

**Design, Synthesis, Antiproliferative and CDK2-Cyclin A Inhibitory Activity  
of Novel Flavopiridol Analogues**

Yu Mi Ahn,<sup>a</sup> Lakshminarayana Vogeti,<sup>a</sup> Chun-Jing Liu,<sup>a</sup> Hari K. R. Santhapuram,<sup>a</sup>  
Jonathan M. White,<sup>a</sup> Veena Vasandani,<sup>b</sup> Lester A. Mitscher,<sup>a</sup> Gerald H. Lushington,<sup>a</sup> Paul R. Hanson,<sup>c</sup>  
Douglas R. Powell,<sup>c</sup> Richard H. Himes,<sup>d</sup> Katherine F. Roby,<sup>c</sup> Qizhuang Ye,<sup>b</sup> and Gunda I. Georg<sup>a,\*</sup>

<sup>a</sup>Department of Medicinal Chemistry, <sup>b</sup>University of Kansas High Throughput Screening Laboratory, <sup>c</sup>Department of Chemistry,

<sup>d</sup>Department of Molecular Biosciences, 1251 Wescoe Hall Drive, University of Kansas, Lawrence, Kansas 66045-7582, USA

<sup>e</sup>Department of Anatomy and Cell Biology University of Kansas Medical Center,  
2008 Wahl Hall East, 3901 Rainbow Boulevard Kansas City, Kansas 66160, USA

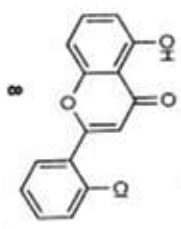
Content:

<sup>1</sup> H NMR 8	p 2	<sup>1</sup> H NMR 19c	p 36
<sup>13</sup> C NMR 8	p 3	<sup>13</sup> C NMR 19c	p 37
<sup>1</sup> H NMR 9a	p 4	<sup>1</sup> H NMR 19d	p 38
<sup>13</sup> C NMR 9a	p 5	<sup>13</sup> C NMR 19d	p 39
<sup>1</sup> H NMR 9b	p 6	<sup>1</sup> H NMR 20a	p 40
<sup>13</sup> C NMR 9b	p 7	<sup>13</sup> C NMR 20a	p 41
<sup>1</sup> H NMR 10	p 8	<sup>1</sup> H NMR 20b	p 42
<sup>13</sup> C NMR 10	p 9	<sup>13</sup> C NMR 20b	p 43
<sup>1</sup> H NMR 12	p 10	<sup>1</sup> H NMR 20c	p 44
<sup>13</sup> C NMR 12	p 11	<sup>13</sup> C NMR 20c	p 45
<sup>1</sup> H NMR 14	p 12	<sup>1</sup> H NMR 21a	p 46
<sup>13</sup> C NMR 14	p 13	<sup>13</sup> C NMR 21a	p 47
<sup>1</sup> H NMR 15a	p 14	<sup>1</sup> H NMR 21b	p 48
<sup>13</sup> C NMR 15a	p 15	<sup>13</sup> C NMR 21b	p 49
<sup>1</sup> H NMR 15b	p 16	<sup>1</sup> H NMR 21c	p 50
<sup>13</sup> C NMR 15b	p 17	<sup>13</sup> C NMR 21c	p 51
<sup>1</sup> H NMR 16	p 18	<sup>1</sup> H NMR 21d	p 52
<sup>13</sup> C NMR 16	p 19	<sup>13</sup> C NMR 21d	p 53
<sup>1</sup> H NMR 17a	p 20	<sup>1</sup> H NMR 22a	p 54
<sup>13</sup> C NMR 17a	p 21	<sup>13</sup> C NMR 22a	p 55
<sup>1</sup> H NMR 17b	p 22	<sup>1</sup> H NMR 22b	p 56
<sup>13</sup> C NMR 17b	p 23	<sup>13</sup> C NMR 22b	p 57
<sup>1</sup> H NMR 17c	p 24	<sup>1</sup> H NMR 22c	p 58
<sup>13</sup> C NMR 17c	p 25	<sup>13</sup> C NMR 22c	p 59
<sup>1</sup> H NMR 17d	p 26	<sup>1</sup> H NMR 22d	p 60
<sup>13</sup> C NMR 17d	p 27	<sup>13</sup> C NMR 22d	p 61
<sup>1</sup> H NMR 17e	p 28	<sup>1</sup> H NMR 23	p 62
<sup>13</sup> C NMR 17e	p 29	<sup>13</sup> C NMR 23	p 63
<sup>1</sup> H NMR 18b	p 30	<sup>1</sup> H NMR 24a	p 64
<sup>13</sup> C NMR 18b	p 31	<sup>13</sup> C NMR 24a	p 65
<sup>1</sup> H NMR 19a	p 32	<sup>1</sup> H NMR 24b	p 66
<sup>13</sup> C NMR 19a	p 33	<sup>13</sup> C NMR 24b	p 67
<sup>1</sup> H NMR 19b	p 34	<sup>1</sup> H NMR 24c	p 68
<sup>13</sup> C NMR 19b	p 35	<sup>13</sup> C NMR 24c	p 69

ppm  
12.5015

2

7.6673  
7.6628  
7.6487  
7.6442  
7.5965  
7.5754  
7.5548  
7.4990  
7.4950  
7.4630  
7.4599  
7.4443  
7.4415  
6.9858  
6.9646  
6.8641  
6.8435  
6.6348  
6.4481  
4.1502  
4.1324  
2.7646  
2.0664  
1.2969  
1.2792  
1.2614  
0.9009



Integral  
0.9445  
1.0000  
1.9505  
1.9919  
0.9710  
0.9551  
0.9062

ppm  
12  
10  
8  
6  
4  
2  
0

Current Data Parameters  
NAME YA-11-95-1R  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20001010  
Time 13.11  
INSTRUM drx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 228.1  
DM 78.000 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

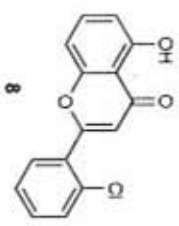
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1320007 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 13.000 ppm  
F1 5201.69 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
FPMCN 0.66500 ppm/cm  
HZCM 266.08646 Hz/cm

- 183.776
- 164.076
- 161.235
- 157.197
- 136.032
- 133.310
- 132.517
- 131.758
- 131.343
- 131.040
- 127.595
- 112.007
- 111.941
- 111.241
- 107.605
- 77.767
- 77.449
- 77.132

ppm 200 175 150 125 100 75 50 25 0



Current Data Parameters  
 NAME VA-11-95-1C  
 EXPNO 1  
 PROCNO 1

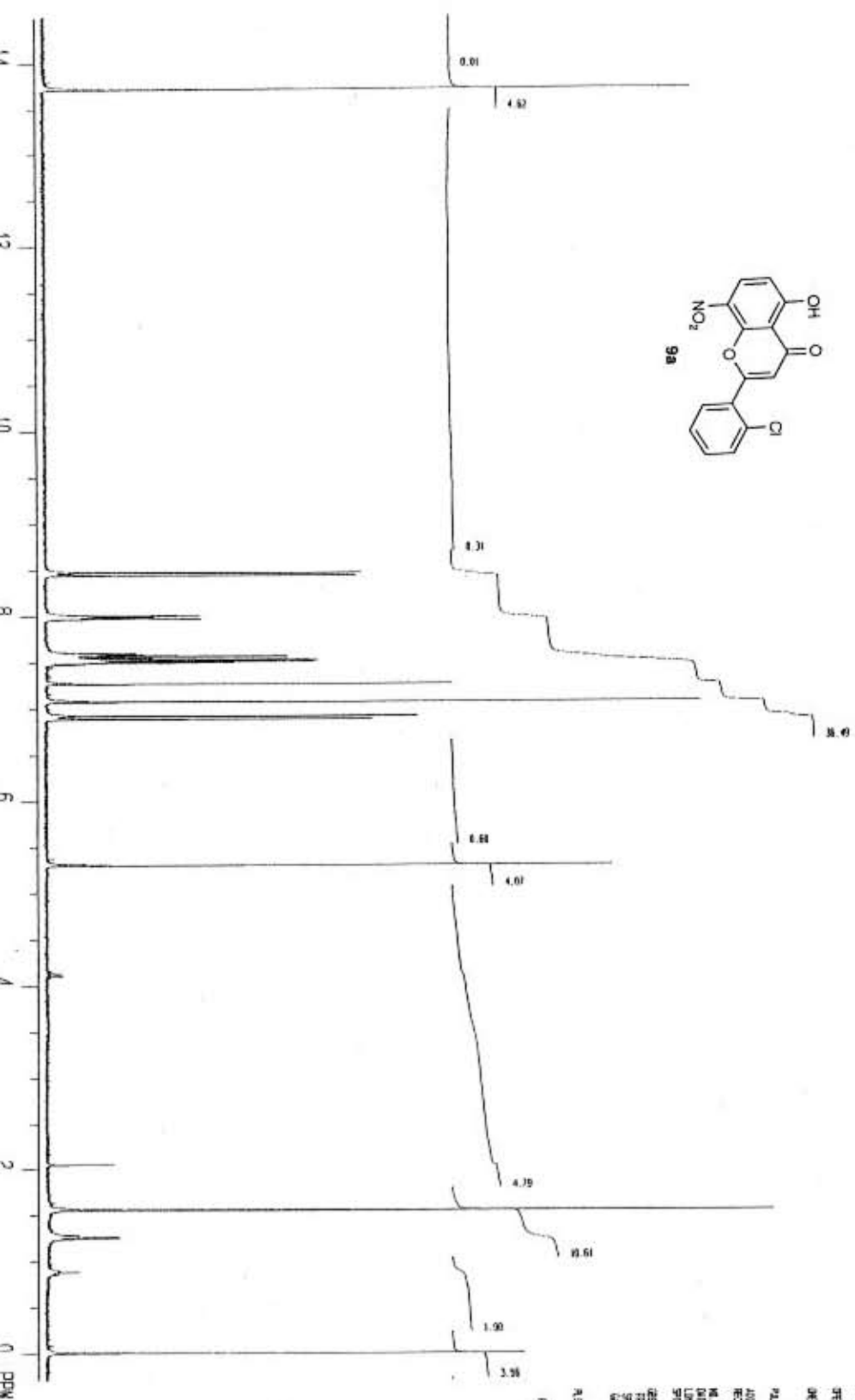
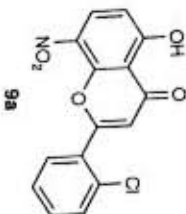
F2 - Acquisition Parameters  
 Date\_ 20081010  
 Time 12.54  
 INSTRUM dx400  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 168  
 DS 2  
 SWH 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156275 sec  
 RG 2896.3  
 DM 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 0.05000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

CHANNEL F1 \*\*\*\*\*  
 NUC1 13C  
 P1 12.30 usec  
 PL1 2.00 dB  
 SFO1 100.6232933 MHz

CHANNEL F2 \*\*\*\*\*  
 CODEPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 0.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.623290 MHz  
 MDW SM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

ID SWS plot parameters  
 CX 20.00 cm  
 FAP 220.036 ppm  
 F1 22138.42 Hz  
 F2P -18.036 ppm  
 F2 -1009.73 Hz  
 PERCHM 11.50359 ppm/cm  
 HCON 1157.40747 Hz/cm



9.01 SCALE  
131.26 MHz  
453.99 MHz  
FID  
14.50  
30 20.000

DATE: 03/11/81  
TIME: 11:30  
INSTR: FTN  
PROC: 100

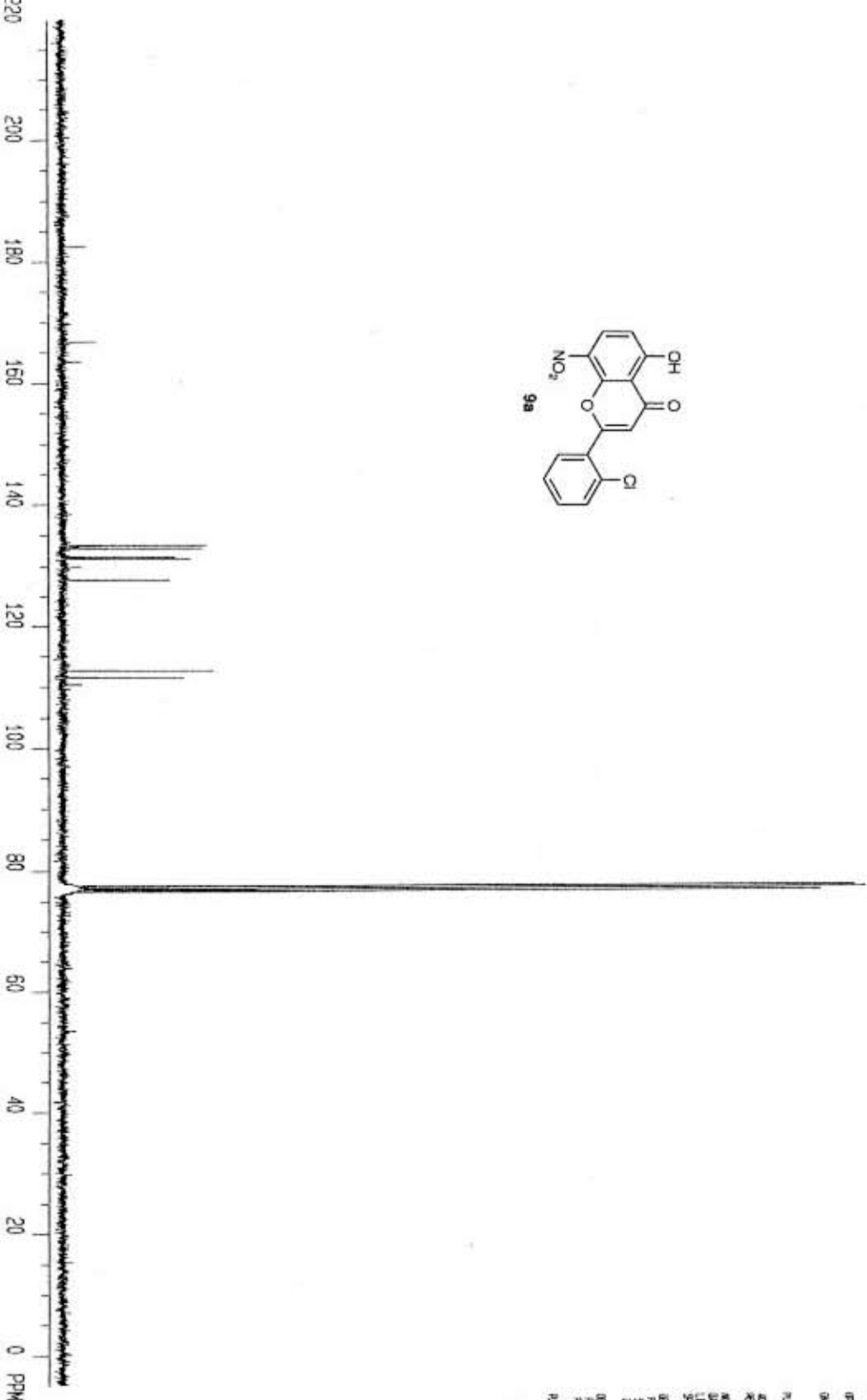
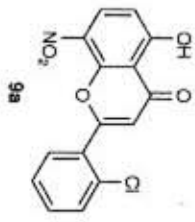
NAME: 9a  
MW: 278.12  
LIT. REF: J. Org. Chem. 46, 1086 (1981)  
ANAL. CALCD: C, 61.87%; H, 2.55%; N, 35.58%  
ANAL. FOUND: C, 61.8%; H, 2.6%; N, 35.6%

PREP: 9a  
YIELD: 100%

03MARB1

GE NMR  
DE PLUS





GE NMR  
GE PLUS

YA.002  
03MAR81

8-41111-1-11111

OPERATOR: SAM

DE PILE: GEORGE

FILE NAME: 5.63.DAT

NO. OF SCANS: 32

ACQ. TIME: 010.20 HRS

ACQ. DATE: 1.00.81

NO. OF TUBES: 2

NO. OF SAMPLES: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1

NO. OF POINTS: 1

NO. OF SPECTRA: 1

NO. OF CHANNELS: 1



GE NMR  
GE PLUS

YA.001  
11APR80

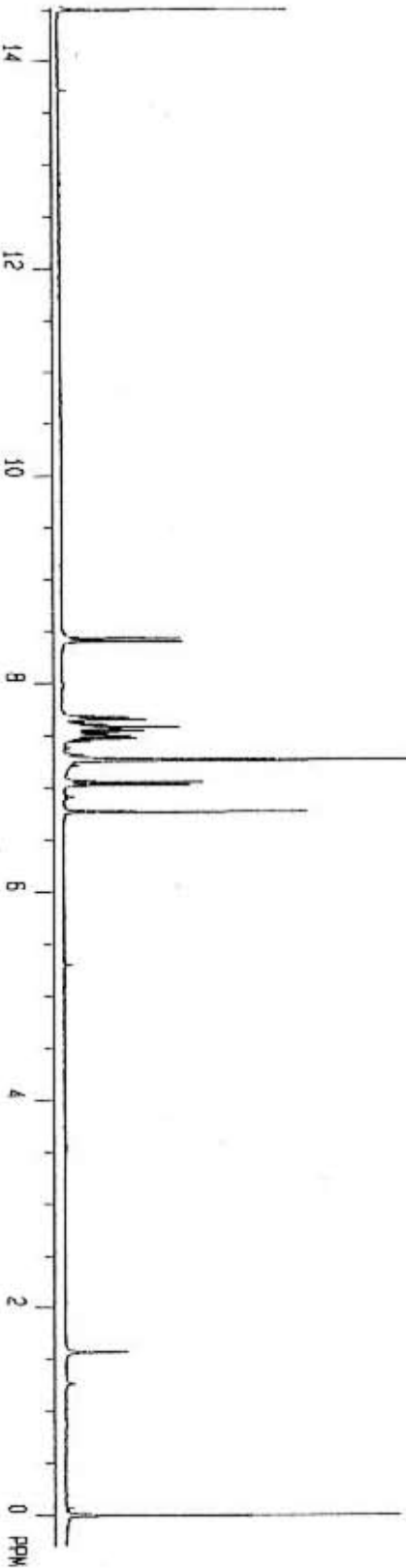
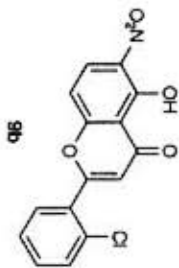
1-ETHYLBENZENE  
DEUTERIUM 5M  
ONE PULSE SEQUENCE

PULSE WIDTH : 4.21 USEC  
ACC. TIME : 30.00 SECS  
RELAX. TIME : 2.27 SEC  
REC'D TIME : 1.75 SEC

NO. OF LINES : 2708  
DATA SIZE : 23.16 K  
LINE RESOLVE : 0.31 HZ  
S/FW RATE : 18.495

OSCILL. : 250.1348000 MC  
FREQ. : 602.418 MC  
SPT. WIDTH : 602.418 MC  
AUX : 83.31

RG1 SCALE  
20.1348000  
FROM : 14.53 PPM  
TO : 1.28 PPM





GE NMR  
GE PLUS

YA.002  
11APR60

4-INDROLOXONE

OPERATOR: SM

DE: PILE 524902

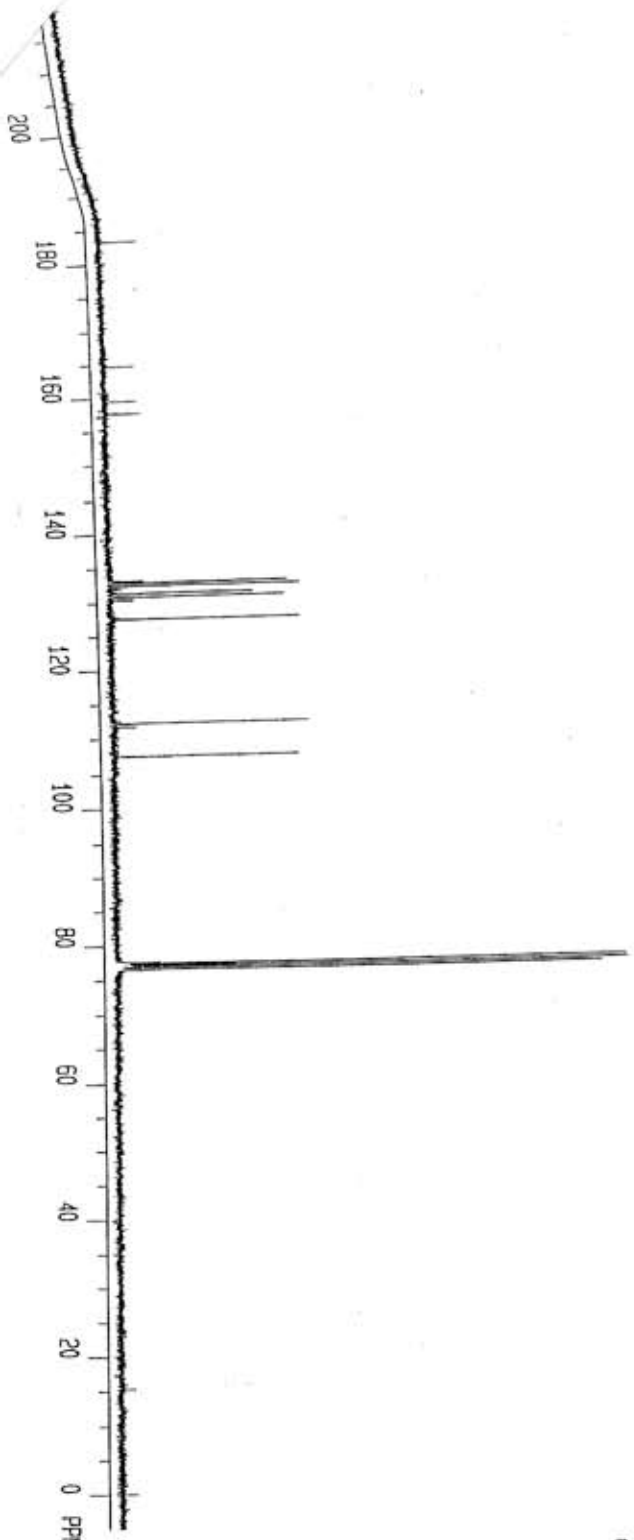
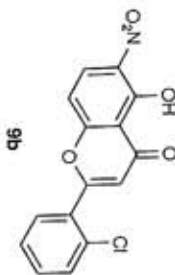
PILE NO: 5.43 SEC  
 NO. OF SPTS: 24 SPTS  
 ACQ. TIME: 815.21 SEC  
 ACQ. TIME: 1.00 SEC  
 NO. OF JETS: 1798  
 SOL. CONC: 10.00  
 LINE WIDTH: 1.00 Hz  
 SPT. RATE: 15 SPTS

DRYING: 75.00000 MC  
 FREQUENCY: 200.00 MC  
 SPT. WIDTH: 20.00 MC  
 SWS: 50.00

DEPARTMENT: STANDARD-16 MODALITY  
 PROJECT: 4400 PPM  
 PAPER: 2700

PLATE SCALE:  
 511.81 Hz/cm  
 FROM 225.00  
 TO 4.50 PPM  
 PPM LISTING

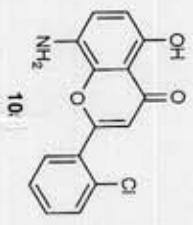
F	HT	PPM
1	3	64
2	102	76.64
3	3	76.62
4	106	77.06
5	25	77.26
6	107	77.49
7	29	107.47
8	4	111.80
9	4	127.42
10	4	127.42
11	4	129.76
12	36	130.71
13	20	131.23
14	42	132.36
15	27	132.86
16	7	133.10
17	7	137.57
18	8	139.43
19	8	139.43
20	8	139.43



Current Data Parameters

NAME YA-11-119-1  
 EXPNO 1  
 PROCNO 1

- ppm
- 13.7402
- 12.8361
- 12.5083
- 12.4840
- 11.9095
- 11.8725
- 11.7452
- 11.7006
- 11.6764
- 11.6515
- 11.6017
- 8.4851
- 8.4619
- 8.1679
- 7.6586
- 7.6542
- 7.6399
- 7.6354
- 7.5698
- 7.5667
- 7.5145
- 7.5104
- 7.4714
- 7.4679
- 7.4529
- 7.4495
- 7.2831
- 7.0716
- 7.0498
- 6.7477
- 6.7259
- 6.5702
- 5.3216
- 4.1680
- 4.1503
- 4.1323
- 4.1146
- 3.7658
- 2.0678
- 1.6134
- 1.2978
- 1.2801
- 1.2732
- 1.2623
- 0.9395
- 0.9206
- 0.9147
- 0.0903



