

Supporting Information

Tethered derivatives of D-glucose and pentacyclic triterpenes for homo/heterobivalent inhibition of glycogen phosphorylase

Keguang Cheng,^a Jun Liu,^b Hongbin Sun,^{*a} Éva Bokor,^c Katalin Czifrák,^c Bálint Kónya,^c Marietta Tóth,^c Tibor Docsa,^d Pál Gergely,^e and László Somsák^{*c}

^a*Center for Drug Discovery, College of Pharmacy, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, China*

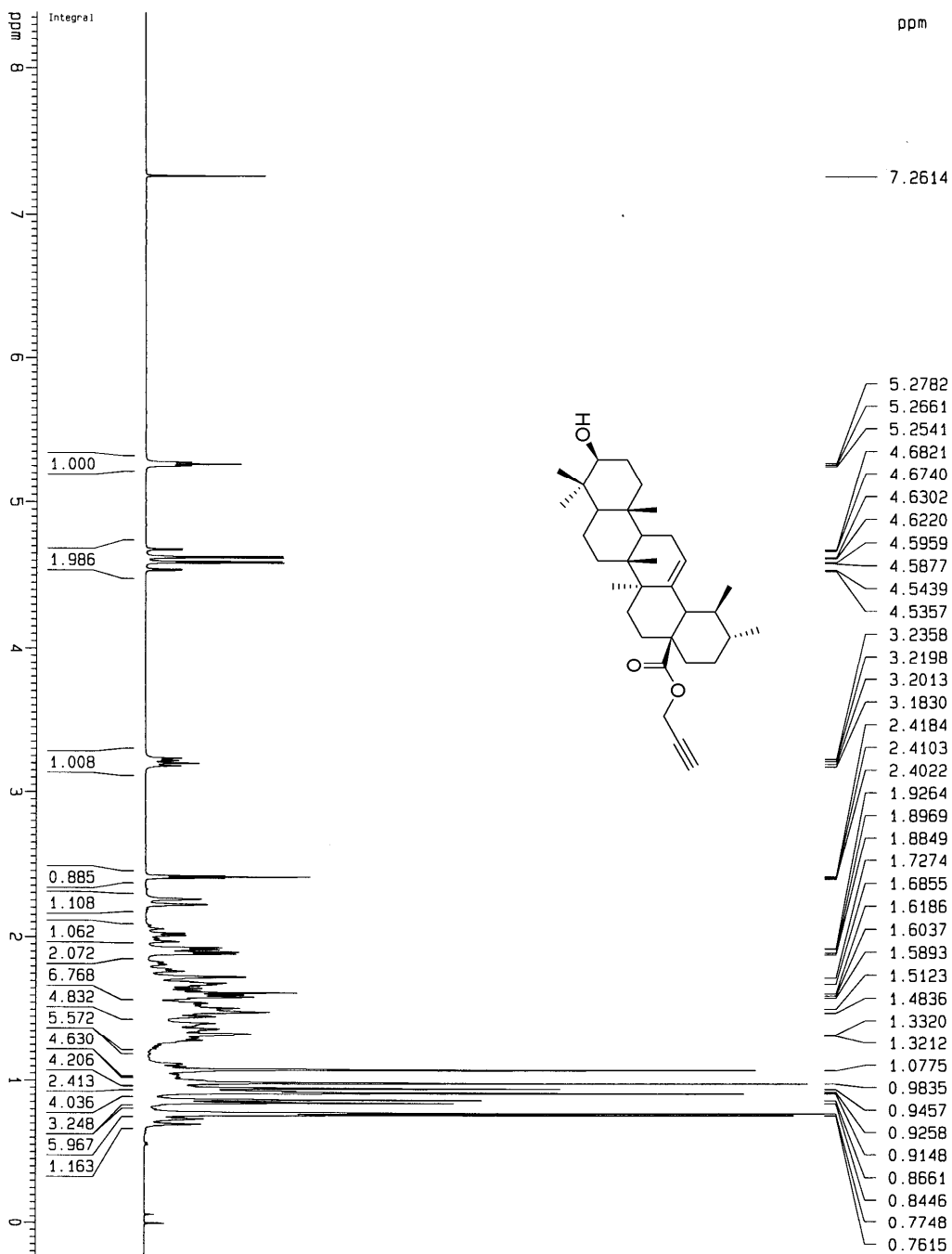
^b*Jiangsu Center for Drug Screening, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, China*

^c*Department of Organic Chemistry, University of Debrecen, POB 20, H-4010 Debrecen, Hungary*

^d*Cell Biology and Signaling Research Group of the Hungarian Academy of Sciences at the Department of Medical Chemistry, Medical and Health Science Centre, University of Debrecen, Egyetem tér 1, H-4032 Debrecen, Hungary*

^e*Department of Medical Chemistry, Medical and Health Science Centre, University of Debrecen, Egyetem tér 1, H-4032 Debrecen, Hungary*

Copies of ¹H NMR and ¹³C NMR spectra of **5, 6, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38**.



Current Data Parameters
 NAME SNO
 EXPRNO 514
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080308
 Time 12.14
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 13512
 SOLVENT CDCl3
 NS 28
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.443695 Hz
 AQ 1.1269507 sec
 RG 32
 DW 83.400 usec
 DE 8.00 usec
 TE 298.0 K
 D1 2.00000000 sec

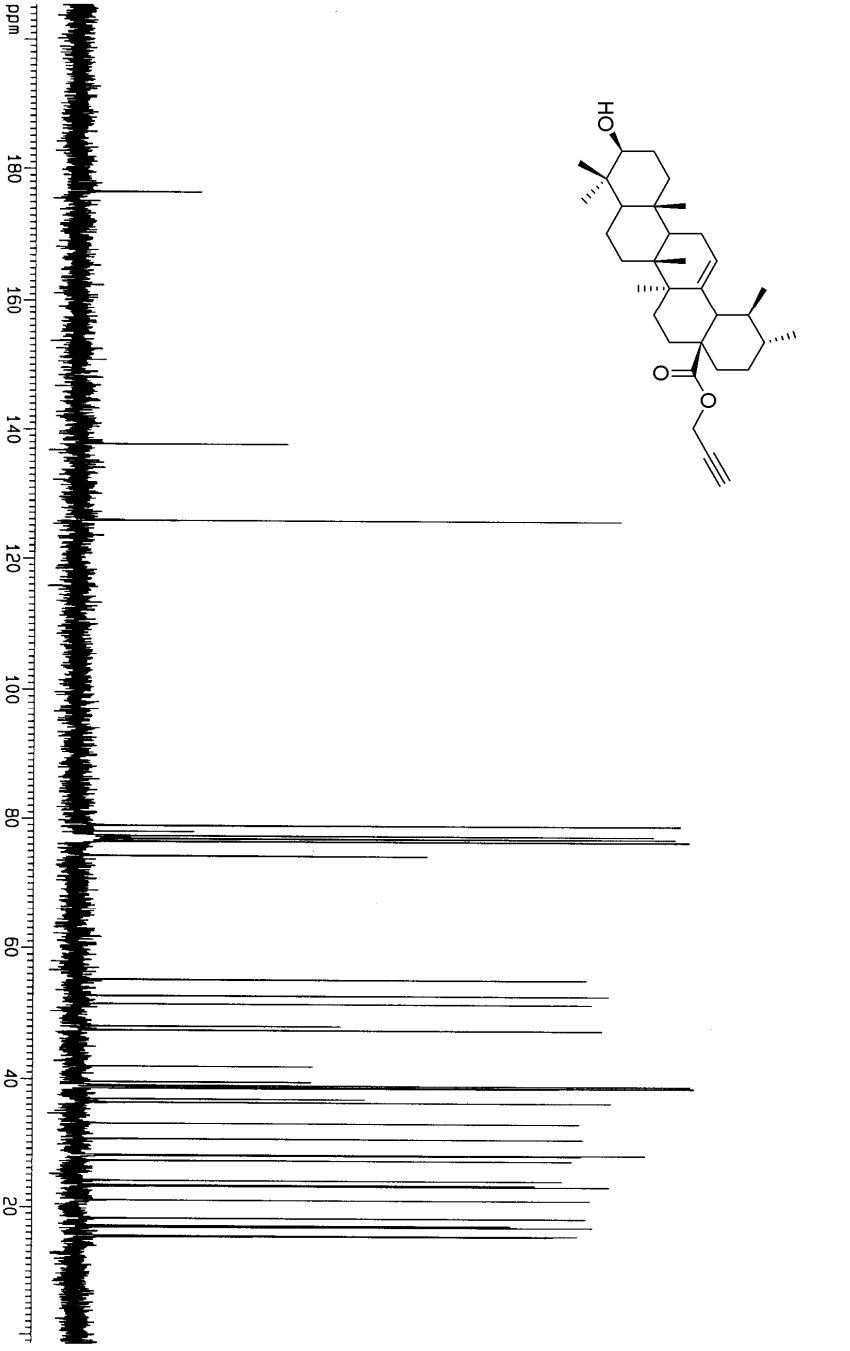
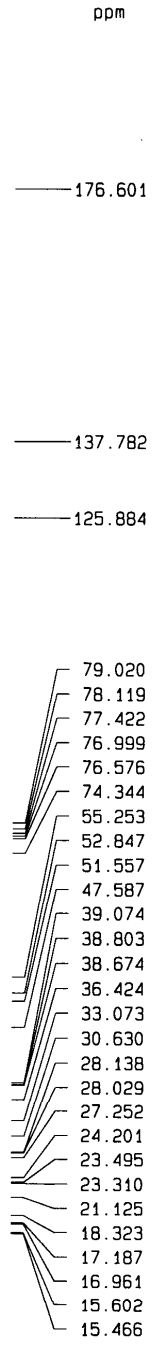
***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1324010 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300120 MHz
 NDM EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters:
 CX 22.00 cm
 CY 12.00 cm
 F1P 8.387 dpm
 F1 2517.21 Hz
 F2P -67.43 Hz
 F2 0.39144 dpm/cm
 HZCM 117.48322 Hz/cm

KELLY-139B 13C-NMR CDCL3 303K AV-300

Current Data Parameters
 NAME SIB
 EXPNO 538
 PROCNO 1



F2 - Acquisition Parameters

Date_ 20080311
 Time 16:31
 INSTRUM spect
 PROBRD 5 mm GNP 1H/13
 PULPROG zgpgc
 TD 32768
 SOLVENT CDCL3
 NS 451
 DS 8
 SFO1 75.4763978 MHz
 SF02 300.1312005 MHz
 FIDRES 0.552895 Hz
 AQ 0.50444468 sec
 RG 409500
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

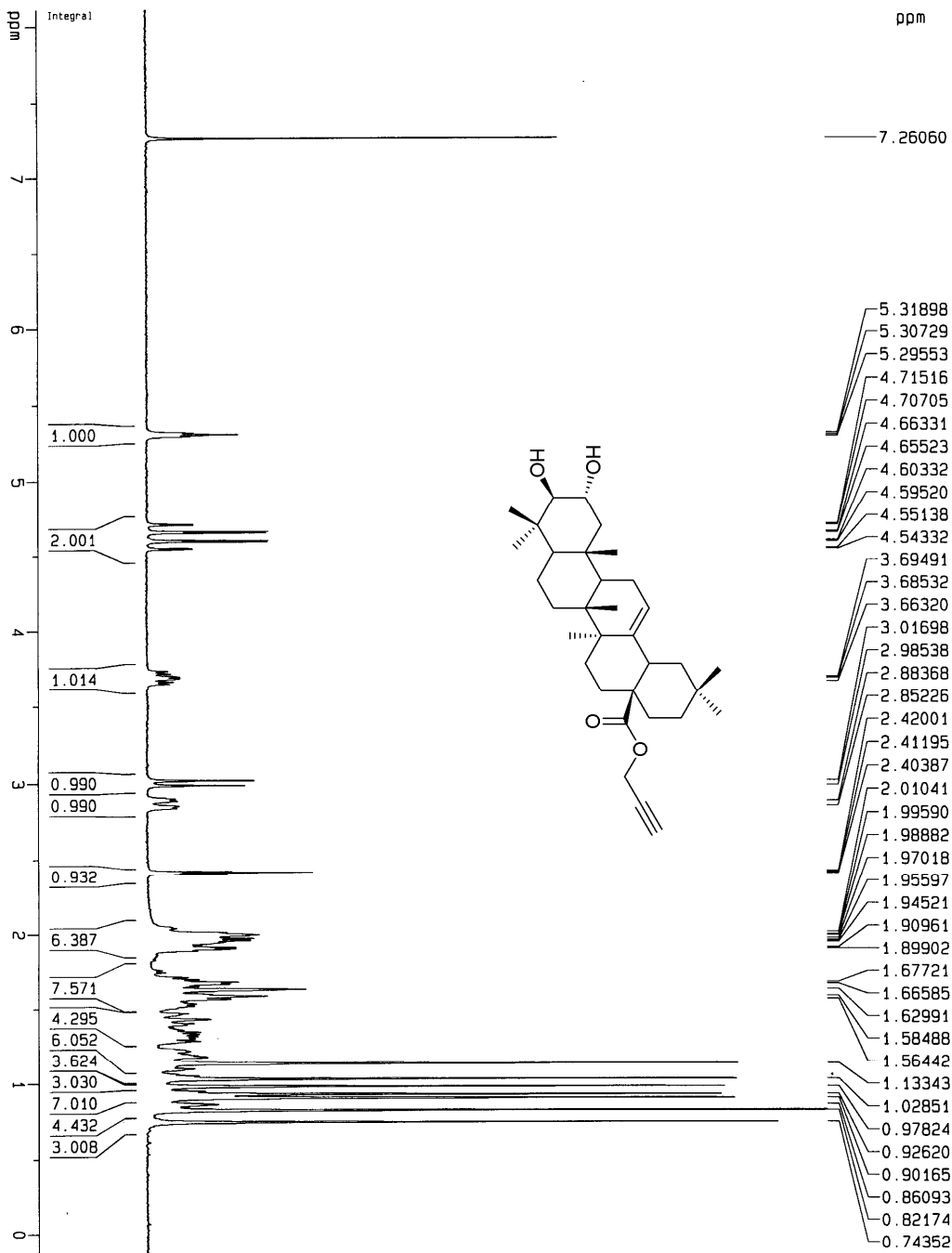
***** CHANNEL f1 *****
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SFO1 75.4763978 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PPRD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677512 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 10.00 cm
 F1P 205.518 ppm
 F1 15510.02 Hz
 F2P -1.459 ppm
 F2 -110.14 Hz
 PPHCM 9.40809 ppm/cm
 HZCM 710.00720 Hz/cm

KELLY-139C 1H-NMR CDCL3 303K AV-300



- 7.26060
- 5.31898
- 5.30729
- 5.29553
- 4.71516
- 4.70705
- 4.66331
- 4.65523
- 4.60332
- 4.59520
- 4.55138
- 4.54332
- 3.69491
- 3.68532
- 3.66320
- 3.01698
- 2.98538
- 2.88368
- 2.85226
- 2.42001
- 2.41195
- 2.40387
- 2.01041
- 1.99590
- 1.98882
- 1.97018
- 1.95597
- 1.94521
- 1.90961
- 1.89902
- 1.67721
- 1.66585
- 1.62991
- 1.58488
- 1.56442
- 1.13343
- 1.02851
- 0.97824
- 0.92620
- 0.90165
- 0.86093
- 0.82174
- 0.74352

Integral

1.000

2.001

1.014

0.990

0.990

0.932

6.387

7.571

4.295

6.052

3.624

3.030

7.010

4.432

3.008

Current Data Parameters

NAME	shb
EXPNO	536
PROCNO	1

F2 - Acquisition Parameters

Date_	20080311
Time	15:57
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	13512
SOLVENT	CDCl3
NS	8
DS	0
SMH	3140.704 Hz
FIDRES	0.232438 Hz
AQ	2.1511605 sec
RG	16
DM	159.200 usec
DE	6.00 usec
TE	298.0 K
D1	2.00000000 sec

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

NUC1	1H
P1	6.00 usec
PL1	-4.00 dB
SFO1	300.1313127 MHz

F2 - Processing parameters

SI	32768
SF	300.1300123 MHz
MDM	EN
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR Plot parameters

CX	22.00 cm
CY	12.00 cm
F1P	8.111 ppm
F1	2434.35 Hz
F2P	-0.141 ppm
F2	-42.41 Hz
PPMCK	0.37510 ppm/cm
HZCM	112.57974 Hz/cm

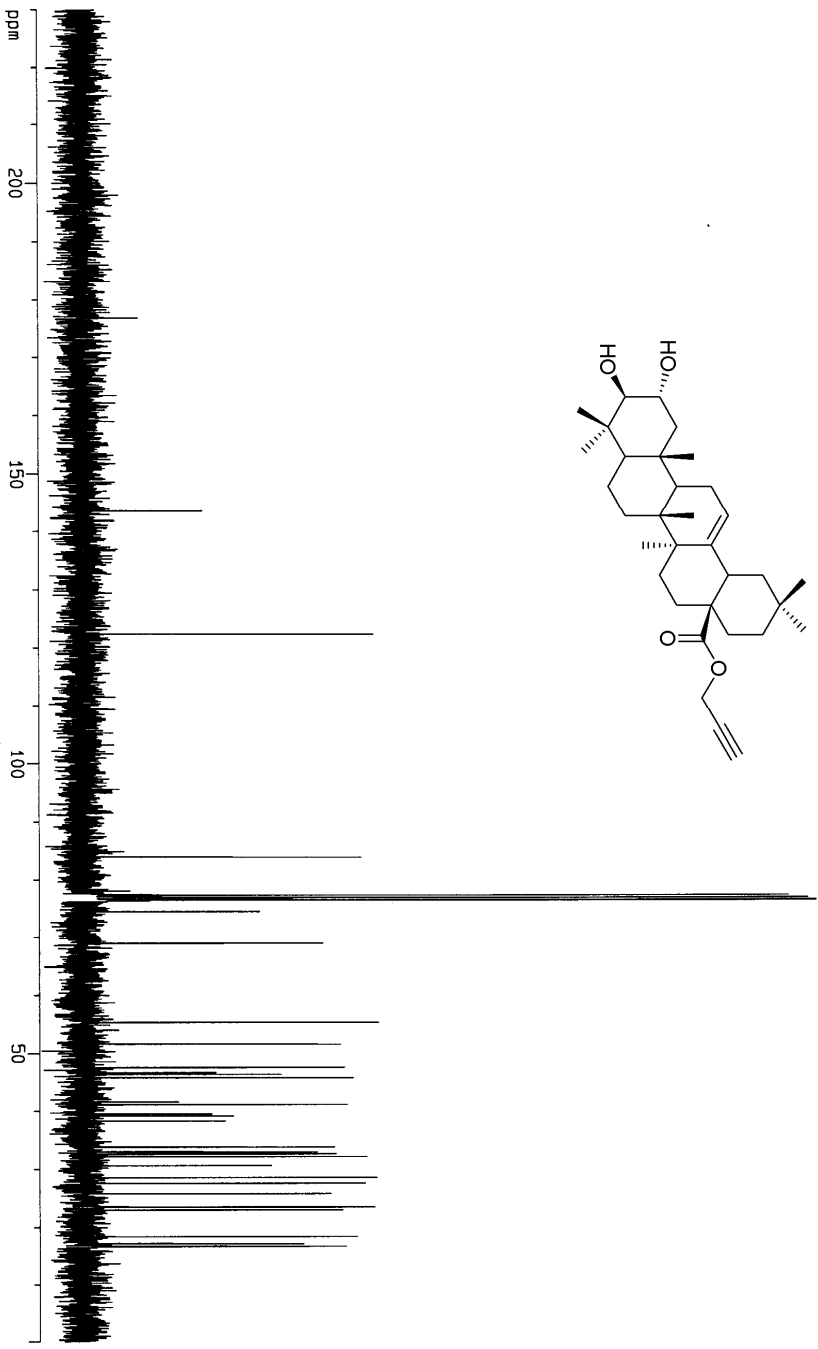
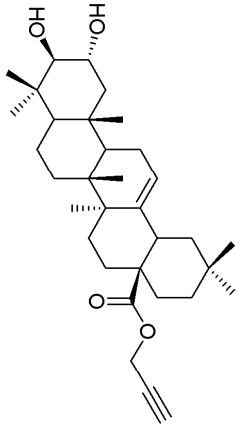
Kelly-139C C13-NMR CDC13 300K AV-300

Current Data Parameters
 NAME shb
 EXPNO 570
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080313
 Time 22.04
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 723
 DS 8
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.904468 sec
 RG 102400
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

ppm

- 176.805
- 143.494
- 122.462
- 84.005
- 78.143
- 77.427
- 77.004
- 76.581
- 74.361
- 68.998
- 55.353
- 51.641
- 47.649
- 46.488
- 45.868
- 41.312
- 33.878
- 33.064
- 32.693
- 32.223
- 28.621
- 27.662
- 25.865
- 23.615
- 23.506
- 23.039
- 18.378
- 17.171
- 16.726
- 16.640

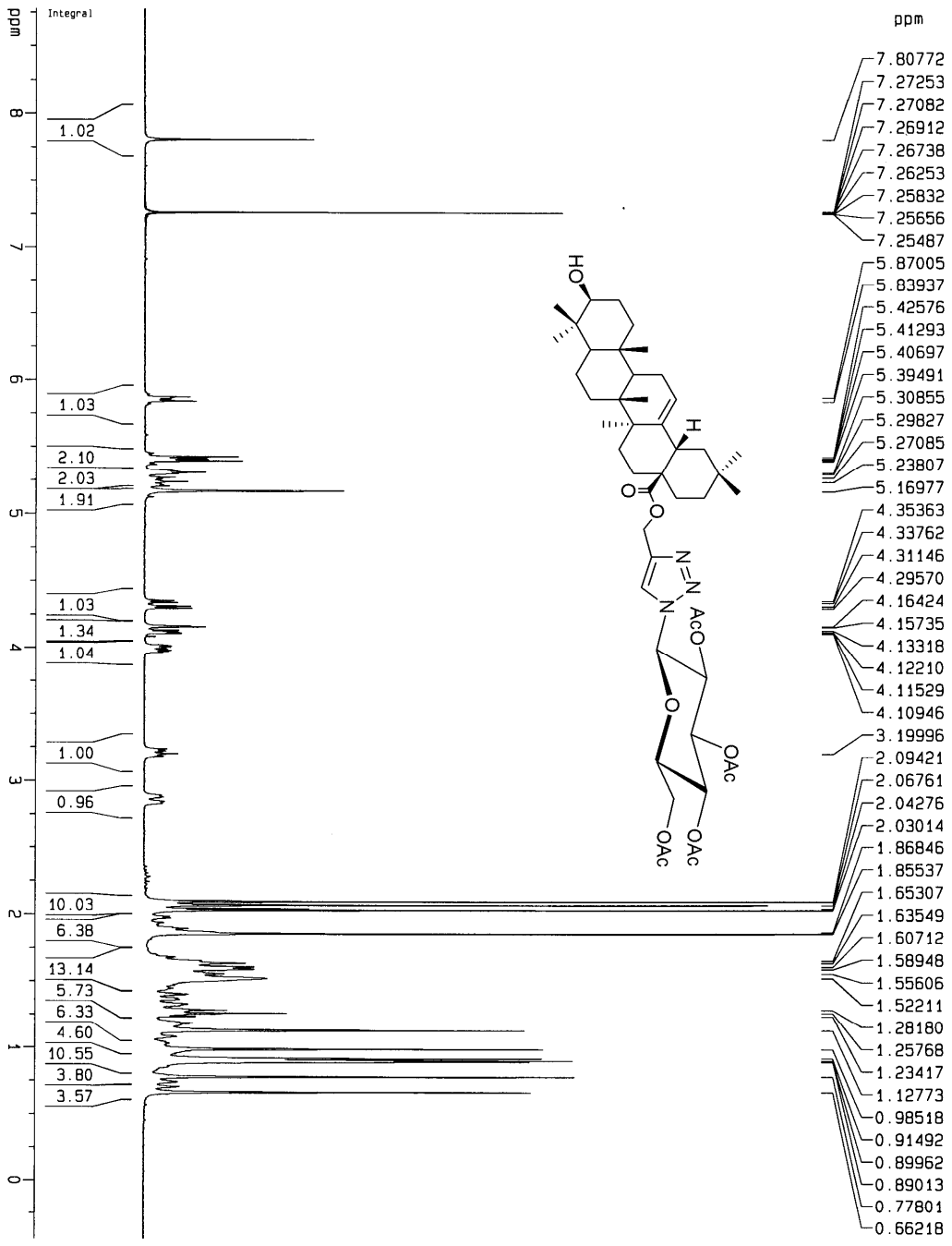


***** CHANNEL f1 *****
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 KGM EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.00 cm
 CY 12.00 cm
 F1P 230.000 ppm
 F1 17357.58 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PPKCM 10.43455 ppm/cm
 HZCM 788.98108 Hz/cm



Current Data Parameters
 NAME sbs
 EXPNO 616
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080320
 Time 22:22
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 11904
 SOLVENT CDCl3
 NS 24
 DS 0
 SWH 2976.190 Hz
 FIDRES 0.250016 Hz
 AQ 1.9999320 sec
 RG 256
 DM 168.000 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1312724 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300115 MHz
 KW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 12.00 cm
 F1P 8.779 ppm
 F1 2634.87 Hz
 F2P -0.448 ppm
 F2 -134.59 Hz
 PPMCK 0.41943 ppm/cm
 HZCM 125.88459 Hz/cm

Keyly-141 C13-NMR CDCl3 300K AV-300

Current Data Parameters
 NAME SIB
 EXNO 631
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20080324
 Time 10:39
 INSTRUM spect
 PROBD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 2304
 DS B
 SH1 18115.941 Hz
 FIDRES 0.55895 Hz
 AQ 0.9044468 sec
 RG 102400
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

==== CHANNEL f1 =====

NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SFO1 75.4763978 MHz

==== CHANNEL f2 =====

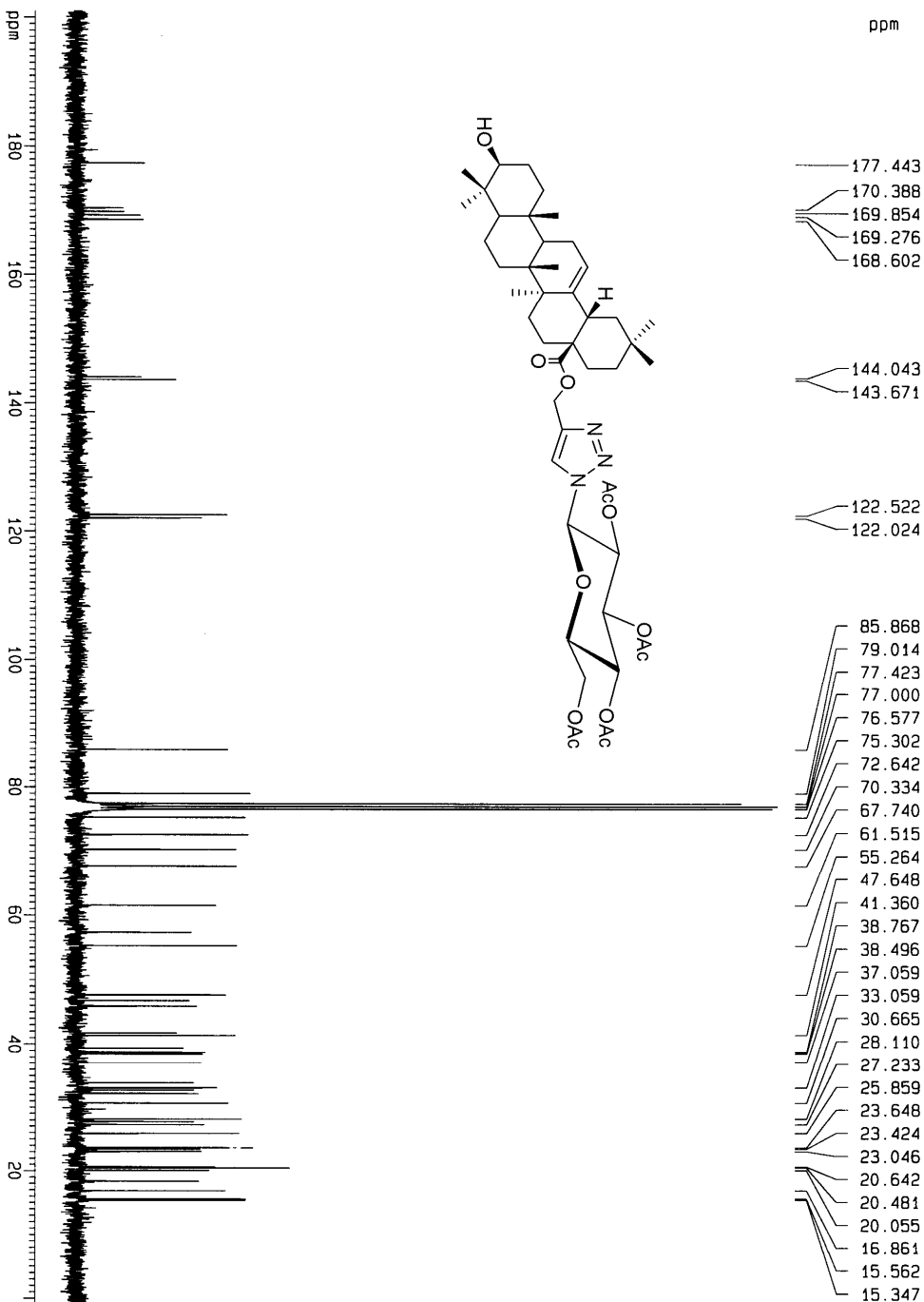
CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PCPD2 -4.00 dB
 PL12 19.25 dB
 SFO2 300.1312005 MHz

