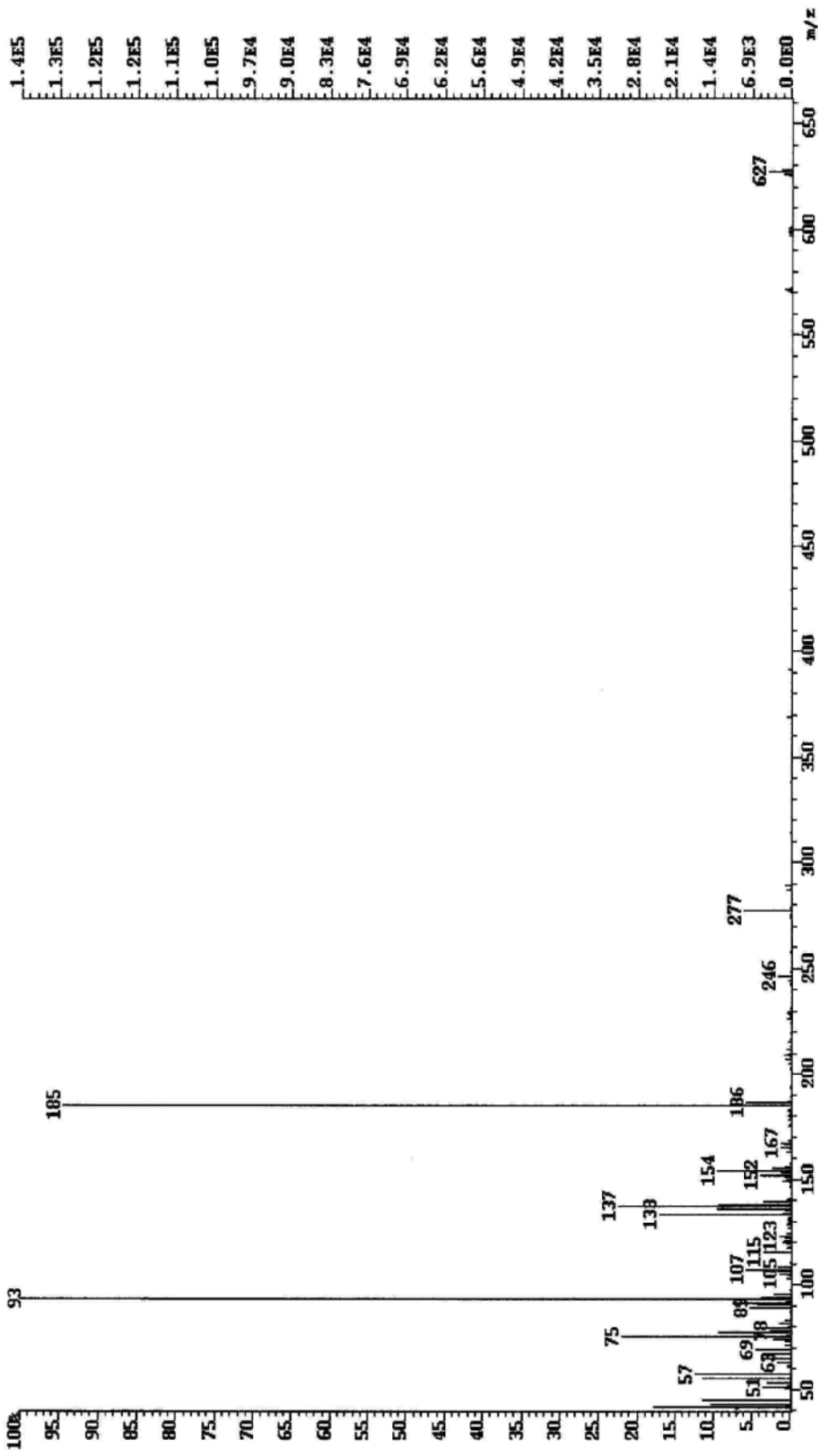
Sample Name: LPC - 8 (KBr)