Integral

7.189

39.265  
 7.615  
 7.221  
 6.793

1.664  
 16.947

1.852  
 11.454

F2 - Acquisition Parameters  
 Date\_ 20001128  
 Time 15.04  
 INSTRUM dxr400  
 PROBRD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.24453 Hz  
 AQ 2.0447731 sec  
 RG 362  
 DW 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec

==== CHANNEL f1 =====  
 NUCL1 1H  
 P1 7.70 usec  
 PL1 -6.00 dB  
 SFO1 400.1320007 MHz

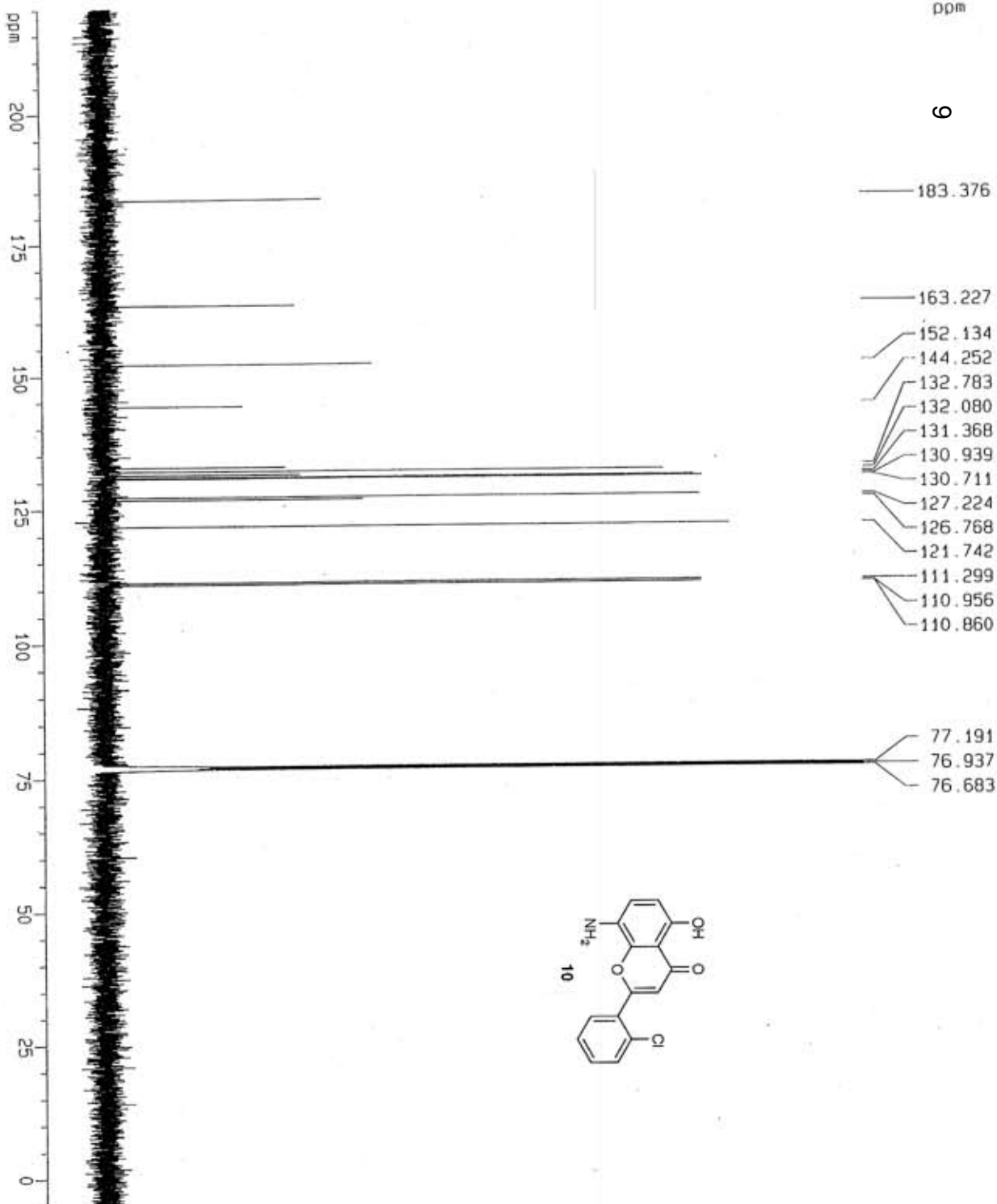
F2 - Processing parameters  
 SI 16384  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 FLF 14.000 ppm  
 F1 5601.82 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPM/CM 0.71500 ppm/cm  
 HZ/CM 286.09296 Hz/cm



ppm

9



183.376

163.227

152.134

144.252

132.783

132.080

131.368

130.939

130.711

127.224

126.768

121.742

111.299

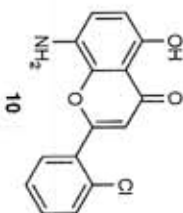
110.956

110.860

77.191

76.937

76.683



Current Data Parameters  
 NAME YA-11-13-1C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20001128  
 Time 18:12  
 INSTRUM spect  
 PPROG 5 ml 800 sb-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 2893  
 DS 4  
 SWH 31446.541 Hz  
 FIDRES 0.473886 Hz  
 AQ 1.0420724 sec  
 RG 3752.6  
 DM 15.500 usec  
 DE 5.00 usec  
 TE 300.0 K  
 D1 0.10000000 sec  
 D11 0.03000000 sec  
 D12 0.00002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 <sup>13</sup>C  
 P1 5.50 usec  
 PL1 5.00 dB  
 SFO1 125.7719472 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*

CPROG2 waltz16  
 NUC2 <sup>1</sup>H  
 P2 55.00 usec  
 PL2 17.50 dB  
 PL12 19.00 dB  
 PL13 30.00 dB  
 SFO2 500.1325000 MHz

F1 - Acquisition parameters

NO 2  
 TO 255  
 SFO1 500.1325 MHz  
 FIDRES 23.475660 Hz  
 SW 12.016 GHz

F2 - Processing parameters

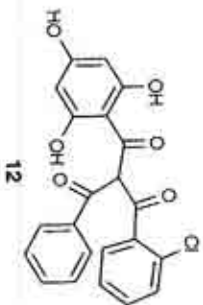
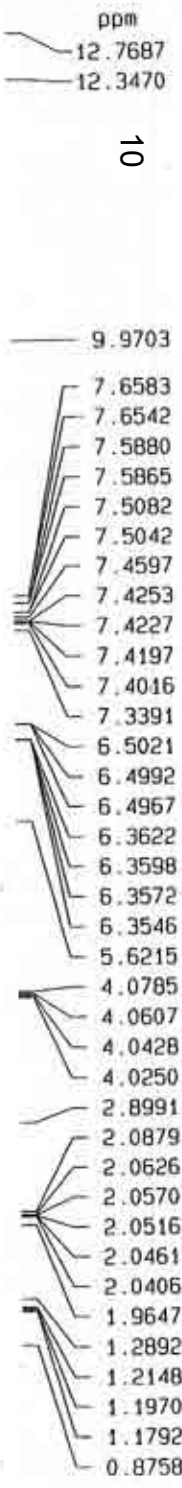
SI 125.7578008 MHz  
 SF 500.1325000 MHz  
 KW EM  
 KSM 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters

SI 125.7578008 MHz  
 SF 500.1325000 MHz  
 KW NO  
 SSB 0  
 LB 0.30 Hz  
 GB 0

F2 - Processing parameters

SI 320.00 MHz  
 SF 27066.71 MHz  
 F2P -5.000 GHz  
 F2 -528.79 Hz  
 PPM 11.25000 ppm/cm  
 NZCM 1434.77537 Hz/cm



Current Data Parameters  
 NAME DBU-slow  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20020919  
 Time 13.40  
 INSTRUM spect  
 PROBNM 5 mm QNP 1H/15  
 PULPROG zg30  
 TD 65536  
 SOLVENT Acetone  
 NS 32  
 DS 2  
 SWH 8278.146 Hz  
 FIDRES 0.125314 Hz  
 AQ 3.5584243 sec  
 RG 352  
 DM 60.400 usec  
 DE 5.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUCl 1H  
 P1 8.70 usec  
 PL1 -4.00 dB  
 SFO1 400.1324710 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1300058 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 7.01 cm  
 F1P 13.000 ppm  
 F1 5201.69 Hz  
 F2P -0.500 ppm  
 F2 -200.06 Hz  
 PPMCK 0.57500 ppm/cm  
 HZCK 270.08177 Hz/cm



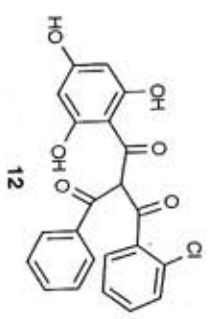
GE NMR  
DE PLUS

LN.002  
12APR80

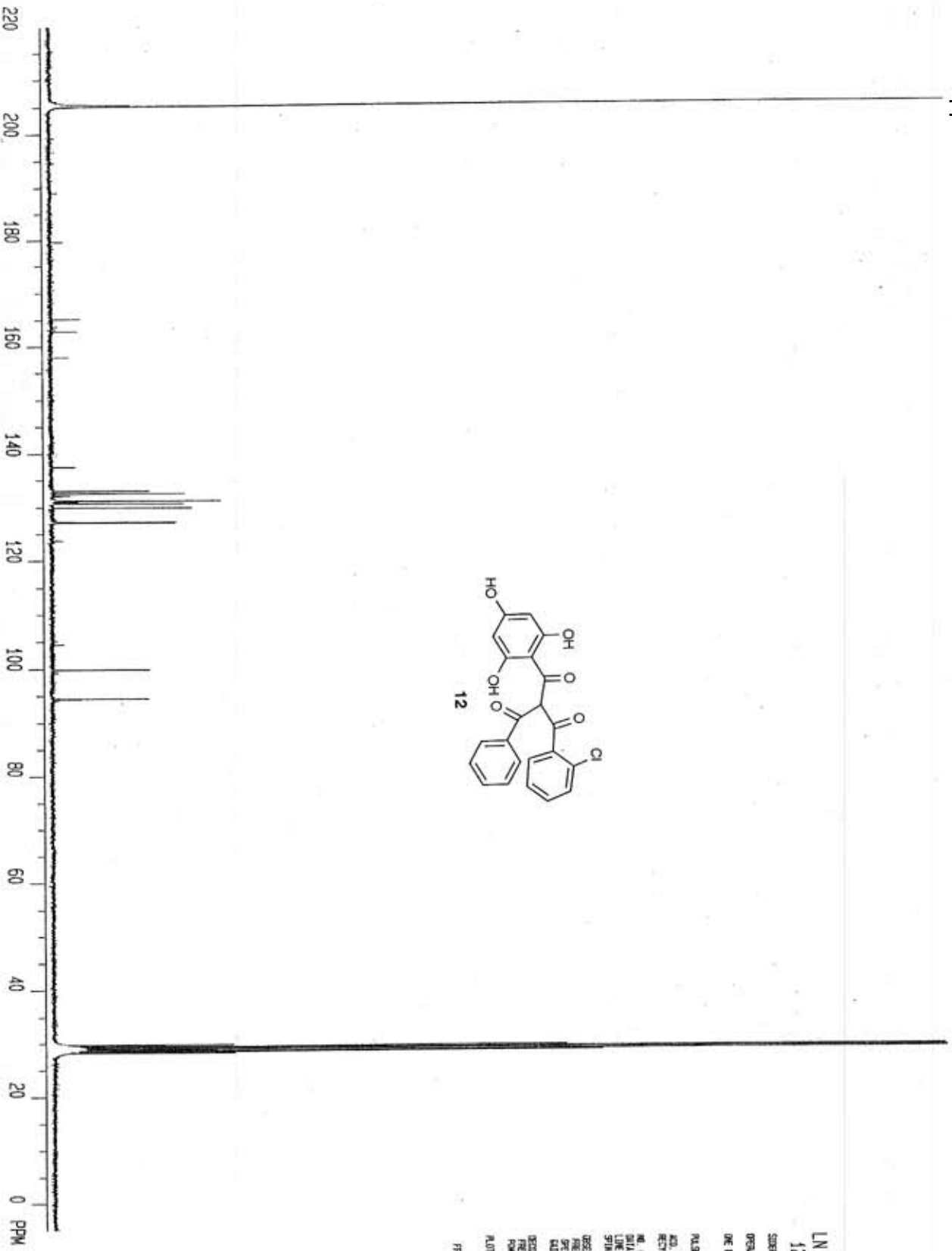
SCANS  
OPERATOR SM  
DE PLUS SCANS

PALE WITH \* 5.63 LBES  
NO. TUB \* 8 CORNERS  
REVOL TIME \* 10.00 SECS  
REVOL TIME \* 1.00 SE  
NO. OF ACQ. \* 7000  
SOLV SITE \* CDCl3  
LINE WIDTH \* 1.00 Hz  
SPIN RATE \* 50000

DESIGN \* T2-480000 M02  
RESIDENCY \* 200000 M2  
SPEC METH \* 200000 M2  
K101 \* 20 M2  
SCALAR STANDBY-16 MODULATION  
FREQUENCY \* 4.000 MHz  
POWER \* 2700  
PULP SCALE  
400.518270  
6.5108 PM/CM  
70 4.18 PM



12



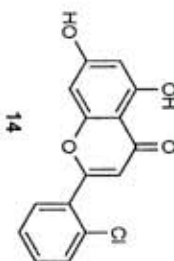
ppm

12

12.7730

9.7560  
7.8180  
7.8155  
7.8001  
7.7966  
7.6685  
7.6521  
7.6482  
7.6437  
7.6301  
7.6265  
7.6100  
7.5846  
7.5808  
7.5663  
7.5627  
7.3529  
6.4959  
6.4682  
6.3092

3.3041  
2.8625  
2.0608  
2.0554  
2.0500  
2.0447  
2.0393  
1.9599



Current Data Parameters  
NAME YA-iii-93-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20020326  
Time 21.04  
INSTRUM drx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT Aceton  
NS 32  
DS 2  
SWH 11990.407 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 256  
DW 41.700 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H

P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1320007 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300065 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters

CX 20.00 cm  
F1P 14.000 ppm  
F1 5601.82 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
PPMCM 0.71500 ppm/cm  
HZCM 286.09296 Hz/cm

Integral

0.5482

0.5219

0.9885

1.9662

1.0178

0.8777

0.9312

0.8867

ppm

12

10

8

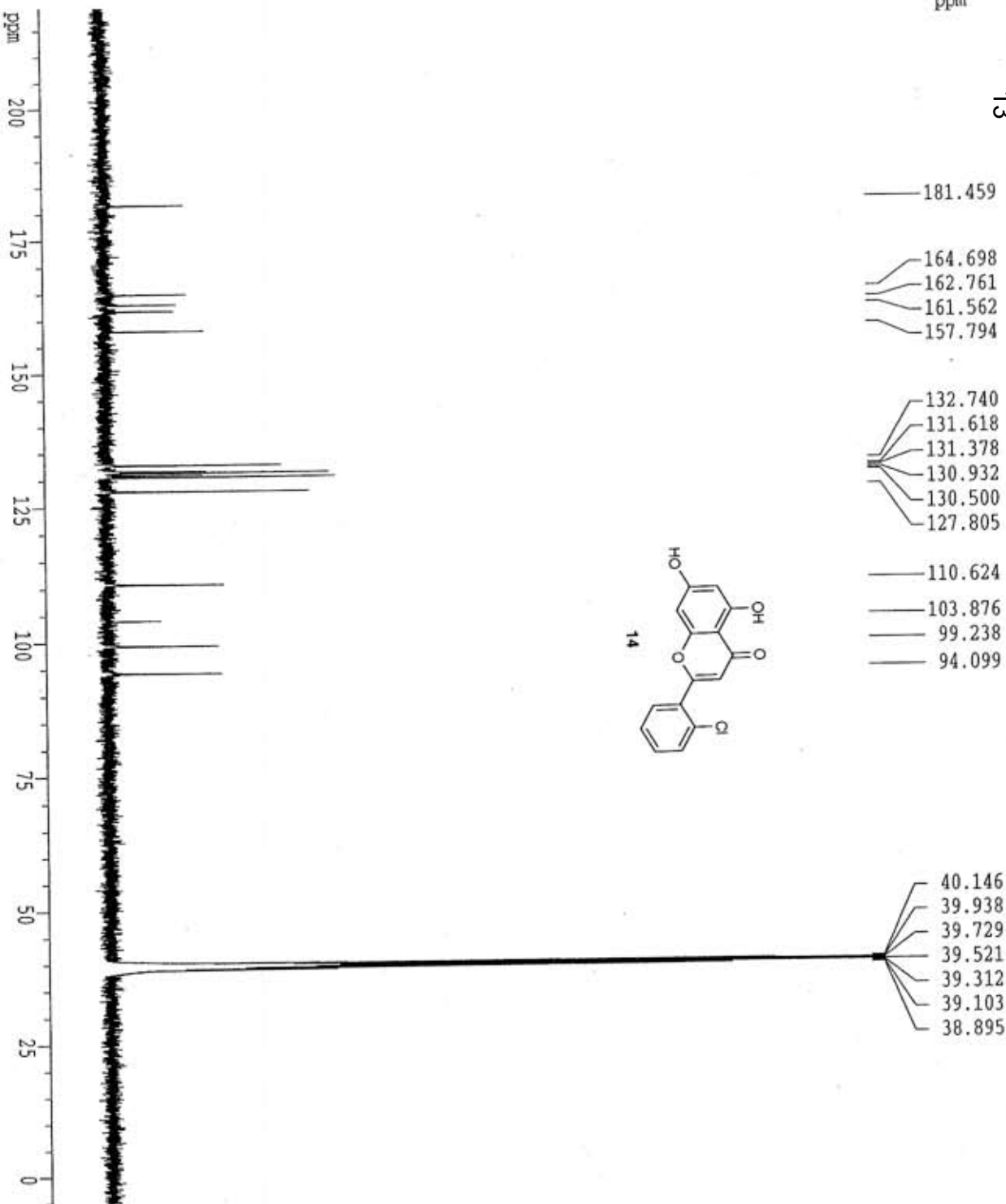
6

4

2

0

ppm



Current Data Parameters  
 NAME YA-iii-93-1C-1  
 EXPMO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20020422  
 Time 22.04

INSTRM drx400  
 PROBRD 5 mm Multinu  
 PULPROG zgpg30  
 TD 65536

SOLVENT ~~DMF-d7~~ DMSO  
 NS 1727

DS 2  
 SFR 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156276 sec

RG 4096  
 DW 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K

D1 0.05000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

----- CHANNEL f1 -----

NUC1 13C  
 P1 12.30 usec  
 PL1 2.00 dB  
 SFO1 100.6232933 MHz

----- CHANNEL f2 -----

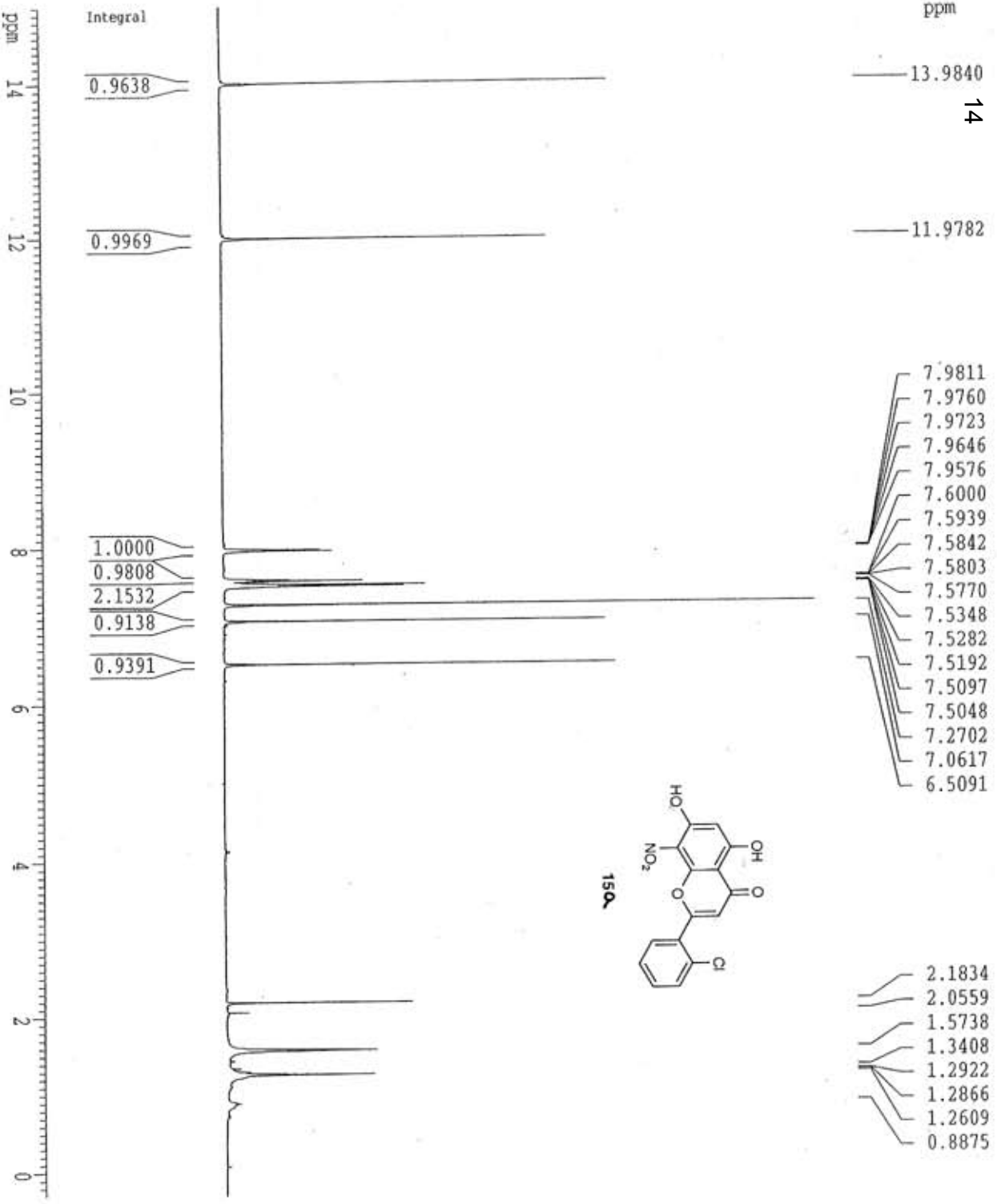
CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 0.00 dB  
 PG12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
 SF 100.6126127 MHz  
 KDM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

ID NMR plot parameters

CX 20.00 cm  
 P1P 220.000 ppm  
 F1 22124.82 Hz  
 F2P -5.000 ppm  
 F2 -503.07 Hz  
 PPMCM 11.25000 ppm/cm  
 HSCM 1131.89417 Hz/cm



Current Data Parameters  
 NAME YA-111-96-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20020323  
 Time 16.48

INSTRUM drx400  
 PROBD 5 mm Multinu  
 PULPROG zg30

TD 32768  
 SOLVENT CDCl3  
 NS 32

DS 2  
 SWH 11990.407 Hz  
 FIDRES 0.365918 Hz

AQ 1.3664756 sec  
 RG 256  
 DW 41.700 usec  
 DE 4.50 usec

TE 300.0 K  
 D1 1.00000000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.70 usec  
 PL1 -6.00 dB  
 SFO1 400.1320007 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300050 MHz

WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 20.00 cm  
 F1P 15.000 ppm  
 F1 6001.95 Hz

F2P -0.300 ppm  
 F2 -120.04 Hz

PPMCK 0.76500 ppm/cm  
 HZCM 306.09943 Hz/cm





Current Data Parameters  
 NAME Yu\_Mi\_4\_19\_05  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20050419

Time 14.10  
 INSTRUM spect  
 PROBRD 5 mm CPDUL 13C  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SFO 10330.578 Hz  
 F1FRES 0.197632 Hz  
 AQ 3.1719923 sec  
 RG 64  
 DM 48.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 MDELST 0.00000000 sec  
 MCNFK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

MUCL 1H  
 P1 15.00 usec  
 PL1 -5.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters

SF 32768  
 SF 500.1300000 MHz  
 MDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