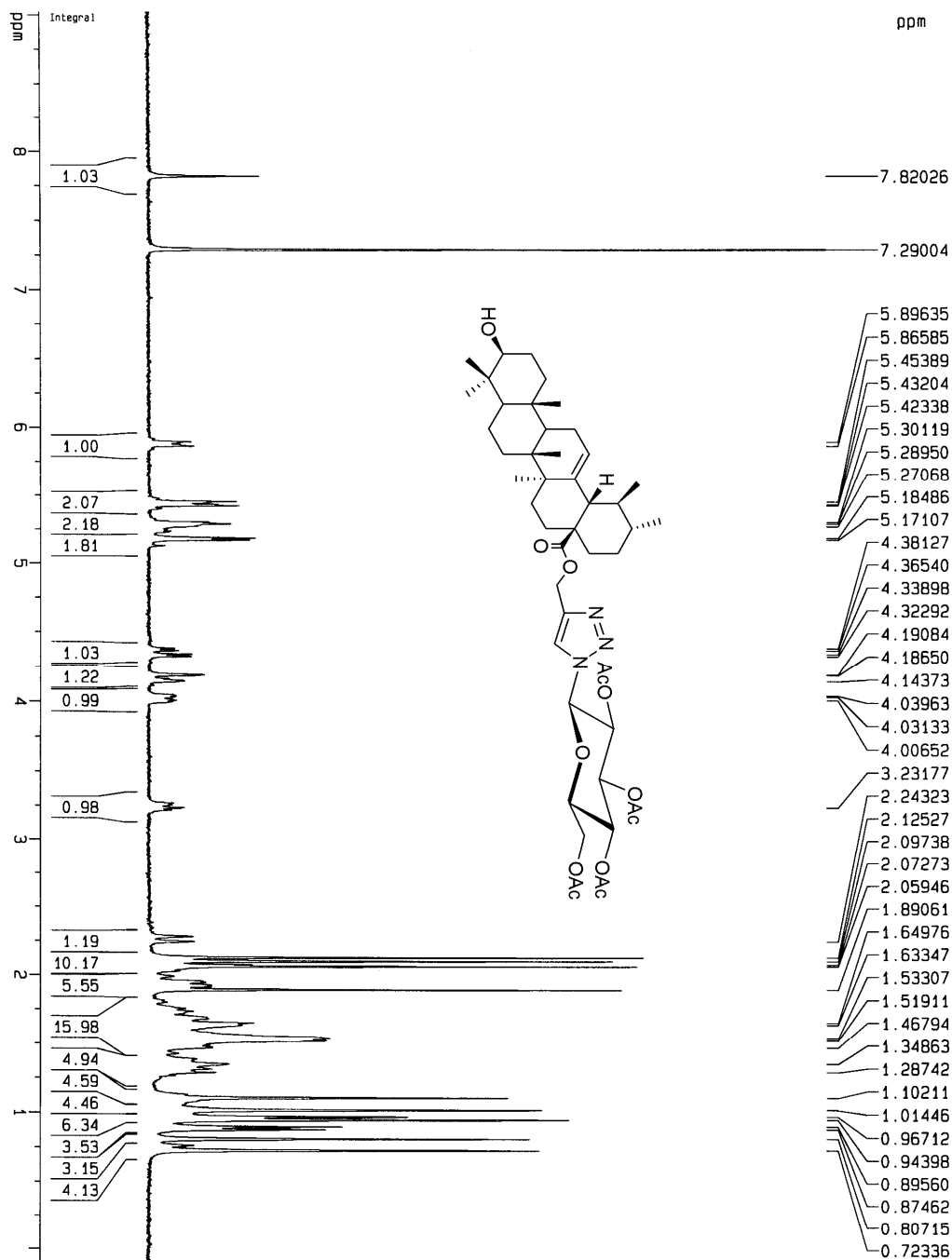
F2 - Processing parameters

S1 32768
 SF 75.4677495 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 22.50 cm
 CY 12.00 cm
 F1P 200.968 ppm
 F1 15166.62 Hz
 F2P -1.222 ppm
 F2 -92.25 Hz
 PPMCH 8.98625 ppm/cm
 HZCM 678.17205 Hz/cm





Current Data Parameters
 NAME S10
 EXRNO 779
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080408
 Time 20:44
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 15242
 SOLVENT CDCl3
 NS 8
 DS 0
 SMH 4139.073 Hz
 FIDRES 0.271557 Hz
 AQ 1.8412835 sec
 RG 1024
 DM 120.800 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.131873 MHz

F2 - Processing parameters
 S1 32768
 SF 300.130036 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 12.00 cm
 F1P 9.021 ppm
 F1 2707.56 Hz
 F2P -0.102 ppm
 F2 -30.52 Hz
 PPMICH 0.41468 ppm/cm
 HZICM 124.45818 Hz/cm

KELLY-145 13C-NMR CDCL3 300K AV-300

Current Data Parameters
 NAME SIB
 EXPNO 830
 PROCNO 1

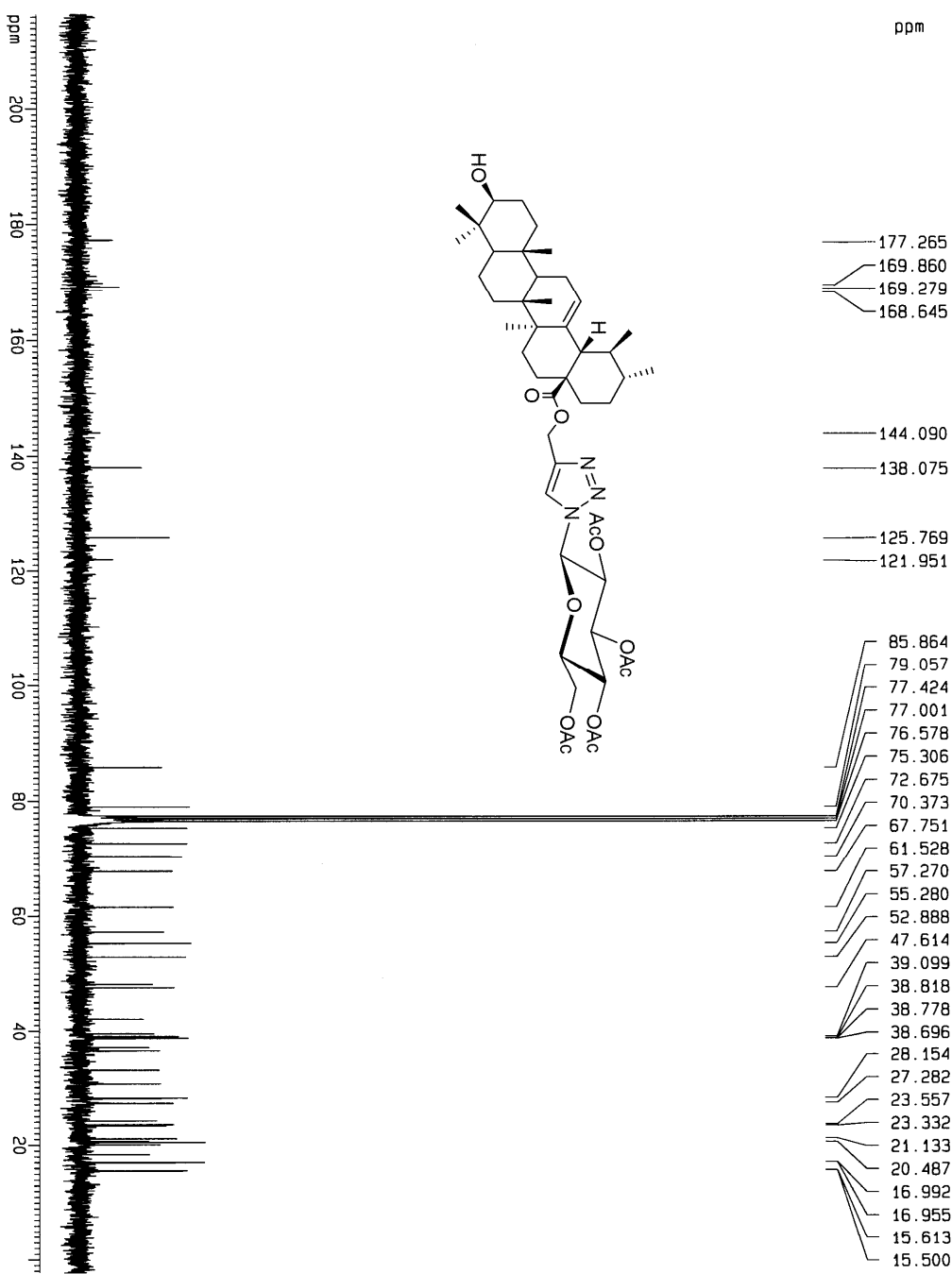
F2 - Acquisition Parameters
 Date_ 20080411
 Time 19:56
 INSTRUM spect
 PROBRW 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 2895
 DS 8
 SMH 21097.047 Hz
 FIDRES 0.643931 Hz
 AQ 0.7766516 sec
 RG 409600
 DW 23.700 usec
 DE 5.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

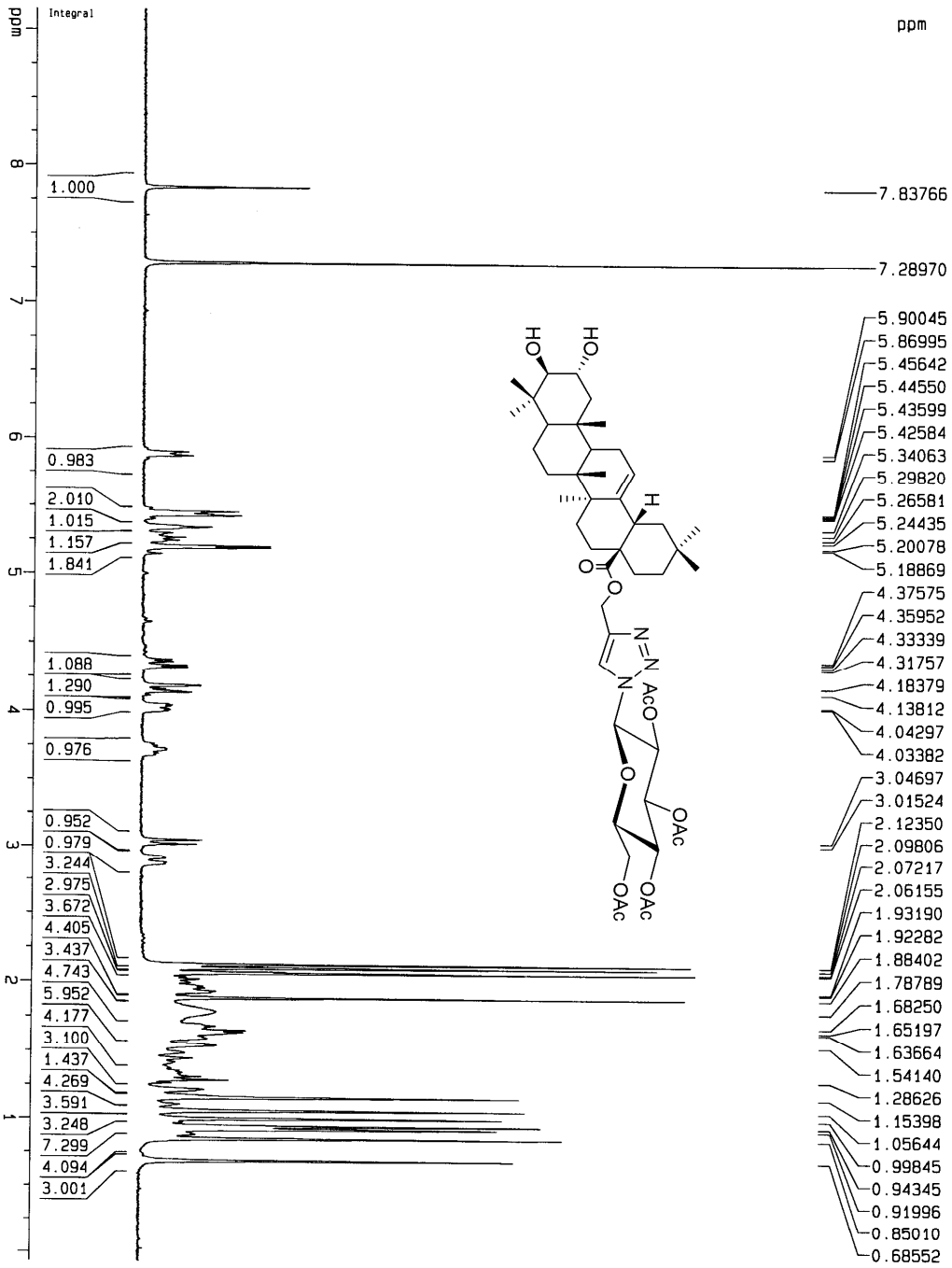
===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 PCPR2 60.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677488 MHz
 MIDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.00 cm
 CY 15.00 cm
 F1P 216.498 ppm
 F1 16336.60 Hz
 F2P -2.309 ppm
 F2 -174.28 Hz
 PPKCH 9.94577 ppm/cm
 HZCH 750.58521 Hz/cm



- 177.265
- 169.860
- 169.279
- 168.645
- 144.090
- 138.075
- 125.769
- 121.951
- 85.864
- 79.057
- 77.424
- 77.001
- 76.578
- 75.306
- 72.675
- 70.373
- 67.751
- 61.528
- 57.270
- 55.280
- 52.888
- 47.614
- 39.099
- 38.818
- 38.778
- 38.696
- 28.154
- 27.282
- 23.557
- 23.332
- 21.133
- 20.487
- 16.992
- 16.955
- 15.613
- 15.500



Current Data Parameters
 NAME sht
 EXPNO 778
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080408
 Time 20:42
 INSTRUM spect
 PROBRD 5 mm QNP
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SMH 4139.073 Hz
 FIDRES 0.271557 Hz
 AQ 1.8412835 sec
 RG 1024
 DM 120.800 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 5.00 usec
 PL1 -4.00 dB
 SF01 300.1317673 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300035 MHz
 KDN EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CT 12.00 cm
 F1P 9.152 ppm
 F1 2746.88 Hz
 F2P -0.069 ppm
 F2 -20.69 Hz
 PPMCN 0.41915 ppm/cm
 HZCN 125.79886 Hz/cm

KELLY-143 1H-NMR CDCL3 300K AV-300

Current Data Parameters
 NAME sfb
 EXPNO 827
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20080411
 Time 9.44
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 1668
 DS 8
 SMH 21097.047 Hz
 FIDRES 0.64831 Hz
 AQ 0.776516 sec
 RG 409600
 DM 23.700 usec
 DE 5.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****

NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4753978 MHz

***** CHANNEL f2 *****

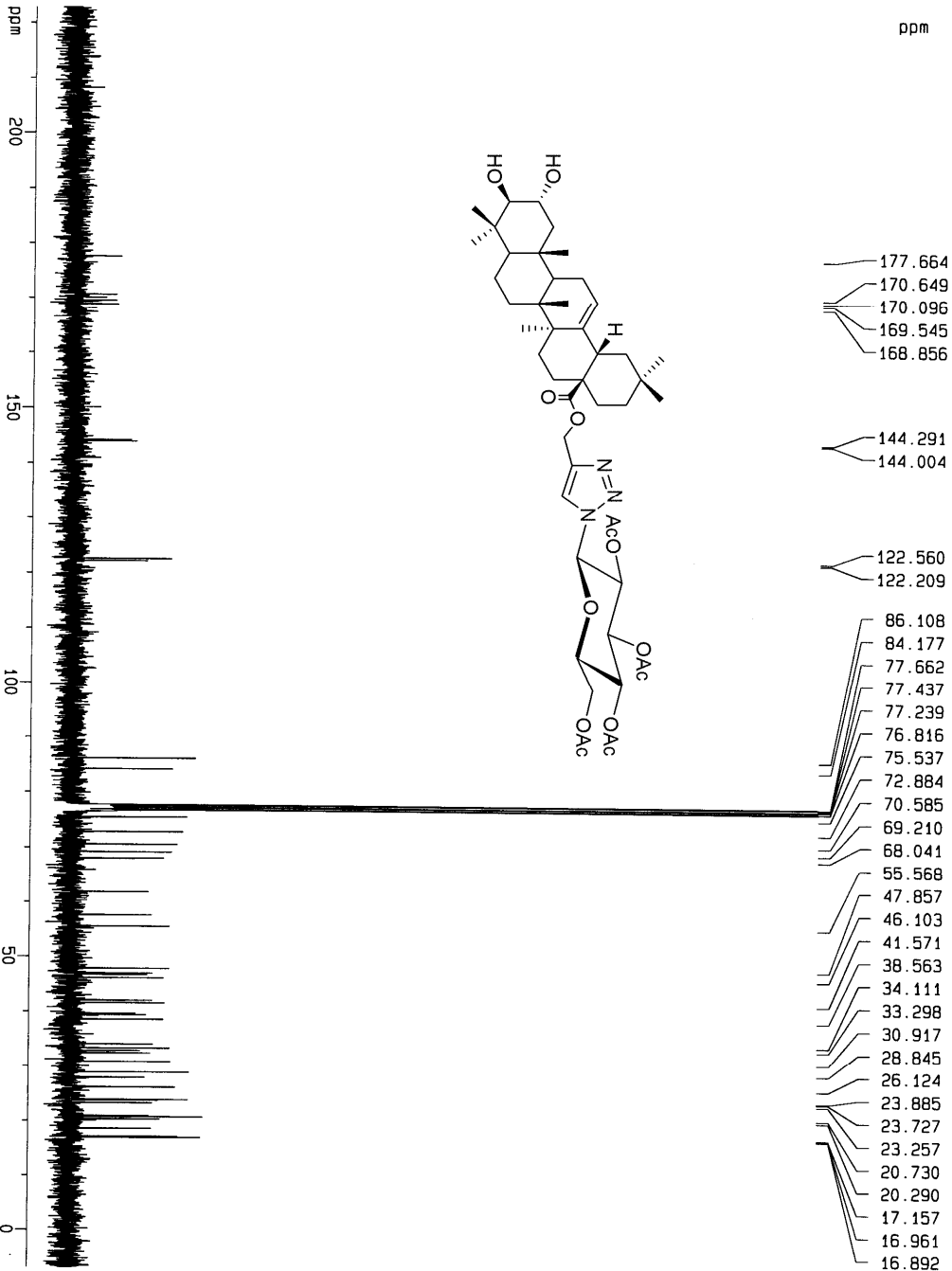
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters

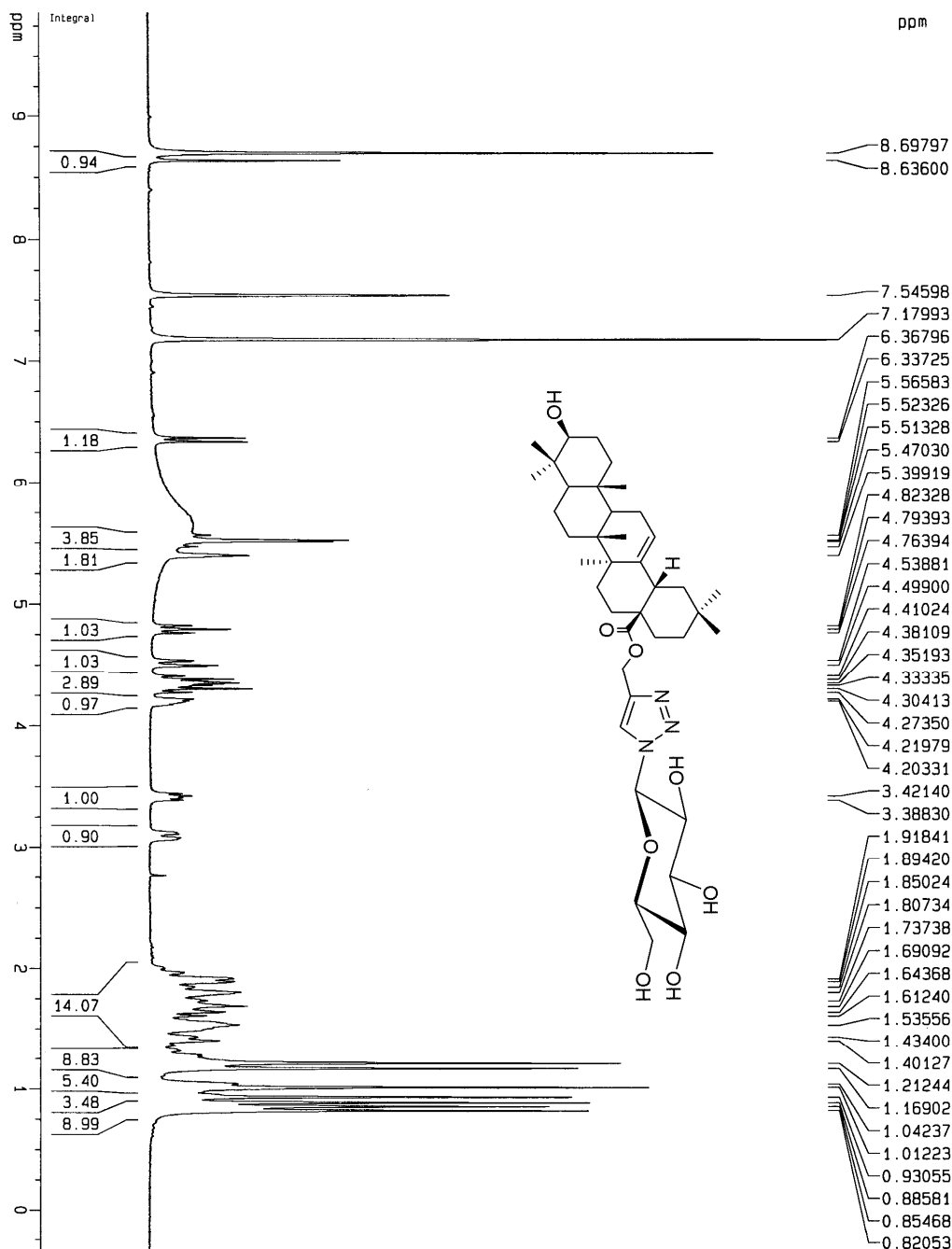
SI 32768
 SF 75.4677310 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters

CX 22.00 cm
 CY 15.00 cm
 F1P 222.938 dBm
 F1 16824.64 Hz
 F2P -6.972 dBm
 F2 -526.20 Hz
 PPMCK 10.45049 dBm/cm
 HZCM 788.67462 Hz/cm



- 177.664
- 170.649
- 170.096
- 169.545
- 168.856
- 144.291
- 144.004
- 122.560
- 122.209
- 86.108
- 84.177
- 77.662
- 77.437
- 77.239
- 76.816
- 75.537
- 72.884
- 70.585
- 69.210
- 68.041
- 55.568
- 47.857
- 46.103
- 41.571
- 38.563
- 34.111
- 33.298
- 30.917
- 28.845
- 26.124
- 23.885
- 23.727
- 23.257
- 20.730
- 20.290
- 17.157
- 16.961
- 16.892



Current Data Parameters
 NAME: 688
 EXPNO: 688
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20080327
 Time: 10.58
 INSTRUM: spect
 PROBO: 5 mm QNP 1H/13
 PULPROG: zg30
 TD: 13512
 SOLVENT: Pyr
 NS: 19
 DS: 0
 SWH: 3378.378 Hz
 FIDRES: 0.250028 Hz
 AQ: 1.9998260 sec
 RG: 287.4
 DW: 148.000 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 2.00000000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 6.00 usec
 PL1: -4.00 dB
 SF01: 300.1315042 MHz

F2 - Processing parameters
 S1: 32768
 SF: 300.1299948 MHz
 MDW: EM
 SSB: 0
 LB: 0.10 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.00 cm
 CY: 12.00 cm
 F1p: 9.862 ppm
 F1: 2959.86 Hz
 F2p: -0.374 ppm
 F2: -112.12 Hz
 PPMCM: 0.46525 ppm/cm
 HZCM: 139.63530 Hz/cm

KELLY-142 13C-NMR PYR-05 300K AV-300

Current Data Parameters
 NAME srb
 EXPNO 694
 PROCNO 1

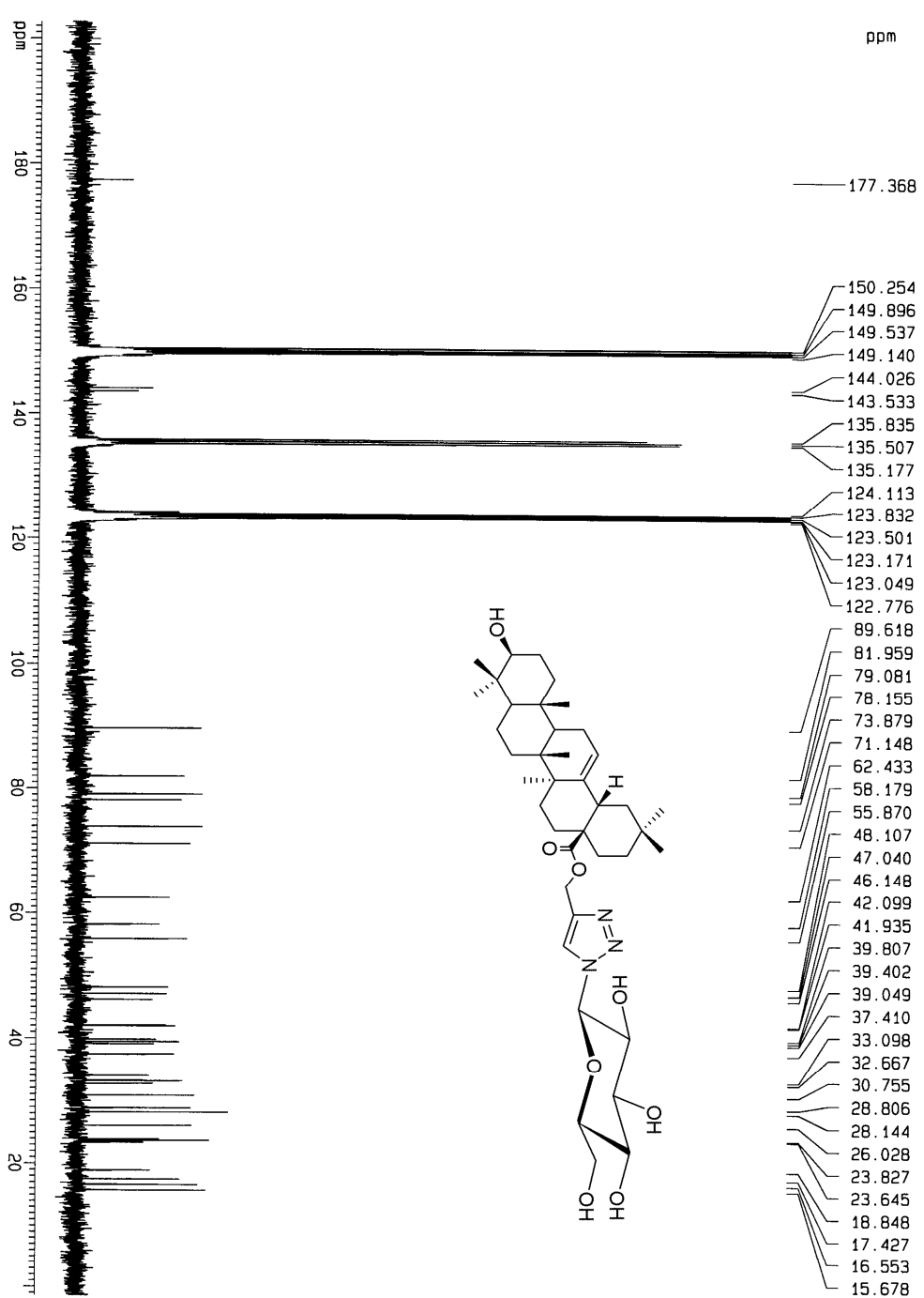
F2 - Acquisition Parameters
 Date_ 20080328
 Time 11:01
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT Pyr
 NS 1088
 DS 8
 SM 18115.941 Hz
 FIDRES 0.552895 Hz
 AQ 0.5044468 sec
 RG 409600
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