检测单位: 国家药物及代谢产物分析研究中心

检测仪器: 美国尼高力公司傅立叶变换红外光谱仪: IMPACT - 400

The IR Spectrum of Compound 2

File: LPC-8 Ident: 2.7 Win 1000PM Acq: 19-MAR-2005 20:24:50 +0:28 Cal: FAB050302
Autospec-UltimaTOF FAB+ Magnet BpM: 93 BpI: 1.38779 TIC: 715578 Flags: HALL
File Text: 6/NBA FAB-MS



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-UltimaTOF FAB+ Voltage BpM:599 BpI:120232 TIC:470540 Flags:NORM
 File Text:HRFAB-MS Created from LPC-8 24_30 PK0(7.3.7,0.0.0.50%,0.0.0.00%,F.F) SPEC(Heights, Centroid)
 Heteroatom Max: 20 Ion: Both Even and Odd

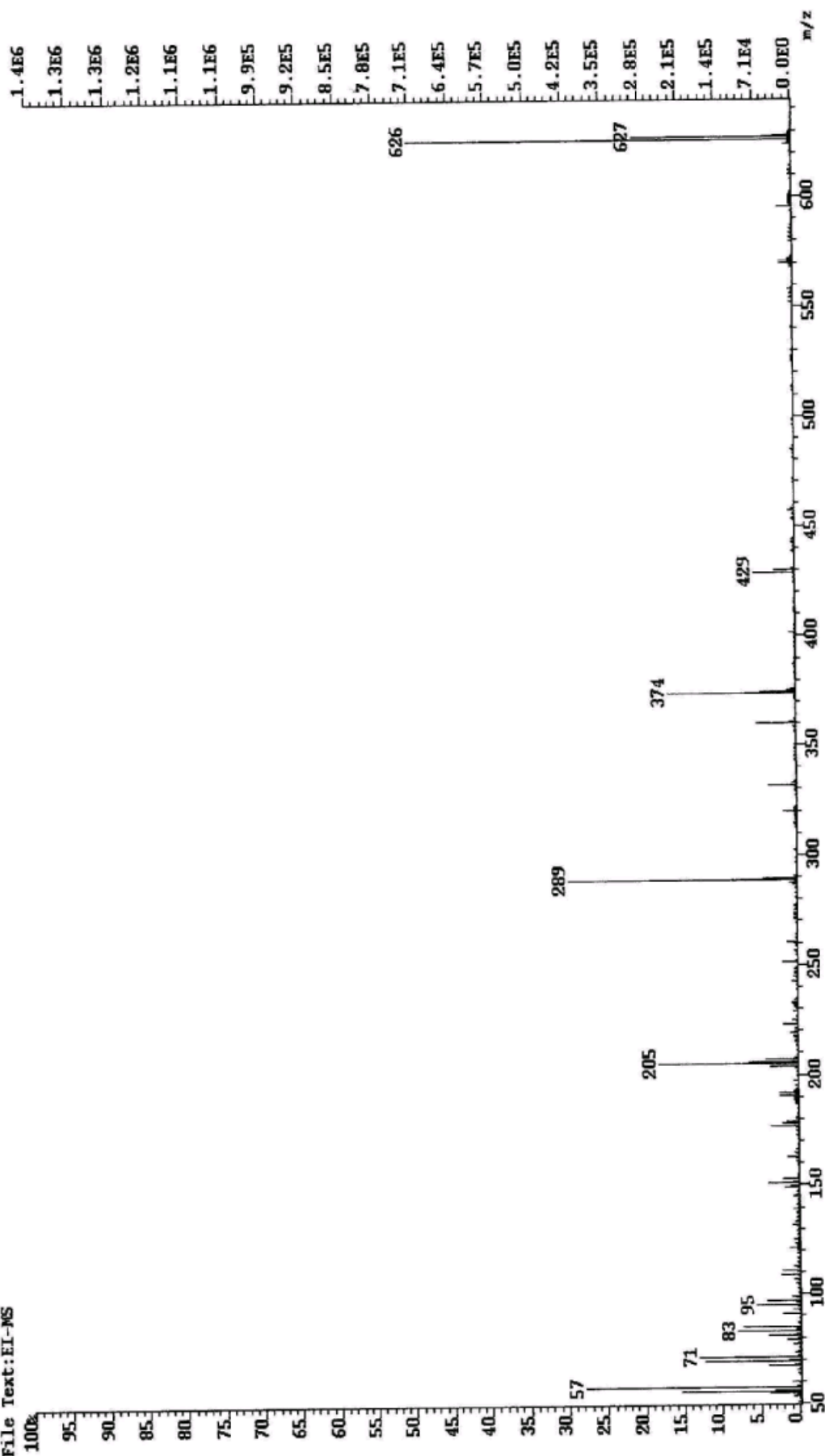
Limits:
 627.382 0.0 -0.5 0 0 5
 627.495 100.0 10.0 30.0 200 400 10
 Mass AREA Pks Std PPN rDa Calc. Mass DBE C H O
 627.426514 25.7 -0.7 -0.4 627.426080 9.5 38 59 7