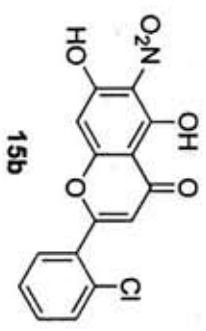
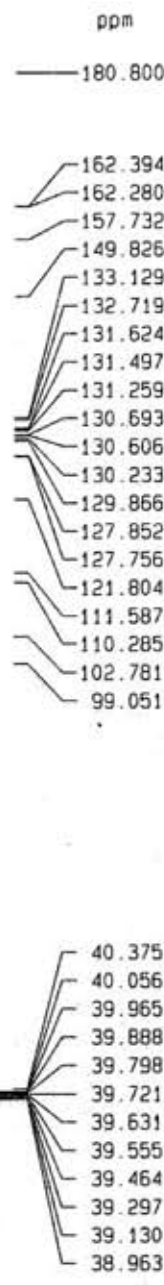
F1 - Processing parameters

SF 1024  
 MC2 9F  
 SF 500.1300000 MHz  
 MDM OSINE  
 SSB 0  
 LB 0.30 Hz  
 GB 0

10 NMR pilot parameters

CX 20.00 cm  
 CY 0.00 cm  
 FIP 14.000 ppm  
 F1 7001.82 Hz  
 F2 -290.06 Hz  
 PPMQ 0.72500 ppm/cm  
 HZCM 362.59424 Hz/cm





Current Data Parameters  
 NAME Yu\_ML\_4\_19\_05  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20090419  
 Time 14.53  
 INSTRUM spect  
 PROBRD 5 mm CPOL 13C  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 2048  
 DS 4  
 SWH 31468.541 Hz  
 FIDRES 0.479636 Hz  
 AQ 1.0420724 sec  
 RG 8192  
 DM 15.900 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 0.15000001 sec  
 d11 0.03000000 sec  
 DELTA 0.05000000 sec  
 ACQRES 0.00000000 sec  
 MCNRC 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 10.00 usec  
 PL1 -4.90 dB  
 SF01 129.7597360 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -5.00 dB  
 PL12 9.54 dB  
 PL13 10.00 dB  
 SF02 500.1329000 MHz

F2 - Processing parameters  
 S1 60636  
 SF 129.7578519 MHz  
 KDN EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

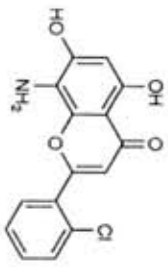
10 NMR plot parameters  
 CX 20.00 cm  
 CI 0.00 cm  
 FIP 150.000 ppm  
 F1 23893.99 Hz  
 F2 -5.000 ppm  
 F2 -628.79 Hz  
 FREQM 9.75000 ppm/cm  
 HZCM 1226.13916 Hz/cm

ppm

18

11.9133

7.8895  
7.8859  
7.8706  
7.8670  
7.6897  
7.6719  
7.6695  
7.6299  
7.6111  
7.6076  
7.5920  
7.5874  
7.5615  
7.5585  
7.5426  
7.5398  
6.5156  
6.3184  
4.0455  
4.0280  
4.0103  
3.9923  
3.3262  
2.5020  
2.4973  
2.4936  
2.4893  
2.0771  
2.0659  
2.0606  
2.0552  
1.9805  
1.1829  
1.1650  
1.1477



ppm

Integral

0.7617

1.0065  
1.0428  
1.0665  
1.0316

1.0342  
1.0653

```

Current Data Parameters
NAME      YA-111-189-1
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20021021
Time     18.50
INSTRUM  drx400
PROBHD   5 mm Multinucl
PULPROG  zg30
TD        32768
SOLVENT  DMSO
NS        32
DS        2
SMH       11185.683 Hz
FIDRES    0.341360 Hz
AQ         1.4647796 sec
RG         228.1
DM         44.700 usec
DE         4.50 usec
TE         300.0 K
D1         1.00000000 sec

***** CHANNEL f1 *****
NUC1      1H
P1        7.70 usec
PL1       -6.00 dB
SFO1      400.1310007 MHz

F2 - Processing parameters
SI         16384
SF         400.1300052 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

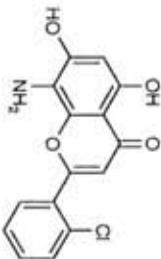
1D NMR plot parameters
CX         20.00 cm
CY         13.22 cm
FIP        14.000 ppm
F1         5601.82 Hz
F2P        -0.300 ppm
F2         -120.04 Hz
PPHMCX     0.71500 ppm/cm
HZCM       286.09296 Hz/cm

```

ppm

19

- 182.333
- 162.681
- 151.900
- 144.097
- 133.045
- 132.073
- 131.978
- 131.470
- 131.033
- 128.210
- 116.840
- 110.424
- 103.973
- 98.987
- 60.225
- 40.608
- 40.400
- 40.191
- 39.982
- 39.774
- 39.565
- 39.356
- 31.168
- 21.236
- 14.557



16

ppm



Current Data Parameters

NAME YA-111-189-1C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20021022  
Time 18.05  
INSTRUM spect  
PROBHD 5 mm QNP 1H/15  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 16384  
DS 4  
SMH 2390.814 Hz  
FIDRES 0.365918 Hz  
AQ 1.3664756 sec  
RG 7298.2  
DM 20.850 usec  
DE 5.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
d12 0.00002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
P1 7.80 usec  
PL1 -2.00 dB  
SF01 100.628298 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
CPOPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -2.00 dB  
PL12 18.22 dB  
PL13 15.00 dB  
SF02 400.1315005 MHz

F2 - Processing Parameters  
SI 32768  
SF 100.6127690 MHz  
KOH EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR Plot Parameters

CK 20.00 cm  
CY 0.00 cm  
F1P 220.000 DDM  
F1 22134.81 Hz  
F2P -503.07 Hz  
F2 11.25000 DDM/cm  
PRMCM 1131.98368 Hz/cm  
HZCM

ppm

20

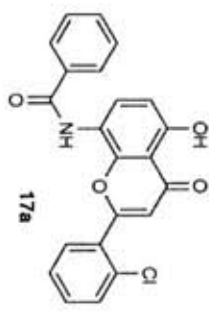
12.0755

8.6312  
 8.6087  
 7.9346  
 7.9164  
 7.9132  
 7.6661  
 7.6511  
 7.6472  
 7.6003  
 7.5942  
 7.5758  
 7.5430  
 7.5232  
 7.5052  
 7.4872  
 7.4681  
 7.4657  
 7.2836  
 6.9470  
 6.9245  
 6.6315  
 4.1527  
 4.1348  
 2.0694  
 1.5856  
 1.3001  
 1.2821  
 1.2745  
 1.2645  
 0.0210

0.9287

1.0000  
 1.0639  
 2.0554  
 7.7493

1.0039  
 0.9444



```

Current Data Parameters
NAME      Hari-IT-44
EXFNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20010118
Time     18.12
INSTRUM  dx400
PROBHD   5 mm Multinu
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       32
DS       2
SWH      8012.820 Hz
FIDRES   0.244532 Hz
AQ       2.0447731 sec
RG       1149.4
DM       62.400 usec
DE       4.50 usec
TE       300.0 K
D1       1.00000000 sec

***** CHANNEL f1 *****
NUC1      1H
P1       7.70 usec
PL1      -6.00 dB
SFO1     400.1320007 MHz

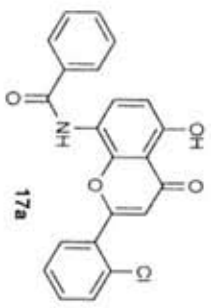
F2 - Processing parameters
SI       16384
SF       400.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       20.00 cm
F1P     14.000 ppm
F1      5601.82 Hz
F2P     -0.300 ppm
F2     -120.04 Hz
PPMCM   0.71500 ppm/cm
HZCM    286.09296 Hz/cm
  
```



Integral

- 182.932
- 163.307
- 156.650
- 146.449
- 134.301
- 132.531
- 132.502
- 132.015
- 131.216
- 131.008
- 130.807
- 128.904
- 128.819
- 128.654
- 127.576
- 126.989
- 118.038
- 113.760
- 111.514
- 111.220
- 110.315
- 77.188
- 77.137
- 76.934
- 76.680



280.082

ppm  
200  
175  
150  
125  
100  
75  
50  
25  
0

Current Data Parameters  
NAME Har1-11-44-1C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20010122  
Time 19.04  
INSTRUM spect  
PROBHD 5 mm BBO BB-  
PULPROG zgpg30  
TO 68.536  
SOLVENT CDCl3  
NS 5123  
DS 4  
SWH 31446.541 Hz  
FIDRES 0.479836 Hz  
AQ 1.0420724 sec  
RG 7299.2  
DM 15.900 usec  
DE 6.00 usec  
TE 300.0 K  
D1 0.10000000 sec  
D11 0.03000000 sec  
D12 0.00020000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 13C  
P1 6.50 usec  
PL1 5.00 dB  
SF01 125.7719472 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
CPOPRG2 waltz16  
NUC2 1H  
PCPD2 95.00 usec  
PL2 17.50 dB  
PL12 19.00 dB  
PL13 30.00 dB  
SF02 500.1325000 MHz

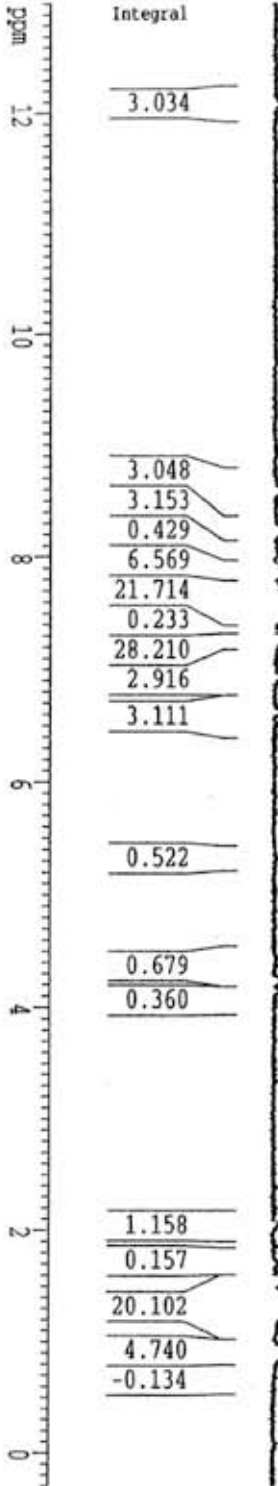
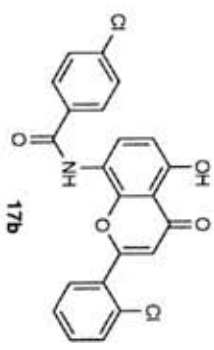
F2 - Processing parameters  
SI 65536  
SF 125.7578008 MHz  
MDM EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.40

10 NMR plot parameters  
CX 20.00 cm  
F1P 220.000 DPK  
F1 27668.71 Hz  
F2P -5.000 DPK  
F2 -628.79 Hz  
PPMCK 11.25000 DPK/cm  
HZCM 1414.77527 Hz/cm

ppm

12.0733

8.6009  
8.5784  
8.2305  
7.8748  
7.8536  
7.6631  
7.6589  
7.6439  
7.6399  
7.6294  
7.6119  
7.6095  
7.5568  
7.5525  
7.5111  
7.4898  
7.4774  
7.4743  
7.2842  
6.9461  
6.9236  
6.6270  
5.3249  
4.1533  
4.1356  
2.0702  
1.5742  
1.3407  
1.3277  
1.3127  
1.3010  
1.2830  
1.2748  
1.2653  
0.9610  
0.9423  
0.9231  
0.9178  
0.9054  
0.8880



Current Data Parameters  
NAME YA-11-143-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20010123  
Time 14.00

INSTRUM drx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3

NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec  
RG 1024  
CW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1320007 MHz

F2 - Processing parameters  
SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 13.000 ppm  
F1 5201.69 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
PPMCM 0.66500 ppm/cm  
HZCM 266.08646 Hz/cm

183.372

163.835

157.267

138.850

133.118

132.888

132.417

131.752

131.541

131.225

129.595

129.080

128.895

128.142

118.276

111.979

111.749

110.793

77.743

77.631

77.426

77.108

76.727

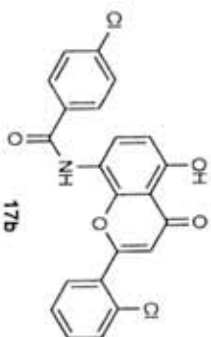
39.117

30.754

29.333

24.137

11.378



Current Data Parameters  
 NAME YA-11-143-1c  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20010124  
 Time 20.15  
 INSTRUM drx400  
 PROBRD 5 mm Multinu  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 30023  
 DS 2  
 SMH 23148.148 Hz  
 FIDRES 0.351213 Hz  
 AQ 1.4156375 sec  
 RG 2048  
 DW 21.500 usec  
 DE 4.50 usec  
 FE 300.0 K  
 D1 0.05000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 13C  
 P1 12.30 usec  
 PL1 2.00 dB  
 SFO1 100.6232933 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*

CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 0.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing Parameters

SI 32768  
 SF 100.6127290 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters

CX 20.00 cm  
 F1P 220.036 ppm  
 F1 22138.42 Hz  
 F2P -10.036 ppm  
 F2 -1009.73 Hz  
 PPMCM 11.50359 ppm/cm  
 HZCM 1157.40747 Hz/cm

ppm

200

175

150

125

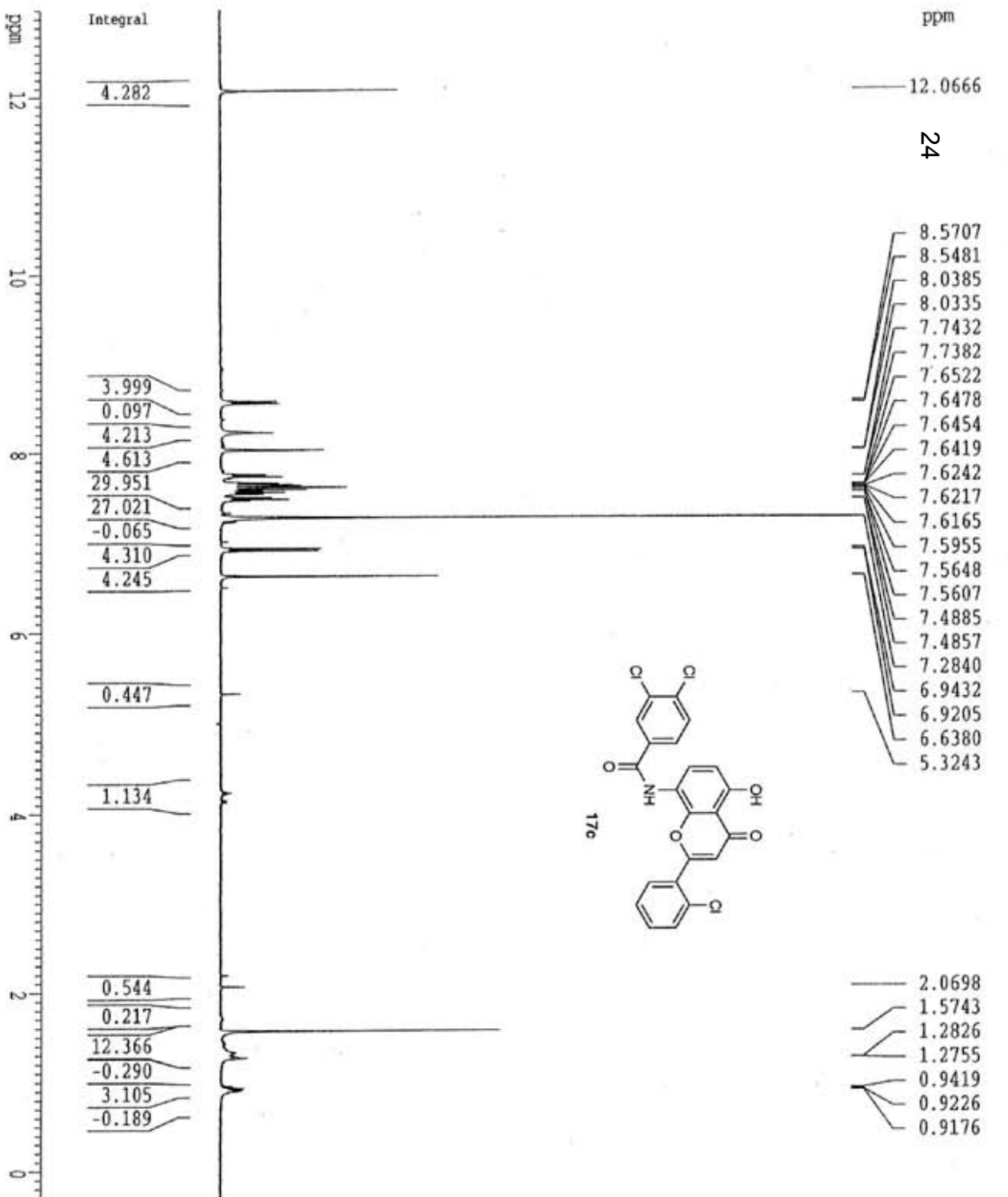
100

75

50

25

0



Current Data Parameters  
 NAME YA-11-144-1  
 EXPNO 1  
 PROCNO 1

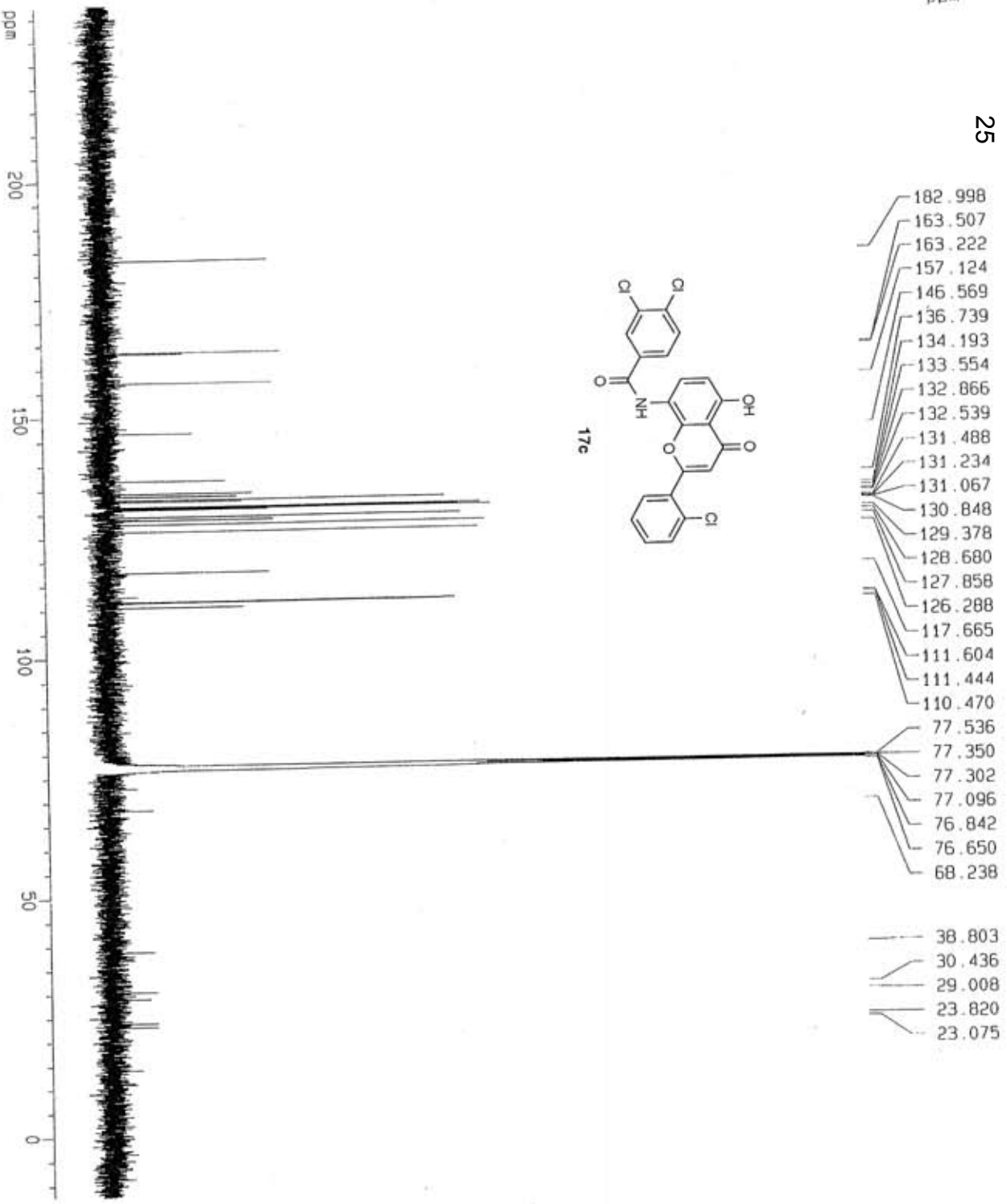
F2 - Acquisition Parameters  
 Date\_ 20010124  
 Time 16.37  
 INSTRUM drx400  
 PROBRD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SMR 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 1024  
 DW 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 7.70 usec  
 PL1 -6.00 dB  
 SF01 400.1320007 MHz

F2 - Processing Parameters  
 SI 16384  
 SF 400.1300000 MHz  
 MDW DM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1 13.000 ppm  
 F2 5201.69 Hz  
 F2P -0.300 ppm  
 PPMCK 0.66500 ppm/cm  
 HZCK 266.08646 Hz/cm





- 182.998
- 163.507
- 163.222
- 157.124
- 146.569
- 136.739
- 134.193
- 133.554
- 132.866
- 132.539
- 131.488
- 131.234
- 131.067
- 130.848
- 129.378
- 128.680
- 127.858
- 126.288
- 117.665
- 111.604
- 111.444
- 110.470
- 77.536
- 77.350
- 77.302
- 77.096
- 76.842
- 76.650
- 68.238
- 38.803
- 30.436
- 29.008
- 23.820
- 23.075

Current Data Parameters  
 NAME YA-11-144-1C  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20010130  
 Time 17.20  
 INSTRUM spect  
 PROBO 5 mm BBO BB-  
 PULPROG zgpg30  
 TO 65536  
 SOLVENT CDCl3  
 NS 45012  
 DS 4  
 SWH 31446.541 HZ  
 FIDRES 0.479836 HZ  
 AQ 1.0420724 sec  
 RG 13004  
 OW 15.900 usec  
 DE 5.00 usec  
 TE 300.0 K  
 O1 0.10000000 sec  
 O11 0.03000000 sec  
 O12 0.000002000 sec

CHANNEL f1

NUC1 13C  
 P1 6.50 usec  
 PL1 5.00 dB  
 SFO1 125.7719472 MHz

CHANNEL f2

CPDPRG2 -waltz16  
 NUC2 1H  
 PCPD2 95.00 usec  
 PL2 17.50 dB  
 PL12 19.00 dB  
 PL13 30.00 dB  
 SFO2 500.1325000 MHz

F2 - Processing parameters

SF 65536  
 SF 125.7577802 MHz  
 NDM EM  
 SSB 0  
 LB 1.00 HZ  
 GB 0  
 PC 1.40

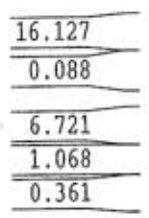
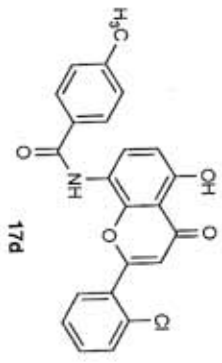
1D NMR plot parameters

CX 20.00 cm  
 F1P 237.682 ppm  
 F1 298990.31 HZ  
 F2P -12.375 ppm  
 F2 -1556.23 HZ  
 PPMCK 12.50282 ppm/cm  
 HZCM 1572.32703 HZ/cm

ppm

26

- 12.0801
- 8.6319
- 8.6095
- 8.2655
- 7.8307
- 7.8109
- 7.6673
- 7.6485
- 7.6246
- 7.6048
- 7.5602
- 7.5419
- 7.5252
- 7.4872
- 7.4684
- 7.4512
- 7.3295
- 7.3099
- 7.2850
- 6.9394
- 6.9169
- 6.6290
- 5.3254



Current Data Parameters  
 NAME YA-i-154-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20010207  
 Time 14.28  
 INSTRUM drx400  
 PROBRD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 1024  
 DW 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec

----- CHANNEL f1 -----  
 NUCL1 1H  
 P1 7.70 usec  
 PL1 -6.00 dB  
 SFO1 400.1320007 MHz

F2 - Processing parameters  
 SI 16384  
 SF 400.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