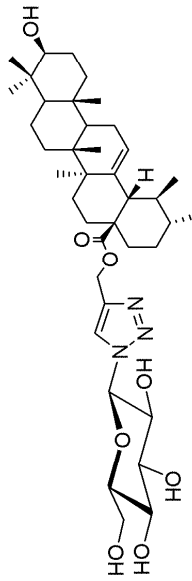
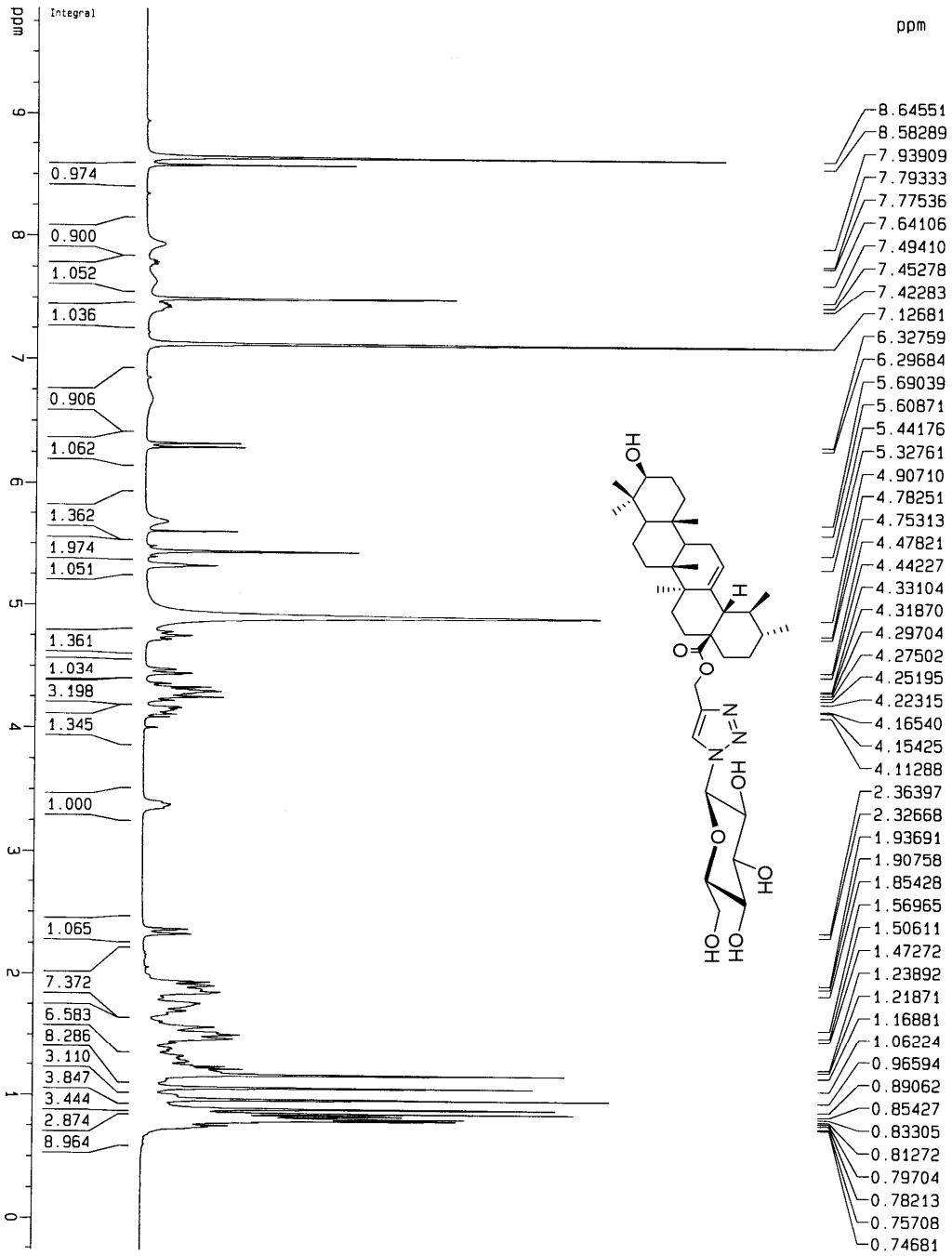
==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.475978 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.132005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.467277 MHz
 MDW FM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 CY 20.00 cm
 F1P 202.677 ppm
 F1 15295.35 Hz
 F2P -1.464 ppm
 F2 -10.47 Hz
 PPMCM 9.07291 ppm/cm
 HZCM 664.71504 Hz/cm





Current Data Parameters
 NAME: shp
 EXPNO: 836
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20080414
 Time: 12.48
 INSTNM: spect
 PROBNM: 5 mm QNP 1H/13
 PULPROG: zg30
 TD: 11414
 SOLVENT: Pyr
 NS: 32
 DS: 0
 SH1: 3910.976 Hz
 FIDRES: 0.33866 Hz
 AQ: 1.4975668 sec
 RG: 322.5
 DM: 131.200 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 2.0000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 6.00 usec
 PL1: -4.00 dB
 SF01: 300.1316115 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1300107 MHz
 WDW: EM
 SSB: 0
 LB: 0.50 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.00 cm
 CY: 12.00 cm
 F1P: 9.658 ppm
 F1: 2956.54 Hz
 F2P: -0.264 ppm
 F2: -79.19 Hz
 PPMICH: 0.46006 ppm/cm
 HZCM: 138.07883 Hz/cm

Kelly-149 C13-NMR CSDJN 300K AV-300

Current Data Parameters
 NAME snb
 EXPNO 856
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20080416
 Time 18.18
 INSTRUM spect
 PROBDW 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT Pyv
 NS 2609
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 102400
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

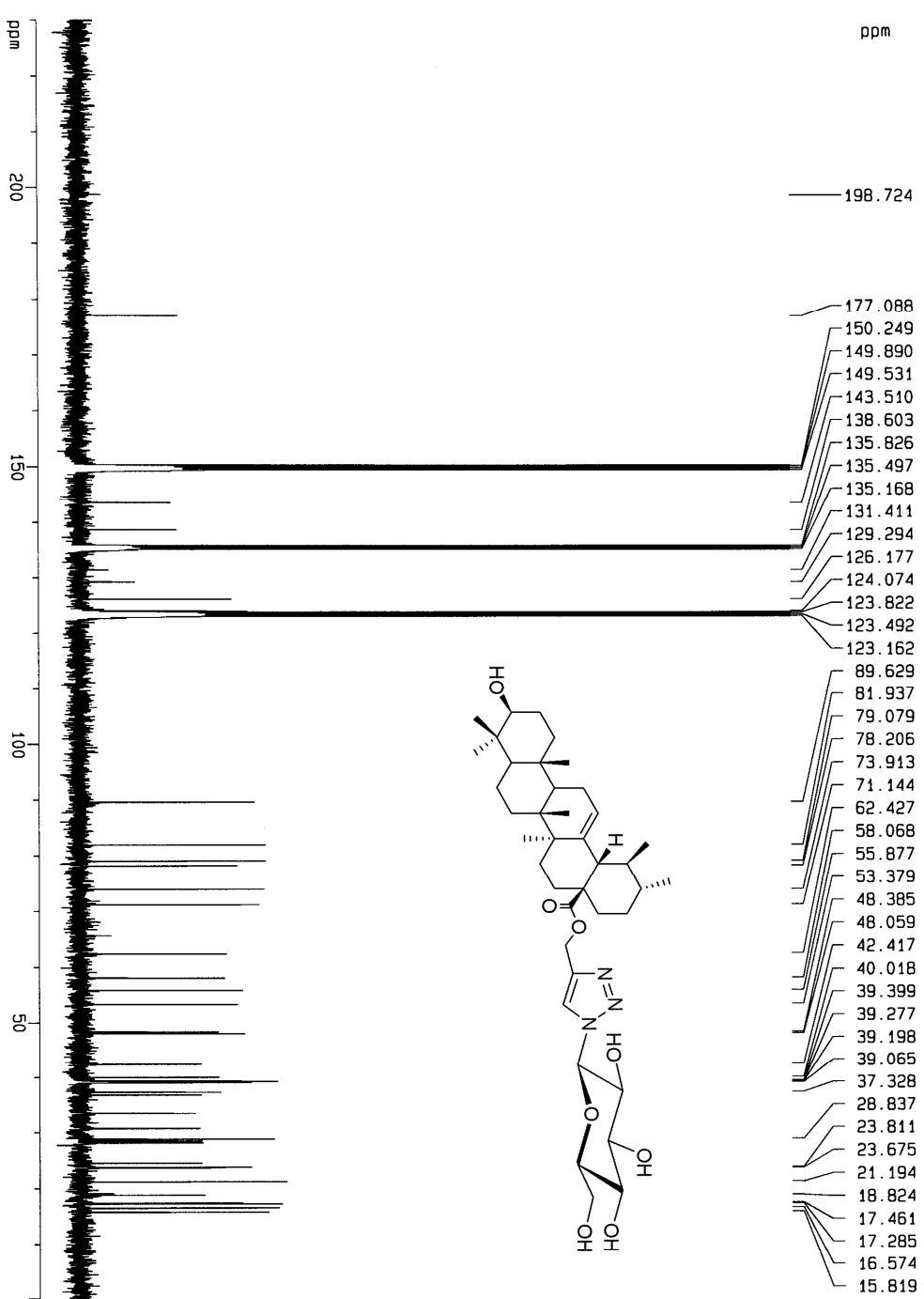
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 POP02 80.00 usec
 PL2 -4.00 dB
 PL12 19.28 dB
 SF02 300.1312005 MHz

F2 - Processing parameters

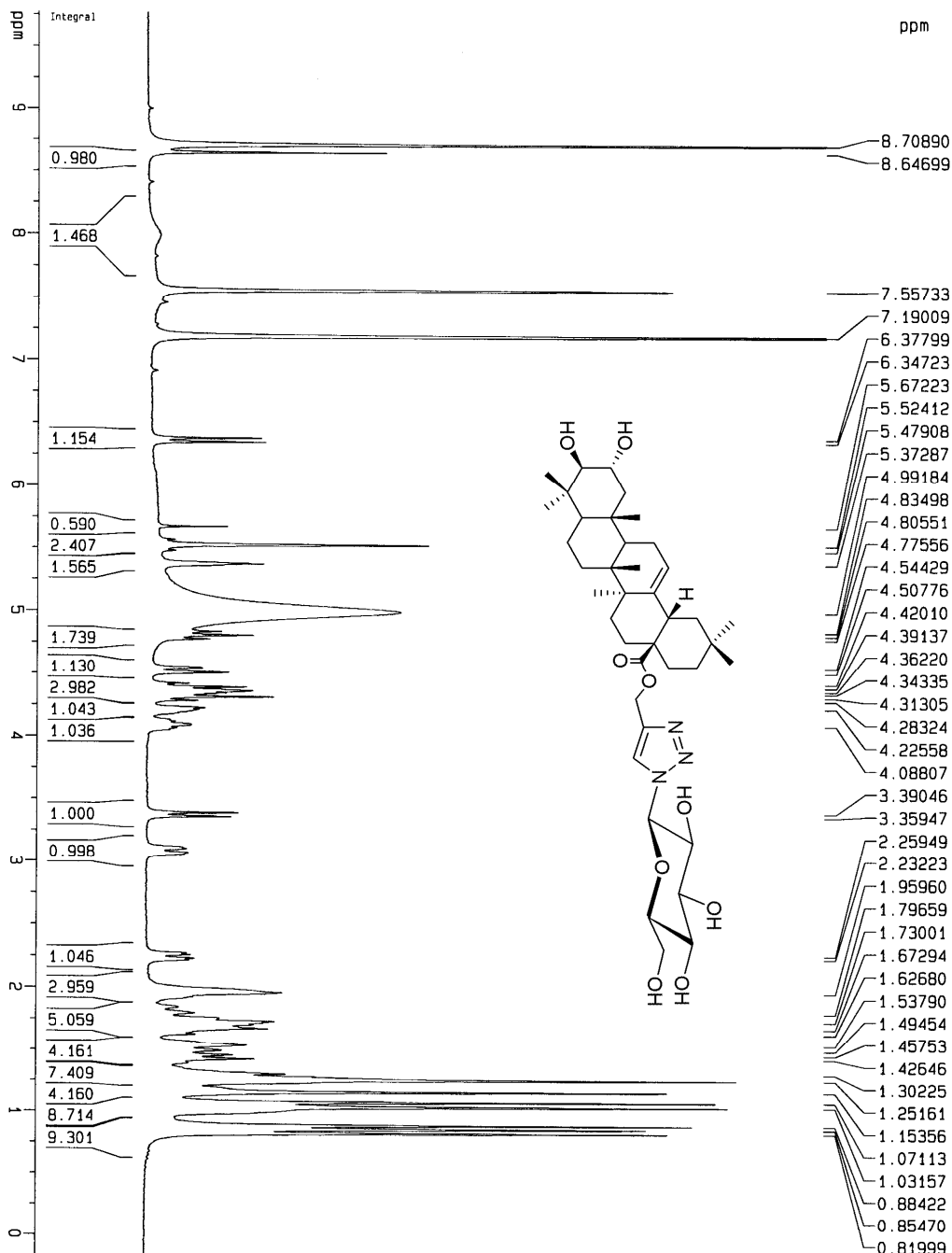
SF 32768
 SF 75.4677277 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters

CX 22.50 cm
 CY 30.00 cm
 F1P 280.000 ppm
 F1 17357.58 Hz
 F2 0.000 ppm
 F2 0.00 Hz
 PPKCM 10.22222 ppm/cm
 HZCM 771.44788 Hz/cm



snb



Current Data Parameters
 NAME shb
 EXPNO 835
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080414
 Time 12.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TO 14.14
 SOLVENT Pyr
 NS 32
 DS 0
 SHF 370.238 Hz
 FIDRES 0.325936 Hz
 AQ 1.5340916 sec
 RG 322.5
 DM 134.400 usec
 DE 5.00 usec
 TE 298.0 K
 D1 2.0000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SFO1 300.1315716 MHz

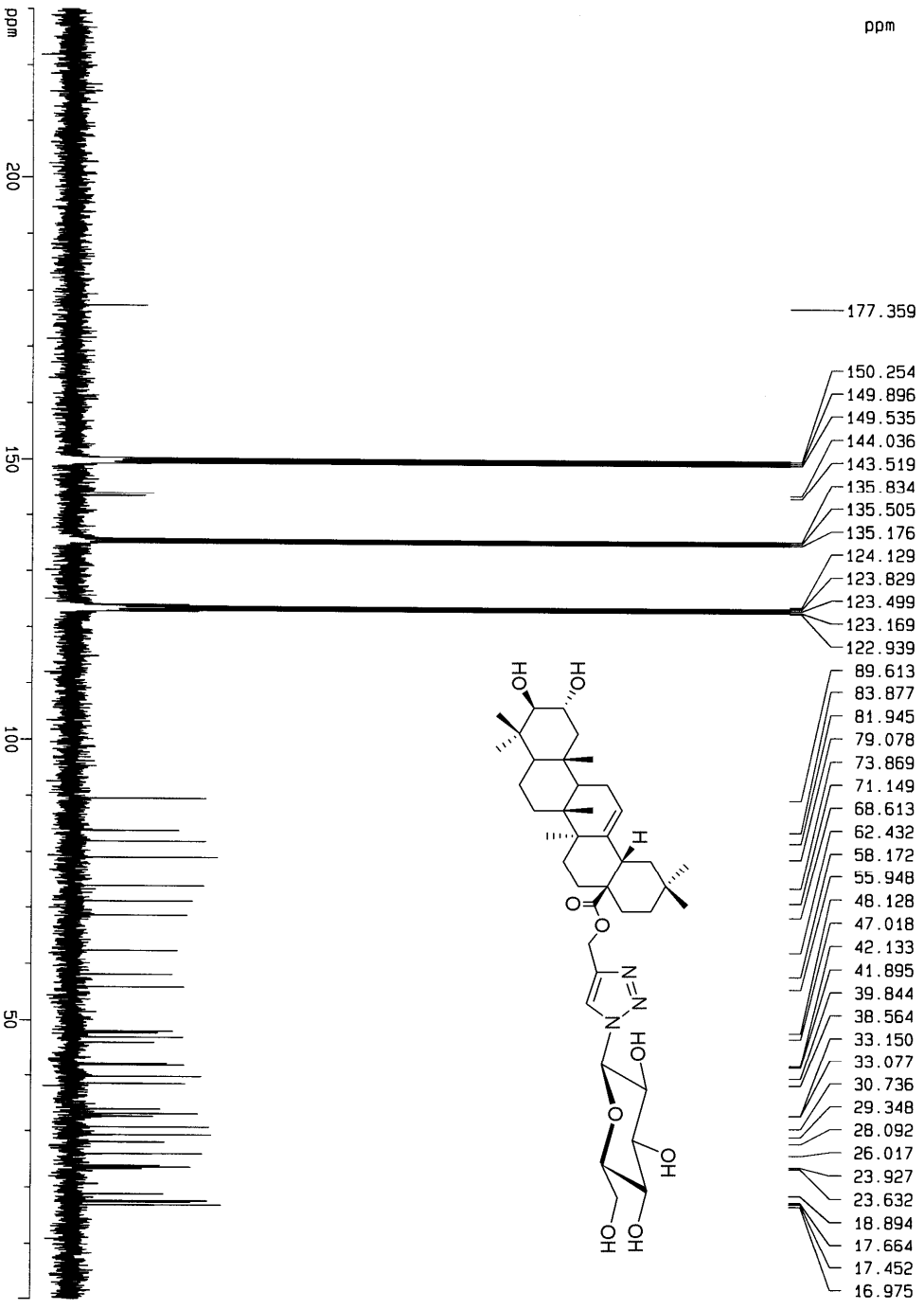
F2 - Processing parameters
 SI 32768
 SF 300.1299916 MHz
 MDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00

1D NMR Plot Parameters
 CX 22.00 cm
 CY 20.00 cm
 F1P 9.771 ppm
 F1 2932.46 Hz
 F2P -0.170 ppm
 F2 -50.92 Hz
 PPMKCM 0.45183 ppm/cm
 HZCM 135.60815 Hz/cm

KELLY-148 C13-NMR CSDEN 300K AV-300

Current Data Parameters
 NAME SNO
 EXPRNO 855
 PROCNO 1

ppm



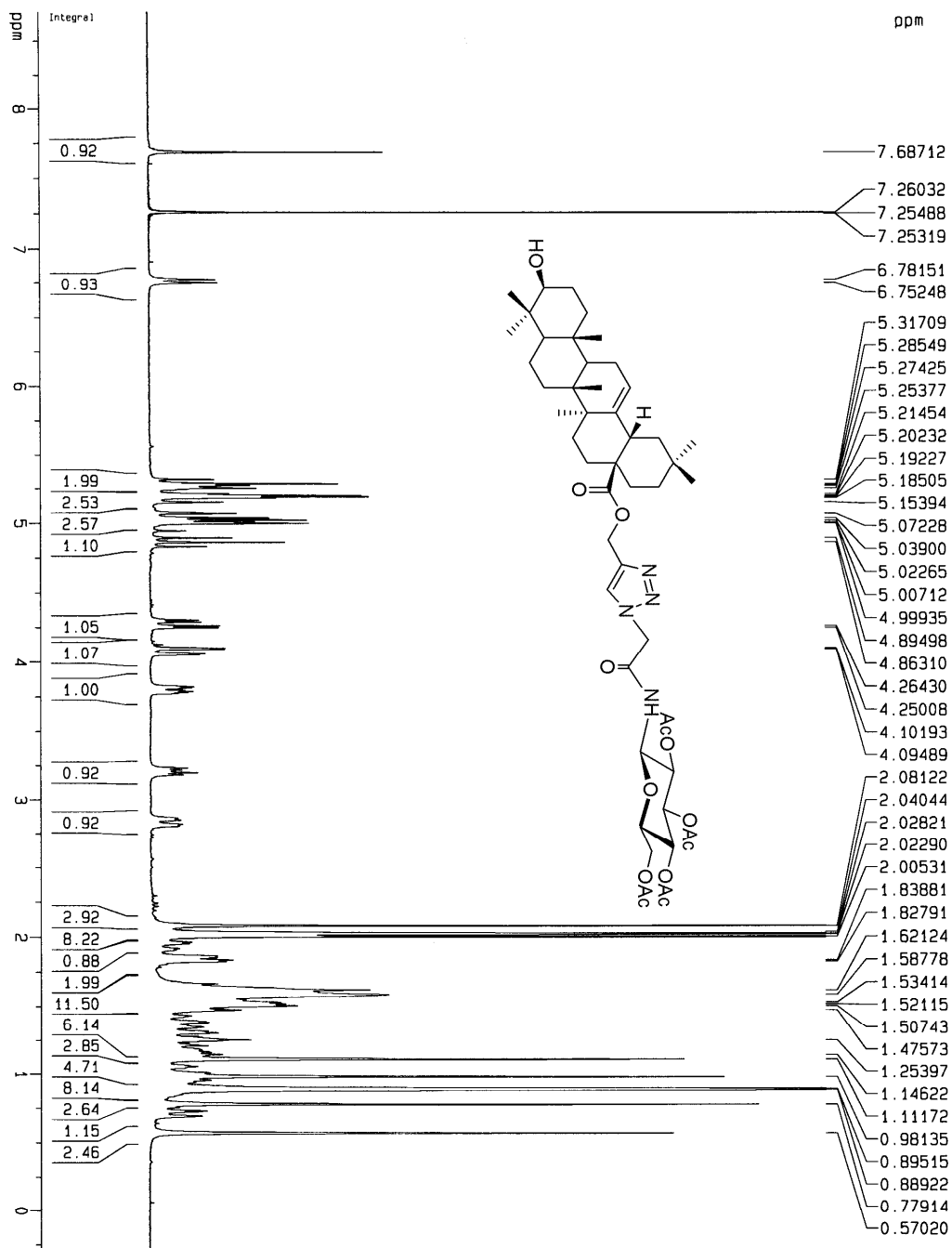
F2 - Acquisition Parameters
 Date_ 20080415
 Time 16.55
 INSTRUM spect
 PROBD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT Pyr
 NS 1384
 DS 8
 SM1 18115.941 Hz
 FIDRES 0.352855 Hz
 AQ 0.3044458 sec
 RG 102400
 DW 27.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.467277 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

sub

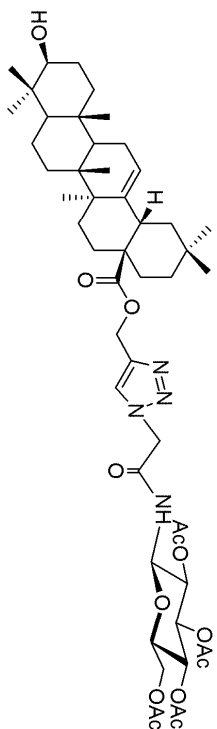
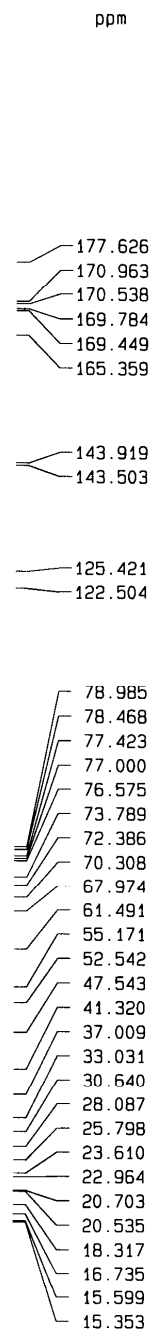


```

Current Data Parameters
NAME          shb
EXPNO        816
PROCNO       1
F2 - Acquisition Parameters
Date_        20080410
Time         11.10
INSTRUM     spect
PROBHD      5 mm QNP 1H/13
PULPROG     zg30
TD           12820
SOLVENT     CDCl3
NS           40
DS           0
SH1         3205.128 Hz
FIDRES      0.250010 Hz
AQ          1.9999700 sec
RG           362
DM          156.000 usec
DE           5.00 usec
TE           298.0 K
D1           2.00000000 sec
===== CHANNEL f1 =====
NUC1         1H
P1           6.00 usec
PL1          -4.00 dB
SFO1         300.1313889 MHz
F2 - Processing parameters
SI           32768
SF           300.1300121 MHz
MVM          EM
SSB          0
LB           0.10 Hz
GB           0
PC           1.00
1D NMR plot parameters
CX           22.00 cm
CY           20.00 cm
F1P         8.712 ppm
F1          2614.84 Hz
F2P         -0.295 ppm
F2          -88.55 Hz
PPKCM       0.40543 ppm/cm
HZCM        122.88142 Hz/cm
  