End of listing

Calculation: Automatic Sort: Deviation

The HRFAB Mass Spectral Data of Compound 2

File: LPC-8 Ident:10 Acq:26-MAR-2006 04:18:47 +0:49 Cal:EI060308
Autospec-UltimaETOF EI+ Magnet BpI:1415462 TIC:9311140 Flags:HALL
File Text:EI-MS



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-HRI
 Autospec-UltimateTOF EI+ Voltage BpM: 598 BpI: 208950 TIC: 813505 Flags: NORM
 File Text: EI-MS Created from LPC-8-HRI 14 S90(L,11) PK0(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 20.0 -0.5 0 0 0
 626.516 100.0 30.0 200 400 20

Mass	3BA Pks	Std	PDM	TDB	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-UltimaETOI 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
 429.310 100.0

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-UltimateTOF EL+ Voltage BpK:381 BpI:123917 TIC:275182 Flags:NUMM
 File Text:EI-MS Created from LPC-8-HR374 13 SW0(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
 374.321 100.0

Mass	RA Pks	Std	BPW	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-UltimateTOF EI+ Voltage BpM:281 BpI:172450 TIC:544577 Flags:NRBM
 File Text:EI-MS Created from LPC-8-HR6 16 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

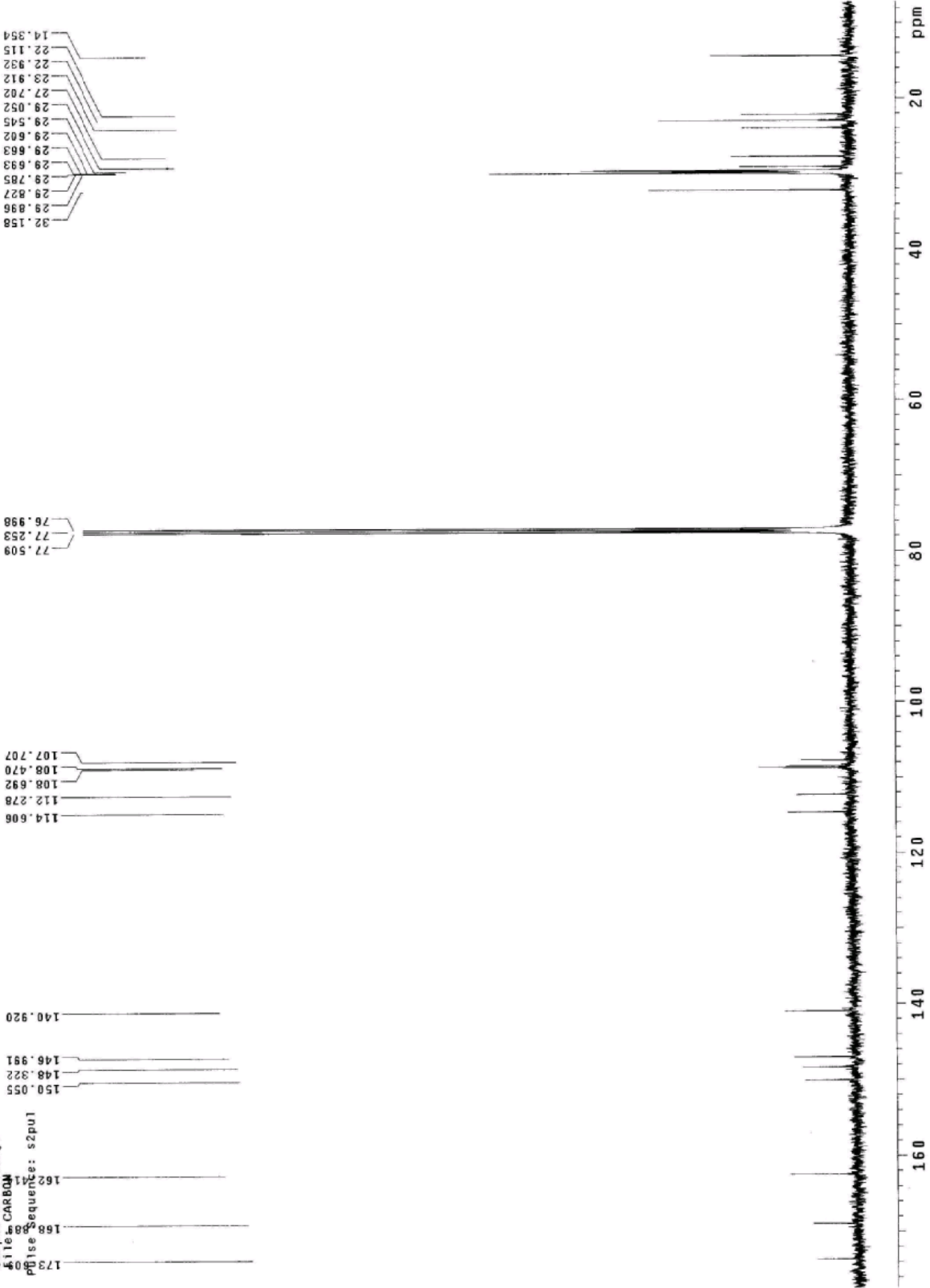
Limits:
 288.990 0.0 -0.5 0 0 0
 289.103 100.0 20.0 20.0 200 400 20