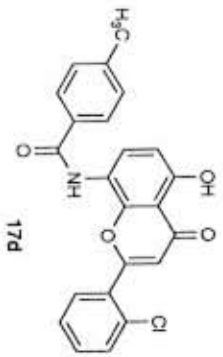
1D NMR plot parameters  
 CX 20.00 cm  
 P1P 14.000 ppm  
 F1 5601.82 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 FWHM 0.71500 ppm/cm  
 HZCM 286.09296 Hz/cm



ppm

27

- 183.117
- 165.465
- 163.445
- 156.662
- 146.536
- 142.776
- 132.668
- 131.605
- 131.372
- 131.174
- 130.998
- 129.632
- 128.745
- 127.733
- 127.160
- 118.355
- 111.658
- 111.362
- 110.466
- 77.352
- 77.098
- 76.844



- 21.606

ppm 200 150 100 50 0



Current Data Parameters  
 NAME VA-11-154-C  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20010207  
 Time 18.36

INSTRUM spect  
 PROCNO 5  
 PULPROG zgpg30  
 TO 65536  
 SOLVENT CDCl3  
 NS 50000  
 DS 4

SM 31446.541 Hz  
 FIDRES 0.479836 Hz  
 AQ 1.0420724 sec  
 RG 6502

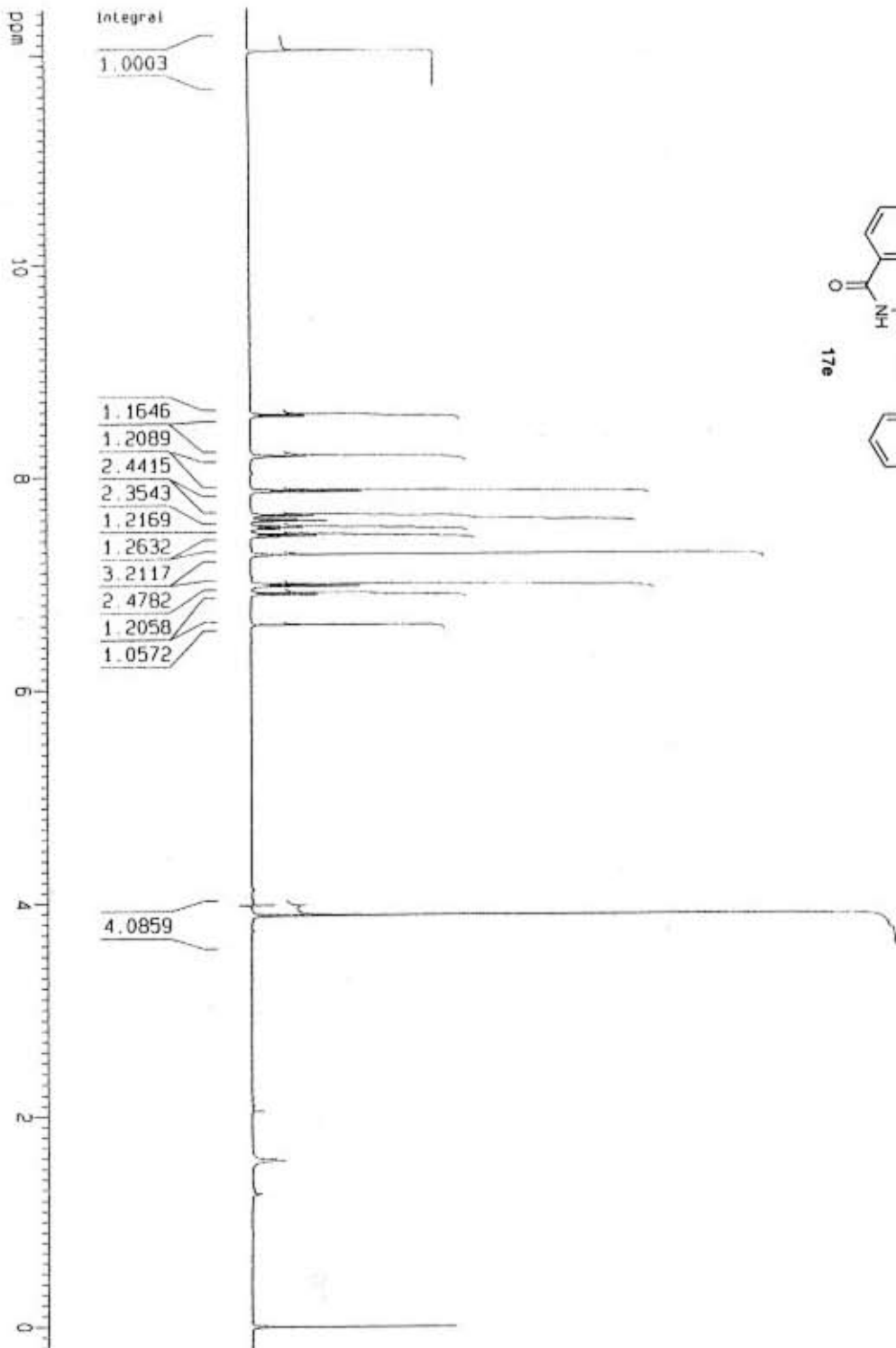
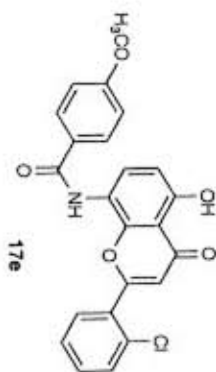
DW 15.900 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 0.10000000 sec  
 D11 0.03000000 sec  
 D12 0.00002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NU1 13C  
 P1 6.50 usec  
 PL1 5.00 dB  
 SF01 125.7719472 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NU2 1H  
 PCPD2 95.00 usec  
 PL2 17.50 dB  
 PL12 19.00 dB  
 PL13 30.00 dB  
 SF02 500.1325000 MHz

F2 - Processing parameters  
 S1 65536  
 SF 125.7577802 MHz  
 WDM EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1p 220.000 ppm  
 F1 27666.71 Hz  
 F2p -1257.56 Hz  
 PPMCH 11.50000 ppm/cm  
 HZCH 1446.21448 Hz/cm



Current Data Parameters  
 NAME 11-KR-46  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20010124  
 Time 9:02  
 INSTRUM spect  
 PULPROG 5 mm BIRD-BB-  
 TD 4930  
 FIDRES 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 15015.015 HZ  
 FIDRES 0.498222 HZ  
 AQ 1.0912344 sec  
 RG 512  
 CW 23.300 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 0.03000000 sec

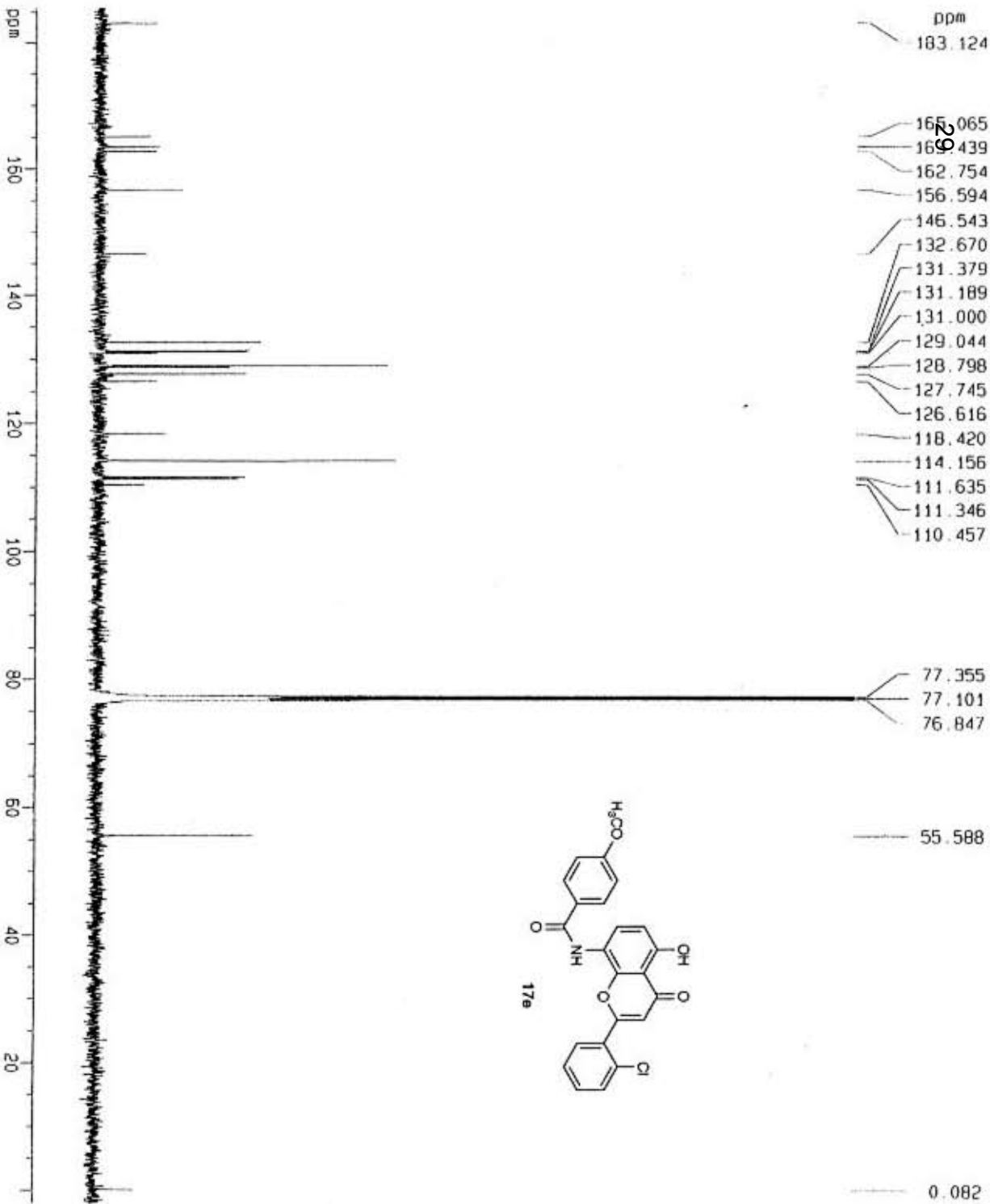
\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 7.70 usec  
 PL1 -4.00 dB  
 SFO1 500.1360008 MHz

F1 - Acquisition Parameters  
 NDO 2  
 TD 256  
 SFO1 500.1325 MHz  
 FIDRES 23.475050 HZ  
 SW 12.016 com

F2 - Processing Parameters  
 SI 32768  
 SF 500.1360123 MHz  
 NQM 0  
 SSB 0  
 LB 0.30 HZ  
 GB 0  
 PC 1.00

F1 - Processing Parameters  
 SI 1024  
 WCZ 0F  
 SF 500.1360000 MHz  
 NQM no  
 SSB 0  
 LB 0.30 HZ  
 GB 0

1D NMR D101 Parameters  
 CX 20.00 cm  
 FIP 12.442 DDM  
 P1 5222.48 HZ  
 F2 -113.88 HZ  
 PPMCN 0.63247 ppm/cg  
 HZCM 319.81680 HZ/cg



Current Data Parameters  
 NAME 11-MR-05  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20010124  
 Time 9:09  
 INSTRUM spect  
 PROBHD 5 mm QNP 5B-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMS-D6  
 CXC13  
 NS 6512  
 DS 4

DE 3146.541 Hz  
 SFO5 0.4790318 Hz  
 AQ 1.0420724 sec  
 RG 3120.5  
 OR 15.500 uSAC  
 DE 6.00 uSAC  
 TE 300.2 K

SI 0.10000000 sec  
 O1 0.03000000 sec  
 O12 0.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 6.50 uSAC  
 PL 5.00 dB  
 SFO1 125.7718472 MHz

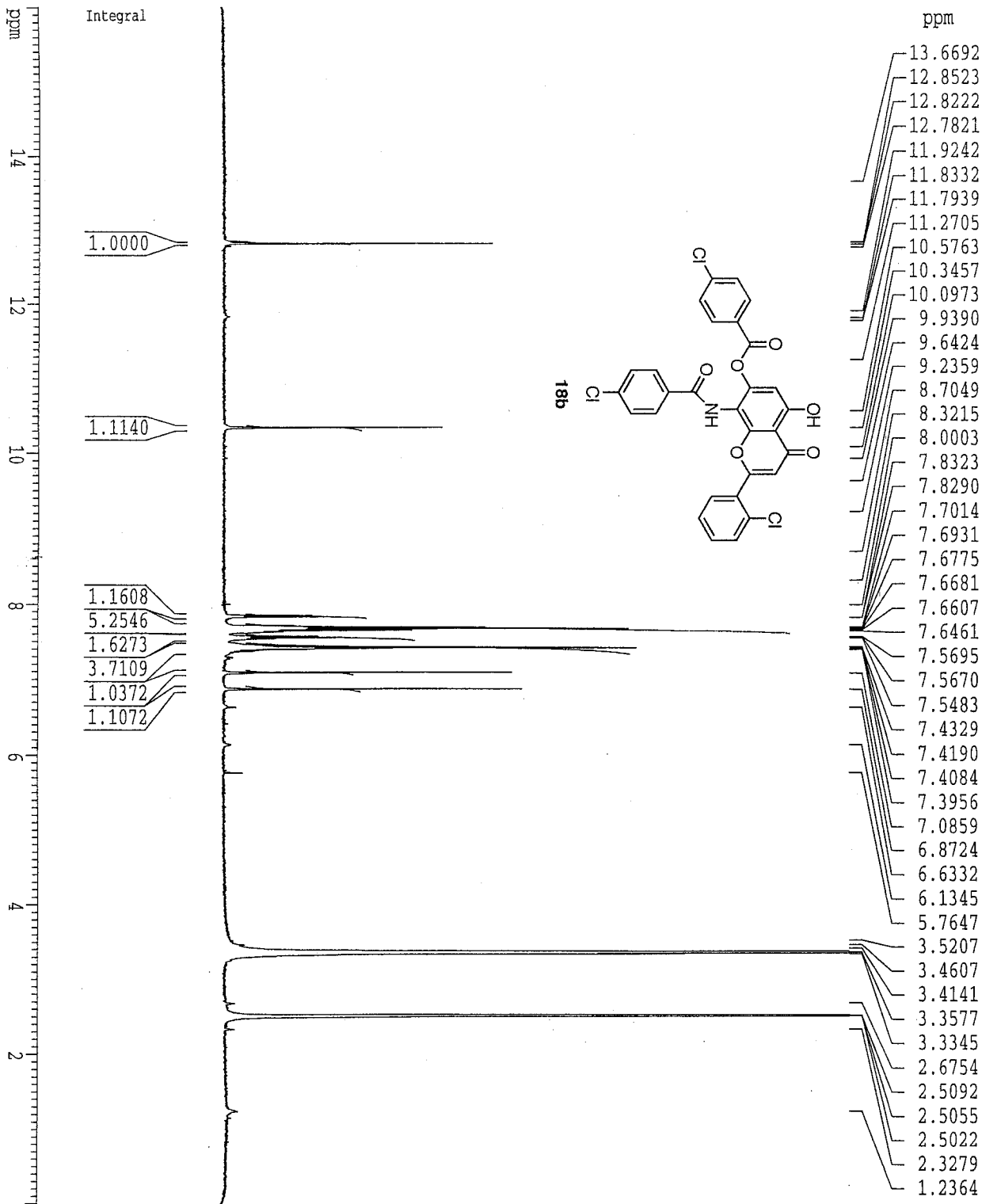
\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PULPROG zgpg30  
 PL2 17.50 dB  
 PL12 19.00 dB  
 PL13 30.00 dB  
 SFO2 500.1325000 MHz

F1 - Acquisition parameters  
 MD 2  
 TD 65536  
 SFO1 500.1325 MHz  
 FIDRES 29.475000 Hz  
 SN 12.016 dB

F2 - Processing parameters  
 SI 65536  
 SF 125.757962 MHz  
 MD 64  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters  
 SI 1024  
 SF 500.130000 MHz  
 MD 64  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 10

10 mad p10t parameters  
 CX 20.00 cm  
 F1P 185.670 ppm  
 F1 23366.43 Hz  
 F2P 2.123 ppm  
 F2 2095.92 Hz  
 SFOC 5.26682000 MHz  
 WDC 1180.5175 Hz/CZ



ppm

13.6692  
12.8523  
12.8222  
12.7821  
11.9242  
11.8332  
11.7939  
11.2705  
10.5763  
10.3457  
10.0973  
9.9390  
9.6424  
9.2359  
8.7049  
8.3215  
8.0003  
7.8323  
7.8290  
7.7014  
7.6931  
7.6775  
7.6681  
7.6607  
7.6461  
7.5695  
7.5670  
7.5483  
7.4329  
7.4190  
7.4084  
7.3956  
7.0859  
6.8724  
6.6332  
6.1345  
5.7647  
3.5207  
3.4607  
3.4141  
3.3577  
3.3345  
2.6754  
2.5092  
2.5055  
2.5022  
2.3279  
1.2364

Integral

1.0000  
1.1140  
1.1608  
5.2546  
1.6273  
3.7109  
1.0372  
1.1072

ppm

14  
12  
10  
8  
6  
4  
2

Current Data Parameters

NAME lc060  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20011212  
Time 10.04  
INSTRUM drx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 64  
DW 78.000 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

===== CHANNEL f1 =====

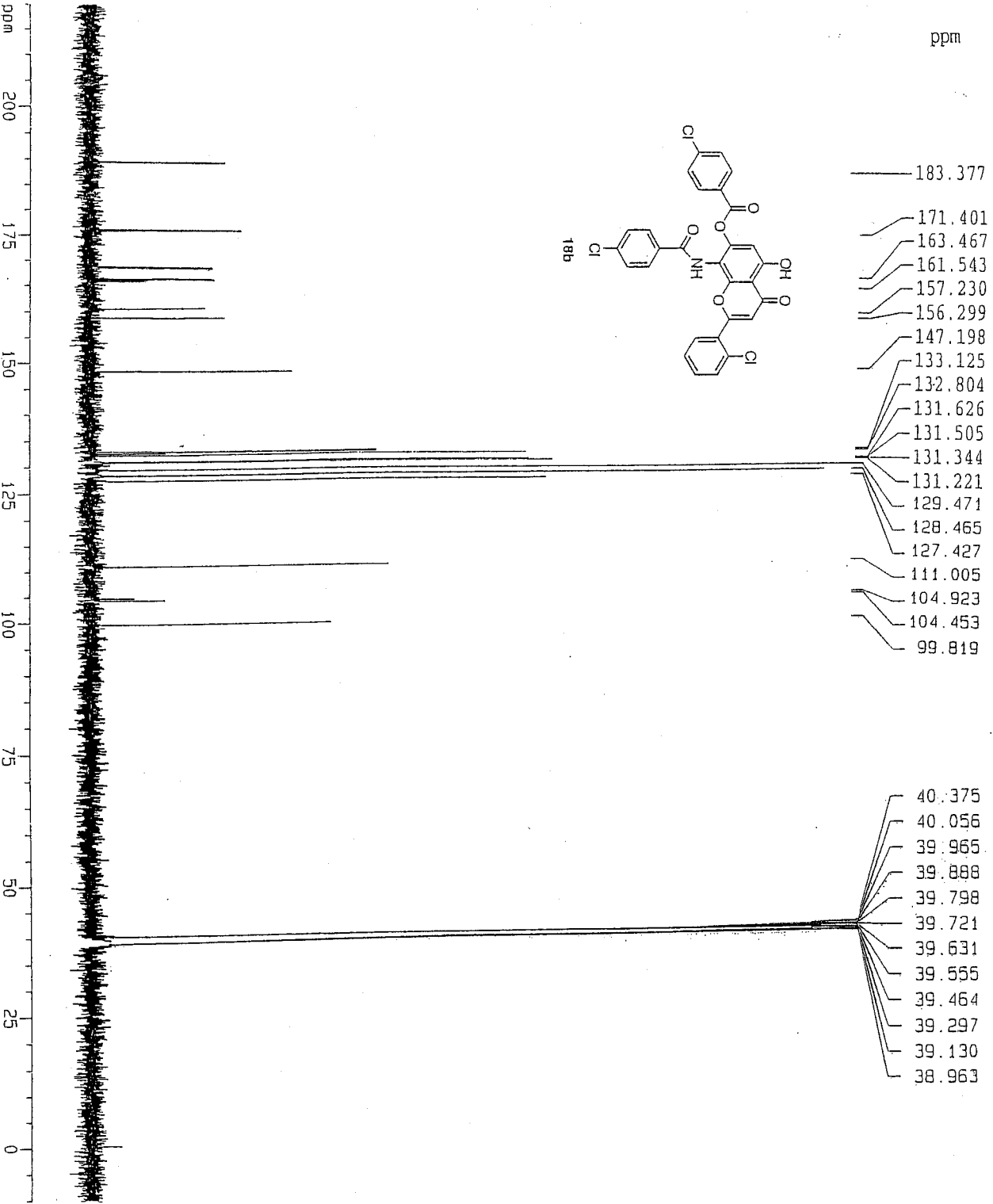
NUC1 1H  
P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1332010 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters

CX 20.00 cm  
F1P 16.010 ppm  
F1 6406.17 Hz  
F2P -0.010 ppm  
F2 -4.09 Hz  
PPMCM 0.80102 ppm/cm  
HZCM 320.51282 Hz/cm



Current Data Parameters  
 NAME LC060  
 EXNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20011212  
 Time 10.04  
 INSTRUM drx400  
 PROBHND 5 mm Multinu  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 2  
 SWH 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156276 sec  
 RG 32768  
 DM 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 0.05000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

==== CHANNEL F1 =====

NUC1 13C  
 P1 12.30 usec  
 PL1 2.00 dB  
 SFO1 100.6232933 MHz

==== CHANNEL F2 =====

CPDPRG2 waltz16  
 NUC2 1H  
 PCPDZ 100.00 usec  
 PL2 0.00 dB  
 PLI2 18.00 dB  
 PLI3 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
 SF 100.6127290 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

ID NMR plot parameters

CX 20.00 cm  
 F1P 215.000 ppm  
 F1 21631.74 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 PPKCM 11.00000 ppm/cm  
 HZCM 1106.73999 Hz/cm

ppm

32

12.1741

8.4931

7.9327

7.9147

7.9113

7.6351

7.6311

7.6161

7.6117

7.5942

7.5910

7.5387

7.5343

7.5288

7.5089

7.4904

7.4651

7.4618

7.2619

6.5296

6.5245

4.1295

4.1117

2.0461

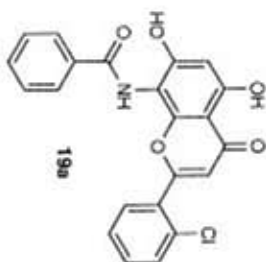
1.2775

1.2595

1.2534

1.2418

0.0002



Integral

1.0555

0.8839

1.0042

2.1081

2.6764

4.9224

2.0116

Current Data Parameters  
 NAME YA-111-192-1  
 EXNO 1  
 PRONO 1

F2 - Acquisition Parameters  
 Date\_ 20021031  
 Time 10.49  
 INSTRUM spect  
 PROBD 5 mm DNP 1H/15  
 PULPROG zg30  
 TD 32768  
 SFOVENT CDC13  
 NS 16  
 DS 2  
 SMH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 405.4  
 DM 52.400 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 8.70 usec  
 PL1 -4.50 dB  
 SF01 400.1320007 MHz