```

Kelly-146 13C-NMR CDCL3 300K AV-300

Current Data Parameters
 NAME snb
 EXPNO 841



```

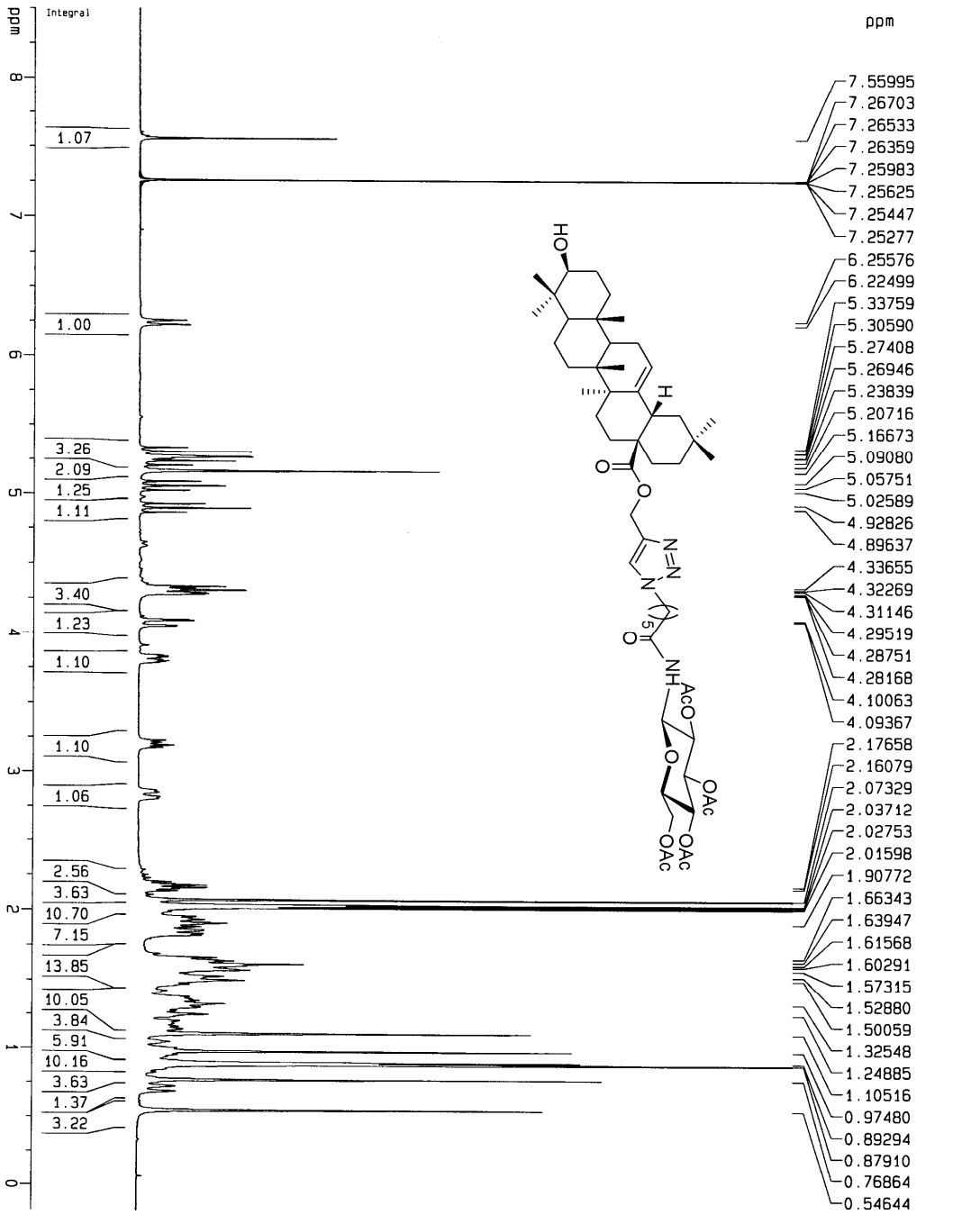
F2 - Acquisition Parameters
Date_      20080414
Time       15.49
INSTRUM    spect
PROBHD     5 mm QNP 1H/13
PULPROG    zgpgc
TD         32768
SOLVENT    CDCl3
NS         1216
DS         8
SMH        21097.047 Hz
FIDRES     0.648931 Hz
AQ         0.7769316 sec
RG         102400
DM         23.700 usec
DE         6.00 usec
TE         300.0 K
D1         2.00000000 sec
d11        0.03000000 sec

===== CHANNEL f1 =====
NUC1       13C
P1         8.00 usec
PL1       -2.00 dB
SFO1       75.4763978 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        -4.00 dB
SFO2       300.1312005 MHz

F2 - Processing parameters
SI         32768
SF         75.4677520 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         22.00 cm
CY         12.00 cm
F1P        220.682 DPM
F1         16654.39 Hz
F2P        -3.576 DPM
F2         -289.89 Hz
PPMCH      10.19357 DPM/cm
HZCM       759.28577 HZ/cm
  
```

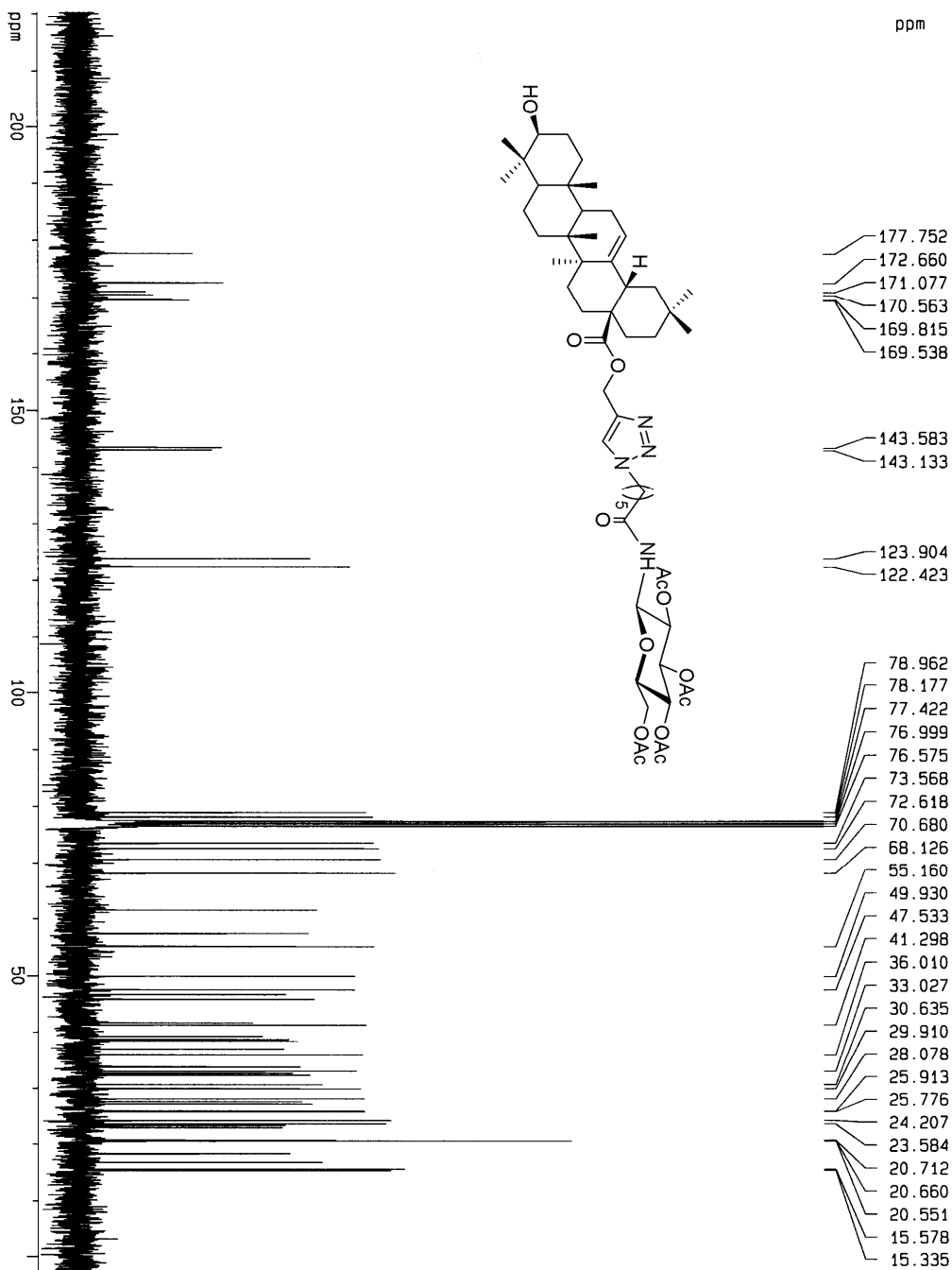


Current Data Parameters
 NAME shb
 EXPNO 817
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20080410
 Time 11:14
 INSTRUM spect
 PROBNM 5 mm QNP 1H/13
 PULPROG zg30
 TO 13020
 SOLVENT CDCl3
 NS 33
 DS 0
 SMH 3255.208 Hz
 FIDRES 0.250016 Hz
 AQ 1.999220 sec
 RB 362
 DM 153.600 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SFO1 300.1314580 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300125 MHz
 MDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 15.00 cm
 F1P 8.503 ppm
 F1 2552.03 Hz
 F2P -0.189 ppm
 F2 -56.70 Hz
 PPHCKM 0.35509 ppm/cm
 HZCM 118.57864 Hz/cm

Ke11y-147 13C-NMR CDCL3 300K AV-300



- 177.752
- 172.660
- 171.077
- 170.563
- 169.815
- 169.538
- 143.583
- 143.133
- 123.904
- 122.423
- 78.962
- 78.177
- 77.422
- 76.999
- 76.575
- 73.568
- 72.618
- 70.680
- 68.126
- 55.160
- 49.930
- 47.533
- 41.298
- 36.010
- 33.027
- 30.635
- 29.910
- 28.078
- 25.913
- 25.776
- 24.207
- 23.584
- 20.712
- 20.660
- 20.551
- 15.578
- 15.335

Current Data Parameters
 NAME shb
 EXPNO 842
 PROCNO 1

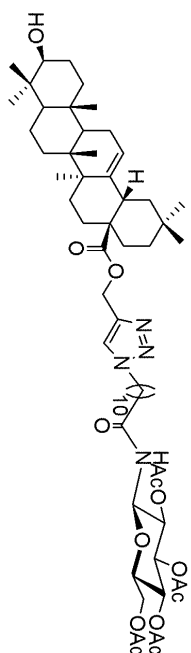
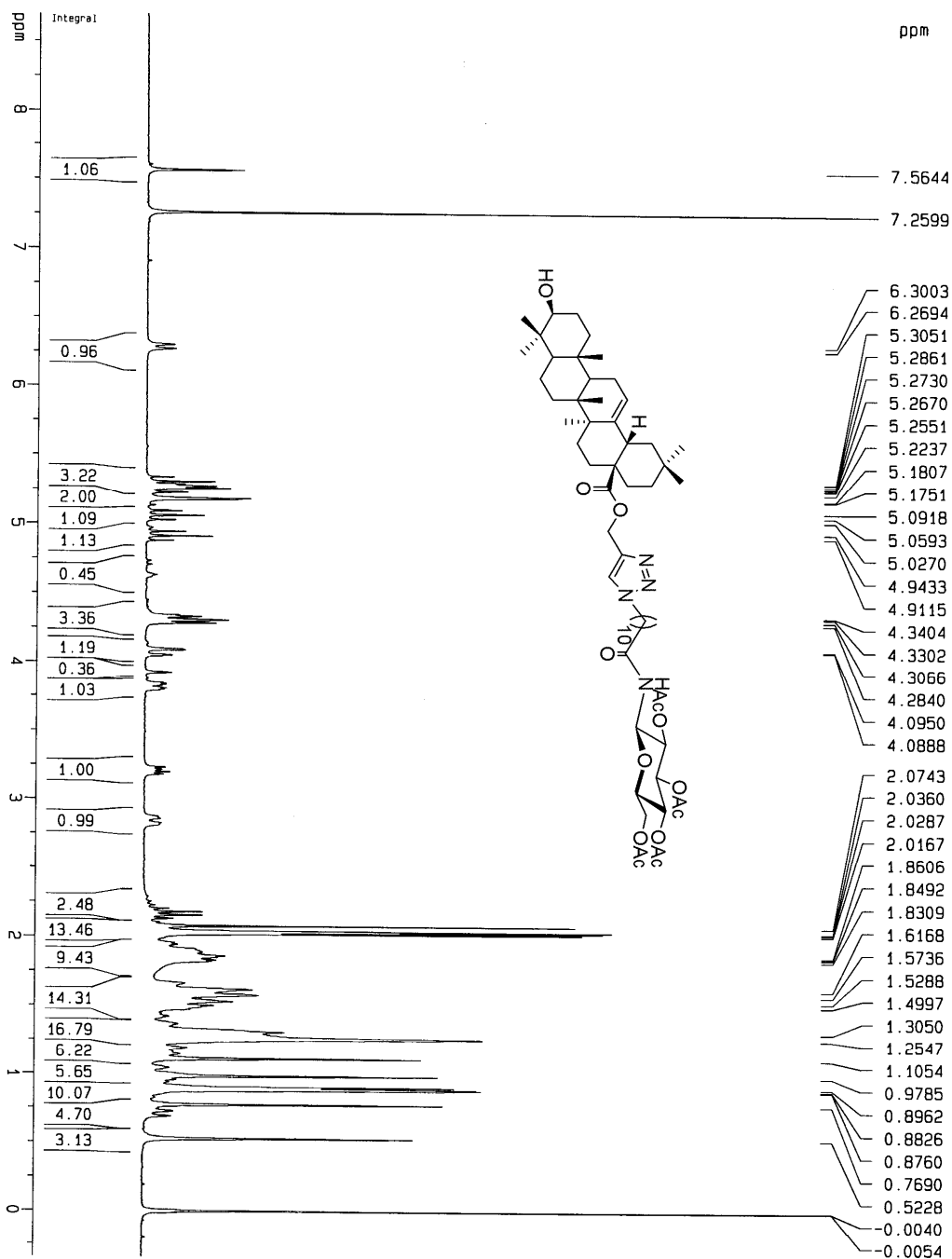
F2 - Acquisition Parameters
 Date_ 20080414
 Time 16.54
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 1531
 DS 8
 SMH 21097.047 Hz
 FIDRES 0.643931 Hz
 AQ 0.776516 sec
 RG 102400
 DM 23.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUCl1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUCl2 1H
 P2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677520 MHz
 EQ EM
 MDM 0
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CK 22.00 cm
 CY 20.00 cm
 F1P 220.339 ppm
 F1 16628.47 Hz
 F2P -2.546 ppm
 F2 -192.15 Hz
 PPMCM 10.13113 ppm/cm
 MZCM 764.57349 Hz/cm



Current Data Parameters

NAME shb

EXPNO 837

PROCNO 1

F2 - Acquisition Parameters

Date_ 20080414

Time 15.36

INSTRUM spect

PROBHD 5 mm QNP 1H/13

PULPROG zg30

TD 13414

SOLVENT CDCl3

NS 16

DS 0

SWH 2997.602 Hz

FIDRES 0.26625 Hz

AQ 1.9039052 sec

RG 512

DM 166.800 usec

DE 6.00 usec

TE 298.0 K

D1 2.00000000 sec

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

NUC1 1H

P1 6.00 usec

PL1 -4.00 dB

SFO1 300.1312599 MHz

F2 - Processing parameters

SF 300.130124 MHz

SI 32768

WDW EM

SSB 0

LB 0.50 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 22.00 cm

CY 12.00 cm

F1P 8.696 ppm

F1 2610.05 Hz

F2P -0.347 ppm

F2 -104.00 Hz

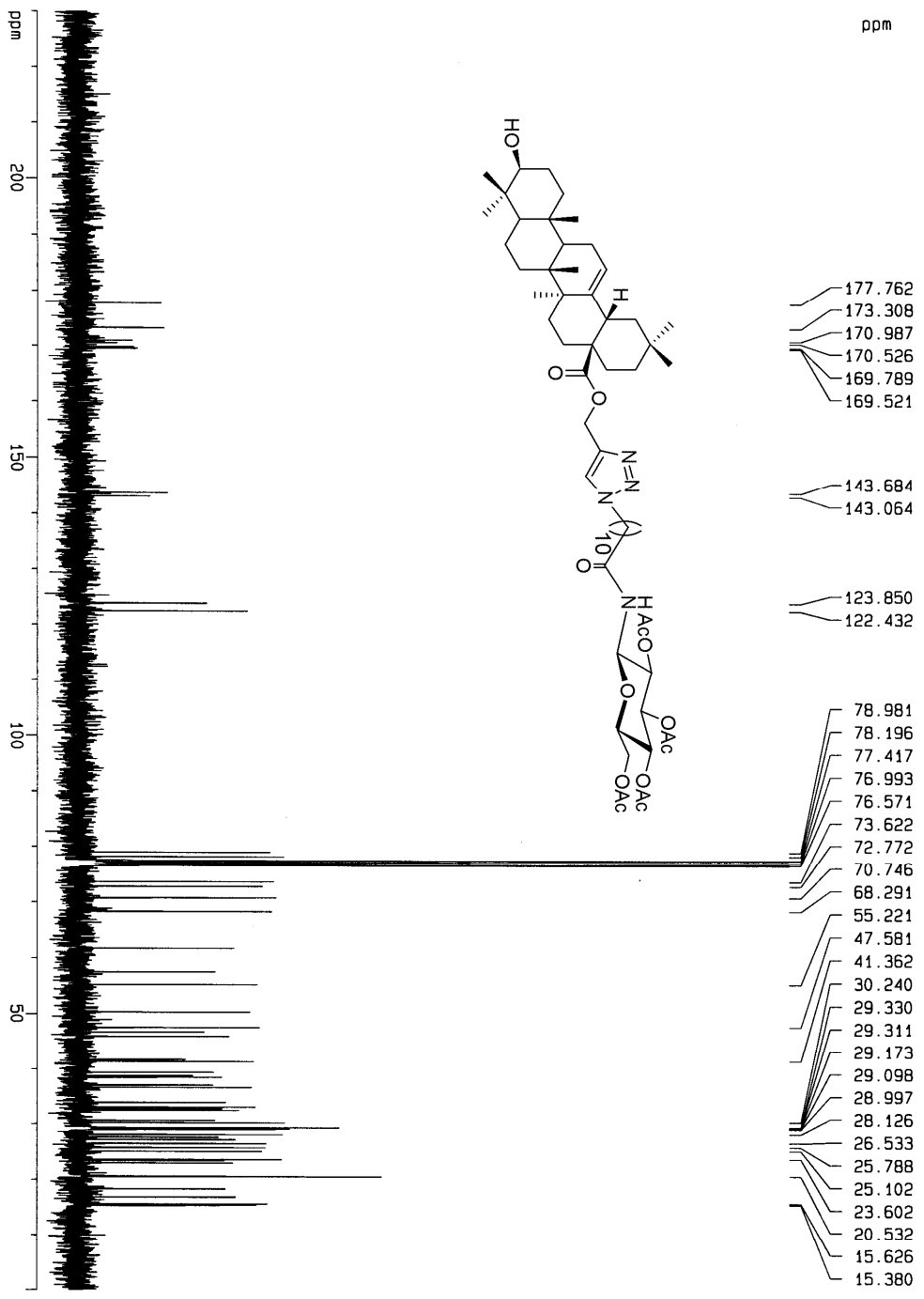
PRNCH 0.4104 ppm/cm

HZCN 123.36568 Hz/cm

KELLY-150 C13-NMR CDCl3 300K AV-300

Current Data Parameters
 NAME S1D
 EXNO 957
 PROCNO 1

ppm



- 177.762
- 173.308
- 170.987
- 170.526
- 169.789
- 169.521
- 143.684
- 143.064
- 123.850
- 122.432
- 78.981
- 78.196
- 77.417
- 76.993
- 76.571
- 73.622
- 72.772
- 70.746
- 68.291
- 55.221
- 47.581
- 41.362
- 30.240
- 29.330
- 29.311
- 29.173
- 29.098
- 28.997
- 28.126
- 26.533
- 25.788
- 25.102
- 23.602
- 20.532
- 15.626
- 15.380

F2 - Acquisition Parameters
 Date_ 20080416
 Time_ 20.25
 INSTRUM spect
 PROBDW 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 2220
 DS B
 SMH 21097.047 Hz
 FIDRES 0.649831 Hz
 AQ 0.7766516 sec
 RG 102400
 DW 23.700 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

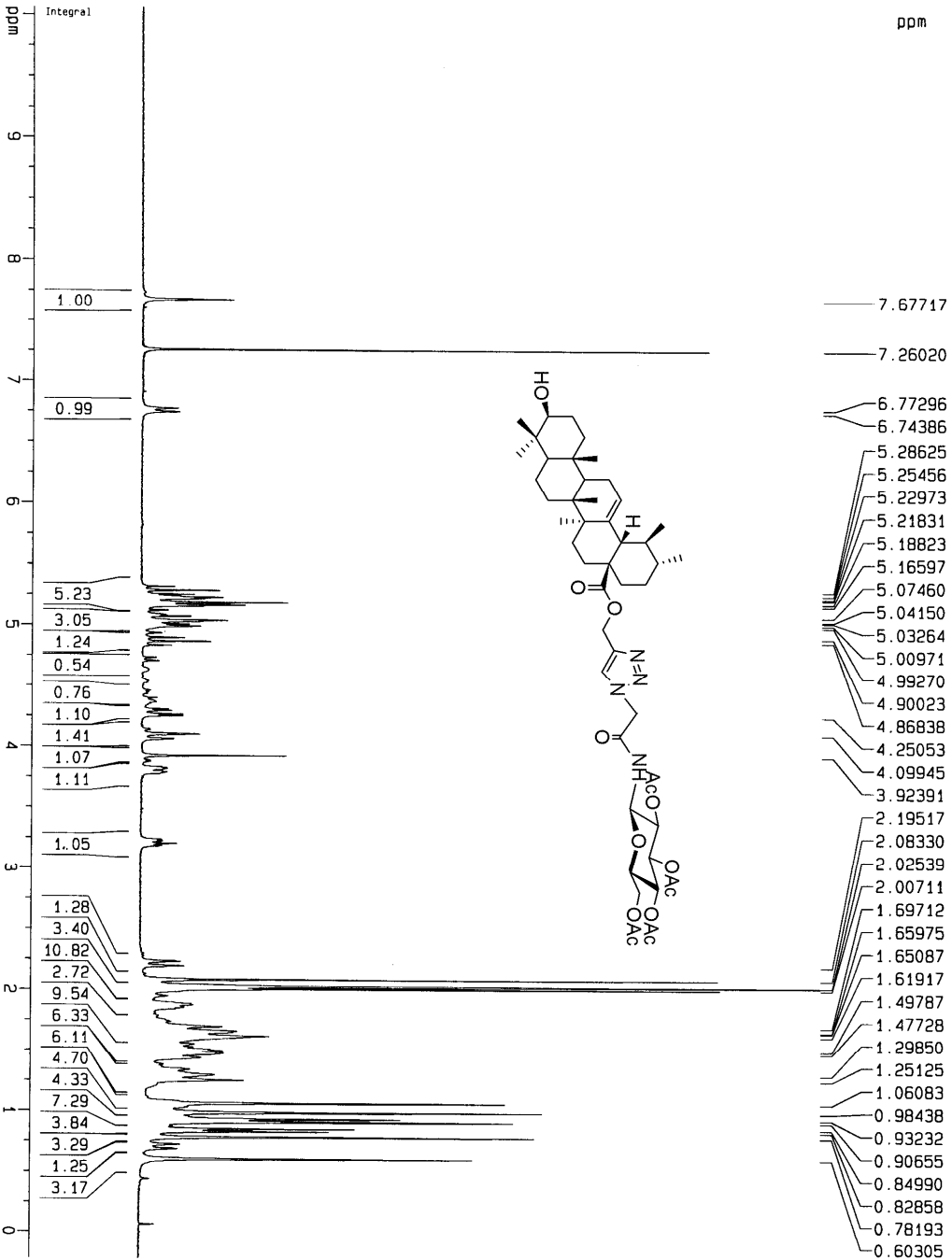
===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SFO1 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677494 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.50 cm
 CY 20.00 cm
 F1P 230.000 ppm
 F1 17357.58 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PNHCM 10.22222 ppm/cm
 HZCM 771.44812 Hz/cm

sub



Current Data Parameters
 NAME: spb
 EXPNO: 890
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20080418
 Time: 23.13
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zg30
 TD: 11414
 SOLVENT: CDCl3
 NS: 16
 DS: 0
 SH1: 5995.204 Hz
 FIDRES: 0.325250 Hz
 AQ: 0.9519776 sec
 RG: 512
 DM: 83.400 usec
 DE: 5.00 usec
 TE: 298.0 K
 D1: 2.0000000 sec

===== CHANNEL f1 =====
 NUC1: 1H
 P1: 6.00 usec
 PL1: -4.00 dB
 SF01: 300.1324010 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1300124 MHz
 MDW: EM
 SSB: 0
 LB: 0.20 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.00 cm
 CY: 12.00 cm
 F1P: 10.062 ppm
 F1: 3080.03 Hz
 F2P: -0.225 ppm
 F2: -67.75 Hz
 PPMCM: 0.46765 ppm/cm
 HZCM: 140.35487 Hz/cm

Key11y-153 C13-NMR CDC13 300K AV-300

Current Data Parameters
 NAME snb
 EXPNO 922
 PROCNO 1

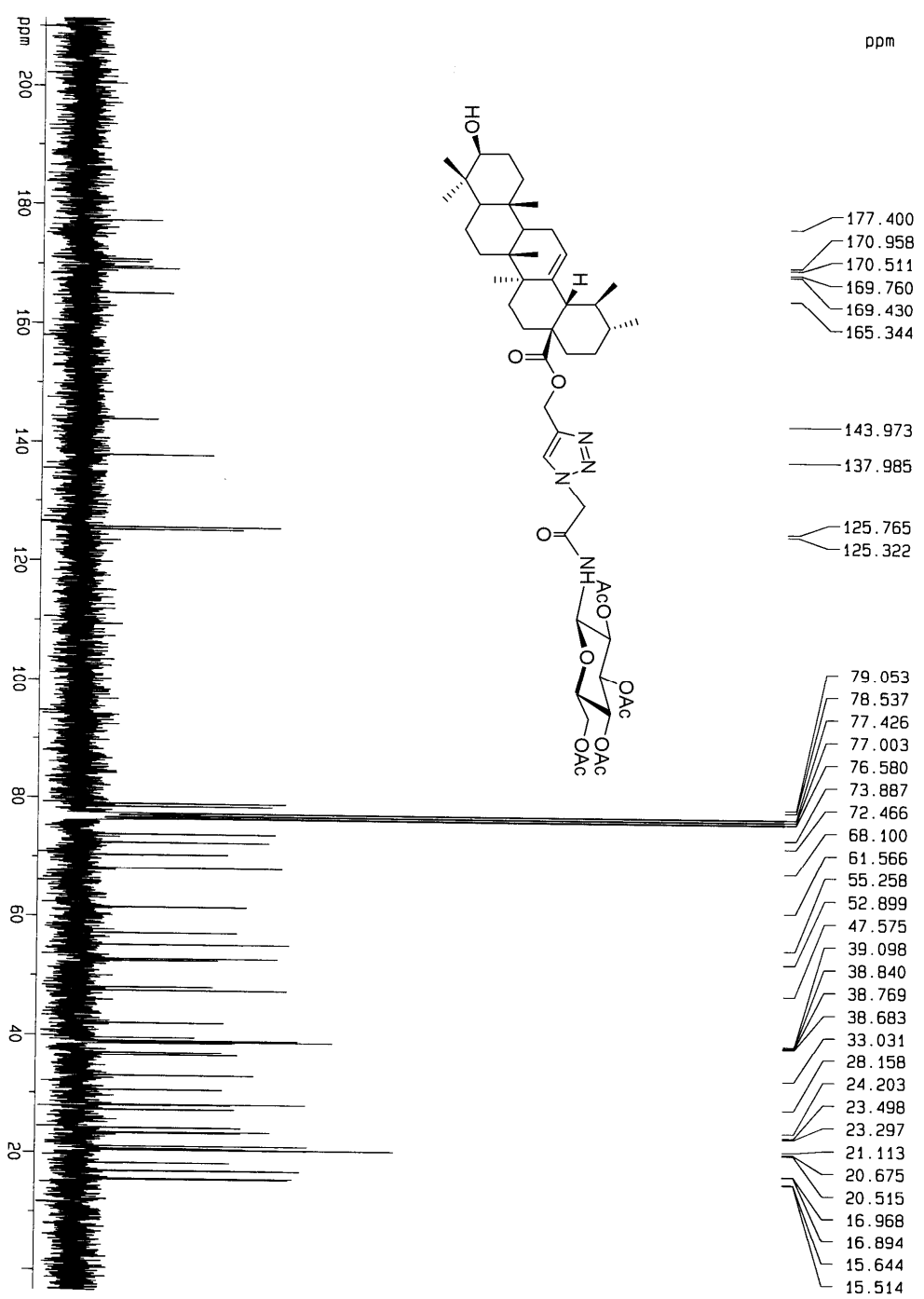
F2 - Acquisition Parameters
 Date_ 20080423
 Time 17.16
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TD 32768
 SOLVENT CDC13
 NS 1403
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 102400
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