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

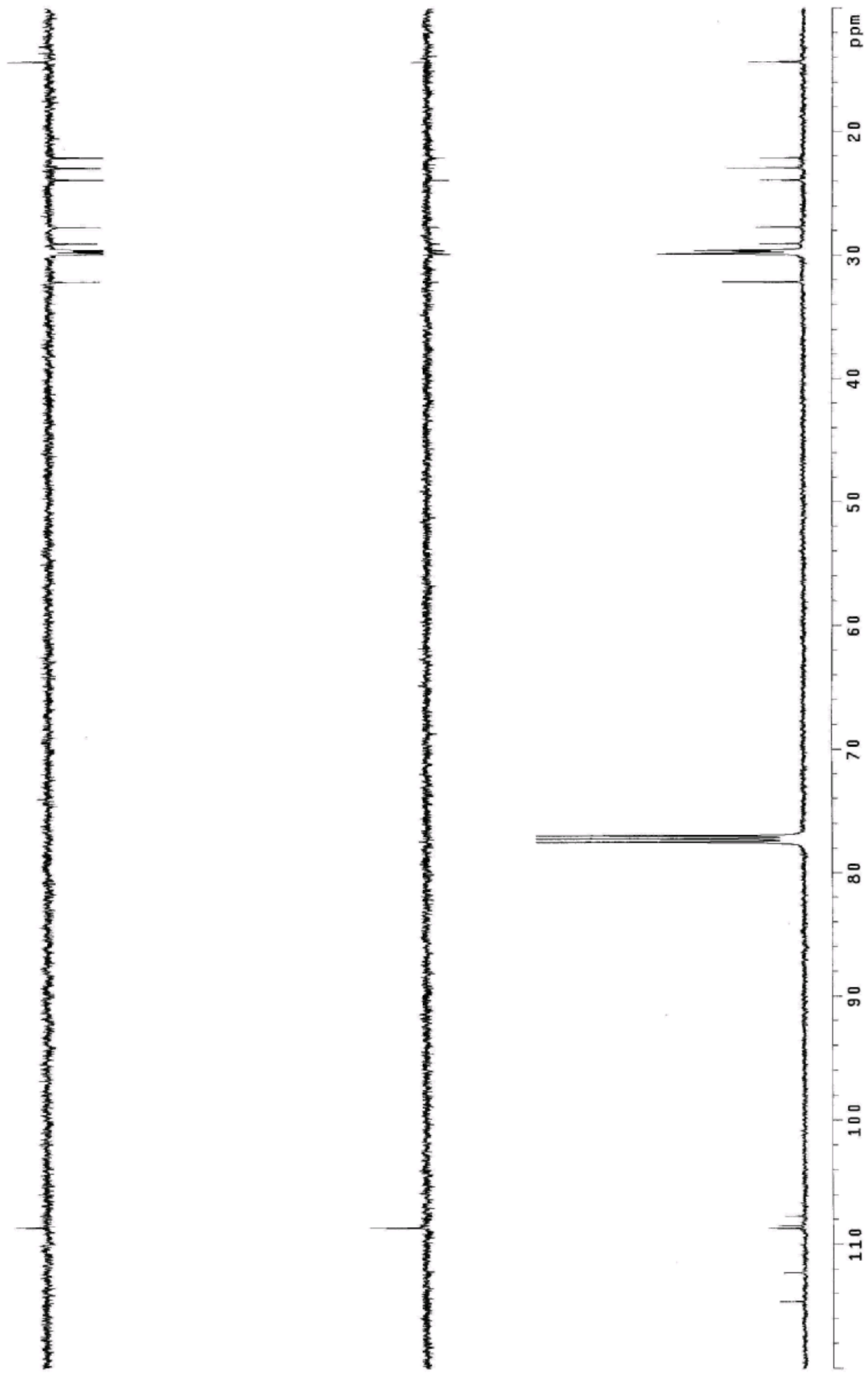
End of Listing Calculation: Automatic Sort: Deviation

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

INOVA-500 13C-NMR LPC-8 IN CDCl3
 Archive directory: /export/home/vnmr1/vnmrSYS/data
 Sample directory:
 File CARBON
 Pulse sequence: s2pu1