F2 - Processing Parameters  
 S1 32768  
 SF 400.1300087 MHz  
 KMK EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR 0101 Parameters  
 CX 20.00 CM  
 CY 0.00 CM  
 F1P 14.000 ppm  
 F1 5601.82 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPMCK 0.71500 ppm/cm  
 KZCM 286.09296 Hz/cm

ppm

12

10

8

6

4

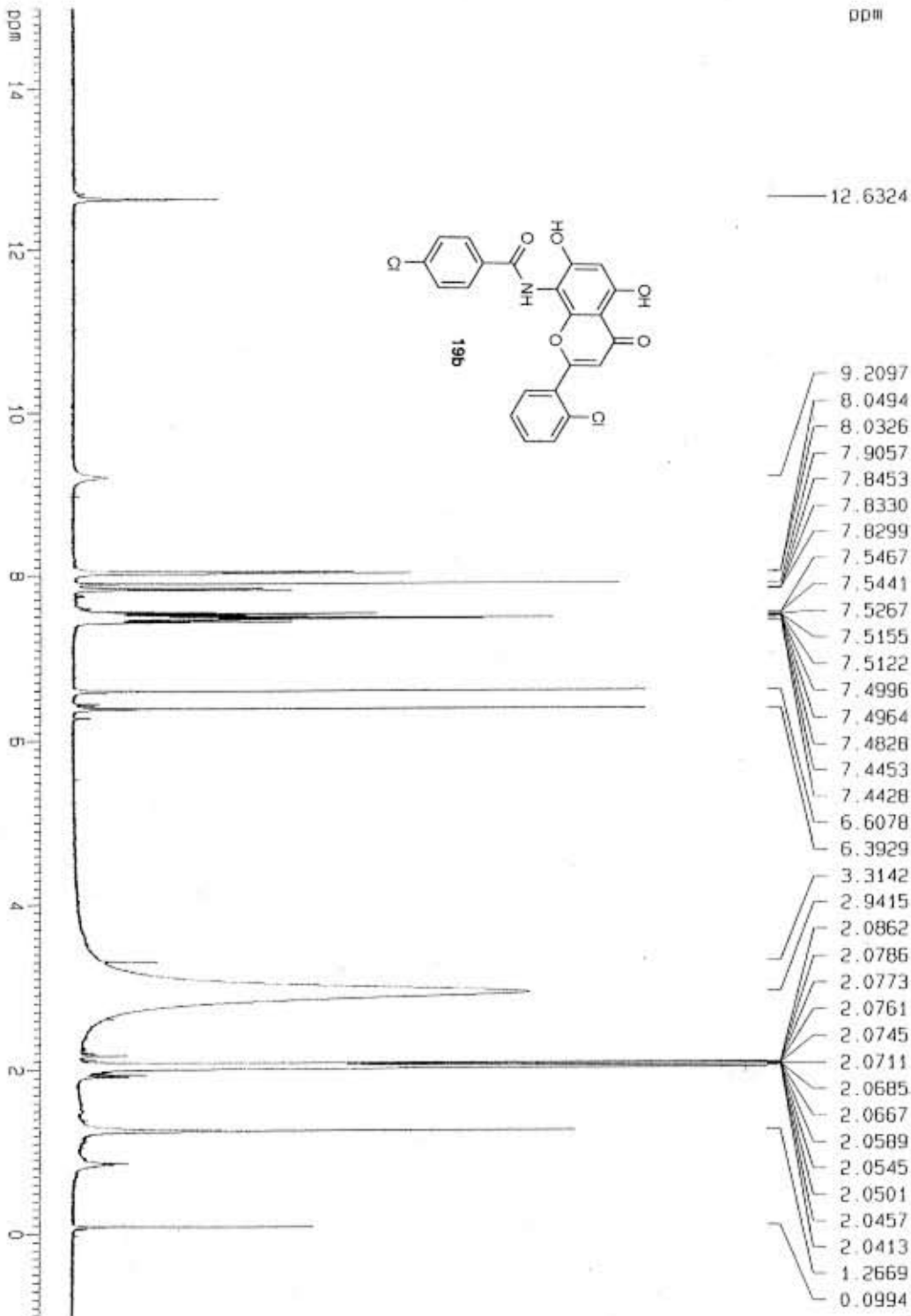
2

0





DDM



Current Data Parameters  
 NAME C1\_1\_149  
 EXPNO 1  
 PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20030515  
 Time 17.49  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zg30  
 TD 32768  
 SOLVENT ACETON  
 NS 32  
 DS 2  
 SMH 10000.000 HZ  
 FIDRES 0.305176 HZ  
 AQ 1.6385000 sec  
 RG 362  
 DW 50.000 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 0.23000000 sec

## \*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 1H  
 P1 7.70 usec  
 PL1 -4.00 dB  
 SFO1 500.1345012 MHz

## F2 - Processing parameters

SI 32768  
 SF 500.1300102 MHz  
 KW EM  
 SSB 0  
 LB 0.30 HZ  
 BB 0  
 PC 1.00

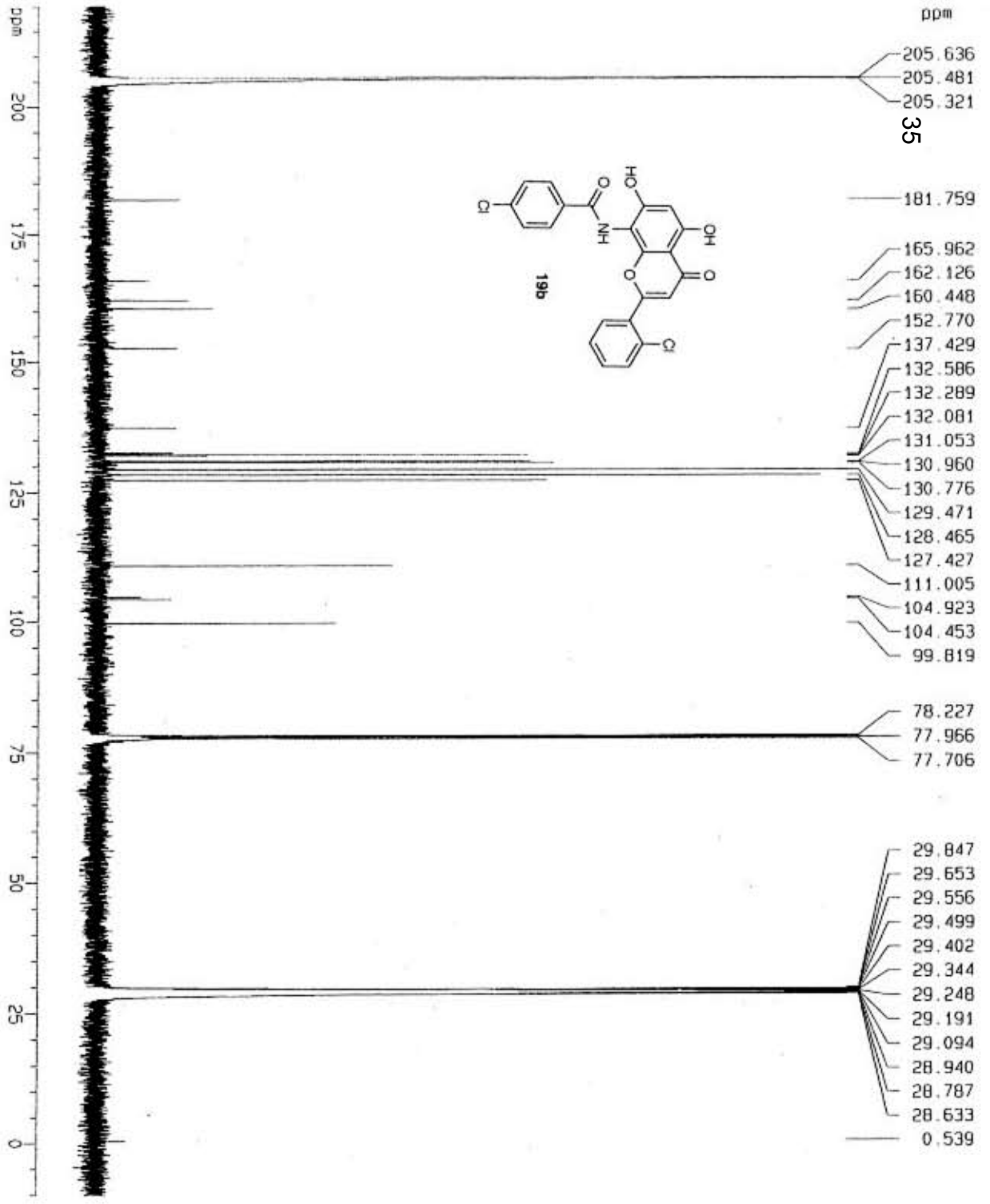
## F1 - Processing parameters

SI 1024  
 KC2 DF  
 SF 500.1300000 MHz  
 WDW OSTINE  
 SSB 0  
 LB 0.30 HZ  
 GB 0

## 1D NMR plot parameters

CX 20.00 cm  
 CV 0.00 cm  
 F1P 15.000 ppm  
 F1 7501.95 HZ  
 F2P -1.018 ppm  
 F2 -509.01 HZ

PPMCK 0.80089 ppm/cm  
 HZCK 400.54816 HZ/cm



F2 - Acquisition Parameters

Date\_ 20020513  
 Time 8:34  
 INSTRUM spect  
 PROCNO 5  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT ACETON  
 NS 40255  
 DS 4  
 SWH 31446.541 Hz  
 FIDRES 0.479826 Hz  
 AQ 1.0420893 sec  
 RG 2048  
 DN 15.900 us/cf  
 DE 5.00 us/cf  
 TE 300.0 K  
 D1 0.10000000 sec  
 D11 0.03000000 sec  
 D12 0.00002000 sec

\*\*\*\*\* CHANNEL F1 \*\*\*\*\*

NUC1 13C  
 P1 10.00 us/cf  
 PL1 5.00 dB  
 SFO1 125.7719472 MHz

\*\*\*\*\* CHANNEL F2 \*\*\*\*\*

CPDPRG2 waltz16  
 NUC2 1H  
 P2 95.00 us/cf  
 PL2 -4.00 dB  
 PL12 19.00 dB  
 PL13 30.00 dB  
 SFO2 500.1325400 MHz

F2 - Processing parameters

SF 65536  
 SF 125.7719408 MHz  
 MDW 5M  
 SSG 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters

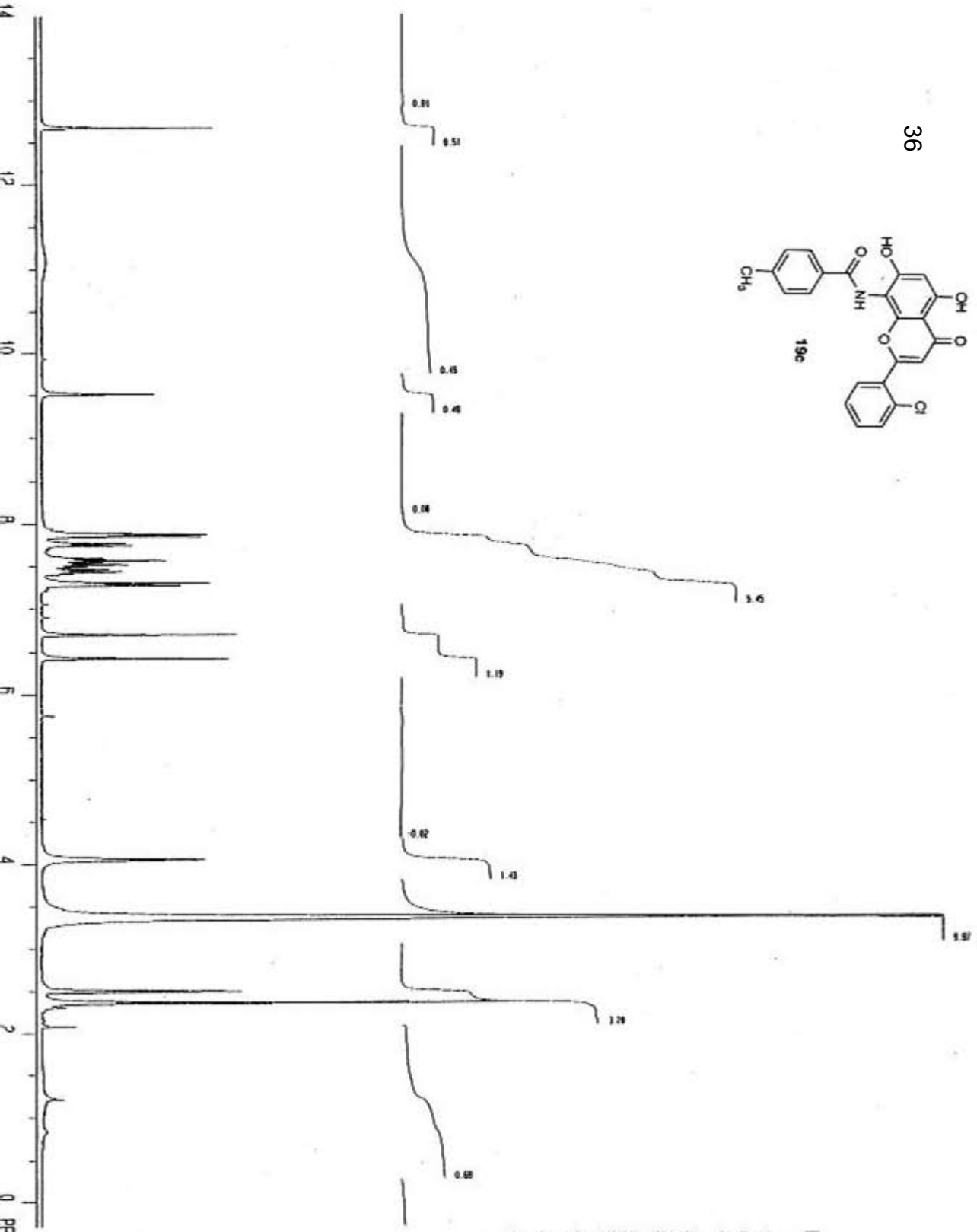
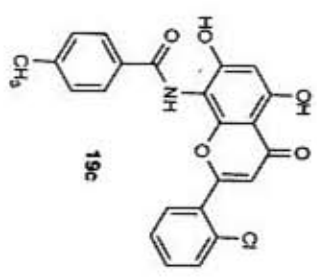
SF 1024  
 OF 0F  
 SF 500.1300000 MHz  
 MDW no  
 SSG 0  
 LB 0.30 Hz  
 GB 0

1D NMR 0101 parameters

CK 20.00 cm  
 CX 0.00 cm  
 F1P 320.000 ppm  
 F1 27866.71 Hz  
 ZPR -10.000 kHz  
 F2 11.30000 ppm/cm  
 SFO1 1469.21472 Hz/cm

1469.21472 Hz/cm

36



GE NMR  
DE PLUS



LN 001  
OSMAY80

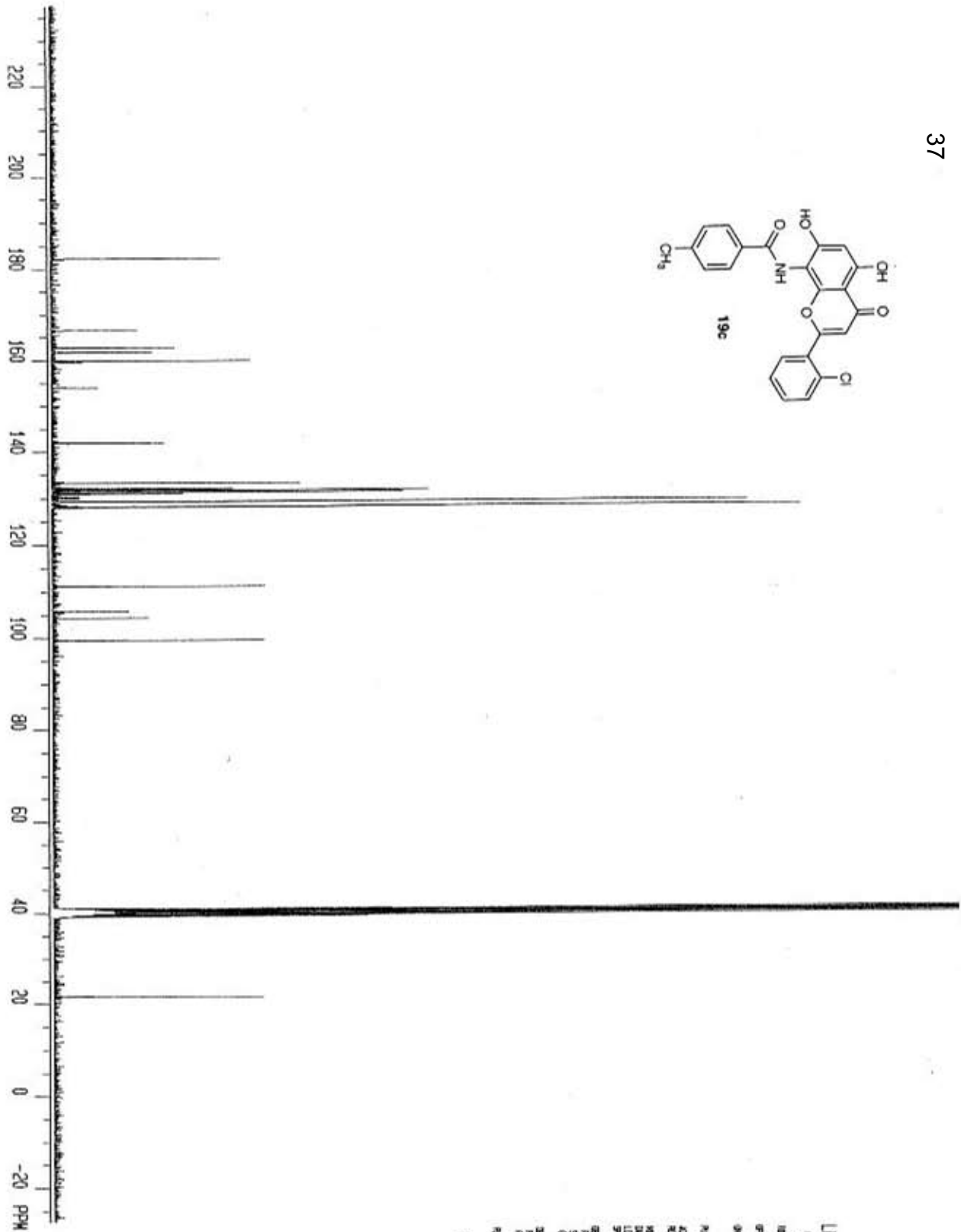
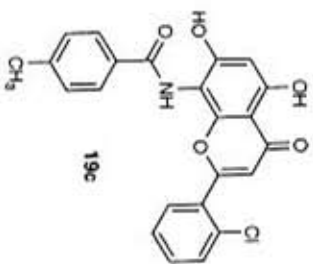
NAME  
OPERATOR SM  
DE FILE SOURCE

PAUSE RECH \* 4.78 SEC  
AQ. TIME \* 30.00 SEC  
RECH. TIME \* 3.71 SEC

NO. OF LINES \* 2728  
DATA FILE NAME \* 19  
SPE. NAME \* 19.PP8

DESIGN \* SM LAMBS M2  
SPE. METHOD \* GDM HC  
GAIN \* 54.31

FLUO SCALE  
SOLVENT  
PWA 54.00  
T0 -28.00 PPM



GE NMR  
DE PLUS

LN.002  
02MAY80

NAME:

FORMULA: C<sub>21</sub>H<sub>15</sub>ClO<sub>3</sub>N

DE PLUS SERVICE

PALE WIDTH \* 1.00000

NO. OF SCANS \* 32

RESOLUTION \* 0.10000

RECORD TIME \* 1.00000

NO. OF LOCKS \* NONE

DATA SIZE \* 32000

LINE WIDTH \* 20.000

SPIN RATE \* 30.000

REFERENCE \* TMS

PROBHD \* 5MM QNP 1H/13

PULPROG \* zgpg30

TD \* 65536

DECOUPLE \* SINGLES - H NOUCLITH

FREQUENCY \* 125.760

PROBHD \* 5MM QNP 1H/13

RG \* 128

RG1 SCALE \* 32768.000

RG2 SCALE \* 1.00000

RG3 SCALE \* 1.00000

RG4 SCALE \* 1.00000

RG5 SCALE \* 1.00000

RG6 SCALE \* 1.00000

RG7 SCALE \* 1.00000

RG8 SCALE \* 1.00000

RG9 SCALE \* 1.00000

RG10 SCALE \* 1.00000

RG11 SCALE \* 1.00000

RG12 SCALE \* 1.00000

RG13 SCALE \* 1.00000

RG14 SCALE \* 1.00000

RG15 SCALE \* 1.00000

RG16 SCALE \* 1.00000

RG17 SCALE \* 1.00000

RG18 SCALE \* 1.00000

RG19 SCALE \* 1.00000

RG20 SCALE \* 1.00000

RG21 SCALE \* 1.00000

RG22 SCALE \* 1.00000

RG23 SCALE \* 1.00000

RG24 SCALE \* 1.00000

RG25 SCALE \* 1.00000

RG26 SCALE \* 1.00000

RG27 SCALE \* 1.00000

RG28 SCALE \* 1.00000

RG29 SCALE \* 1.00000

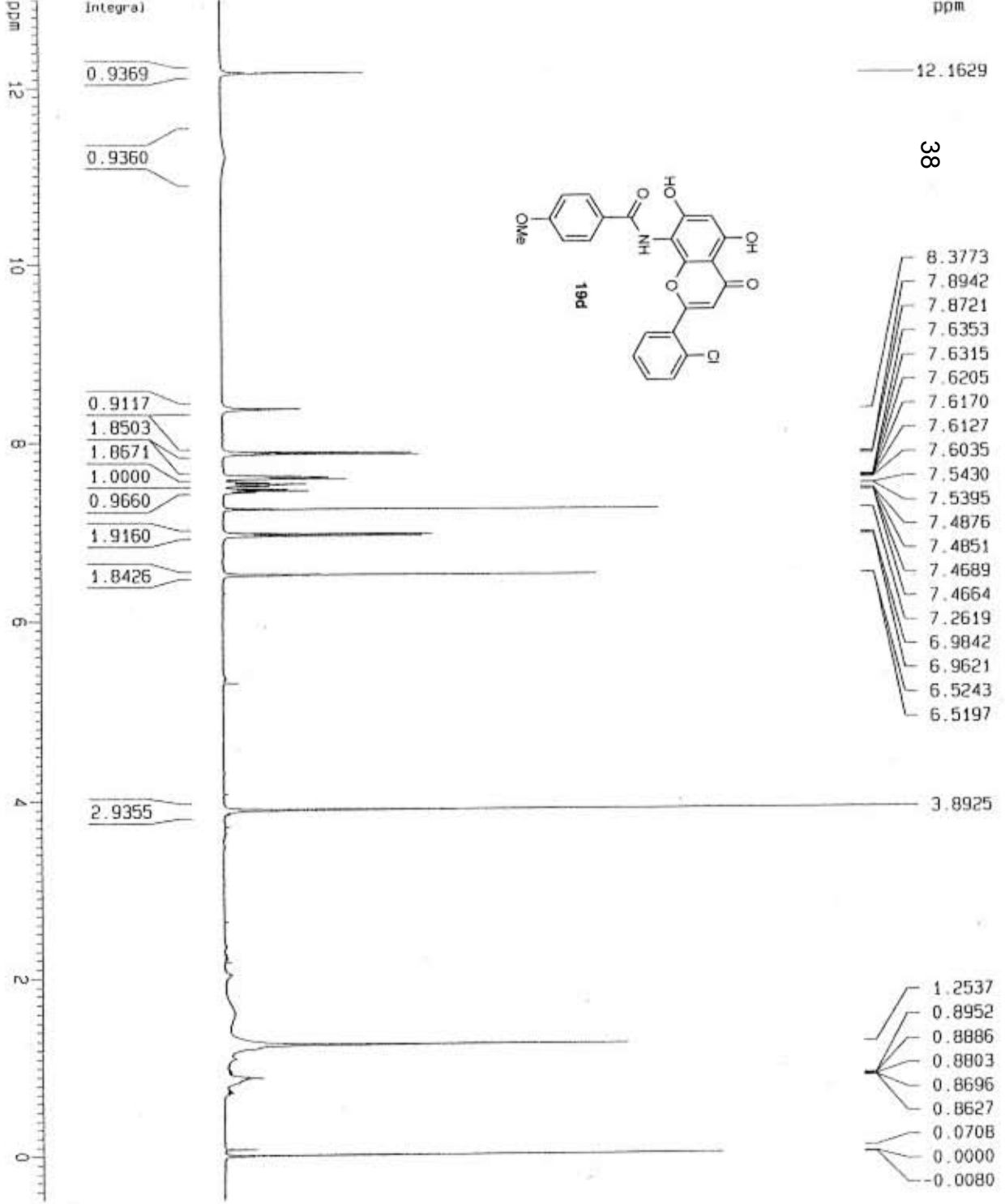
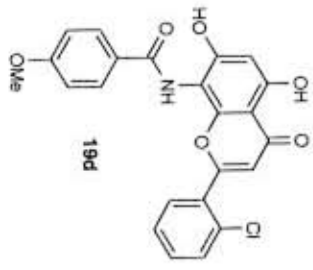
RG30 SCALE \* 1.00000

RG31 SCALE \* 1.00000

RG32 SCALE \* 1.00000

RG33 SCALE \* 1.00000

RG34 SCALE \* 1.00000



NAME: Methoxy amide  
EXPNO: 1  
PROCNO: 1

F2 - Acquisition Parameters  
Date\_: 20021101  
Time: 19.00  
INSTRUM: spect  
PROBHD: 5 mm QNP 1H/15  
PULPROG: zg30  
TD: 65536  
SOLVENT: CDCl3  
NS: 32  
DS: 2  
SWH: 8278.146 Hz  
FIDRES: 0.126314 Hz  
AQ: 3.9584243 sec  
RG: 456.1  
DM: 60.400 usec  
DE: 6.00 usec  
TE: 300.0 K  
D1: 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1: 1H  
P1: 8.70 usec  
PL1: -4.00 dB  
SFO1: 400.1324710 MHz