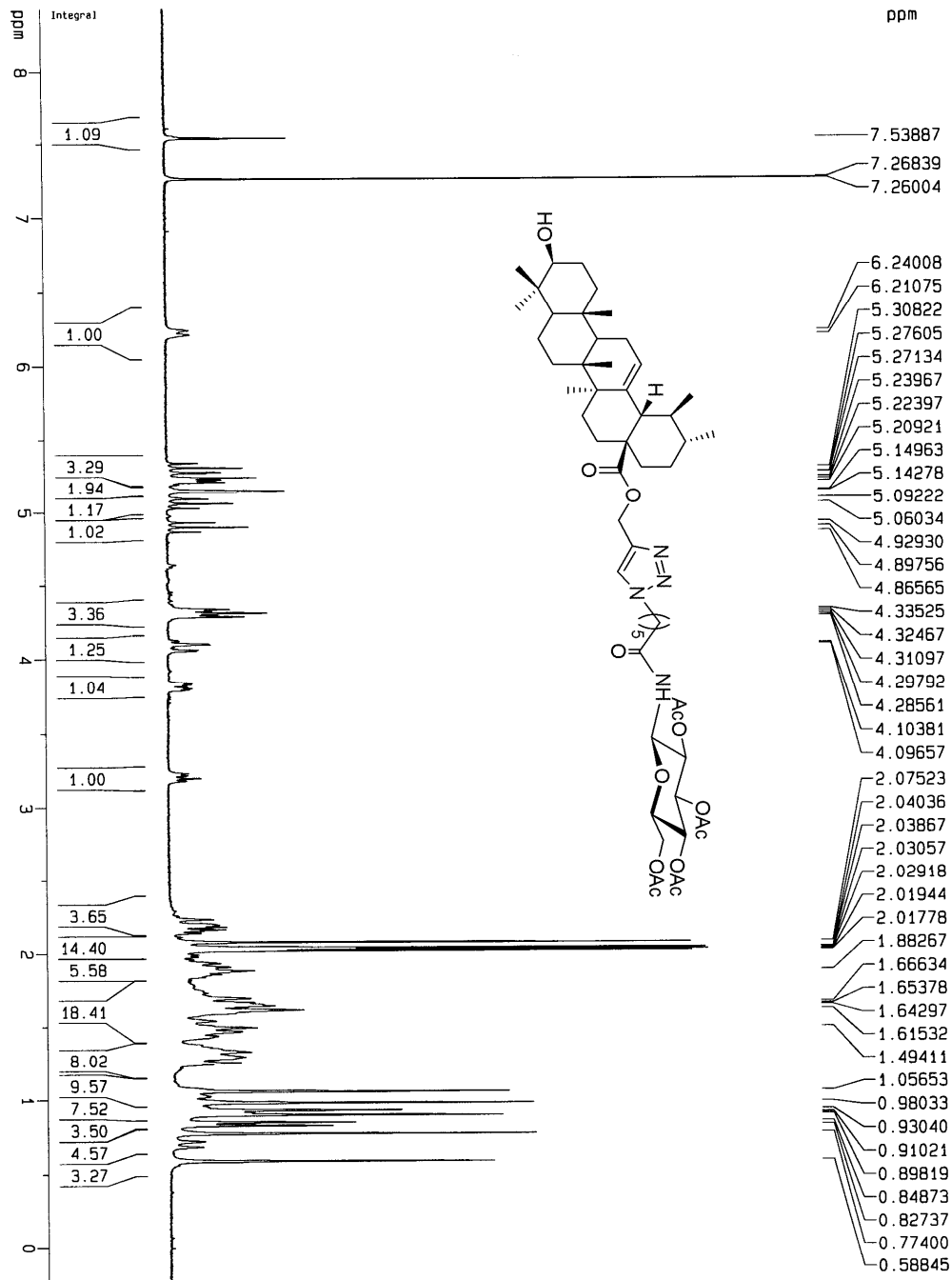
F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 KOP EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.50 cm
 CY 50.00 cm
 F1P 211.351 ppm
 F1 15950.22 Hz
 F2P -3.459 ppm
 F2 -261.01 Hz
 PPGCM 9.54711 ppm/cm
 HZCM 720.45902 Hz/cm



sub

Kelly-154 H1-NMR CDCl3 300K AV-300



Current Data Parameters
 NAME SHB
 EXPNO 878
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080417
 Time 15:57
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 18382
 SOLVENT CDCl3
 NS 16
 DS 0
 SMH 3063.726 Hz
 FIDRES 0.166670 Hz
 AQ 2.3999924 sec
 RG 4456.1
 DM 163.200 usec
 DE 6.00 usec
 TE 303.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1312980 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300124 MHz
 MDW EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 15.00 cm
 F1P 8.425 ppm
 F2P 2528.84 Hz
 F2 -0.231 ppm
 PPM1CM 0.39530 ppm/cm
 HZCM 118.10055 Hz/cm

sub

KELLY-154 C13-NMR CDCl3 300K AV-300

Current Data Parameters
 NAME smp
 EXPNO 896
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20080421
 Time 11:18
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1829
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.5044468 sec
 RG 102400
 DW 27.500 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

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

NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4753978 MHz

===== CHANNEL f2 =====

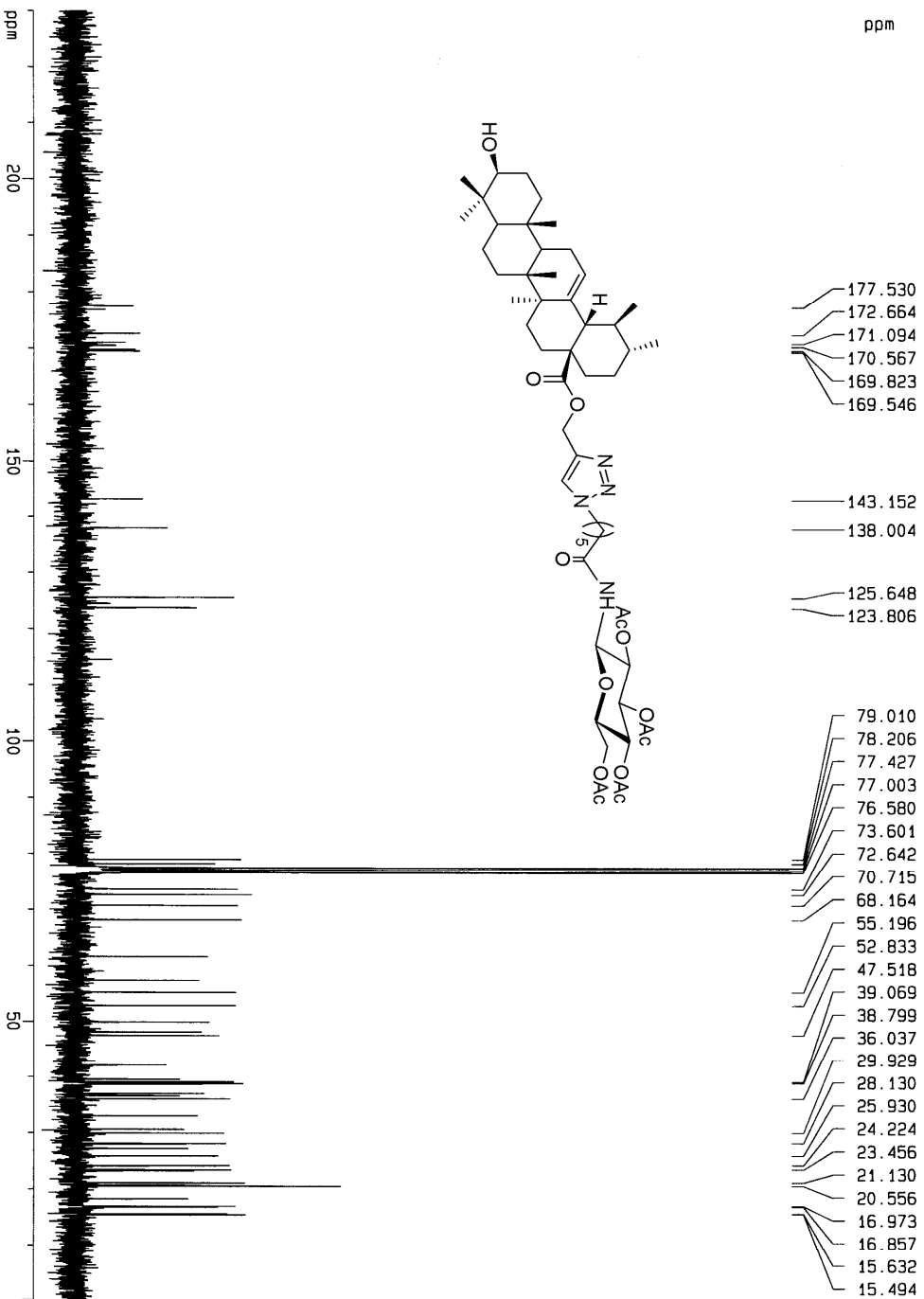
CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters

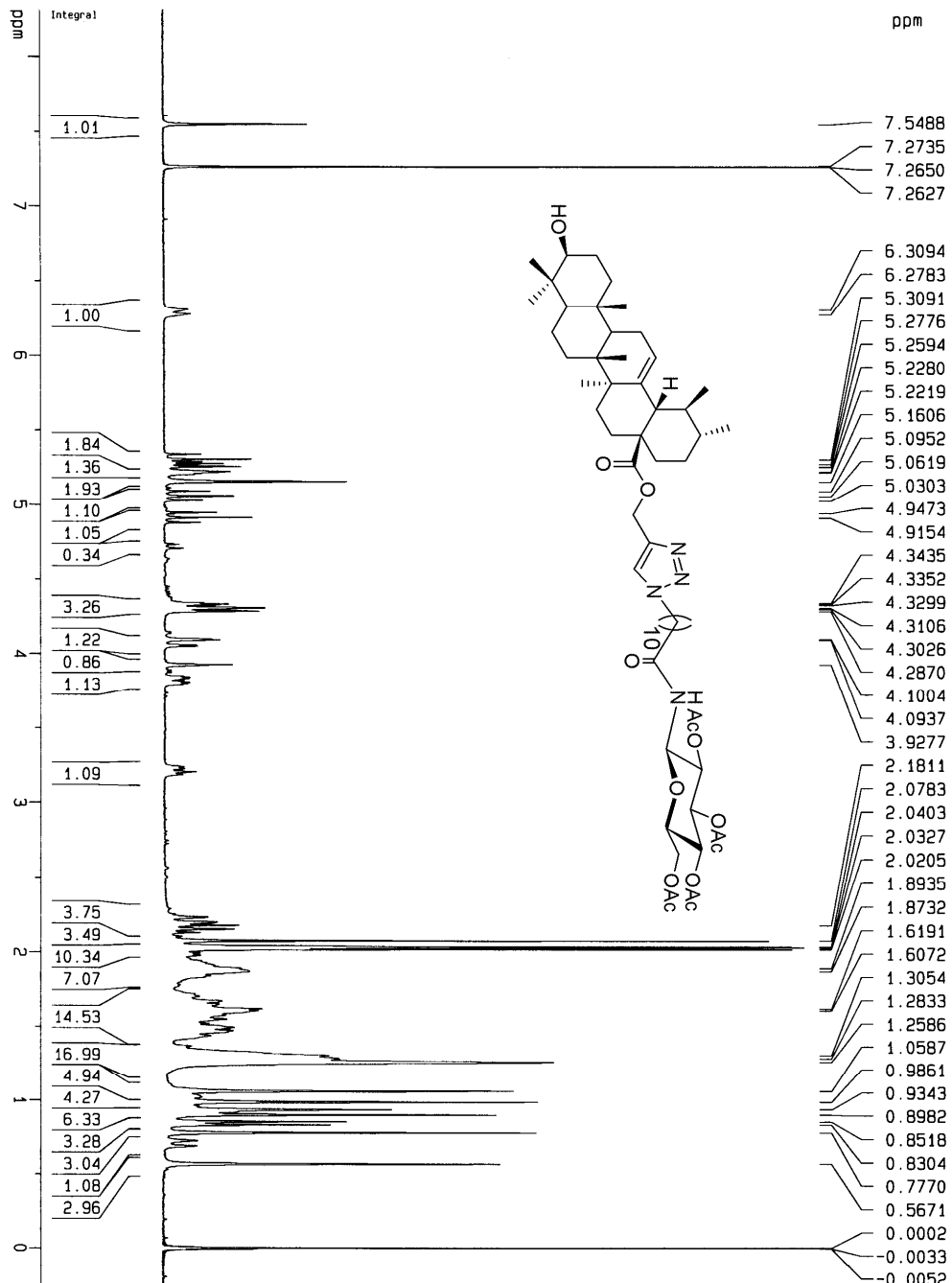
SI 32768
 SF 75.467506 MHz
 WDW EM
 SSF 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters

CX 22.50 cm
 CY 20.00 cm
 F1P 230.000 ppm
 F1 17357.58 Hz
 F2P 0.000 ppm
 F2 10.2222 ppm/cm
 HZCM 771.44806 Hz/cm



KE11Y-155 H1-NMR CDCL3 300K AV-300



7.5488
7.2735
7.2650
7.2627
6.3094
6.2783
5.3091
5.2776
5.2594
5.2280
5.2219
5.1606
5.0952
5.0619
5.0303
4.9473
4.9154
4.3435
4.3352
4.3299
4.3106
4.3026
4.2870
4.1004
4.0937
3.9277
2.1811
2.0783
2.0403
2.0327
2.0205
1.8935
1.8732
1.6191
1.6072
1.3054
1.2833
1.2586
1.0587
0.9861
0.9343
0.8982
0.8518
0.8304
0.7770
0.5671
0.0002
0.0033
0.0052

Integral
1.01
1.00
1.84
1.36
1.93
1.10
1.05
0.34
3.26
1.22
0.86
1.13
1.09
3.75
3.49
10.34
7.07
14.53
16.99
4.94
4.27
6.33
3.28
3.04
1.08
2.96

Current Data Parameters
NAME
SIB
EXPNO 860
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080416
Time 22:22
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 7630
TO 12164
SOLVENT CDCl3
NS 22
DS 0
SWH 3041.363 Hz
FIDRES 0.260030 Hz
AQ 1.9998116 sec
RG 256
DM 164.400 usec
DE 6.00 usec
TE 303.0 K
D1 2.00000000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 6.00 usec
PL1 -4.00 dB
SFO1 300.1314230 MHz

F2 - Processing parameters
SI 32768
SF 300.1300111 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

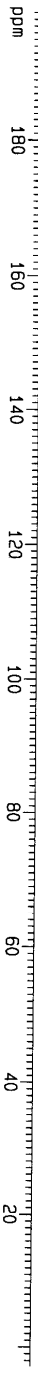
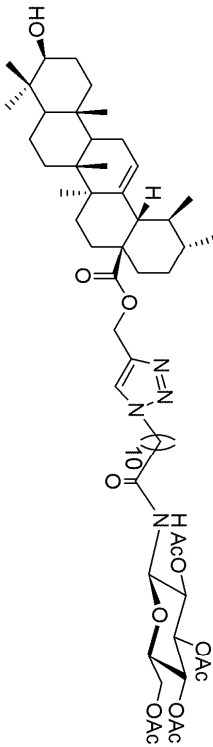
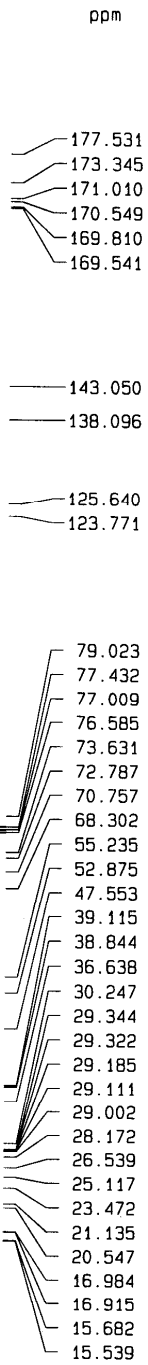
1D NMR plot parameters
CX 22.00 cm
CY 15.00 cm
F1P 8.315 ppm
F1 2495.54 Hz
F2P -0.293 ppm
F2 -97.29 Hz
PPMCH 0.39117 ppm/cm
HZCM 117.40135 Hz/cm

sub

KELLY-155 1H-NMR CDCL3 300K AV-300

Current Data Parameters
 NAME shb
 EXPNO 888
 PROCNO 1

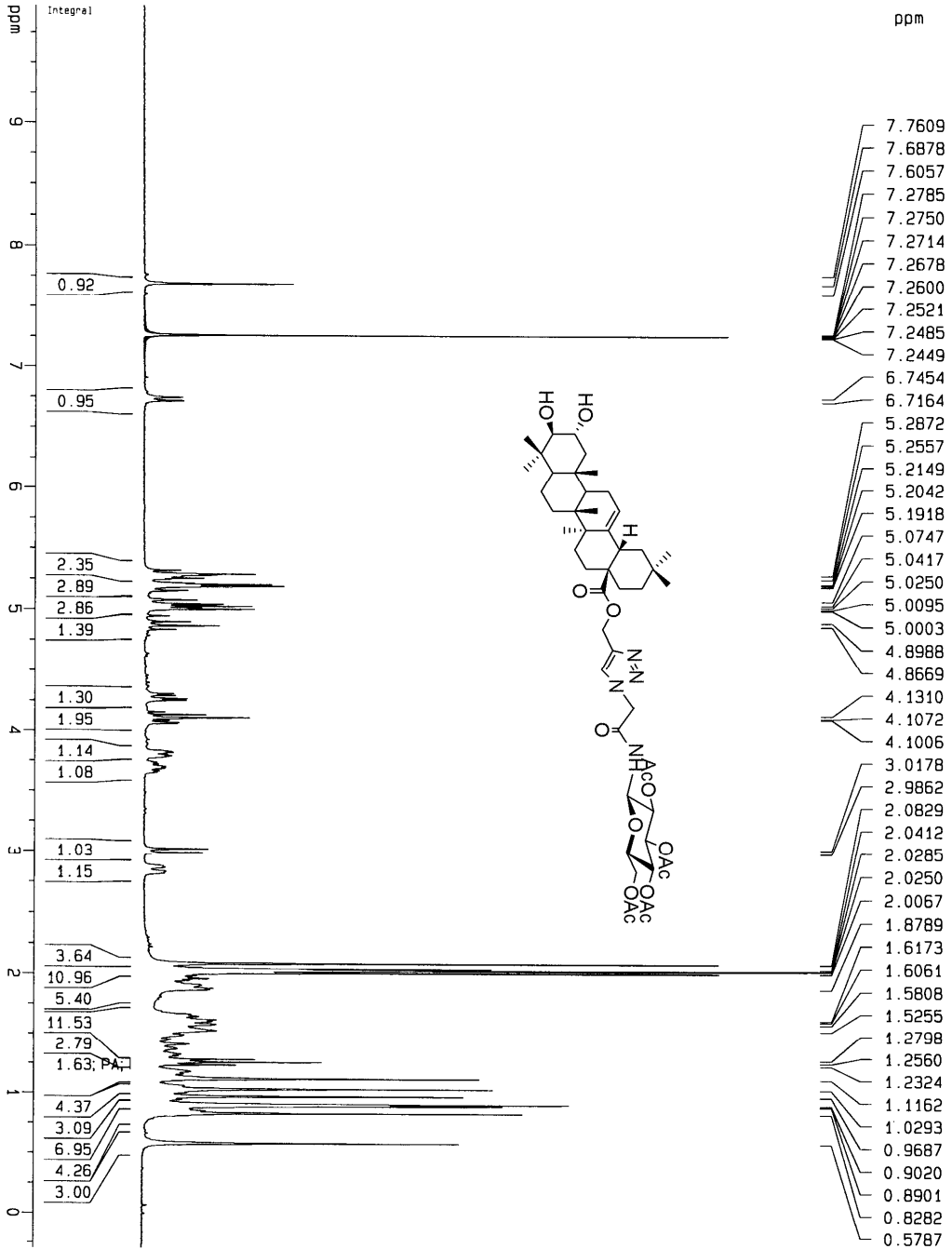
F2 - Acquisition Parameters
 Date_ 20080418
 Time 16:11
 INSTRUM spect
 PROBNM 5 mm QNP 1H/13
 PULPROG zgpg
 TO 32768
 SOLVENT CDCl3
 NS 2079
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.55285 Hz
 AQ 0.9044468 sec
 RG 10240
 DM 27.680 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec



==== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz
 F2 - Processing parameters
 SI 32758
 SF 75.4677484 MHz
 MDK EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 CY 20.00 cm
 F1p 199.905 ppm
 F1 15096.40 Hz
 F2p -2.914 ppm
 F2 -219.89 Hz
 PPMCM 9.01418 ppm/cm
 HZCM 880.27972 Hz/cm

KELLY-156 1H-NMR CDCL3 300K AV-300



ppm

7.7609
7.6878
7.6057
7.2785
7.2750
7.2714
7.2678
7.2600
7.2521
7.2485
7.2449
6.7454
6.7164
5.2872
5.2557
5.2149
5.2042
5.1918
5.0747
5.0417
5.0250
5.0095
5.0003
4.8988
4.8669
4.1310
4.1072
4.1006
3.0178
2.9862
2.0829
2.0412
2.0285
2.0250
2.0067
1.8789
1.6173
1.6061
1.5808
1.5255
1.2798
1.2560
1.2324
1.1162
1.0293
0.9687
0.9020
0.8901
0.8282
0.5787

Integral

0.92
0.95
2.35
2.89
2.86
1.39
1.30
1.95
1.14
1.08
1.03
1.15
3.64
10.96
5.40
11.53
2.79
1.63; PA
4.37
3.09
6.95
4.26
3.00

ppm

Current Data Parameters

NAME sld
EXPNO 891
PROCNO 1

F2 - Acquisition Parameters

Date_ 20080418
Time 23:21
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zg30
TD 11414
SOLVENT CDCl3
NS 16
DS 0
SMH 5995.204 Hz
FIDRES 0.525250 Hz
AQ 0.9519776 sec
RG 512
DE 83.400 usec
TE 298.0 K
D1 2.00000000 sec

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

NUC1 1H
P1 6.00 usec
PL1 -4.00 dB
SFO1 300.1324010 MHz

F2 - Processing parameters

SF 300.1300124 MHz
SI 32768
SF 300.1300124 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

1D NMR plot parameters

CH 22.00 cm
CY 12.00 cm
F1P 9.970 ppm
F1 2992.30 Hz
F2P -0.295 ppm
F2 -88.57 Hz
PPMCM 0.46560 ppm/cm
HZCM 140.03949 Hz/cm

Kelly-156 C13-NMR CDCl3 300K AV-300

Current Data Parameters
 NAME shb
 EXPNO 923
 PROCNO 1

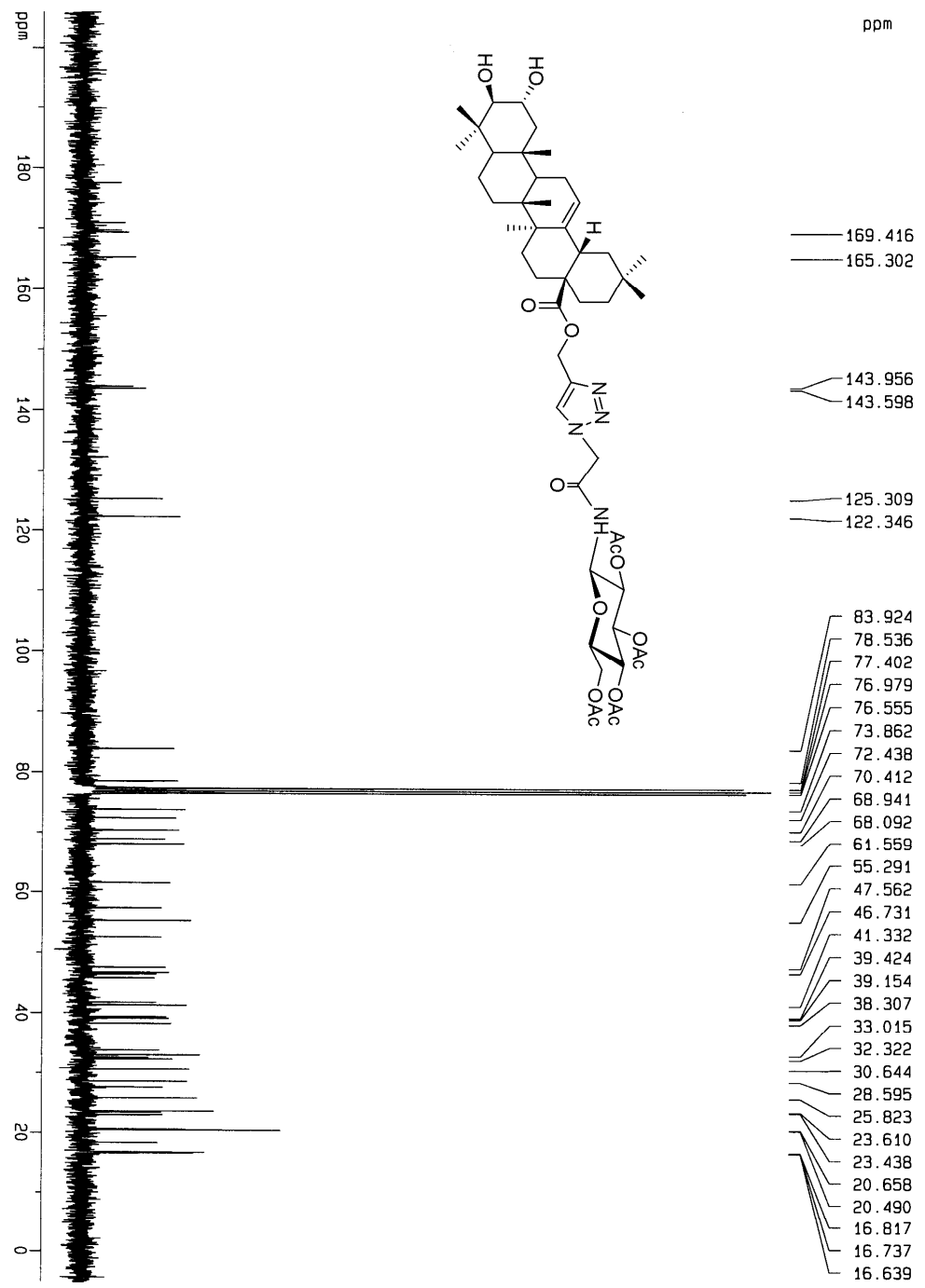
F2 - Acquisition Parameters
 Date_ 20080423
 Time 18.27
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1498
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.552865 Hz
 AQ 0.904468 sec
 RG 102400
 DW 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

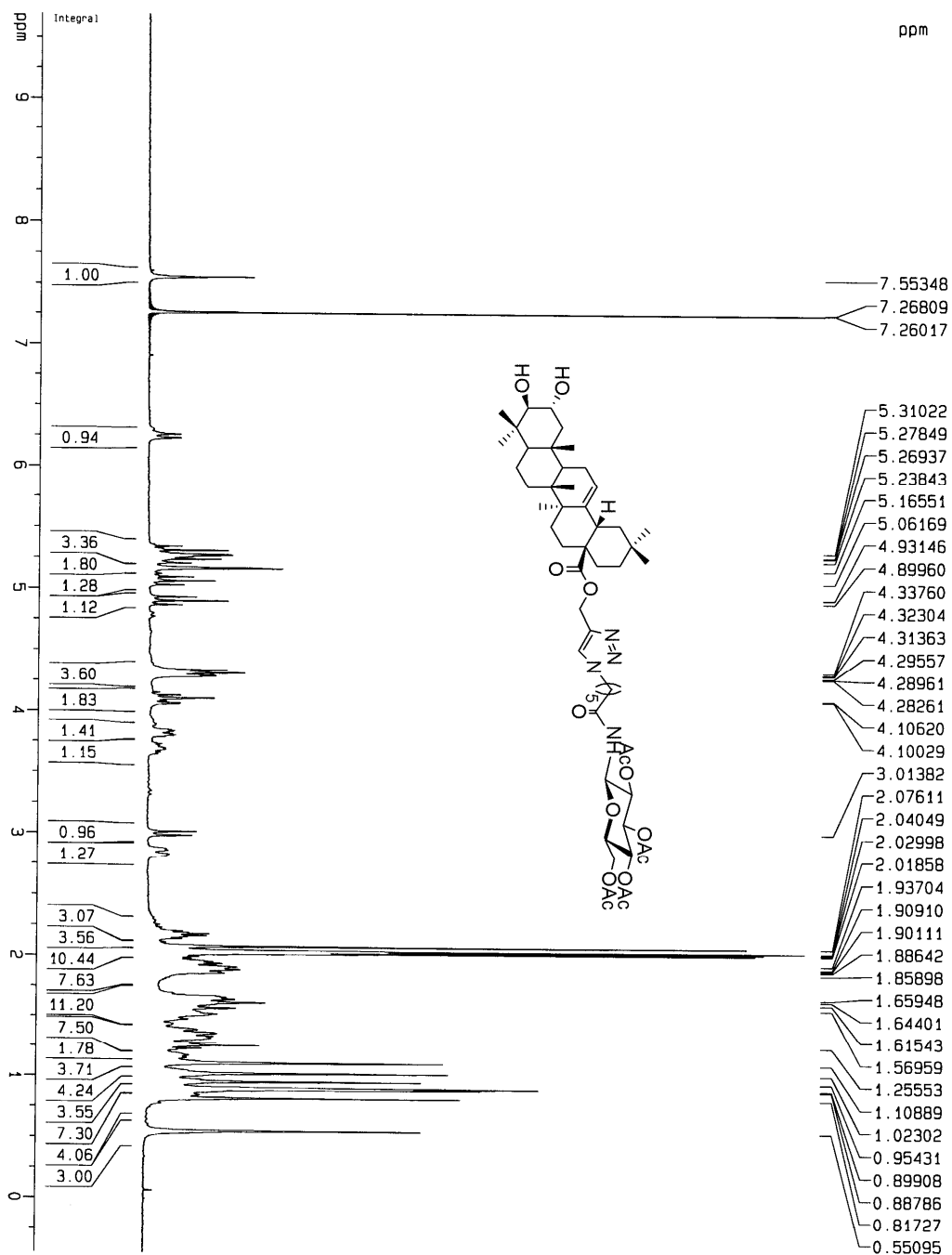
***** CHANNEL f1 *****
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4753978 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.467506 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.50 cm
 CY 12.00 cm
 FIP 206.001 ppm
 F1 15546.46 Hz
 F2 -5.153 ppm
 PPGM 9.36909 ppm/cm
 HZCM 706.27124 Hz/cm