The ¹³C NMR Spectrum of Compound 2



The DEPT Spectrum of Compound 2

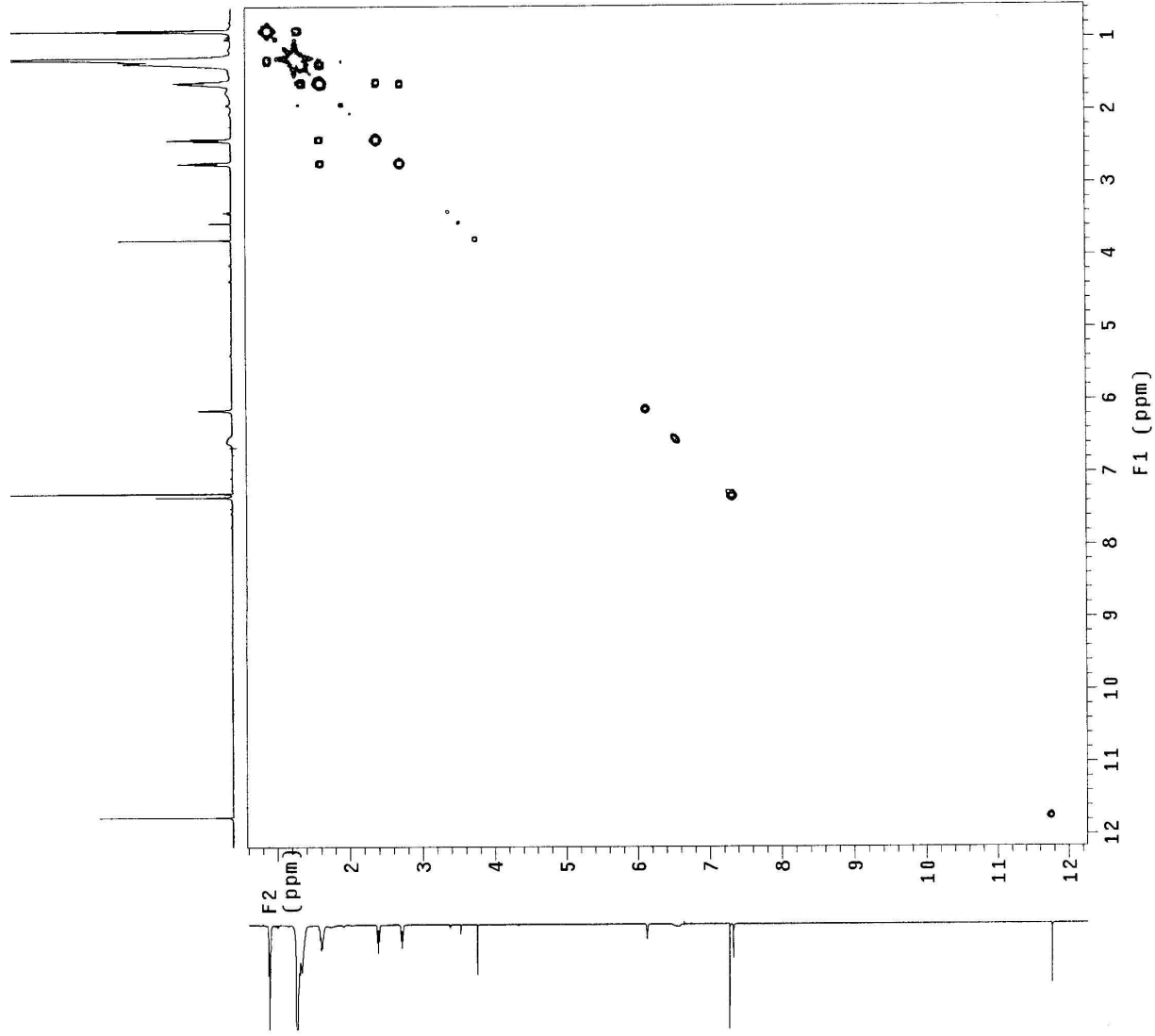
INOVA-501 gCOSY LPC-8 IN CDCL3 04.11.25

File: PROTON

Solvent: CDCl3
Temp. 25.0 C / 298.1 K
INOVA-500 ¹H 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
F1 size 2048 x 2048
Total time 12 min, 0 sec