F2 - Processing Parameters  
SI: 32768  
SF: 400.130085 MHz  
WDW: EM  
SSB: 0  
LB: 0.30 Hz  
GB: 0  
PC: 1.00

1D NMR plot parameters  
CX: 20.00 cm  
CY: 14.48 cm  
F1P: 13.000 ppm  
F1: 5201.59 Hz  
F2P: -0.500 ppm  
F2: -200.06 Hz  
SFOCM: 0.67500 ppm/cm  
HZCM: 270.08777 Hz/cm



GE NMR  
DE PLUS

LN. 002  
09APR80

INSTR. JNM-FX

PRESSURE 5MM

DE PULSE SOURCE

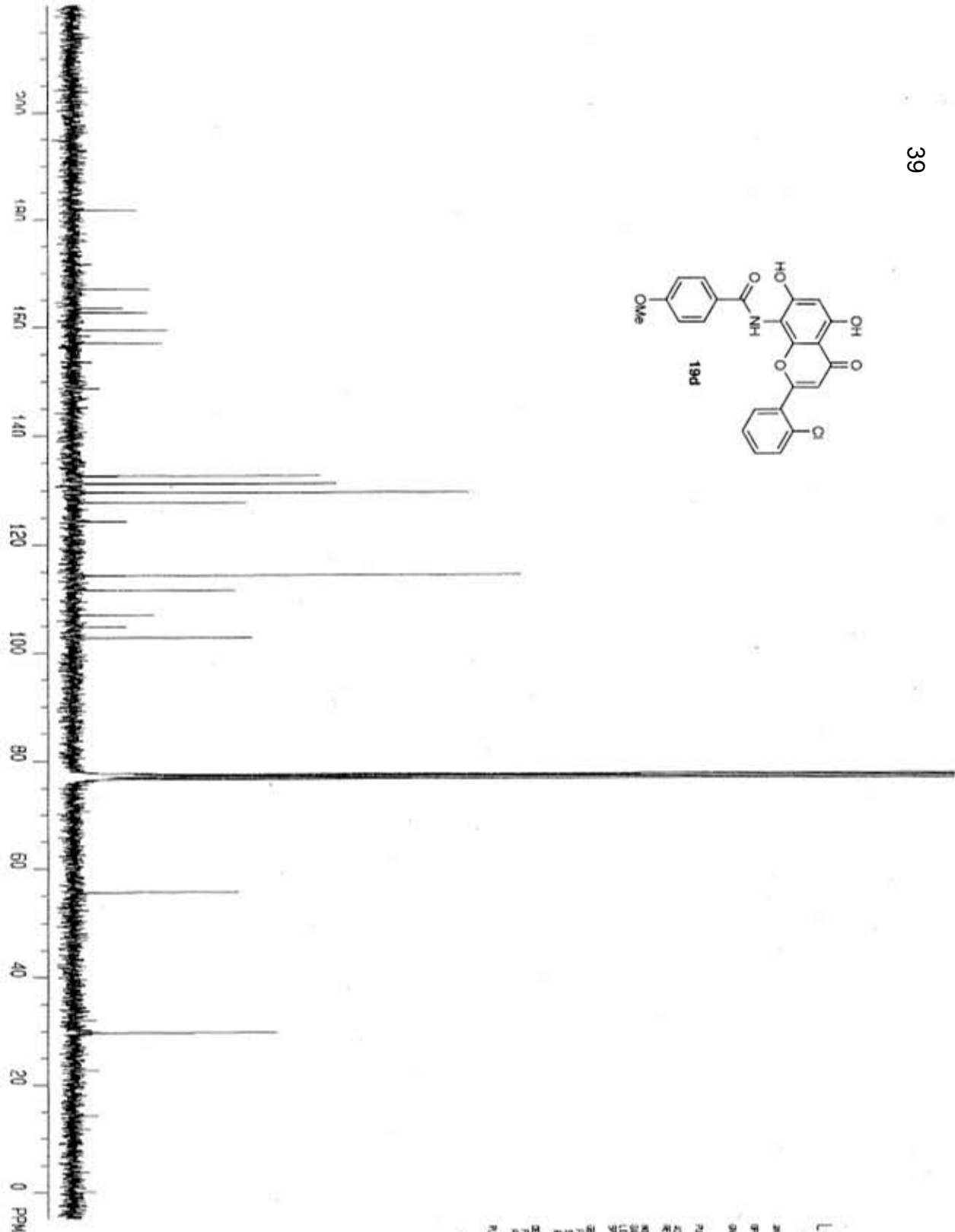
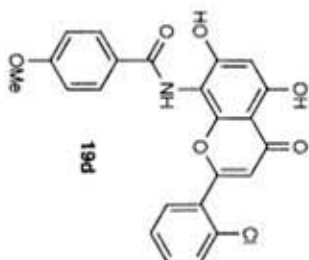
PALE 4000 \* 5.81 SEC  
 QZ 100 \* 80.20 SEC  
 RECHUF TUE \* 1.00 SEC

NO OF ACQ \* 10000  
 QZ1 TIME \* 20.00  
 LINE NUMBER \* 20.00  
 SPIN RATE \* 10.00

ORGANIC  
 PREPARED \* N. AMONIA INC  
 SPEC METHOD \* 2000.00  
 EXCH \* 50.00

EXPERIMENT STANDARDIZATION  
 FREQUENCY \* 4.000 MHz  
 PULSE \* 2.00

RF STATE  
 QZ 50.00 MHz  
 FREQ 1.000 MHz  
 TRAN 20.00  
 TO 4.000 MHz



ppm 12 10 8 6 4 2 0

Integral

0.8891

1.0000  
0.9705  
2.0314  
1.0043  
0.9585  
0.8795

4.1148

4.1414

ppm

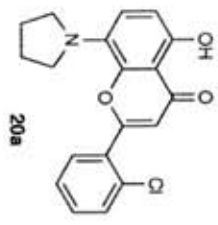
12.0185

40

7.6596  
7.6553  
7.6411  
7.6366  
7.5733  
7.5566  
7.5537  
7.4978  
7.4934  
7.4639  
7.4604  
7.4450  
7.4420  
7.0951  
7.0730  
6.7952  
6.7731  
6.5977

3.3551  
3.3391  
3.3232

1.9695  
1.9609  
1.9533  
1.9458  
1.9372



Current Data Parameters  
NAME YA-11-179-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20010307  
Time 11.16

INSTRUM drx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3

DS 16  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec  
RG 228.1  
DW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1320007 MHz

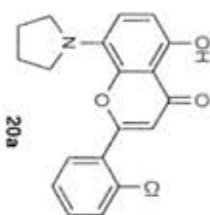
F2 - Processing parameters  
SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ID NMR plot parameters  
CX 20.00 cm  
FLP 13.000 ppm  
P1 5201.69 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
PENCN 0.65500 ppm/cm  
HZCM 266.08646 Hz/cm



ppm

184.199  
41  
163.454  
152.934  
147.634  
133.176  
132.353  
132.234  
131.731  
131.218  
131.059  
127.587  
121.896  
112.100  
111.852  
111.264  
77.766  
77.449  
77.131  
51.400  
25.316



ppm  
175  
150  
125  
100  
75  
50  
25  
0

Current Data Parameters

NAME VA-11-17a-1C  
EXNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20010307  
Time 11.19  
INSTRUM dx400  
PROBHD 5 mm Multinu  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 485  
DS 2  
SMB 23148.148 Hz  
FIDRES 0.353213 Hz  
AQ 1.4158276 sec  
RG 1024  
DM 21.600 usec  
DE 4.50 usec  
TE 300.0 K  
D1 0.05000000 sec  
d11 0.03000000 sec  
d12 0.00002000 sec

\*\*\*\*\* CHANNEL F1 \*\*\*\*\*

NUC1 13C  
P1 12.30 usec  
PL1 2.00 dB  
SFO1 100.6232933 MHz

\*\*\*\*\* CHANNEL F2 \*\*\*\*\*

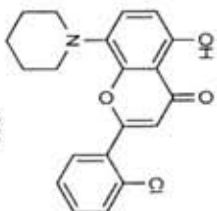
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 0.00 dB  
PL12 18.00 dB  
PL13 18.00 dB  
SFO2 400.1318005 MHz

F2 - Processing parameters

SI 32768  
SF 100.6127290 MHz  
KHZ BW  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR plot parameters

CX 20.00 cm  
FIP 210.000 ppm  
F1 21128.87 Hz  
F2p -5.000 ppm  
F2 -503.06 Hz  
FREQCN 10.75000 ppm/cm  
HZCN 1081.58651 Hz/cm



7.7718  
7.7667  
7.7536  
7.7482  
7.5794  
7.5635  
7.5605  
7.4981  
7.4932  
7.4778  
7.4729  
7.4585  
7.4545  
7.2912  
7.2693  
6.8037  
6.7818  
6.7648  
5.3179

3.0284  
3.0157  
3.0026  
1.7695  
1.7548  
1.7410  
1.7281  
1.7139  
1.6754  
1.6158  
1.6006  
1.5868  
1.5723

Integral

0.9060

1.0000

0.9546

2.0139

1.1255

0.9714

0.8846

4.1095

4.1891

2.0931

Current Data Parameters  
NAME YA-11-180-1  
EXTNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20010307  
Time 17.11

INSTRUM drx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2

SMH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec

RG 228.1  
DW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.000000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 IR

P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1320007 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ID NMR plot parameters

CX 20.00 cm  
F1P 13.000 ppm  
F1 5201.69 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
PCHCM 0.66500 ppm/cm  
HZCM 266.08646 Hz/cm

ppm  
12  
10  
8  
6  
4  
2  
0

ppm

43  
184.191

163.221

155.617

150.274

134.528

133.214

132.453

131.809

131.455

131.216

127.588

126.132

112.228

111.798

111.061

77.769

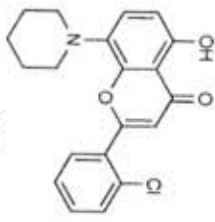
77.451

77.133

53.787

26.812

24.597



ppm  
175  
150  
125  
100  
75  
50  
25  
0

Current Data Parameters  
 NAME YA-11-180-1C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20010307  
 Time 17.14

INSTRUM dtx400  
 PROBRD 5 mm Multinu  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 289

DS 2  
 SWH 23148.148 Hz  
 FIDRES 0.352113 Hz  
 AQ 1.4156276 sec  
 RG 4096

TDW 21.500 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 0.05000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 12.30 usec  
 PL1 2.00 dB  
 SFO1 100.6212933 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCP02 100.00 usec  
 PL2 0.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127290 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CK 20.00 cm  
 F3P 210.000 ppm  
 F1 21128.67 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 SFOCK 10.75000 ppm/cm  
 HZCM 1081.58691 Hz/cm

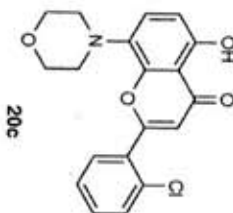
ppm

12.2226

44

7.7160  
7.7117  
7.6973  
7.6928  
7.5741  
7.5713  
7.5183  
7.5141  
7.4849  
7.4813  
7.4661  
7.4629  
7.3003  
7.2831  
7.2784  
6.8285  
6.8065  
6.7165

3.8739  
3.8626  
3.8511  
3.0985  
3.0871  
3.0758



Integral

0.9059

1.0000

0.9729

1.0431

1.0397

1.1427

0.9800

0.8907

4.1468

4.1333

Current Data Parameters  
NAME YA-11-1996-1  
EXMNO 177 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20010305

Time 16.30  
INSTRUM dtx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SMH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec  
RG 228.1  
DW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

----- CHANNEL f1 -----

NUC1 1H  
P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1320007 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

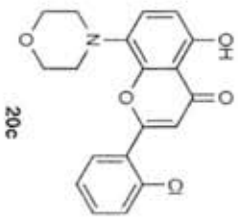
1D NMR plot parameters

CX 20.00 cm  
F1P 13.000 ppm  
F1 5201.69 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
PPMCM 0.66500 ppm/cm  
HZCM 266.08646 Hz/cm

ppm 12 10 8 6 4 2 0

ppm

- 184.033
- 45
- 163.489
- 156.248
- 150.373
- 133.141
- 132.894
- 132.622
- 131.774
- 131.496
- 131.170
- 127.697
- 126.151
- 112.274
- 111.839
- 111.271
- 77.767
- 77.449
- 77.132
- 67.619
- 52.543



ppm



Current Data Parameters  
 NAME YA-11-176-1C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20010305  
 Time 16.35  
 INSTRUM dx400  
 PROBRD 5 mm Multinu  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 355  
 DS 2  
 SWH 23148.148 Hz  
 FIDRES 0.359213 Hz  
 AQ 1.4156276 sec  
 RG 1024  
 DW 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 0.05000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

CHANNEL f1

NUC1 13C  
 P1 12.30 usec  
 PL1 2.00 dB  
 SFO1 100.6219933 MHz

CHANNEL f2

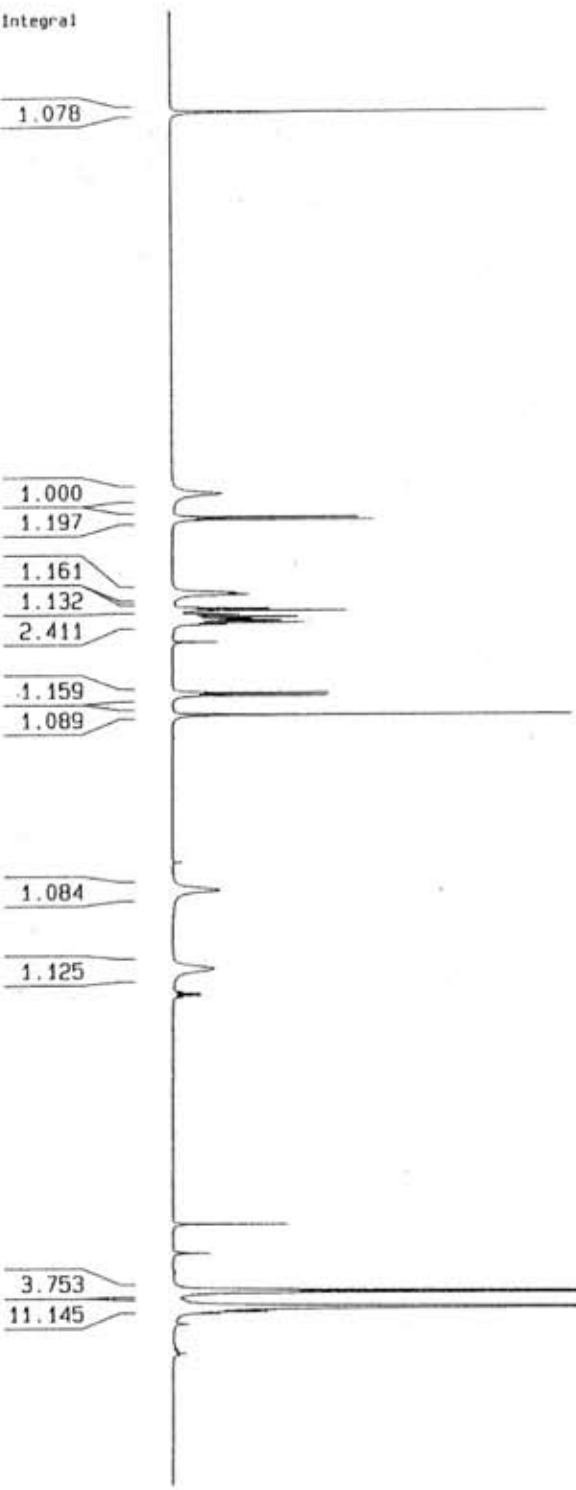
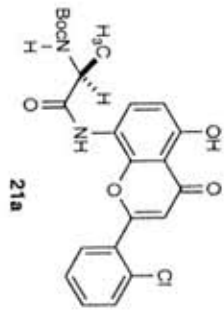
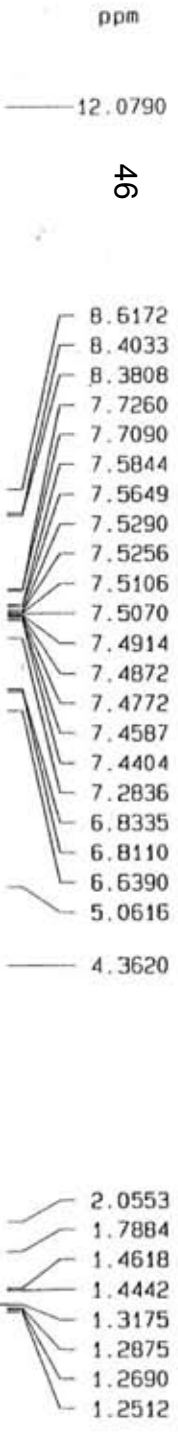
CPDPRG2 waltz16  
 NUC2 1H  
 PCP02 100.00 usec  
 PL2 0.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768  
 SF 100.6127290 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

ID NMR plot parameters

SI 20.00 cm  
 CX 210.000 ppm  
 F1 21128.67 Hz  
 F2 -5.000 ppm  
 PPMCK 10.75000 ppm/cm  
 HZCM 1081.58691 Hz/cm



Current Data Parameters  
 NAME YA-11-171-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 1010227  
 Time 15.27  
 INSTRUM drx400  
 PROBRD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SMH 6012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 161.3  
 DM 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec  
 P1 7.70 usec  
 DE 4.50 usec  
 SFO1 400.132007 MHz  
 NUC1 1H  
 PL1 -6.00 dB

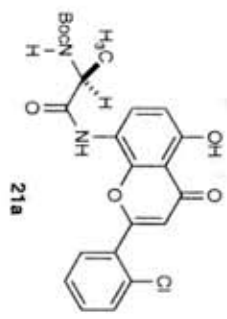
F2 - Processing parameters  
 SI 16384  
 SF 400.130000 MHz  
 MDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 13.000 ppm  
 F1 5201.65 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPMCM 0.66500 DPM/CM  
 HZCM 255.06546 HZ/CM

ppm

47

- 185.379
- 171.381
- 163.464
- 157.096
- 156.219
- 147.029
- 133.170
- 132.812
- 131.523
- 131.197
- 128.930
- 127.862
- 118.162
- 112.159
- 111.435
- 110.735
- 80.832
- 77.777
- 77.460
- 77.141
- 51.211
- 28.528
- 18.082
- 14.609



ppm

Current Data Parameters  
 NAME YA-11-171-1C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 1010227  
 Time 15:32  
 INSTRUM drx400  
 PROBHD 5 mm NUI11nu  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 854  
 DS 2  
 SWH 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156276 sec  
 RG 1024  
 DM 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 d11 0.0200000 sec  
 d12 0.0000200 sec  
 PL13 18.00 dB  
 D1 0.05000000 sec

CPDPRG2 waltz16  
 PCPD2 100.00 usec  
 SF02 400.1315005 MHz  
 NUC2 1H  
 PL2 0.00 dB  
 PL12 18.00 dB  
 P1 12.30 usec  
 DE 4.50 usec  
 SF01 100.6232933 MHz  
 NUC1 13C  
 PL1 2.00 dB

F2 - Processing Parameters  
 SI 32768  
 SF 100.6127290 MHz  
 MDK EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters

CX 20.00 cm  
 F1P 210.000 ppm  
 F1 21128.67 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 PPRCK 10.75000 ppm/cm  
 HZCM 1081.58691 Hz/cm

ppm

4.8

12.8537

8.4577

8.4353

8.0481

7.6218

7.6029

7.5866

7.5667

7.5496

7.5355

7.5314

7.4850

7.4701

7.4667

7.2845

7.1953

7.1761

7.1572

7.1129

6.8646

6.8420

6.5962

5.3226

5.0833

4.4965

3.9957

3.9791

3.1754

3.1604

1.6278

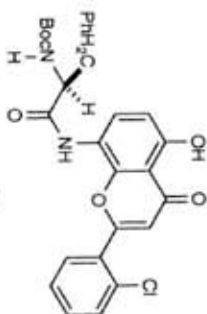
1.3283

1.2797

1.2742

0.9832

0.9664



Integral

1.0000

1.0183

1.0168

4.4614

5.1674

1.1667

1.0444

0.9341

1.0299

2.0867

9.7979

Current Data Parameters  
 NAME YA-11-164-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 1010219  
 Time 17.59  
 INSTRUM drx400  
 PROBRD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2

SMH 8012.820 Hz  
 FIDRES 0.244532 Hz

AQ 2.0447731 sec

RG 456.1

DM 62.400 usec

DE 4.50 usec

TE 300.0 K

D1 1.00000000 sec

P1 7.70 usec

DE 4.50 usec

SFO1 400.1320007 MHz

M/CI 1H

PL1 -6.00 dB

F2 - Processing parameters

SF 400.1300000 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

10 NMR plot parameters

CX 20.00 cm

F1P 13.000 ppm

F1 5201.65 Hz

F2P -0.300 ppm

F2 -120.04 Hz

PPMCM 0.56500 ppm/cm

HZCM 266.08646 Hz/cm

ppm

12

10

8

6

4

2

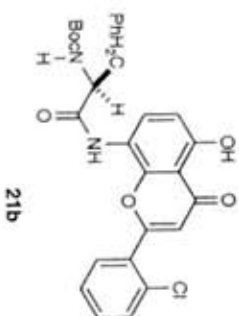
0



ppm

49

183.327  
169.961  
163.468  
157.057  
146.592  
136.625  
133.157  
132.838  
131.632  
131.419  
131.171  
129.612  
129.099  
128.533  
127.909  
127.435  
117.857  
112.011  
111.493  
110.673  
80.896  
77.751  
77.433  
77.116  
57.123  
38.741  
28.538  
19.451



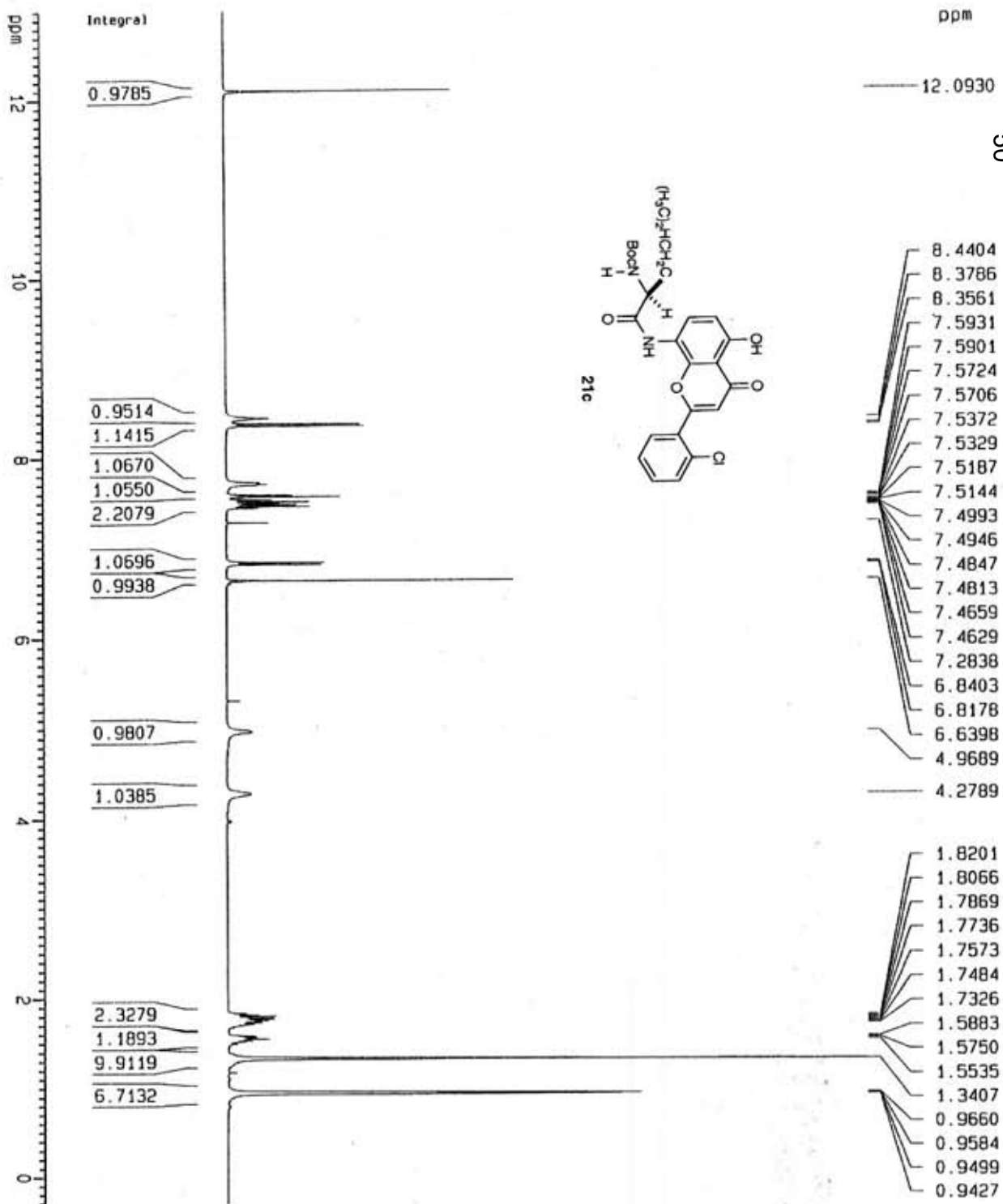
ppm

Current Data Parameters  
NAME YA-11-16A-1C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 10:02:18  
Time 18.03  
INSTRUM drx400  
PROBHD 5 mm NUT11nu  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1895  
DS 2  
SWH 231.48148 Hz  
FIDRES 0.353213 Hz  
AQ 1.4156276 sec  
RG 1024  
DM 21.500 usec  
DE 4.50 usec  
TE 300.0 K  
D11 0.0300000 sec  
D12 0.0000200 sec  
PL13 18.00 dB  
D1 0.05000000 sec  
CPOPRG2 waltz16  
PCPD2 100.00 usec  
SF02 400.1315005 MHz  
NUC2 1H  
PL2 0.00 dB  
PL12 18.00 dB  
P1 12.30 usec  
DE 4.50 usec  
SF01 100.6232933 MHz  
NUC1 13C  
PL1 2.00 dB