Current Data Parameters
 NAME shb
 EXPNO 882
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080418
 Time 23.18
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zg30
 TD 13414
 SOLVENT CDCl3
 NS 16
 DS 0
 SMH 5995.204 Hz
 FIDRES 0.528250 Hz
 AQ 0.9519776 sec
 RG 512
 DM 83.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SFO1 300.1324010 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300124 MHz
 MDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 12.00 cm
 F1P 9.693 ppm
 F1 2909.03 Hz
 F2P -0.457 ppm
 F2 -137.14 Hz
 PPHCM 0.46134 ppm/cm
 HZCM 138.46245 Hz/cm

Kelly-157 C13-NMR CDC13 300K AV-300

Current Data Parameters
 NAME srb
 EXPNO 924
 PROCNO 1

F2 - Acquisition Parameters

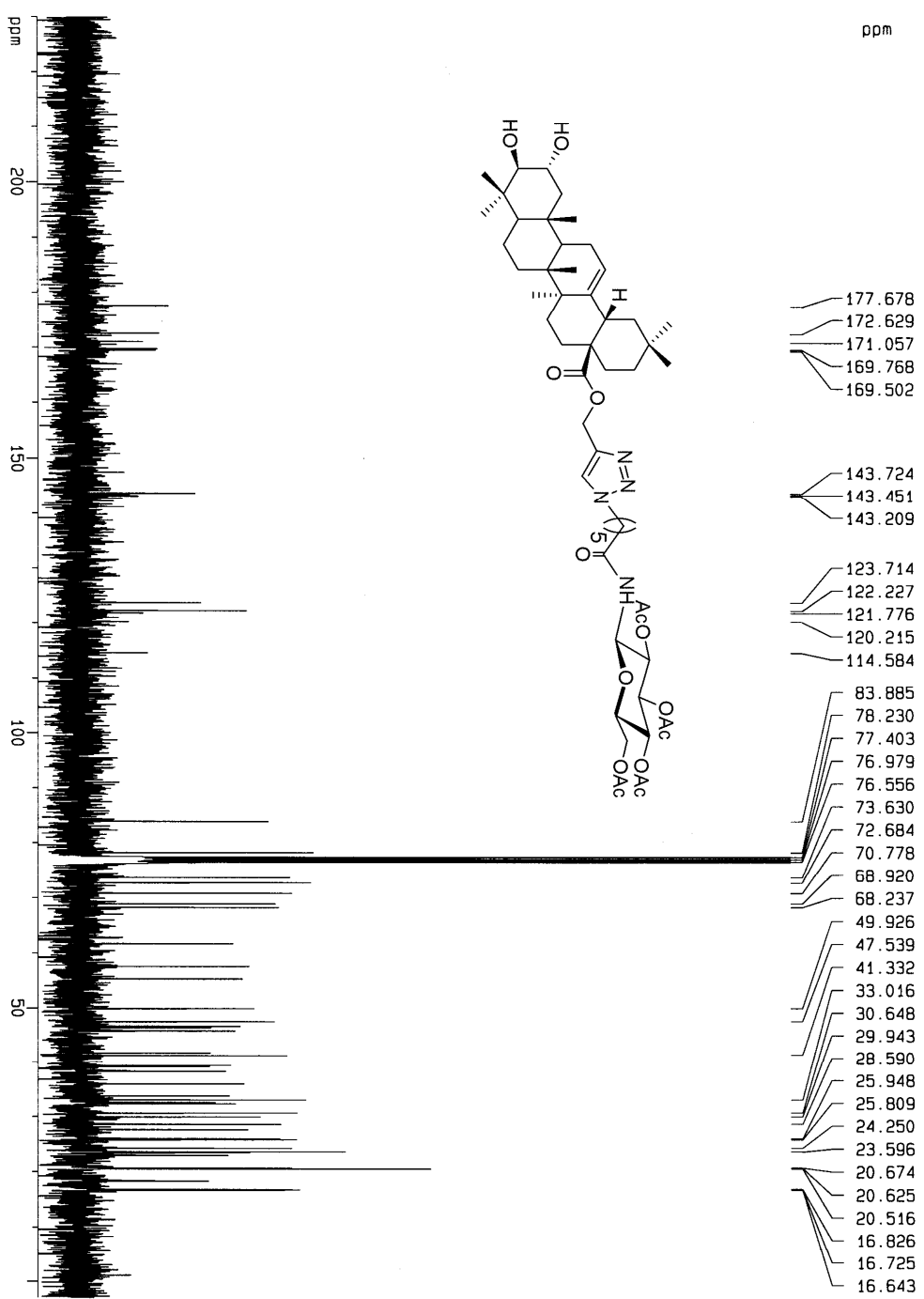
Date_ 20080423
 Time 20:01
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpgc
 TO 32768
 SOLVENT CDCl3
 NS 2163
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 102400
 DW 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

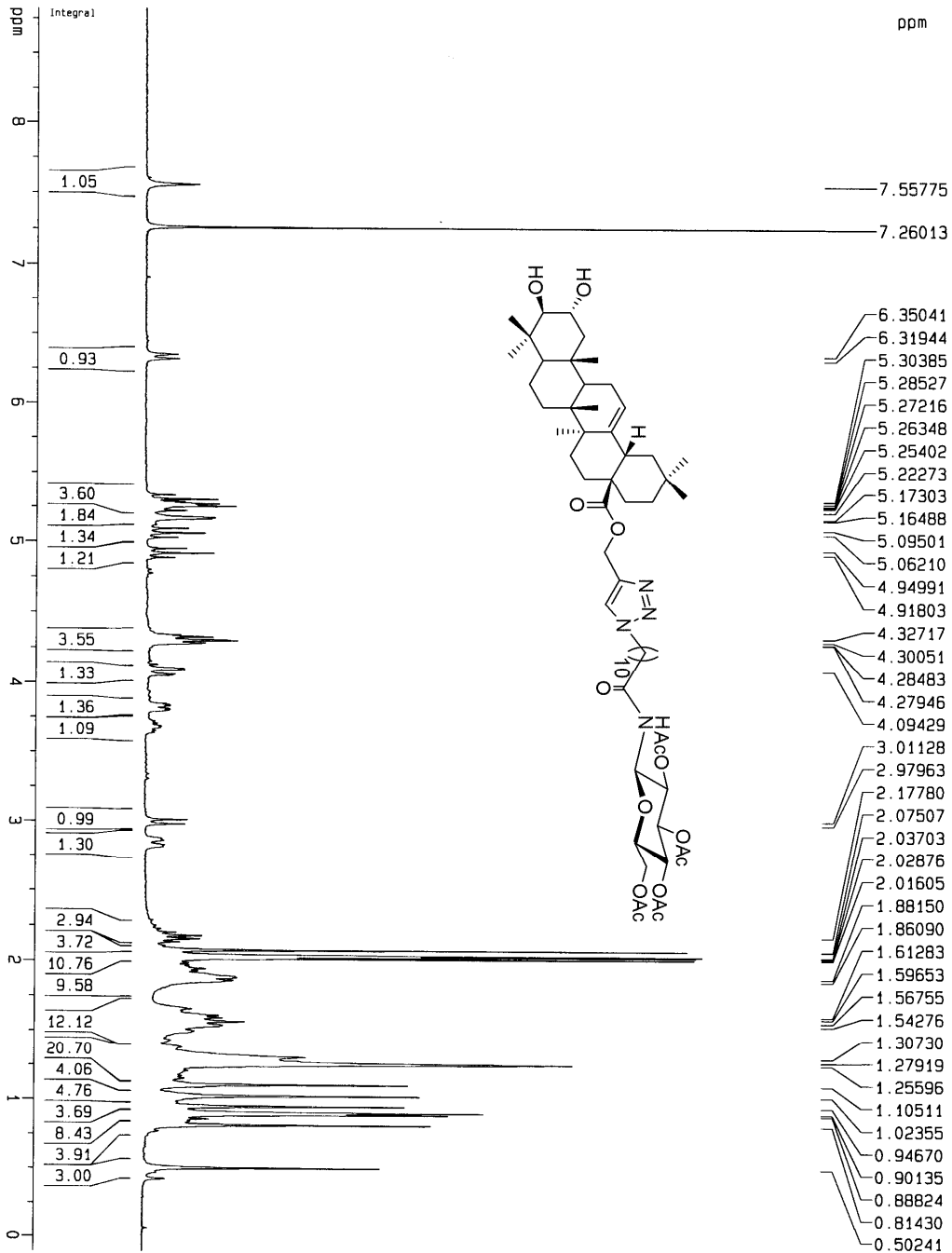
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PPRP2 80.00 usec
 PL2 -4.00 dB
 PL12 19.29 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677506 MHz
 NQW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.50 cm
 CY 30.00 cm
 F1P 230.000 ppm
 F1 17357.58 Hz
 F2P -3.000 ppm
 F2 -226.40 Hz
 PPGCM 10.35656 ppm/cm
 HZCM 781.51050 Hz/cm



srb



Current Data Parameters
 NAME shb
 EXPNO 893
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080418
 Time 23:26
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 14144
 SOLVENT CDCl3
 NS 16
 DS 0
 SMI 4166.667 Hz
 FIDRES 0.365049 Hz
 AQ 1.3697300 sec
 RG 512
 DM 120.000 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1314990 MHz

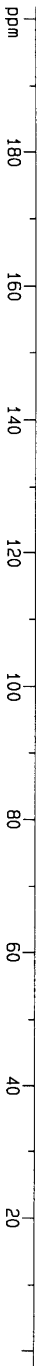
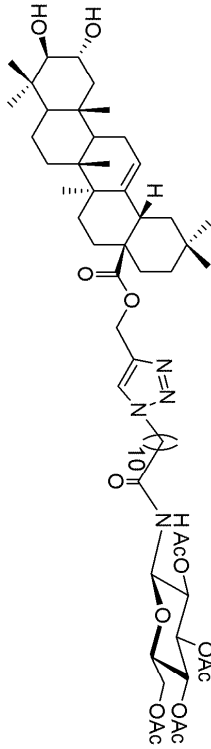
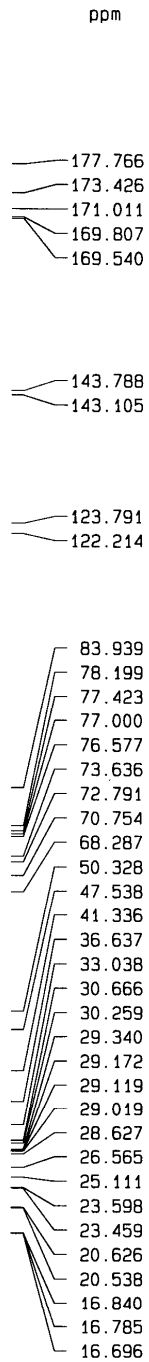
F2 - Processing parameters
 SI 32768
 SF 300.1300124 MHz
 MDN EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00

1D NMR Plot parameters
 CX 62.00 cm
 CY 12.00 cm
 F1P 8.825 ppm
 F1 2648.79 Hz
 F2P -0.108 ppm
 F2 -32.54 Hz
 PRACH 0.40693 ppm/cm
 HZCM 121.87850 Hz/cm

KELLY-158 C13-NMR CDCl3 300K AV-300

Current Data Parameters
 NAME s1b
 EXPNO 925
 PROCNO 1

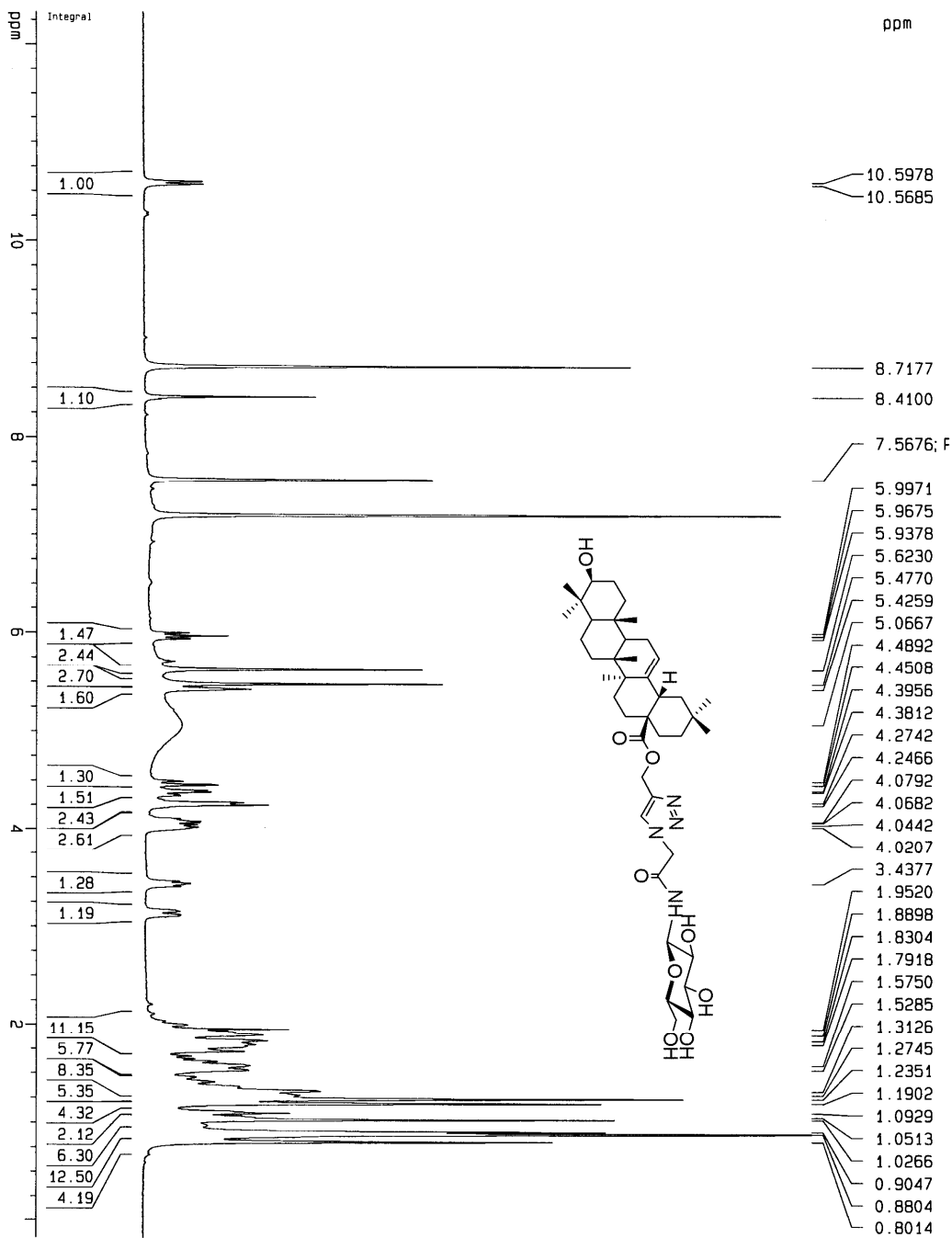
F2 - Acquisition Parameters
 Date_ 20080424
 Time 8.18
 INSTRUM spect
 PROCNO 5
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 2620
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 102400
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec



F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters:
 CX 22.50 cm
 CY 12.00 cm
 F1P 201.817 ppm
 F1 15230.67 Hz
 F2P -2.898 ppm
 F2 -218.66 Hz
 PPKCM 9.09842 ppm/cm
 HZCM 686.63751 Hz/cm

sub



Current Data Parameters
 NAME SMO
 EXNO 50
 PROCNO 1

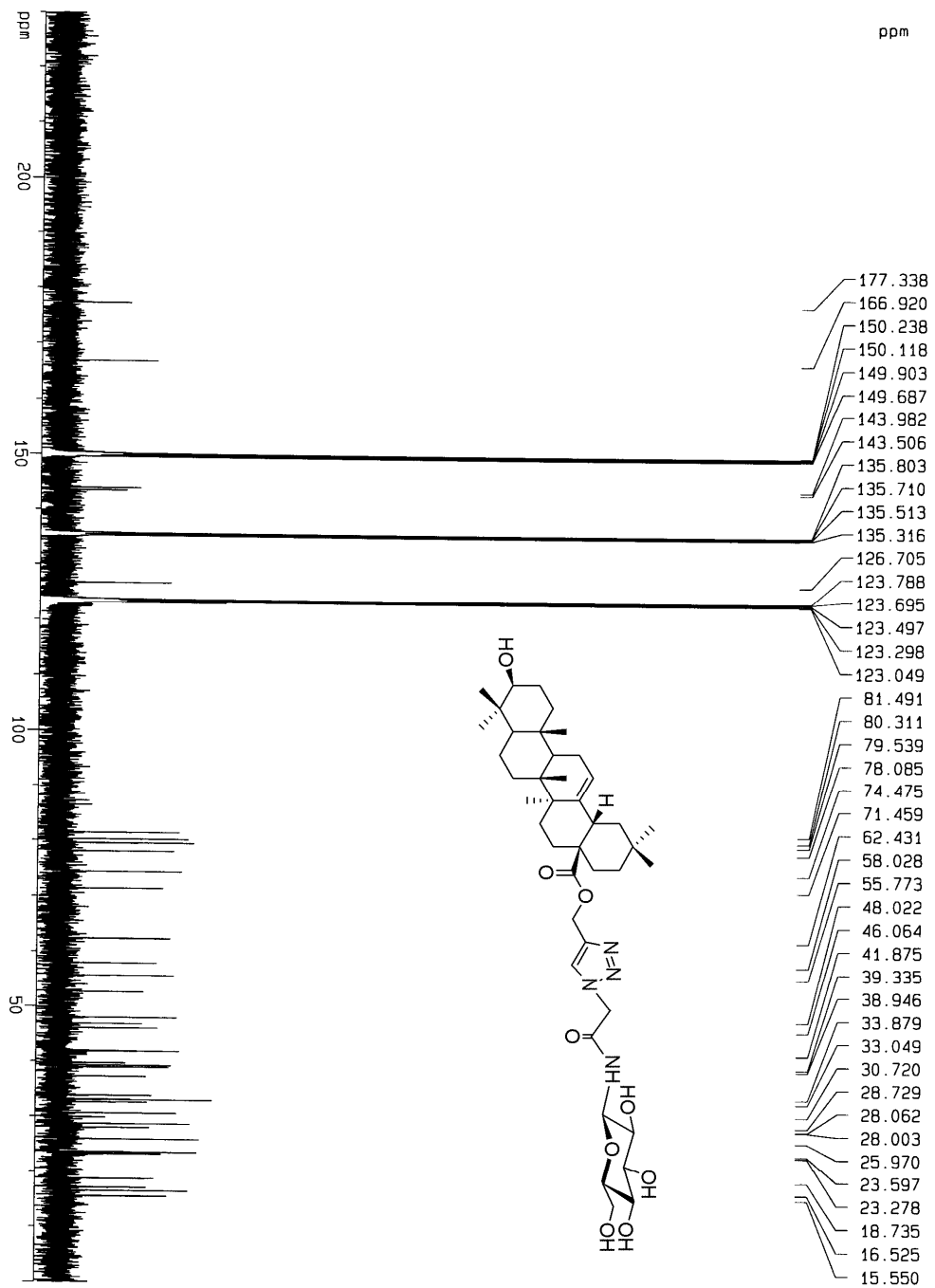
F2 - Acquisition Parameters
 Date_ 20080415
 Time 13.18
 INSTRUM Spect
 PROHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 11414
 SOLVENT Pyr
 NS 16
 DS 0
 SHW 5995.204 Hz
 FIDRES 0.528260 Hz
 AQ 0.9519776 sec
 RG 322.5
 DW 83.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 2.00000000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1324010 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299889 MHz
 MCM EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 15.00 cm
 F1P 12.331 ppm
 F1 3701.03 Hz
 F2P -0.184 ppm
 F2 -55.17 Hz
 PPMCM 0.56888 ppm/cm
 HZCM 170.73676 Hz/cm

Kelly-151 C13-NMR C5D5N 30K AV-500



- 177.338
- 166.920
- 150.238
- 150.118
- 149.903
- 149.687
- 143.982
- 143.506
- 135.803
- 135.710
- 135.513
- 135.316
- 126.705
- 123.788
- 123.695
- 123.497
- 123.298
- 123.049
- 81.491
- 80.311
- 79.539
- 78.085
- 74.475
- 71.459
- 62.431
- 58.028
- 55.773
- 48.022
- 46.064
- 41.875
- 39.335
- 38.946
- 33.879
- 33.049
- 30.720
- 28.729
- 28.062
- 28.003
- 25.970
- 23.597
- 23.278
- 18.735
- 16.525
- 15.550

Current Data Parameters
 NAME 80804
 EXPNO 105
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080417
 Time 15.02
 INSTRUM svs00
 PROBHD 5 mm QNP 1H/15
 PULPROG zgpg
 TD 32768
 SOLVENT Pyr
 NS 662
 DS 8
 SWH 30229.746
 FIDRES 0.922539
 AQ 0.5420493
 RG 102400
 DW 16.540
 DE 20.67
 TE 308.0
 D1 1.50000000
 D11 0.03000000

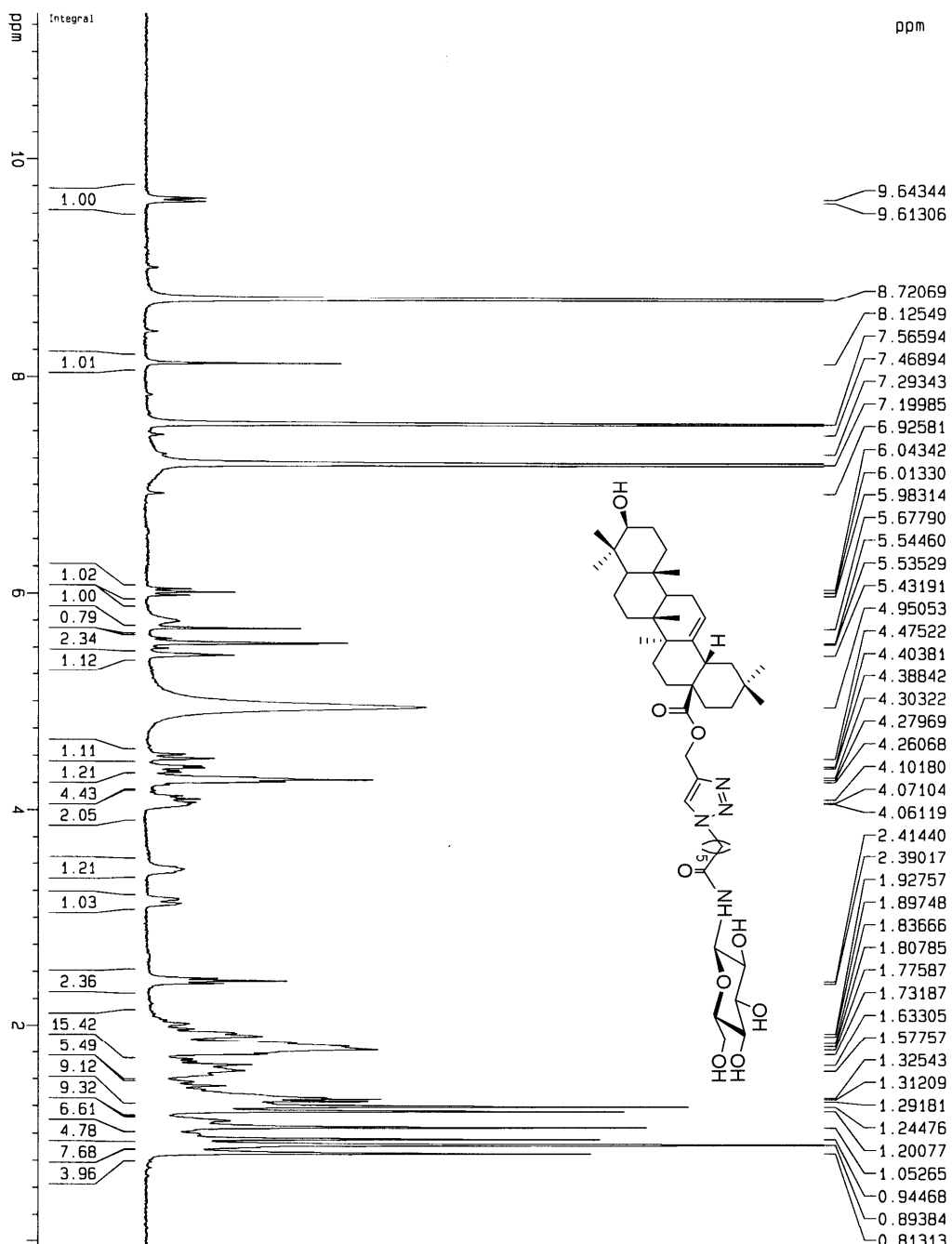
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50
 PL1 -2.00
 SF01 125.772011

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00
 PL2 -5.00
 PL12 10.92
 SF02 500.1320005

F2 - Processing parameters
 SI 32768
 SF 125.7577605
 MDW EM
 SSB 0
 LB 1.00
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.00
 CY 30.00
 F1P 230.000
 F1 28924.29
 F2P 0.000
 F2 0.000
 PPMCM 10.45455
 HZCM 1314.74036

Sub



```

Current Data Parameters
NAME          shb
EXPNO        851
PROCNO       1

F2 - Acquisition Parameters
Date_         20080415
Time          13:27
INSTRUM      spect
PROBHD       5 mm QNP 1H/13
PULPROG      zg30
TD            11414
SOLVENT      Pyr
NS            32
DS            0
SH1           4496.403 Hz
FIDRES        0.393938 Hz
AQ            1.2692968 sec
RG            322.5
DE            111.200 usec
TE            298.0 K
D1            2.00000000 sec

***** CHANNEL f1 *****
NUC1          1H
P1            6.00 usec
PL1           -4.00 dB
SF01         300.1317419 MHz

F2 - Processing parameters
SI            32768
SF            300.1299895 MHz
WDW           EM
SSB           0
LB            0.50 Hz
GB            0
PC            1.00

1D NMR plot parameters
CX            22.00 cm
CY            50.00 cm
F1P           11.355 ppm
F1            3408.02 Hz
F2P           -0.097 ppm
F2            -28.16 Hz
PP4CK        0.35205 ppm/cm
HZCM         156.23543 Hz/cm
    
```

Kel11y-152 C13-NMR CSD5N 303K AV-500

Current Data Parameters
 NAME 40804
 EXPNO 106
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080417
 Time 15.29