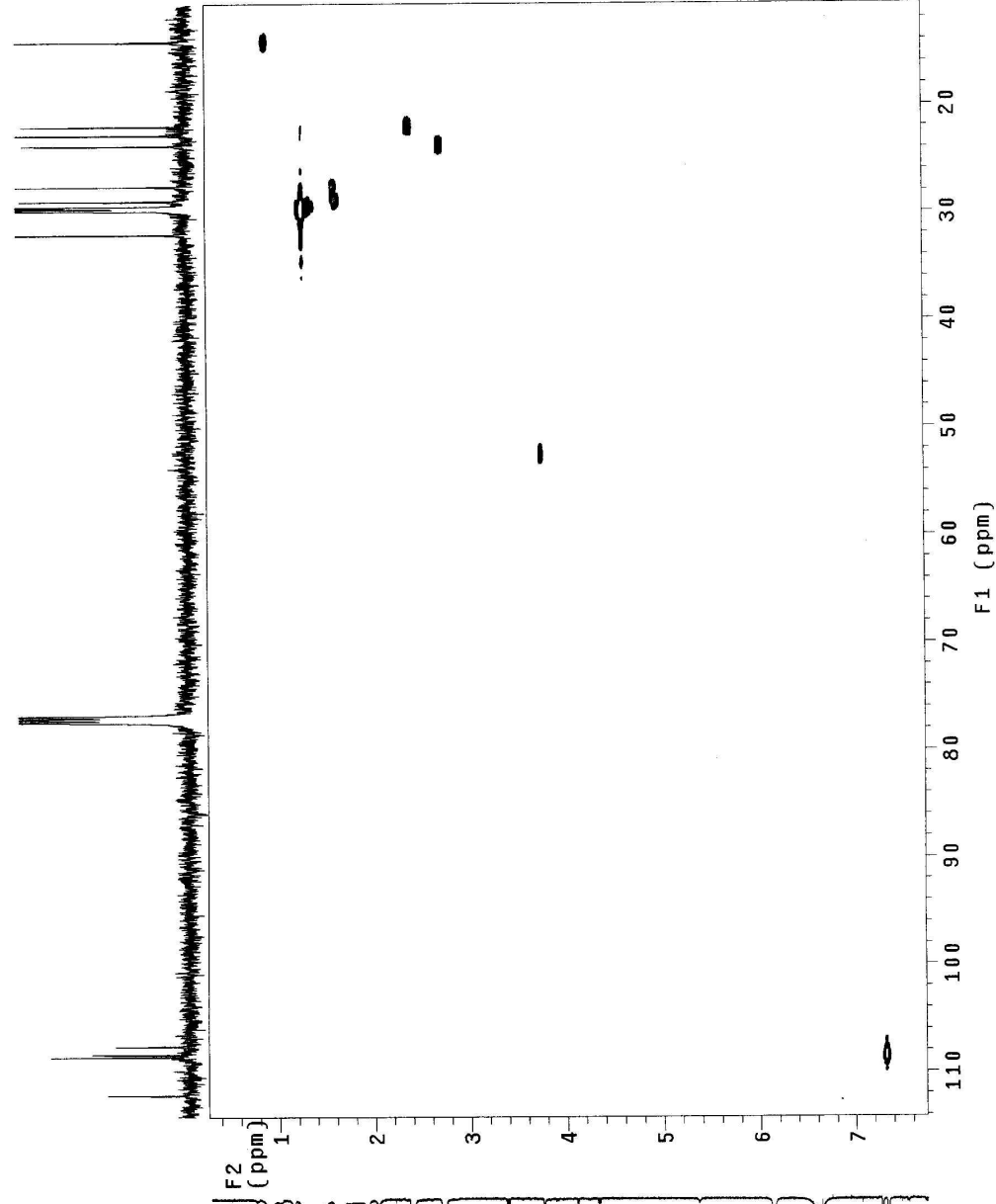


The ¹H-¹H gCOSY Spectrum of Compound 2

File: PROTON

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

Relax. delay 1.000 sec
Acq. time 0.238 sec
Width 4293.7 Hz
2D Width 23201.9 Hz
64 repetitions
256 increments
OBSERVE H1, 499.7450328 MHz
DECOUPLE C13, 125.6725540 MHz
Power 48 dB
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.059 sec
F1 DATA PROCESSING
Sine bell 0.006 sec
FT size 2048 x 2048
Total time 5 hr, 59 min, 5 sec