F2 - Processing parameters  
SI 32768  
SF 100.6127290 MHz  
KOHM EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

10 NMR plot parameters  
CX 20.00 cm  
F1P 210.000 ppm  
F1 21128.67 Hz  
F2P -5.000 ppm  
F2 -503.06 Hz  
PPMCK 10.75000 ppm/cm  
HZCK 1081.58691 Hz/cm



Current Data Parameters  
 NAME YA-11-155-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 1010220  
 Time 11.17

INSTRUM drx400  
 PROCNO 5 mm Multinu  
 PULPROG zg30  
 TO 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2

SWH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 114  
 DM 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K

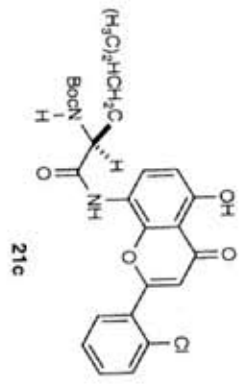
D1 1.00000000 sec  
 P1 7.70 usec  
 DE 4.50 usec  
 SF01 400.1320007 MHz  
 NUC1 1H  
 PL1 -6.00 dB

F2 - Processing parameters  
 SI 16384  
 SF 400.1300000 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 20.00 cm  
 F1P 13.000 ppm  
 F1 5201.69 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPMCK 0.66500 ppm/cm  
 HZCM 266.08646 Hz/cm

51

- 183.386
- 171.365
- 163.485
- 157.210
- 156.289
- 147.149
- 133.138
- 132.813
- 131.512
- 131.238
- 129.173
- 127.891
- 118.031
- 112.165
- 111.461
- 110.746
- 80.747
- 77.770
- 77.453
- 77.135
- 54.189
- 41.345
- 28.552
- 25.225
- 23.336
- 22.378



Current Data Parameters  
 NAME YA-11-165-1C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 10/02/20  
 Time 11:22  
 INSTRUM dry400  
 PROBHD 5 mm WJ11nu  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT COCl3  
 NS 877  
 DS 2

SWH 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156276 sec  
 RG 1024

DM 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 d11 0.0200000 sec  
 d12 0.0000200 sec  
 PL13 18.00 dB  
 D1 0.05000000 sec

PROGNAME waltz16  
 PCPD2 100.00 usec  
 SF02 400.1315005 MHz  
 NUC2 1H

PL2 0.00 dB  
 PL12 18.00 dB  
 P1 12.30 usec  
 DE 4.50 usec

SF01 100.6232933 MHz  
 NUC1 13C  
 PL1 2.00 dB

F2 - Processing parameters

S1 32758  
 SF 100.6127290 MHz  
 MDK EM  
 SSB 0  
 LB 1.00 HZ  
 GB 0  
 PC 1.40

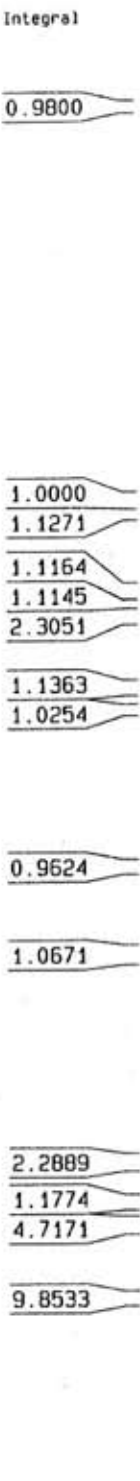
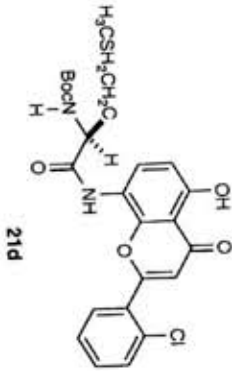
10 NMR Plot Parameters

CX 20.00 cm  
 F1P 210.000 ppm  
 F1 21128.67 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 PPMCH 10.75000 ppm/cm  
 HZCH 1081.58691 Hz/cm

ppm

52

12.1093  
8.5217  
8.4191  
8.3966  
7.7233  
7.7057  
7.6003  
7.5807  
7.5466  
7.5423  
7.5279  
7.5239  
7.5087  
7.5042  
7.4945  
7.4915  
7.4758  
7.4731  
7.2840  
6.8630  
6.8405  
6.6472  
5.3198  
5.2443  
4.4706  
4.4544  
2.6291  
2.6120  
2.5956  
2.5795  
2.2299  
2.2121  
2.1951  
2.0676  
2.0441  
2.0262  
2.0085  
1.4630  
1.3569  
1.2947  
1.2767



## Current Data Parameters

NAME YA-11-188-2  
EXPNO 1  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 1010321  
Time 18.15  
INSTRUM drx400  
PROBHD 5 mm WJltinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec  
RG 322.5  
DM 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.0000000 sec  
P1 7.70 usec  
DE 4.50 usec  
SF01 400.1320007 MHz  
NUC1 1H  
PL1 -6.00 dB

## F2 - Processing parameters

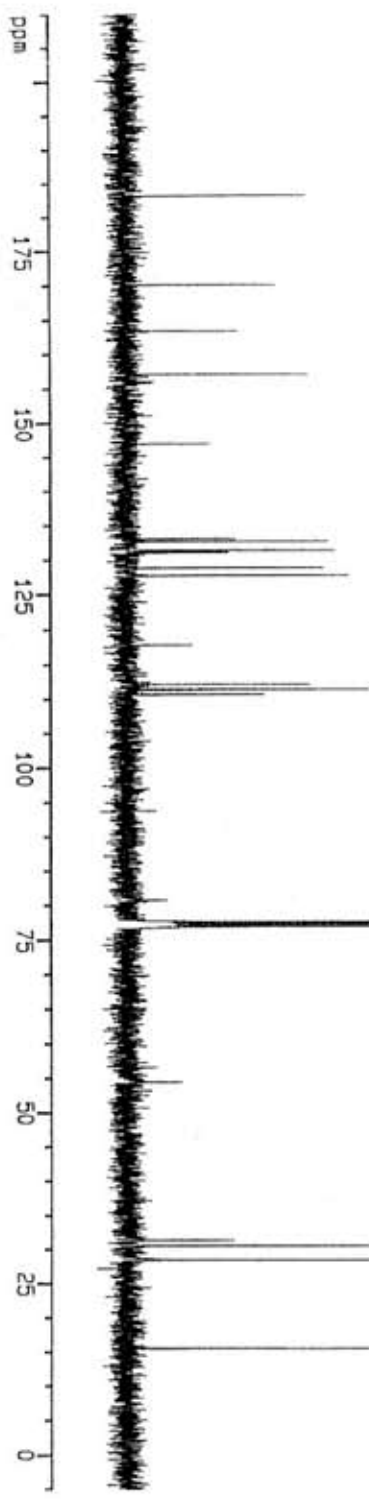
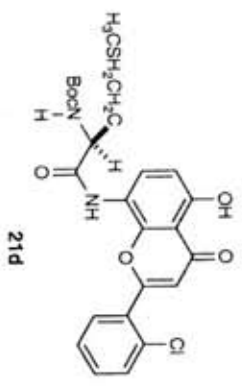
SI 16384  
SF 400.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

## 1D NMR plot parameters

CX 20.00 cm  
F1P 13.000 ppm  
F1 5201.69 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
PPMCM 0.66500 ppm/cm  
HZCM 266.08646 Hz/cm

ppm

- 183.532
- 170.094
- 163.298
- 157.078
- 146.856
- 133.014
- 132.626
- 131.311
- 131.262
- 130.998
- 128.767
- 127.663
- 117.695
- 112.028
- 111.291
- 110.560
- 80.697
- 77.551
- 77.233
- 76.915
- 54.330
- 31.260
- 30.475
- 28.361
- 15.429



Current Data Parameters  
 NAME YA-11-188-2C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

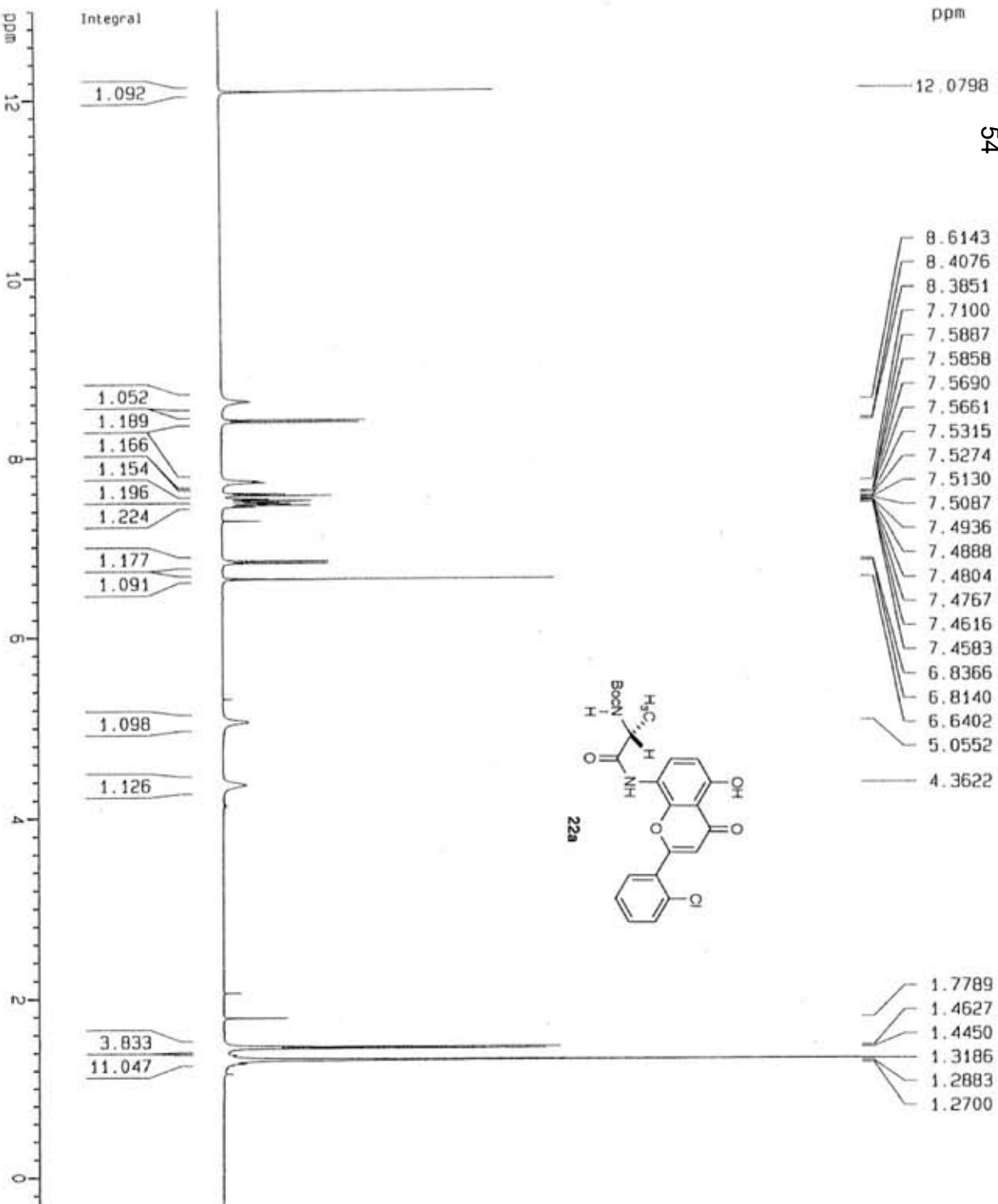
Date\_ 1010322  
 Time 10.13  
 INSTRUM drx400  
 PROBHD 5 mm Multinu  
 PULPROG zgpg30  
 TD 65536  
 TO  
 SOLVENT CDCl3  
 NS 1024  
 DS 2  
 SWH 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156276 sec  
 RG 1290.2  
 DM 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 PL13 18.00 dB  
 O1 0.05000000 sec  
 CPDPRG2 waltz16  
 PCPD2 100.00 usec  
 SF02 400.1315005 MHz  
 NUC2 1H  
 PL2 0.00 dB  
 PL12 18.00 dB  
 P1 12.30 usec  
 DE 4.50 usec  
 SF01 100.6232933 MHz  
 NUC1 13C  
 PL1 2.00 dB

F2 - Processing parameters

SI 32768  
 SF 100.6127503 MHz  
 KHM EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

10 NMR plot parameters

CX 20.00 cm  
 F1P 210.000 DPM  
 F1 21126.68 Hz  
 F2P -5.000 DPM  
 F2 -503.06 Hz  
 PPMCK 10.75000 ppm/cm  
 HZCM 1081.58704 Hz/cm



Current Data Parameters  
 NAME VA-11-170-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 1010226  
 Time 18.06  
 INSTRUM drx400  
 PROBNM 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.044773; sec  
 RG 161.3  
 DW 52.400 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 1.0000000 sec  
 P1 7.70 usec  
 DE 4.50 usec  
 SFO1 400.1320007 MHz  
 NUC1 1H  
 PL1 -6.00 dB

F2 - Processing parameters  
 SI 15384  
 SF 400.1300000 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 F1P 13.000 ppm  
 F1 5201.69 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPMCM 0.65500 ppm/cm  
 HZCM 266.06546 Hz/cm

ppm

183.984

171.374

163.467

157.091

156.227

147.021

133.171

132.813

131.525

131.200

128.920

127.863

118.172

112.160

111.441

110.736

80.853

77.776

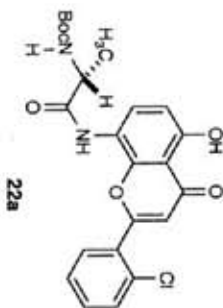
77.458

77.140

51.230

28.530

18.080



ppm

Current Data Parameters  
 NAME YA-11-170-1C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 1010226  
 Time 18.09  
 INSTRUM drx400  
 PROBNM 5 ml Multinu  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 705  
 DS 2

SWH 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156275 sec  
 RG 4096

DW 21.800 usec  
 DE 4.50 usec  
 TE 300.0 K  
 d11 0.0300000 sec  
 d12 0.0000200 sec  
 PL13 16.00 dB  
 O1 0.05000000 sec  
 CPROG2 wait15

PCPD2 100.00 usec  
 SF02 400.1315005 MHz  
 NUC2 1H  
 PL2 0.00 dB  
 PL12 16.00 dB  
 P1 12.20 usec  
 DE 4.50 usec  
 SF01 100.6232933 MHz  
 NUC1 13C  
 PL1 2.00 dB

F2 - Processing Parameters  
 SI 32768  
 SF 100.6127290 MHz  
 KDN EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters

CX 20.000 cm  
 F1P 210.000 dm  
 F1 21128.67 Hz  
 F2p -5.000 dm  
 F2 -503.06 Hz  
 PPMCM 10.75000 ppm/cm  
 HCM 1081.58691 Hz/cm

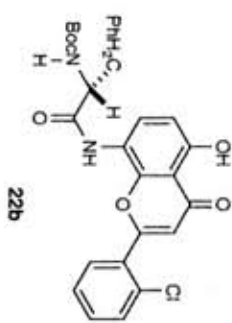
ppm  
12  
10  
8  
6  
4  
2  
0

Integral

0.9446  
1.0000  
1.0054  
4.2375  
5.1189  
1.0397  
0.9567  
0.8974  
1.0209  
2.1106  
9.2184

ppm  
12.0528  
56

8.4515  
8.4288  
8.0590  
7.6048  
7.6014  
7.5664  
7.5632  
7.5321  
7.5279  
7.4856  
7.4817  
7.4668  
7.4633  
7.2835  
7.2149  
7.1944  
7.1749  
7.1560  
6.8597  
6.8371  
6.5939  
5.0974  
4.5141  
4.4995  
3.1759  
3.1600  
2.0665  
1.6536  
1.4299  
1.3260  
1.2981  
1.2795



Current Data Parameters  
NAME YA-11-160-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20010214  
Time 20.39  
INSTRUM drx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SFR 8013.820 Hz  
FIDRES 0.244512 Hz  
AQ 2.0447731 sec  
RG 256  
DW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
NUC1 1H  
P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.132007 MHz

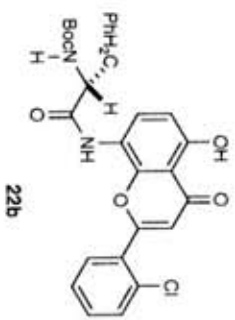
F2 - Processing parameters  
SI 16384  
SF 400.1300000 MHz  
MVM EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

ID NMR plot parameters  
CX 20.00 cm  
F1P 13.000 ppm  
F1 5201.69 Hz  
F2P -0.300 ppm  
F2 -120.04 Hz  
PPMCK 0.66500 ppm/cm  
HZCM 266.08646 Hz/cm



57

- 183.328
- 169.979
- 163.471
- 157.055
- 155.911
- 146.601
- 136.639
- 133.152
- 132.846
- 131.633
- 131.425
- 131.160
- 129.617
- 129.102
- 128.545
- 127.915
- 127.436
- 117.855
- 112.011
- 111.489
- 110.669
- 80.874
- 77.762
- 77.443
- 77.126
- 57.130
- 38.740
- 28.541



NAME: YA-II-160-1C  
 EXPNO: 1  
 PROCNO: 1

F2 - Acquisition Parameters

Date\_: 20010214  
 Time: 20.44  
 INSTRUM: drx400  
 PROBRD: 5 mm Multinu  
 PULPROG: zgpg30  
 TD: 65536  
 SOLVENT: CDCl3  
 NS: 3185  
 DS: 2  
 SWH: 23148.148 Hz  
 FIDRES: 0.351213 Hz  
 AQ: 1.4156276 sec  
 RG: 2048  
 DW: 21.600 usec  
 DE: 4.50 usec  
 TE: 300.0 K  
 D1: 0.05000000 sec  
 d11: 0.03000000 sec  
 d12: 0.00002000 sec

CHANNEL F1

NUC1: 13C  
 P1: 12.30 usec  
 PL1: 2.00 dB  
 SFO1: 100.6212933 MHz

CHANNEL F2

CPDPRG2: waltz16  
 NUC2: 1H  
 PCP02: 100.00 usec  
 PL2: 0.00 dB  
 PL12: 18.00 dB  
 PL13: 18.00 dB  
 SFO2: 400.1316005 MHz

F2 - Processing parameters

SI: 32768  
 SF: 100.6127290 MHz  
 WDW: EM  
 SSB: 0  
 LB: 1.00 Hz  
 GB: 0  
 PC: 1.40

ID NMR plot parameters

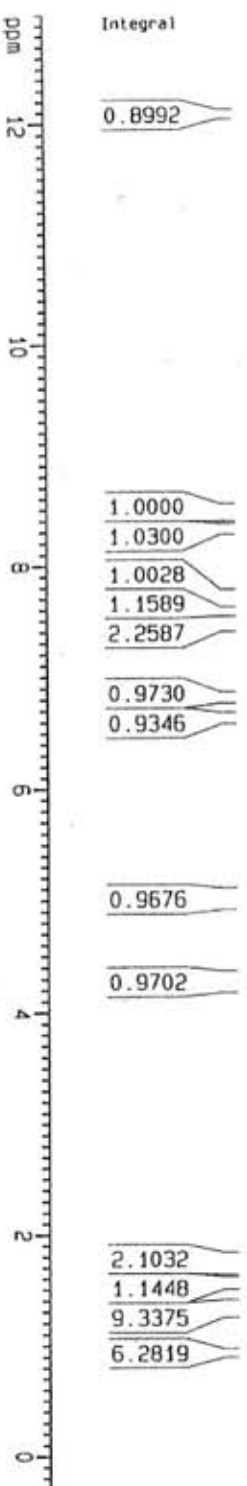
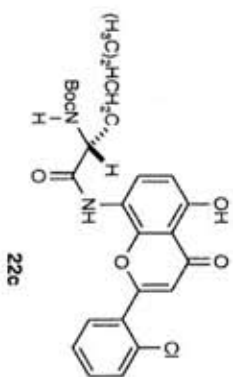
CK: 20.00 cm  
 P1P: 220.000 ppm  
 F1: 22134.86 Hz  
 F2P: -5.000 ppm  
 PCWK: 11.2500 ppm/cm  
 HZCM: 1131.89319 Hz/cm

ppm

12.0910

58

- 8.4684
- 8.3441
- 8.3216
- 7.7012
- 7.5811
- 7.5781
- 7.5613
- 7.5586
- 7.5262
- 7.5218
- 7.5077
- 7.5034
- 7.4883
- 7.4837
- 7.4740
- 7.4706
- 7.4553
- 7.4522
- 6.8223
- 6.7998
- 6.6343
- 5.3091
- 5.0293
- 5.0140
- 2.0522
- 1.8507
- 1.7969
- 1.7773
- 1.7638
- 1.5525
- 1.4792
- 1.3358
- 1.0558
- 1.0399
- 0.9877
- 0.9710
- 0.9584
- 0.9503
- 0.9424
- 0.9346



Integral

0.8992

1.0000

1.0300

1.0028

1.1589

2.2587

0.9730

0.9346

0.9676

0.9702

2.1032

1.1448

9.3375

6.2819

Current Data Parameters  
 NAME YA-11-167-1H  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 1010221  
 Time 18.13

INSTRUM drx400  
 PROBD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2

SMH 8012.820 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 90.5  
 DM 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K

D1 1.00000000 sec  
 P1 7.70 usec  
 DE 4.50 usec  
 SF01 400.1320007 MHz  
 NUC1 1H  
 PL1 -6.00 dB

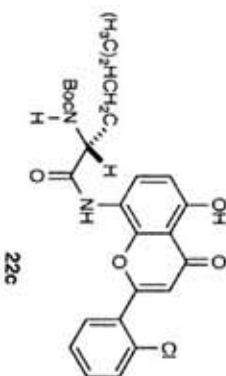
F2 - Processing parameters  
 SI 16384  
 SF 400.1300000 MHz  
 KW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 13.000 ppm  
 F1 5201.69 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPM/CM 0.56500 ppm/cm  
 HZ/CM 266.08646 Hz/cm

ppm

59

171.401  
163.467  
161.543  
157.230  
156.299  
147.198  
133.125  
132.804  
131.626  
131.505  
131.344  
131.221  
129.229  
127.886  
118.009  
117.020  
114.063  
112.157  
111.441  
110.740  
80.719  
77.779  
77.461  
77.143  
72.322  
54.187  
41.354  
28.782  
28.553  
28.311  
25.222  
23.702  
23.338  
22.378  
22.056  
19.437



ppm

```

Current Data Parameters
NAME      YA-II-167-1C
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20010228
Time     17.28
INSTRUM  drx400
PROBHD   5 mm Multinu
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       1287
DS       2
SMR      23148.148 Hz
FIDRES   0.351213 Hz
AQ       1.4156276 sec
RG        8192
DM       21.600 usec
DE       4.50 usec
TE       300.0 K
D1       0.05000000 sec
d11      0.03000000 sec
d12      0.00002000 sec

***** CHANNEL f1 *****
NUC1     13C
P1       12.30 usec
PL1      2.00 dB
SFO1     100.6232933 MHz

***** CHANNEL f2 *****
CPDPRG2  waltz16
NUC2     1H
PCPD2    100.00 usec
PL2      0.00 dB
PL12     18.00 dB
PL13     18.00 dB
SFO2     400.1316005 MHz

F2 - Processing parameters
SI       32768
SF       100.6127290 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

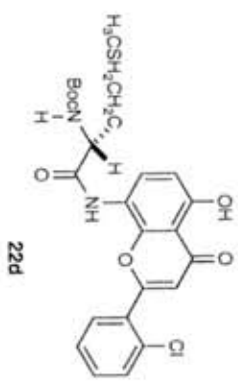
ID NMR plot parameters
CX       20.00 cm
FLP      210.000 ppm
F1       21128.67 Hz
F2P      -5.000 ppm
F2       -503.06 Hz
PPMCKM  10.75000 ppm/cm
H2CKM   1081.58691 Hz/cm
  