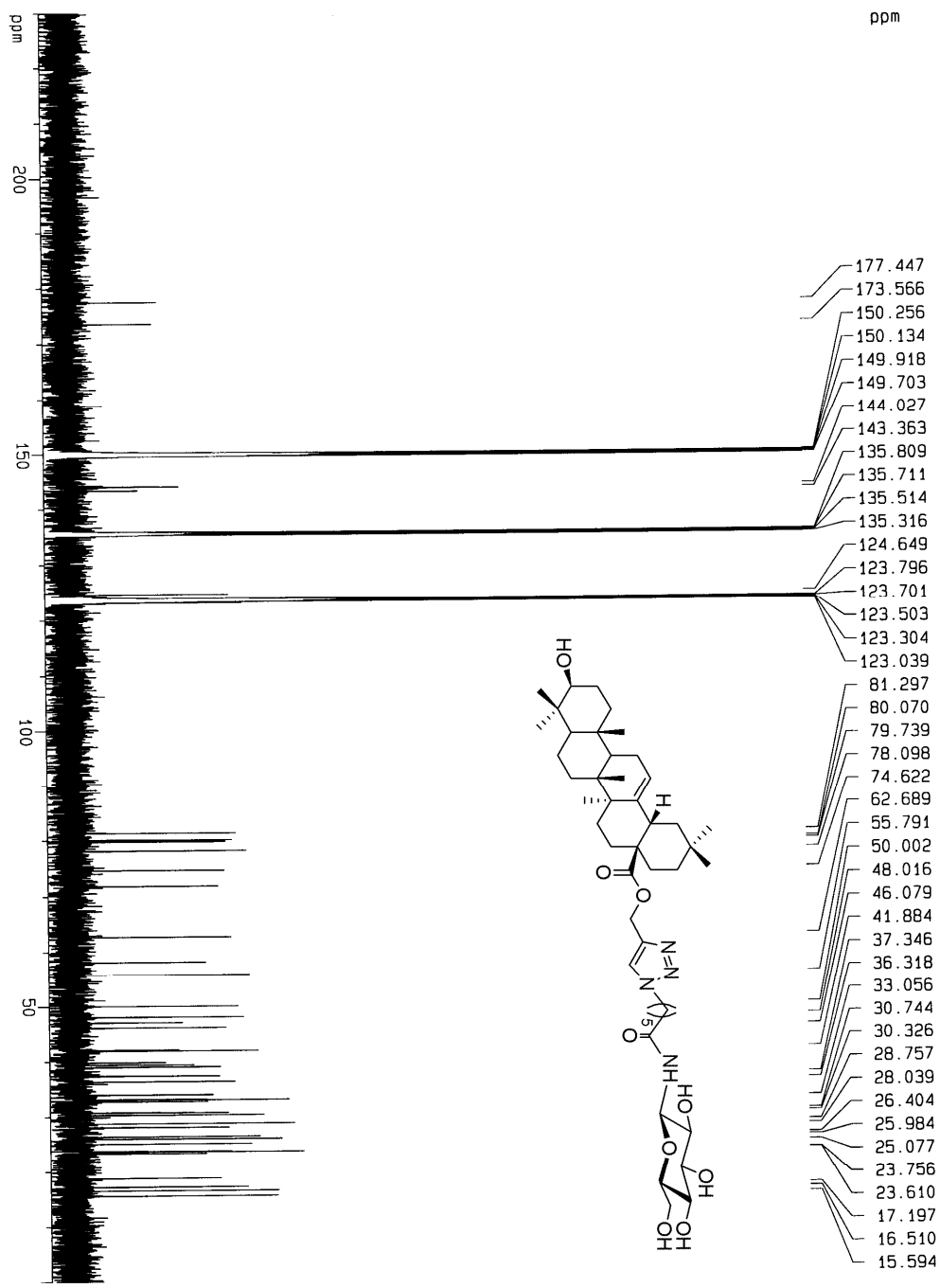
INSTRUM a3500
 PULPROG 5 mm QNP 1H/15
 PULPROG 29dc
 TD 32768
 SOLVENT Pyz
 NS 2576
 DS 8
 SWH 30229.746
 FIDRES 0.322939
 AQ 0.5420493
 RG 102400
 DM 16.540
 DE 20.67
 TE 309.0
 O1 1.50000000
 O1 0.03000000
 d11

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50
 PL1 -2.00
 RF1 125.7722011
 SF01

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00
 PL2 -5.00
 PL12 10.92
 SF02 500.1320005

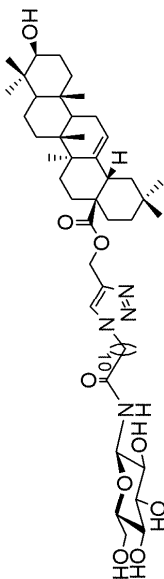
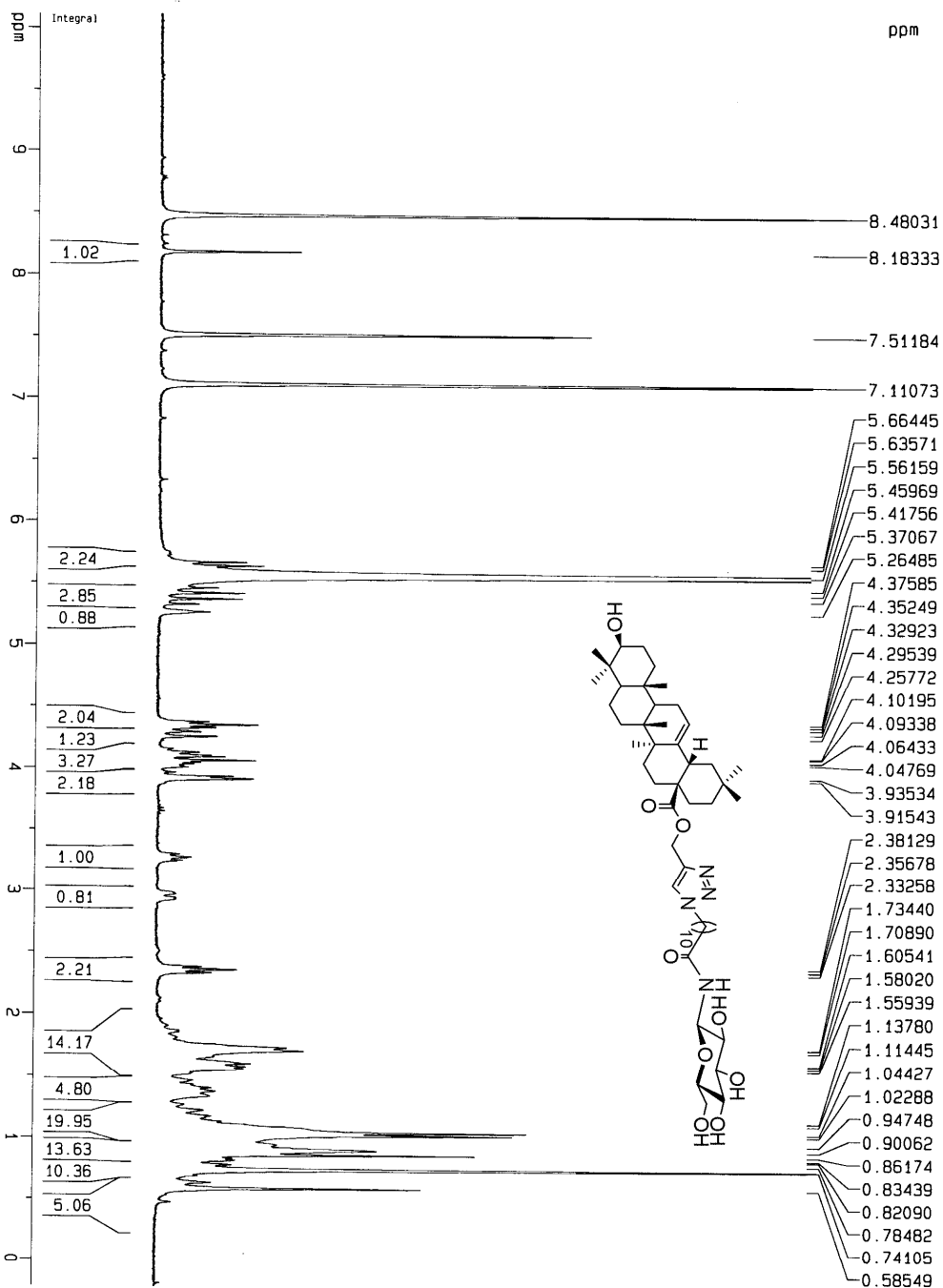
F2 - Processing parameters
 SI 32768
 SF 125.757587
 NDM EM
 SSB 0
 LB 1.00
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.00
 CY 60.00
 F1P 230.000
 F1 26924.29
 F2P 0.000
 F2 10.45455
 PPMCK 1314.74036
 HZCM



Sub

Kelly-159 H1-NMR +D2O C505N 300K AV-30C



Current Data Parameters
 NAME snb
 EXPNO 919
 PROCNO 1

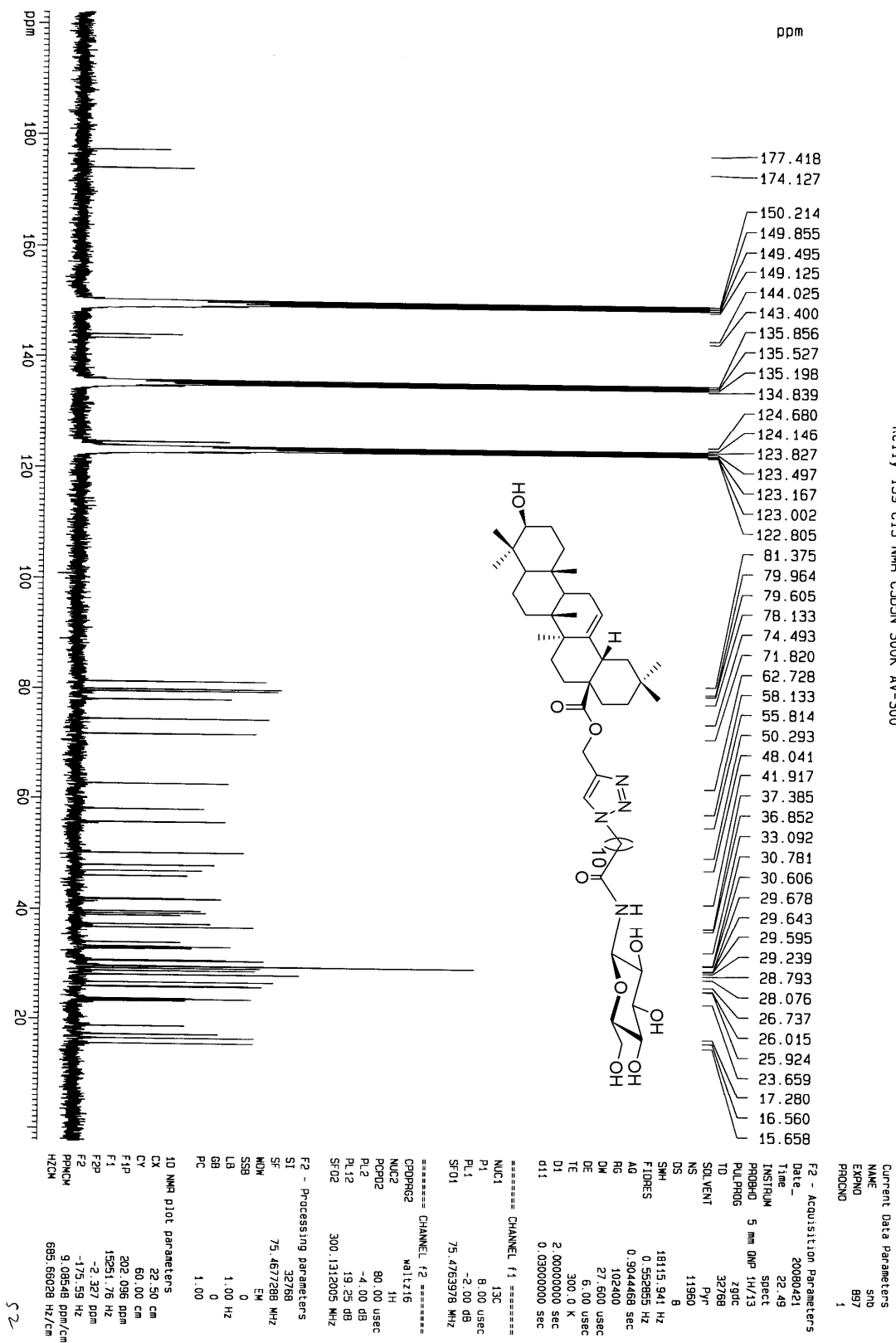
F2 - Acquisition Parameters
 Date_ 20080423
 Time 16.29
 INSTRUM spect
 PULPROG 5 mm QNP 1H/13
 TD 2030
 SOLVENT H₂O
 NS 32
 DS 0
 SMH 3906.250 Hz
 FIDRES 0.162896 Hz
 AQ 3.0694900 sec
 RG 287.4
 DM 128.000 usec
 DE 6.00 usec
 TE 303.0 K
 D1 2.00000000 sec

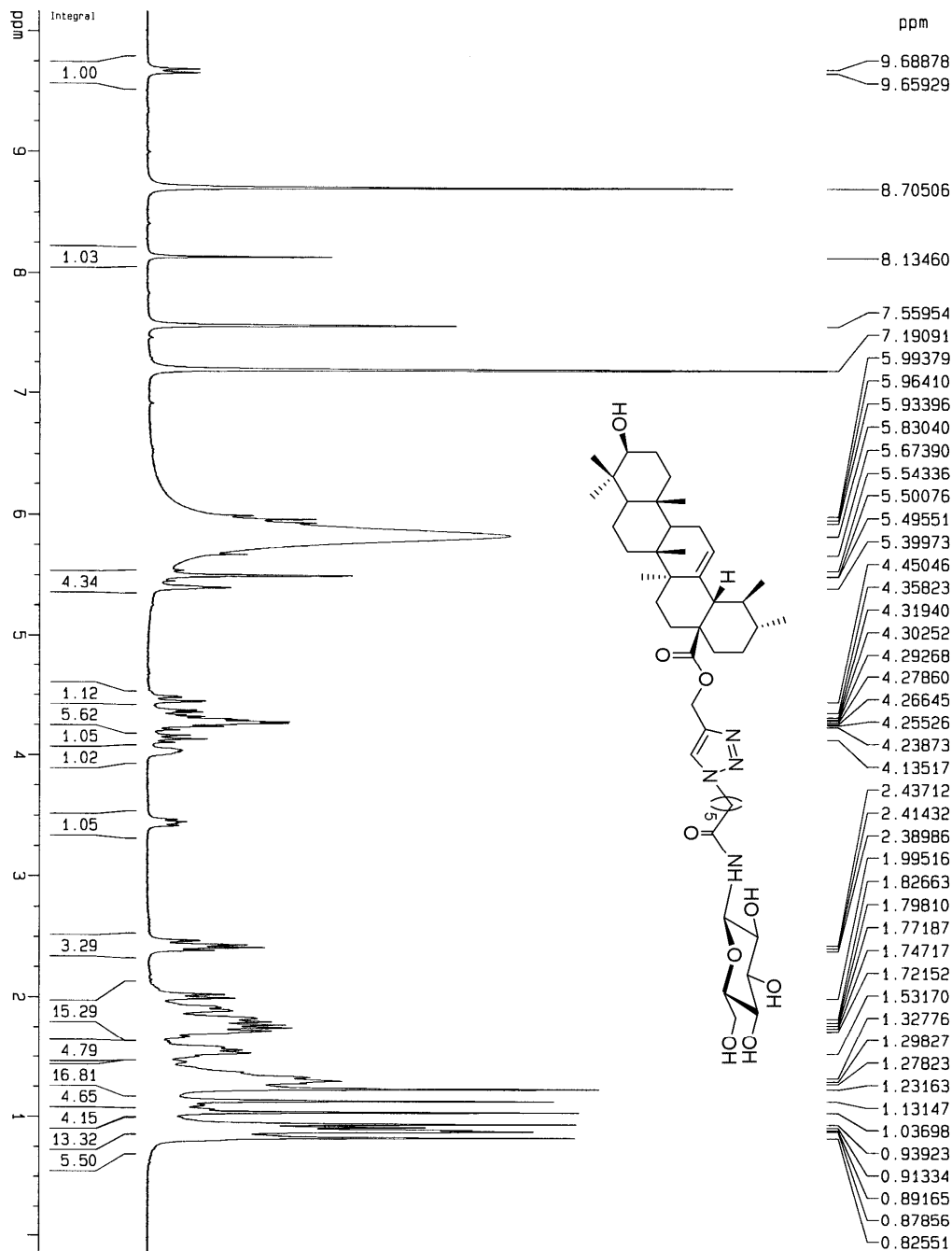
***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SFO1 300.1317408 MHz

F2 - Processing parameters
 S1 32789
 SF 300.1300150 MHz
 MDM EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 150.00 cm
 F1P 10.114 ppm
 F1 3035.419 Hz
 F2P -0.225 ppm
 F2 -67.61 Hz
 PPM/CM 0.46995 ppm/cm
 HZ/CM 141.04880 Hz/cm

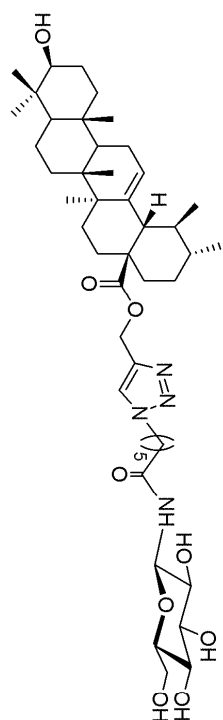
SMN





ppm

9.68878
9.65929
8.70506
8.13460
7.55954
7.19091
5.99379
5.96410
5.93396
5.83040
5.67390
5.54336
5.50076
5.49551
5.39973
4.45046
4.35823
4.31940
4.30252
4.29268
4.27860
4.26645
4.25526
4.23873
4.13517
2.43712
2.41432
2.38986
1.99516
1.82663
1.79810
1.77187
1.74717
1.72152
1.53170
1.32776
1.29827
1.27823
1.23163
1.13147
1.03698
0.93923
0.91334
0.89165
0.87856
0.82551



Current Data Parameters
 NAME: shb
 EXPNO: 918
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20080423
 Time: 16:20
 INSTRUM: spect
 PROBHD: 5 mm QNP 1H/13
 PULPROG: zg30
 TD: 2880
 SOLVENT: Pyr
 NS: 16
 DS: 0
 SMH: 3981.988 Hz
 FIDRES: 0.161884 Hz
 AQ: 3.0886741 sec
 RG: 256
 DM: 128.800 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 2.00000000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 6.00 usec
 PL1: -4.00 dB
 SFO1: 300.1315926 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.129914 MHz
 WDW: EM
 SSB: 0
 LB: 0.20 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.00 cm
 CY: 12.00 cm
 F1P: 10.166 ppm
 F1: 3051.11 Hz
 F2P: -0.144 ppm
 F2: -43.13 Hz
 PPM/CM: 0.46862 ppm/cm
 HZ/CM: 140.64766 Hz/cm

Sub

kelly-161 13C-NMR CDCL3 303K AV-300

Current Data Parameters
 NAME snb
 EXPNO 941
 PROCNO 1

F2 - Acquisition Parameters

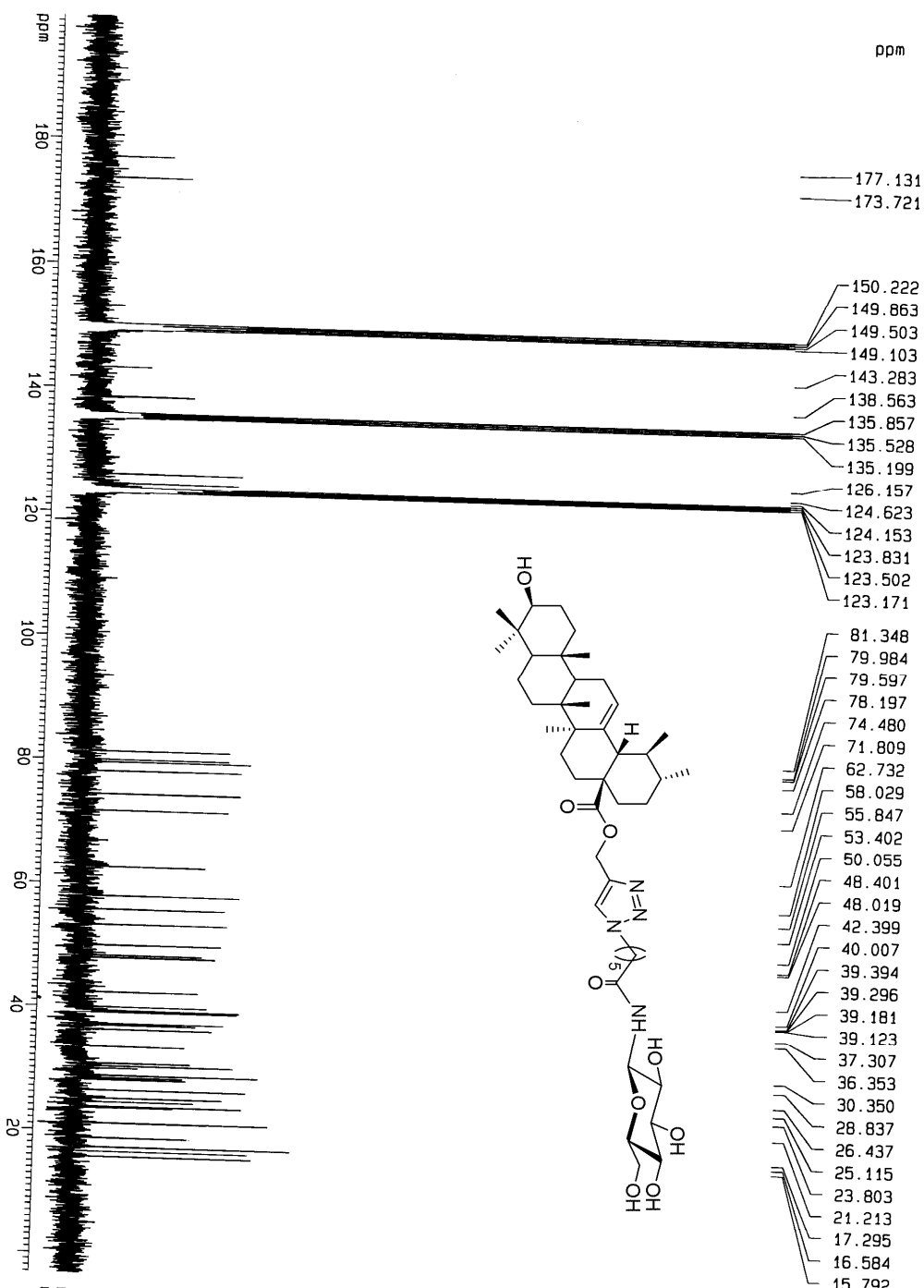
Date_ 20080425
 Time 11.38
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 32768
 SOLVENT FYP
 NS 1189
 DS 8
 SWH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 409600
 DW 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SFO1 75.4763978 MHz

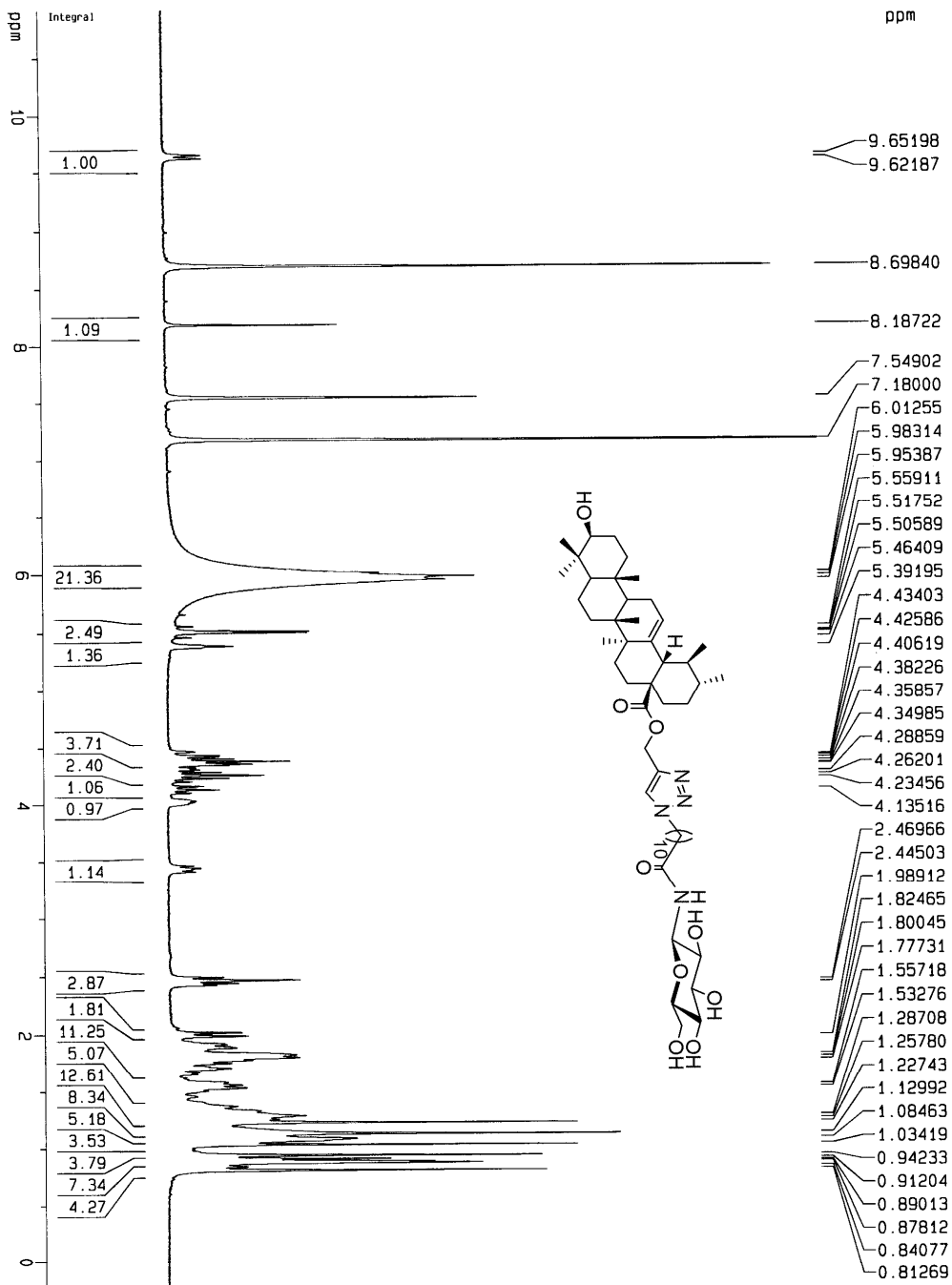
===== CHANNEL f2 =====
 CPOPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.467282 MHz
 KDW EN
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 22.50 cm
 CY 30.00 cm
 F1P 199.848 ppm
 F1 15082.09 Hz
 F2P -3.184 ppm
 F2 -240.27 Hz
 PPMCN 9.02364 ppm/cm
 HZCM 690.99390 Hz/cm



Kel11y-160 H1-NMR C5D5N 300K AV-300



Current Data Parameters
 NAME sfo
 EXPNO 934
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080424
 Time 14:13
 INSTRUM Spect
 PROBDH 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 15430
 SOLVENT Pyv
 NS 16
 DS 0
 SWH 3858.025 Hz
 FIDRES 0.250034 Hz
 AQ 1.9997780 sec
 RG 256
 DM 129.600 usec
 DE 6.00 usec
 TE 303.0 K
 D1 2.00000000 sec