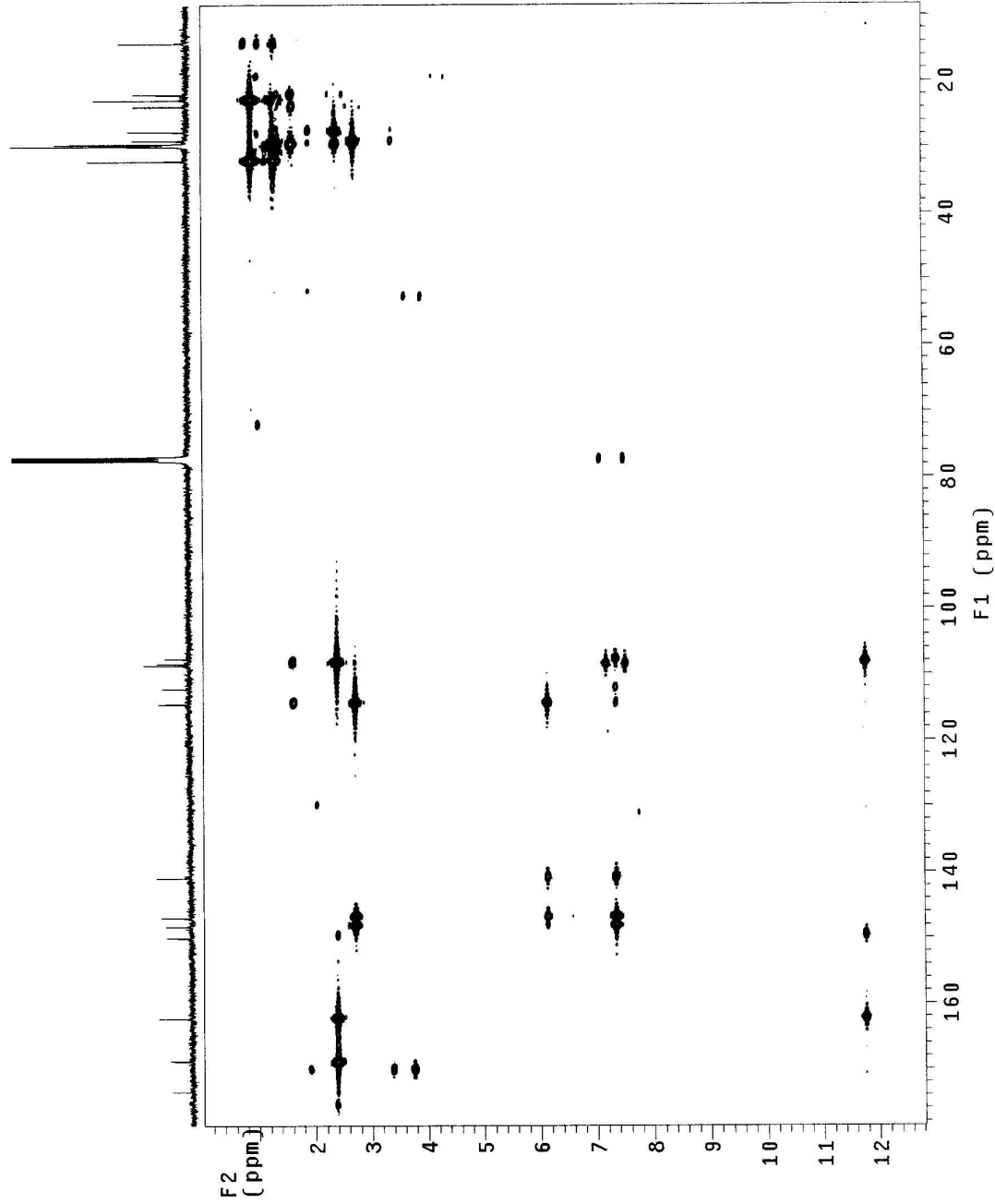


The gHSQC Spectrum of Compound 2

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
F1 size 2048 x 4096
Total time 10 hr, 38 min, 23 sec



The gHMBC Spectrum of Compound 2