```

ppm

12.1077

60

8.5297  
 8.4075  
 8.3849  
 7.7042  
 7.5993  
 7.5962  
 7.5767  
 7.5432  
 7.5387  
 7.5247  
 7.5202  
 7.5053  
 7.5006  
 7.4918  
 7.4884  
 7.4730  
 7.4701  
 7.2841  
 6.8567  
 6.8343  
 6.6453  
 5.3178  
 4.1441  
 4.1261  
 2.6265  
 2.6092  
 2.5942  
 2.5776  
 2.2281  
 2.2103  
 2.1934  
 2.0651  
 2.0423  
 2.0245  
 2.0067  
 1.7030  
 1.3550  
 1.2926  
 1.2745  
 1.2570



ppm 12 10 8 6 4 2 0

Integral

1.0067

1.0000

1.1191

1.0638

1.0523

2.2522

1.0705

1.0071

0.9264

1.0529

2.2593

1.2046

4.8138

9.8716

Current Data Parameters  
 NAME VA-11-187-2  
 EXNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20010321  
 Time 18.48  
 INSTRUM dx400  
 PROBRD 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.830 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 322.5  
 DW 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 7.70 usec  
 PL1 -6.00 dB  
 SFO1 400.132007 MHz

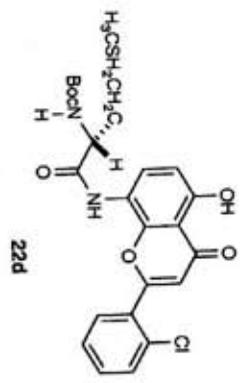
F2 - Processing parameters  
 SI 16384  
 SF 400.1300000 MHz  
 WDM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 13.000 ppm  
 F1 5201.69 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPMCK 0.66500 ppm/cm  
 HZCK 266.08646 Hz/cm

ppm

61

- 183.143
- 170.111
- 163.288
- 157.081
- 155.956
- 146.873
- 133.002
- 132.618
- 131.302
- 131.255
- 130.984
- 128.793
- 127.656
- 117.669
- 112.017
- 111.276
- 110.552
- 80.678
- 77.547
- 77.230
- 76.913
- 54.341
- 31.262
- 30.465
- 28.354
- 15.422



\*\*\*\*\* CHANNEL F1 \*\*\*\*\*  
 NAME VA-11-187-2C  
 EXPRNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20010321  
 Time 18.51  
 INSTRUM dirx400  
 PROBRD 5 mm Multin  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 678  
 DS 2

SMR 23148.148 Hz  
 FIDRES 0.353213 Hz  
 AQ 1.4156276 sec  
 RG 2048  
 DW 21.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 0.05000000 sec  
 D11 0.03000000 sec  
 D12 0.00002000 sec

\*\*\*\*\* CHANNEL F2 \*\*\*\*\*  
 GEPRG2 valcx16  
 NUC1 13C  
 P1 12.30 usec  
 PL1 2.00 dB  
 SFO1 100.6232933 MHz

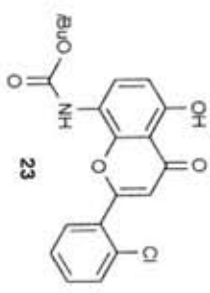
PCPD2 100.00 usec  
 PL2 0.00 dB  
 PL12 18.00 dB  
 PL13 18.00 dB  
 SFO2 400.1316005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6127510 MHz  
 MDW BM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

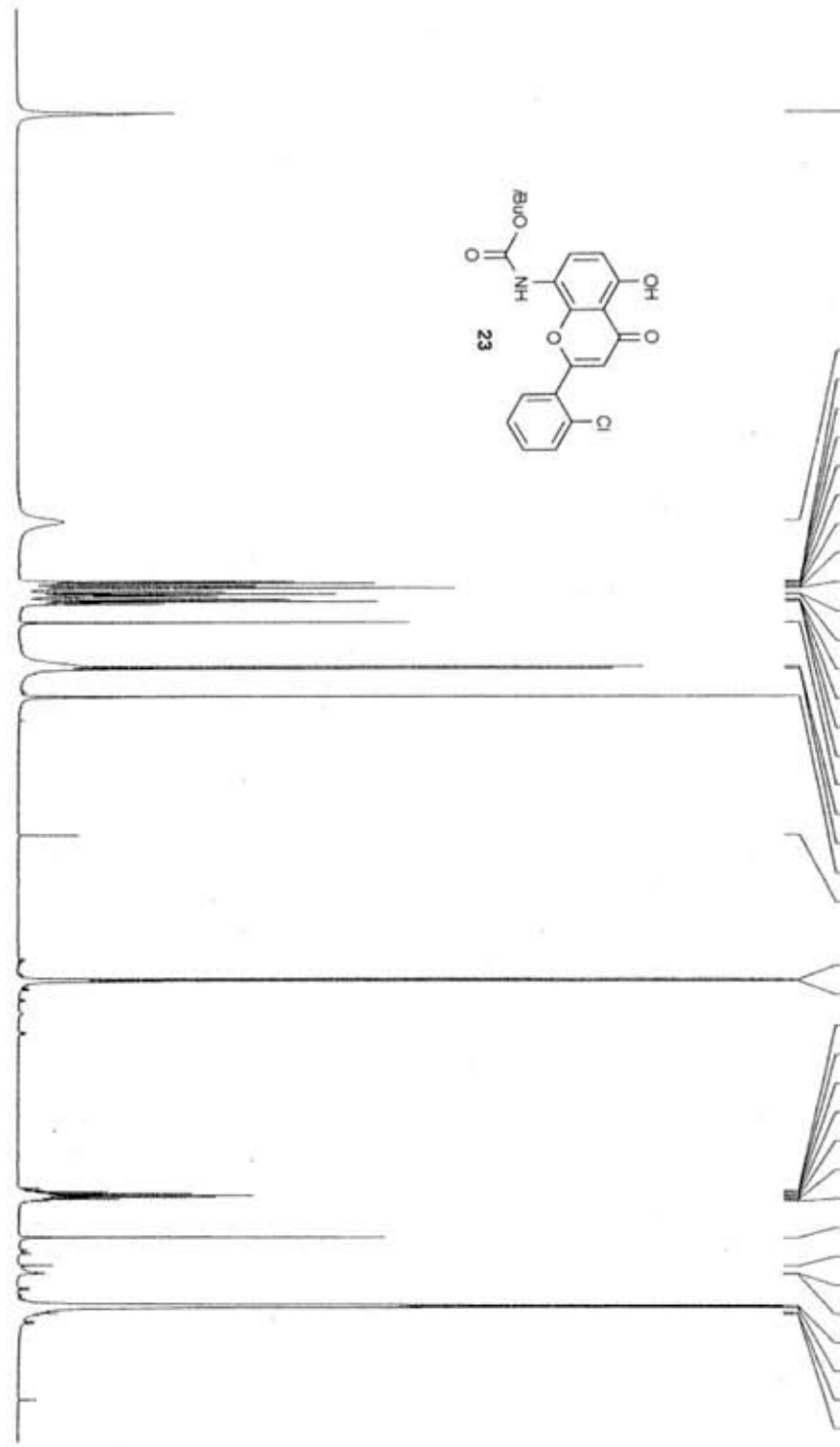
1D NMR plot parameters  
 CX 20.00 cm  
 F1P 210.000 ppm  
 F1 21128.58 Hz  
 F2P -5.000 ppm  
 F2 -503.06 Hz  
 PPRCM 10.75000 ppm/cm  
 SFCM 1081.58704 Hz/cm

ppm

12.0146  
62



- 8.2217
- 7.6606
- 7.6564
- 7.6416
- 7.6375
- 7.6156
- 7.6129
- 7.5958
- 7.5928
- 7.5428
- 7.5385
- 7.4929
- 7.4896
- 7.4739
- 7.4707
- 7.2838
- 6.8783
- 6.8557
- 6.6035
- 5.3220
- 3.9945
- 3.9779
- 2.0507
- 2.0338
- 2.0170
- 2.0003
- 1.9834
- 1.9666
- 1.9500
- 1.6133
- 1.3487
- 1.2805
- 1.2726
- 0.9823
- 0.9654
- 0.9199
- 0.9028



Current Data Parameters  
 NAME YA-11-156-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 1010220  
 Time 16.57

INSTRUM drx400  
 PROCNO 5 mm Multinu  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 2

SWH 6012.620 Hz  
 FIDRES 0.244532 Hz  
 AQ 2.0447731 sec  
 RG 362  
 DM 62.400 usec  
 DE 4.50 usec  
 TE 300.0 K

D1 1.00000000 sec  
 P1 7.70 usec  
 DE 4.50 usec  
 SF01 400.1320007 MHz  
 NUC1 1H  
 PL1 -6.00 dB

F2 - Processing parameters  
 SI 16384  
 SF 400.1300000 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

10 NMR plot parameters  
 CX 20.00 cm  
 F1P 13.000 ppm  
 F1 5201.69 Hz  
 F2P -0.300 ppm  
 F2 -120.04 Hz  
 PPMCK 0.66500 ppm/cm  
 HZCM 266.08646 Hz/cm

266.08646 Hz/cm

ppm

183.148

63

163.696

133.278

132.868

131.626

131.328

131.293

127.870

111.983

111.585

110.800

77.753

77.435

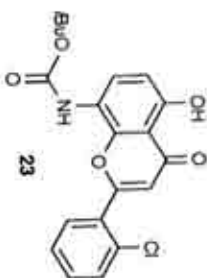
77.118

76.854

72.148

28.357

19.452



Current Data Parameters  
 NAME YA-11-156-1C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 1010221

Time 17.16

INSTRUM drx400

PROBHD 5 mm Multinu

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 2239

DS 2

SWH 23148.148 Hz

FIDRES 0.353213 Hz

AQ 1.4156276 sec

RG 8192

DW 21.500 usec

DE 4.50 usec

TE 300.0 K

d11 0.0300000 sec

d12 0.0000200 sec

PL13 18.00 dB

D1 0.05000000 sec

CPDPRG2 waltz16

PCPD2 100.00 usec

SFO2 400.1315005 MHz

MUCC 1H

PL2 0.00 dB

PL12 18.00 dB

P1 12.30 usec

DE 4.50 usec

SFO1 100.6232933 MHz

MUCC 13C

PL1 2.00 dB

F2 - Processing Parameters

SI 32758

SF 100.6127290 MHz

MOM EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

F1P 210.000 ppm

F1 21129.57 Hz

F2P -5.000 ppm

F2 -503.06 Hz

PPHCK 10.75000 ppm/cm

HZCK 1081.98691 Hz/cm

ppm

175

150

125

100

75

50

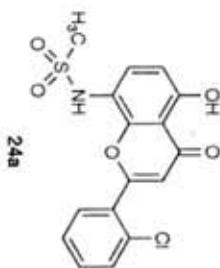
25

0

ppm

64  
12.570

7.8049  
7.7825  
7.6387  
7.6347  
7.6197  
7.6158  
7.5806  
7.5771  
7.5681  
7.5500  
7.5462  
7.4971  
7.4782  
7.4745  
7.2700  
6.8899  
6.8677  
6.6098  
6.5355  
5.3083  
4.1522  
4.1345  
4.1165  
4.0986  
3.4980  
3.3731  
3.3585  
2.9879  
2.0522  
1.6018  
1.2832  
1.2651  
1.2476



Integral

0.9325

1.0000  
1.2403  
1.8027  
1.1221  
0.9949  
0.9326  
0.9221

3.0968

```

Current Data Parameters
NAME      VA-11-20-3
EXPMO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20011001
Time     16.50
INSTRUM  drx400
PROBHD   5 mm Multinu
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       2
SMR      8012.820 Hz
FIDRES   0.244532 Hz
AQ       2.0447731 sec
RG       228.1
RC       62.400 usec
DE       4.50 usec
TE       300.0 K
D1       1.00000000 sec

===== CHANNEL f1 =====
NUC1      1H
P1       7.70 usec
PL1      -6.00 dB
SFO1     400.1320007 MHz

F2 - Processing Parameters
SI       16384
SF       400.1300053 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

ID NMR Plot Parameters
CX       20.00 cm
F1P      14.000 ppm
F1       5601.82 Hz
F2P      -0.300 ppm
F2       -120.04 Hz
PPMCKM  0.71500 ppm/cm
HZCM    286.09296 Hz/cm
  
```

ppm

12

10

8

6

4

2

0



65

182.992

163.779

159.243

149.243

132.928

132.892

132.119

131.334

131.043

130.914

127.851

115.668

112.226

112.133

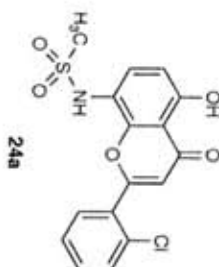
110.922

77.484

77.230

76.975

40.150



ppm

```

NAME          YA-11-20-3C
EXPNO        3
PROCNO       1
----- F2 - Acquisition Parameters -----
Date_        20011001
Time         18.12
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TC           65536
SOLVENT      CDCl3
NS           1429
DS           4
SWH          31468.541 Hz
FIDRES      0.475636 Hz
AQ          1.5420863 sec
RG           3251
SQ           15.900 uSFC
DE          6.00 uSFC
TE          300.2 K
D1          0.10000000 sec
d11         0.00000000 sec
d12         0.00000000 sec
----- CHANNEL f1: -----
NUC1         13C
P1          6.50 uSFC
PL1         5.00 dB
SFO1        125.7715472 MHz
----- CHANNEL f2: -----
CPDPRG2      waltz16
NUC2         1H
P2          85.00 uSFC
PL2         17.50 dB
PL12        19.00 dB
PL13        30.00 dB
SFO2        500.1325000 MHz
----- F1 - Acquisition Parameters -----
AQ          2.00000000 sec
SFO1        500.1325 MHz
FIDRES      23.475060 Hz
SFO         12.016 ppm
----- F2 - Processing Parameters -----
SI          65536
SF          125.7577538 MHz
KOH         EM
SFO         0
LB          1.00 Hz
GB          0
PC          1.40
----- F1 - Processing Parameters -----
SI          1024
SF          500.1300000 MHz
KOH         AC
SFO         0
LB          0.30 Hz
GB          0
ID name plot parameters
CX          30.00 cm
CY          13.69 cm
CZ          220.000 ppm
F1P         27568.71 Hz
F2P         5.000 ppm
SFOC1       -628.79 Hz
SFOC2       11.25000 ppm/cw
NUC1C       13C13.77480 Hz/cw

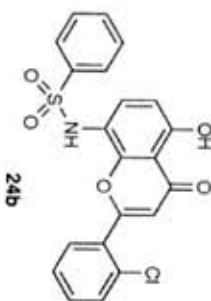
```

ppm

66 2493

7.7920  
7.7698  
7.6019  
7.5992  
7.5812  
7.5781  
7.5496  
7.5455  
7.5207  
7.3955  
7.3310  
7.3280  
7.2700  
7.2028  
7.1824  
7.1635  
6.8581  
6.8359  
6.4762  
5.3078  
4.1522  
4.1345  
4.1166  
4.0986

2.0523  
1.6145  
1.2823  
1.2647  
1.2582  
1.2467



Integral

0.9231

1.0000  
1.8881  
2.0643  
2.0593  
1.0538  
1.9810  
0.9866  
0.9390  
0.9163

12  
10  
8  
6  
4  
2  
0

Current Data Parameters  
NAME VA-11-19-3  
EXTNO 1  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20011002  
Time 17.30  
INSTRUM dx400  
PROBHD 5 mm Multinu  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.244532 Hz  
AQ 2.0447731 sec  
RG 228.1  
TDW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 1.00000000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 1H  
P1 7.70 usec  
PL1 -6.00 dB  
SFO1 400.1320007 MHz

F2 - Processing parameters

SI 16384  
SF 400.1300053 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters

CX 20.00 cm  
F1p 14.000 ppm  
F1 5601.82 Hz  
F2p -0.100 ppm  
F2 -120.04 Hz  
P1PCM 0.71500 ppm/cm  
H2CM 286.09296 Hz/cm

67

182.837

163.036

159.492

149.731

139.029

133.906

133.266

132.789

132.725

131.286

130.922

130.535

128.927

127.537

127.215

115.214

111.950

111.798

110.477

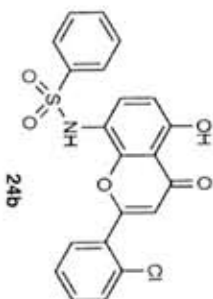
77.544

77.227

76.909

29.909

14.404



Current Data Parameters  
 NAME VA-111-19-3C  
 EXTNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20011002  
 Time 17.33

INSTRUM dtx400

PROBHD 5 mm Nalima

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 556

DS 2

SMR 23148.148 Hz

PTDRES 0.353213 Hz

AQ 1.4156276 sec

RG 8192

DM 21.500 usec

DE 4.50 usec

TE 300.0 K

D1 0.05000000 sec

D11 0.03000000 sec

D12 0.00002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 13C

P1 12.30 usec

PL1 2.00 dB

SFO1 100.6232933 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*

CPDPRG2 waltz16

NUC2 1H

PCPD2 100.00 usec

PL2 0.00 dB

PL12 18.00 dB

PL13 18.00 dB

SFO2 400.1318005 MHz

F2 - Processing parameters

SI 3756

SP 100.6127503 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

ID NMR plot parameters

CX 20.00 cm

F1P 220.000 ppm

F1 22134.80 Hz

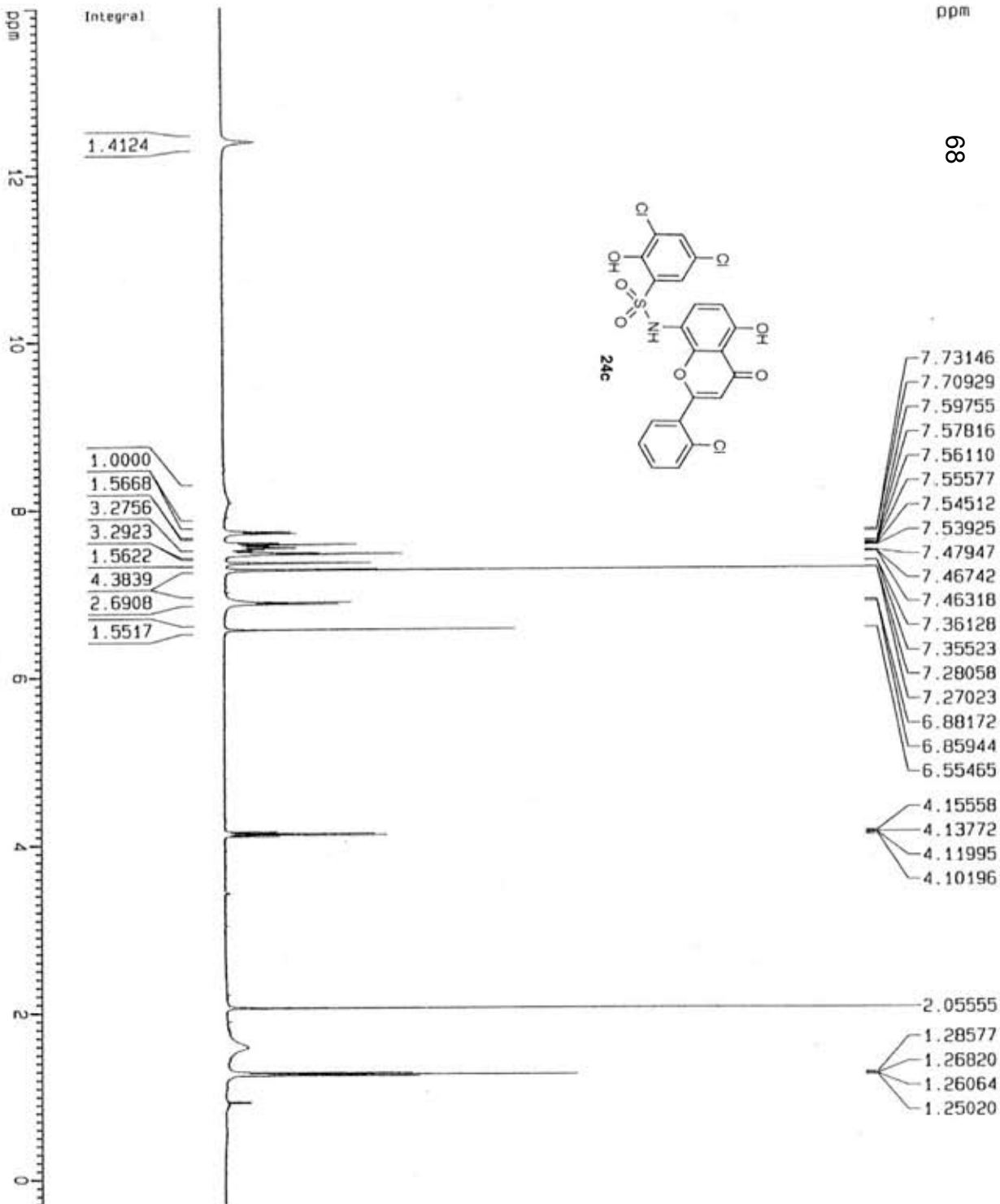
F2P -5.000 ppm

F2 -503.07 Hz

PPMKV 11.25000 ppm/cm

HDCK 1131.89343 Hz/cm





Current Data Parameters  
 NAME - YA-111-28-2  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 1011012

Time 11.43

INSTRUM drx400

PROBHD 5 mm Multinu

PULPROG zg30

TD 32768

SOLVENT CDCl3

NS 16

DS 2

SMH 8012.820 Hz

FIDRES 0.244532 Hz

AQ 2.044731 sec

RG 256

DM 62.400 usec

DE 4.50 usec

TE 300.0 K

D1 1.00000000 sec

P1 7.70 usec

DE 4.50 usec

SF01 400.1320007 MHz

NUC1 1H

PL1 -6.00 dB

F2 - Processing parameters

SI 16394

SF 400.1300053 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

F1P 14.000 ppm

F1 5601.82 Hz

F2P -0.300 ppm

F2 -120.04 Hz

PPMCM 0.71500 ppm/cm

HZCM 266.09296 Hz/cm

ppm

69

182.713

163.310

160.658

134.972

134.896

132.994

132.749

131.621

130.800

130.286

127.880

126.871

125.498

124.161

113.410

112.297

112.078

110.704

77.486

77.231

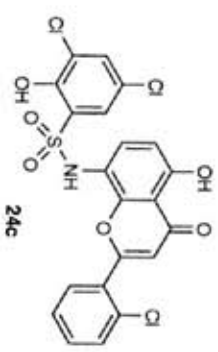
76.978

76.640

60.630

21.276

14.421



Current Data Parameters  
 NAME YA-111-28-2C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20011013  
 Time 14.11  
 INSTRUM spect  
 PROBHD 5 mm BBO BB-1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 5000  
 DS 4  
 SWH 31446.541 Hz  
 FIDRES 0.479836 Hz  
 AQ 1.0420883 sec  
 RG 5160.6  
 DW 15.900 usec  
 DE 6.00 usec  
 TE 300.0 K  
 D1 0.10000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 6.50 usec  
 PL1 5.00 dB  
 SF01 125.7719472 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 95.00 usec  
 PL2 17.50 dB  
 PL12 19.00 dB  
 PL13 30.00 dB  
 SF02 500.1325000 MHz

F2 - Processing parameters  
 S1 65536  
 SF 125.7577624 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 CY 0.00 cm  
 FIP 220.000 ppm  
 F1 27666.71 Hz  
 F2 -5.000 ppm  
 F2 -628.79 Hz  
 PPMCM 11.25000 ppm/cm  
 HZCM 1414.77478 Hz/cm