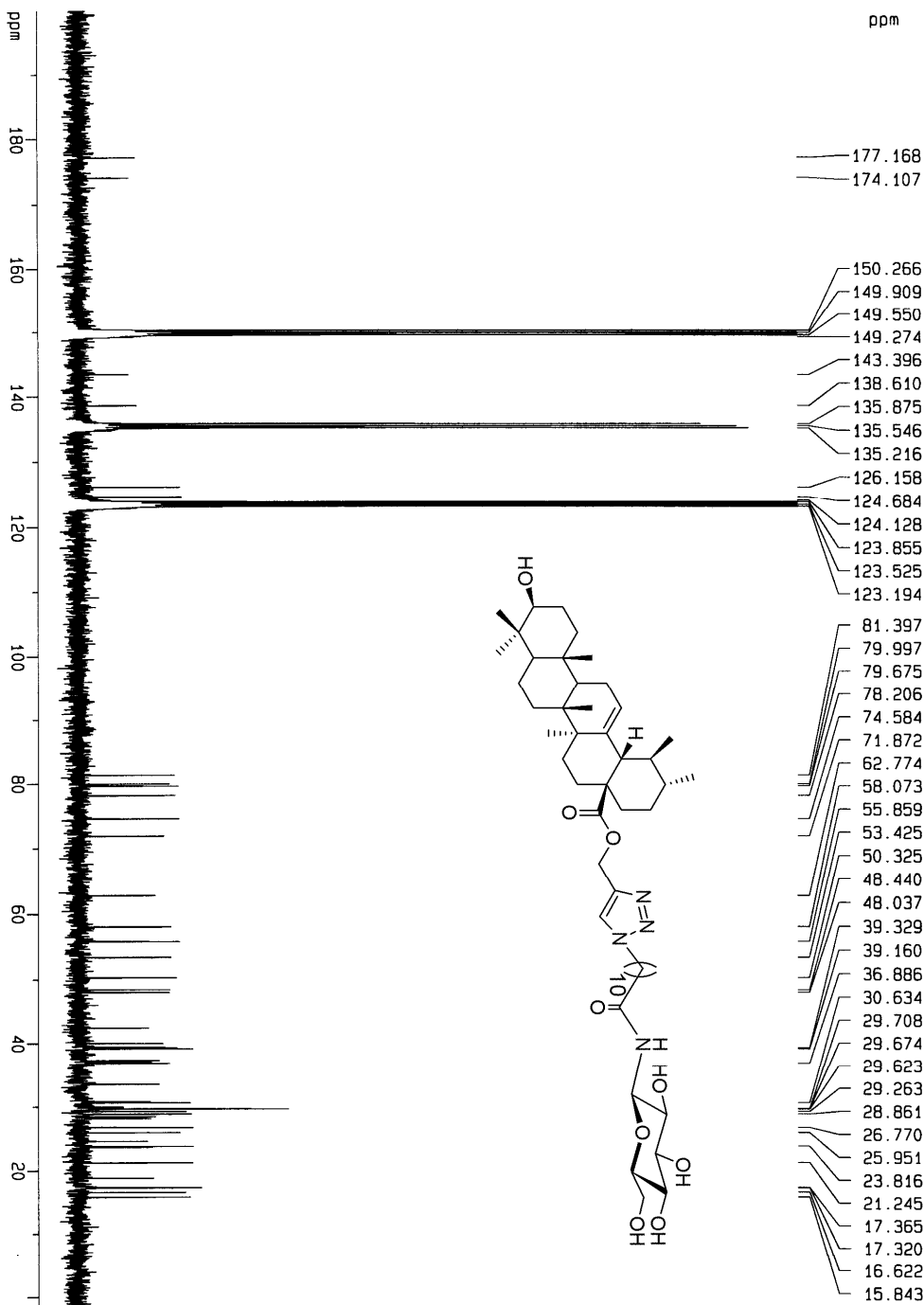
===== CHANNEL f1 =====
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1317627 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299946 MHz
 NDM CK
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 12.00 cm
 FIP 10.922 ppm
 F1 3277.91 Hz
 F2 -0.256 ppm
 F2 -70.82 Hz
 PPMCH 0.50716 ppm/cm
 HZCM 152.21498 Hz/cm

sub

Kelly-160 13C-NMR PYR-D5 300K AV-300



Current Data Parameters
 NAME smp
 EXPRNO 958
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080429
 Time 16:29
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 32768
 SOLVENT pyr
 NS 1290
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.582865 Hz
 AQ 0.304469 sec
 RG 102400
 DW 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

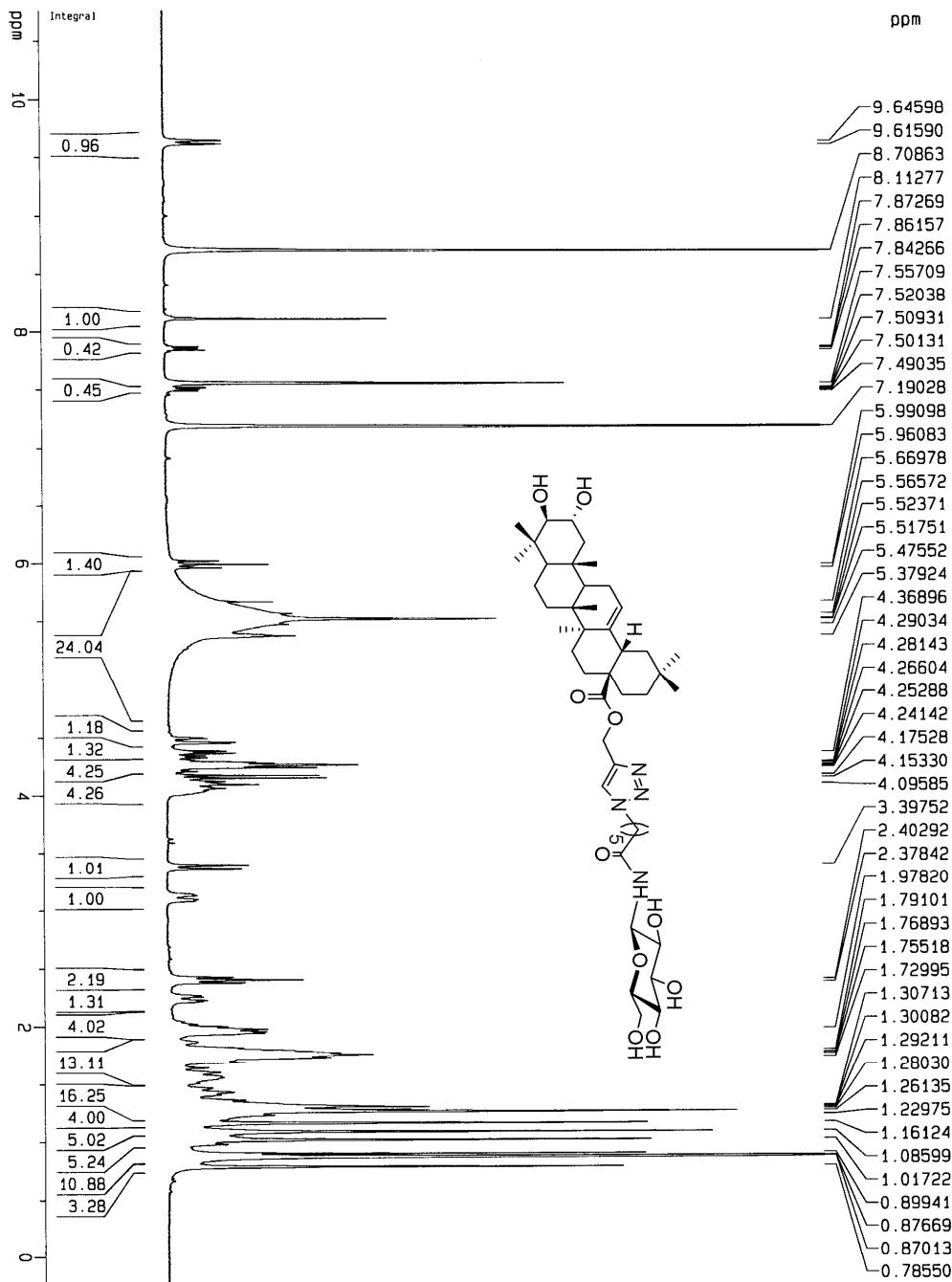
***** CHANNEL f1 *****
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4753978 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing Parameters
 SI 32768
 SF 75.4676127 MHz
 MDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters:
 CX 22.50 cm
 CY 20.00 cm
 F1p 199.959 ppm
 F1 15090.46 Hz
 F2p -1.354 ppm
 F2 -102.18 Hz
 PRICK 8.94726 ppm/cm
 HZCM 675.22839 Hz/cm

KELLY-163 1H-NMR PYR-D5 303K AV-300



Current Data Parameters
 NAME: spb
 EXPNO: 947
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20080425
 Time: 18.07
 INSTRUM: spect
 PROBRD: 5 mm QNP 1H/13
 PULPROG: zg30
 TO: 1312
 SOLVENT: Pyr
 NS: 32
 DS: 0

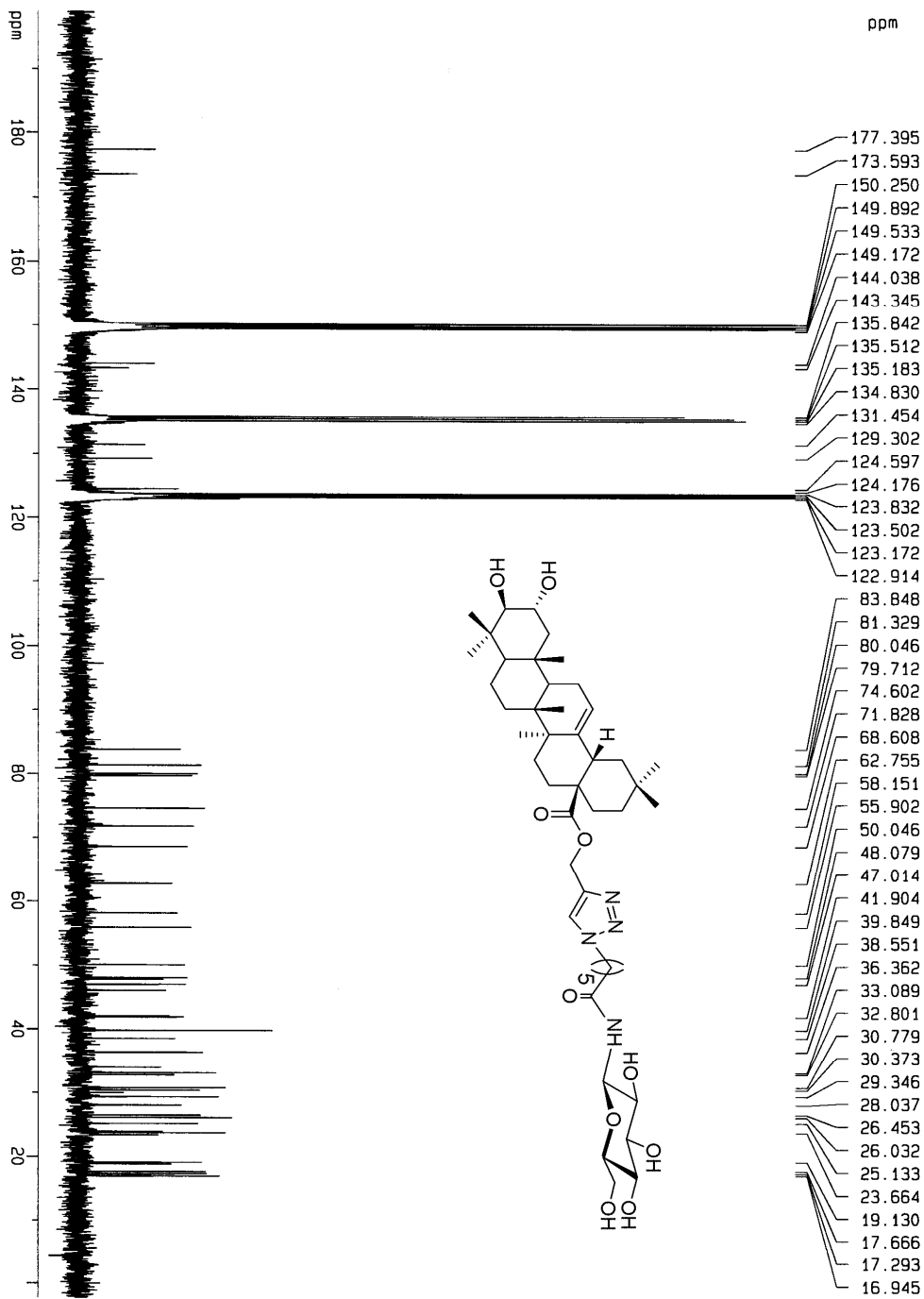
SWH: 5341.880 Hz
 FIDRES: 0.395143 Hz
 AQ: 1.2647732 sec
 RG: 362
 DM: 93.600 usec
 DE: 6.00 usec
 TE: 303.0 K
 D1: 2.00000000 sec

***** CHANNEL f1 *****
 NUC1: 1H
 P1: 6.00 usec
 PL1: -4.00 dB
 SFO1: 300.1324245 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1299317 MHz
 MDW: EM
 SSB: 0
 LB: 0.10 Hz
 GB: 0
 PC: 1.00

1D NMR plot parameters
 CX: 22.00 cm
 CY: 15.00 cm
 F1P: 10.767 ppm
 F1: 3231.57 Hz
 F2P: -0.253 ppm
 F2: -75.90 Hz
 PUNCH: 0.50092 ppm/cm
 HZCM: 150.33986 Hz/cm

KELLY-163 13C-NMR PYR-D5 300K AV-300



Current Data Parameters

NAME	shb
EXPNO	970
PROCNO	1

F2 - Acquisition Parameters

Date_	20080429
Time	21.35
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg
TD	32768
SOLVENT	PYR
NS	929
DS	8
SMH	18115.941 Hz
FIDRES	0.552655 Hz
AQ	0.5044468 sec
RG	102400
DW	27.600 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec

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

NUC1	13C
P1	8.00 usec
PL1	-2.00 dB
SFO1	75.4763978 MHz

===== CHANNEL f2 =====

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	-4.00 dB
PL12	19.25 dB
SFO2	300.1312005 MHz

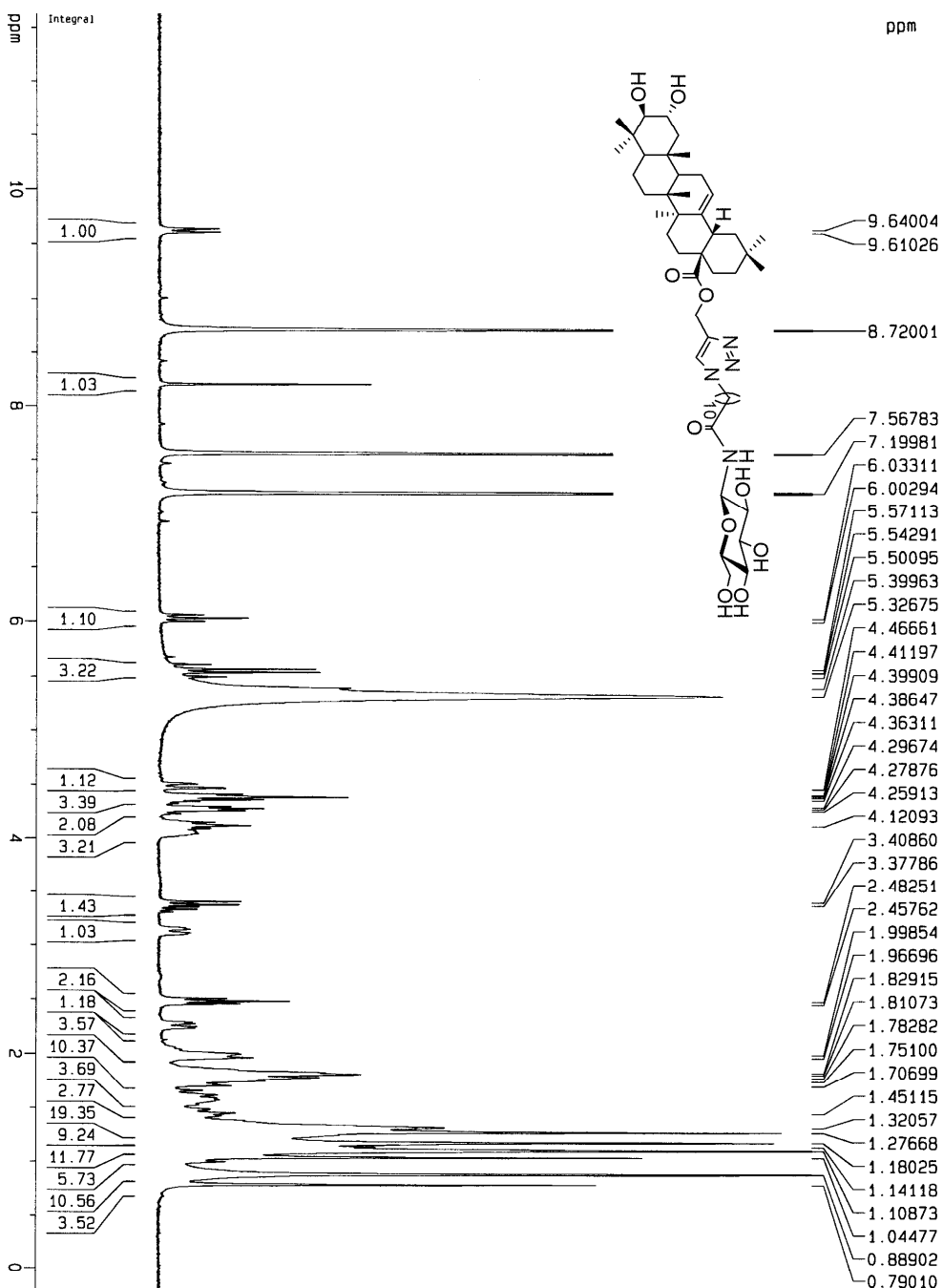
F2 - Processing parameters

SI	32768
SF	75.467277 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.00

10 NMR plot parameters

CX	22.50 cm
CY	20.00 cm
F1P	199.001 ppm
F1	15018.16 Hz
F2P	-2.312 ppm
F2	-174.48 Hz
PRNOM	8.94725 ppm/cm
HZCM	675.22839 Hz/cm

KELLY-164 1H-NMR PYR-D5 303K AV-300



Current Data Parameters
 NAME sn5
 EXPNO 945
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080425
 Time 15:58
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 13812
 SOLVENT P13
 NS 32
 DS 0
 SMH 5341.880 Hz
 FIDRES 0.395343 Hz
 AQ 1.264722 sec
 RG 1024
 DM 93.600 usec
 DE 5.00 usec
 TE 303.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1324245 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299887 MHz
 MVM EM
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.00 cm
 CY 30.00 cm
 F1p 11.630 ppm
 F1 3450.44 Hz
 F2p -0.222 ppm
 F2 -66.66 Hz
 PPMCM 0.539172 ppm/cm
 HZCM 161.66605 Hz/cm

Kelly-164 13C-NMR PYR-D5 300K AV-300

Current Data Parameters
 NAME shb
 EXPNO 971
 PROCNO 1

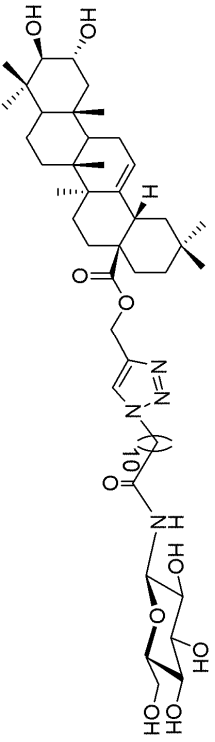
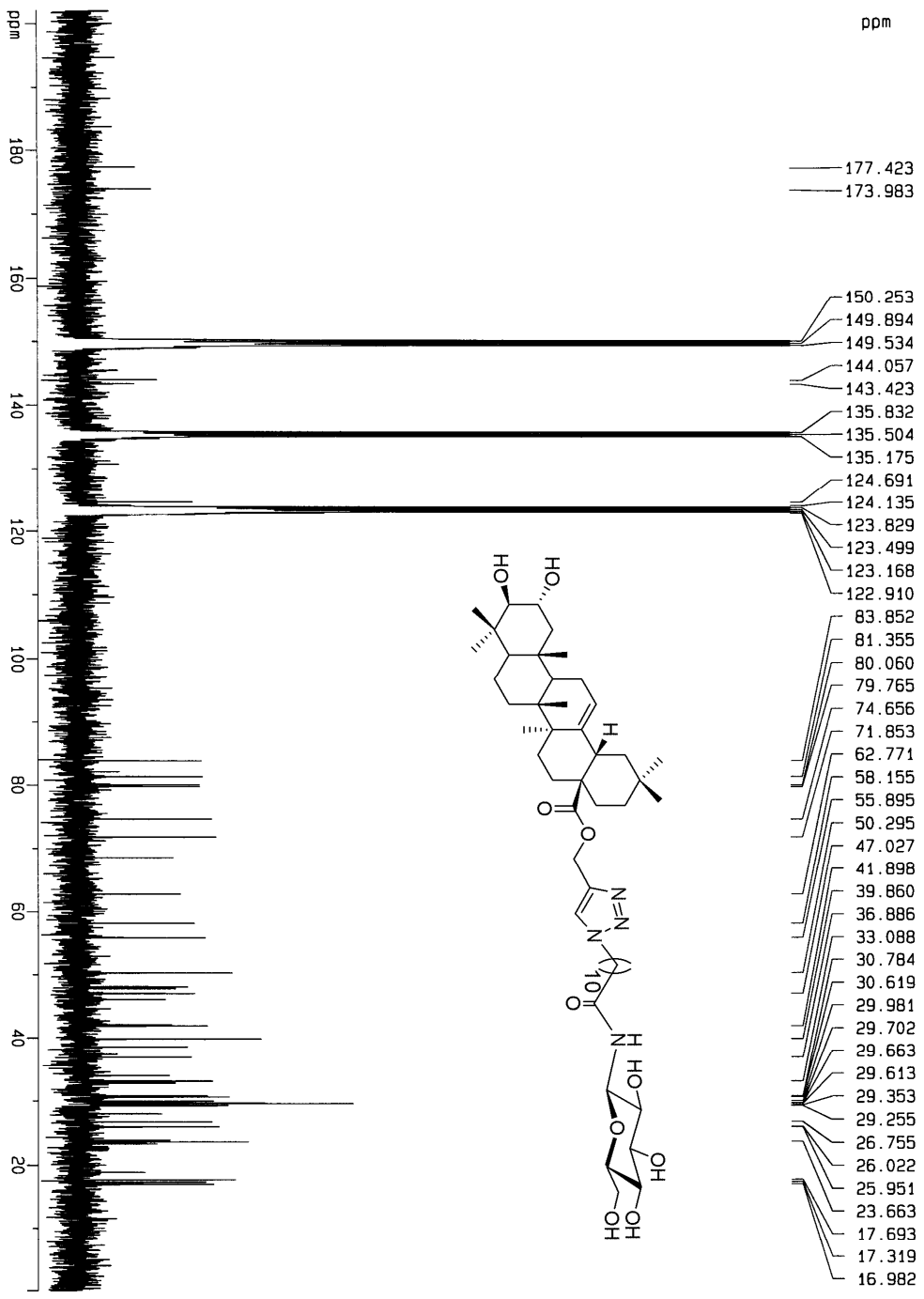
F2 - Acquisition Parameters
 Date_ 20080429
 Time 22:17
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg
 TO 32768
 SOLVENT pyr
 NS 2110
 DS 8
 SFORES 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.59044468 sec
 RG 102400
 DW 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SF01 75.4763978 MHz

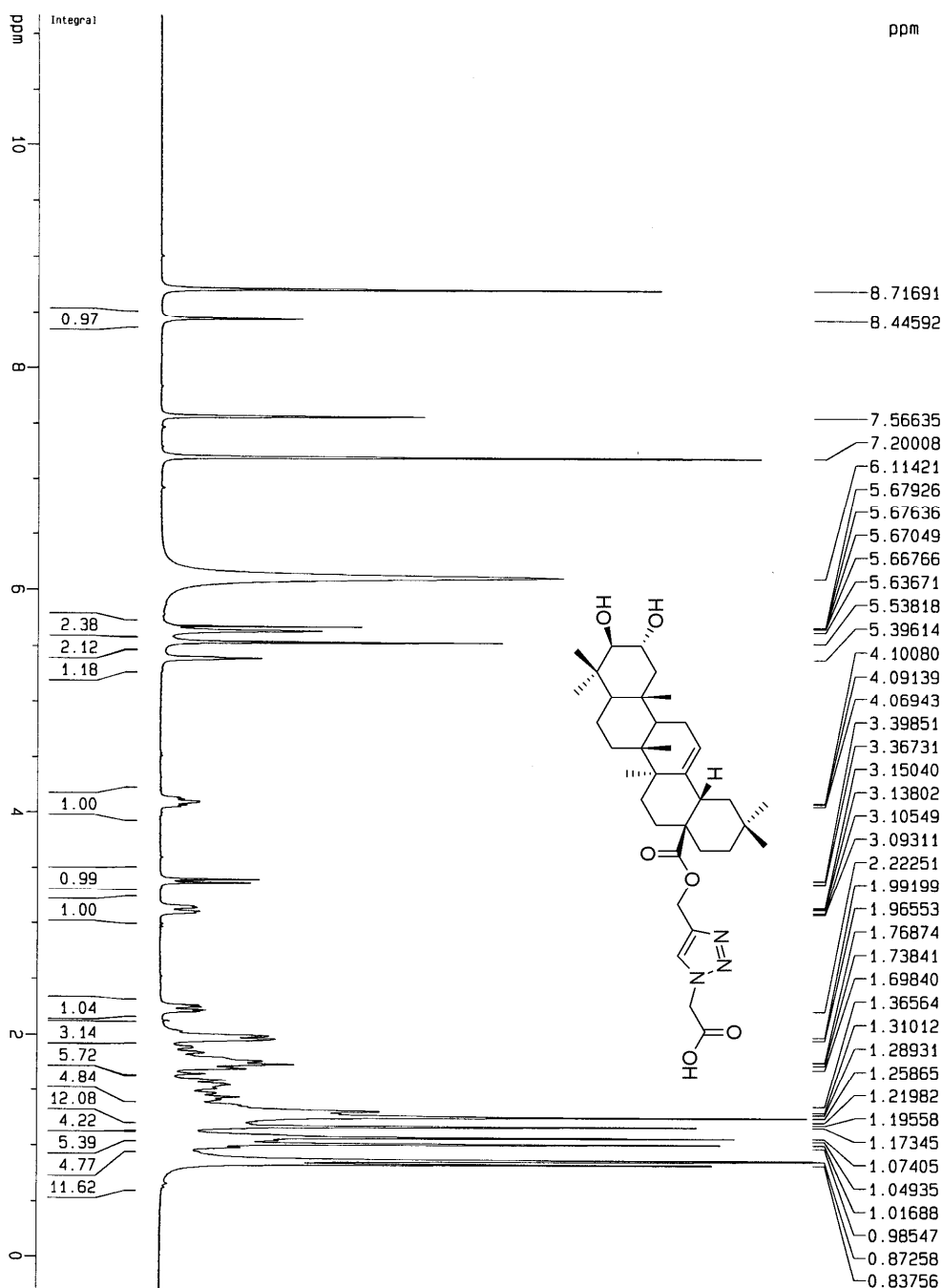
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677277 MHz
 MDW FM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.50 cm
 CY 50.00 cm
 F1p 202.111 ppm
 F1 15252.87 Hz
 F2p -3.78 Hz
 F2 -8.98495 ppm/cm
 PPMCH 678.07355 Hz/cm
 HZCM



KELLY-162 1H-NMR PYR-05 303K AV-300



Current Data Parameters
 NAME SHD
 EXPNO 946
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080425
 Time 16:12
 INSTRUM spect
 PROBRD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 2930
 FIDRES 1.264722 sec
 AQ 1.264722 sec
 RG 302
 DW 93.600 usec
 DE 6.00 usec
 TE 303.0 K
 D1 2.00000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 6.00 usec
 PL1 -4.00 dB
 SF01 300.1324245 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1299887 MHz
 KW 0
 SSB 0
 LB 0.10 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 22.00 cm
 CY 15.00 cm
 FIP 11.172 ppm
 F1 3353.45 Hz
 F2 -0.305 ppm
 PPMCM 0.52171 ppm/cm
 HZCM 156.58017 Hz/cm

KELLY-162 13C-NMR PYR-D5 300K AV-300

Current Data Parameters
 NAME snb
 EXPNO 969
 PROCNO 1

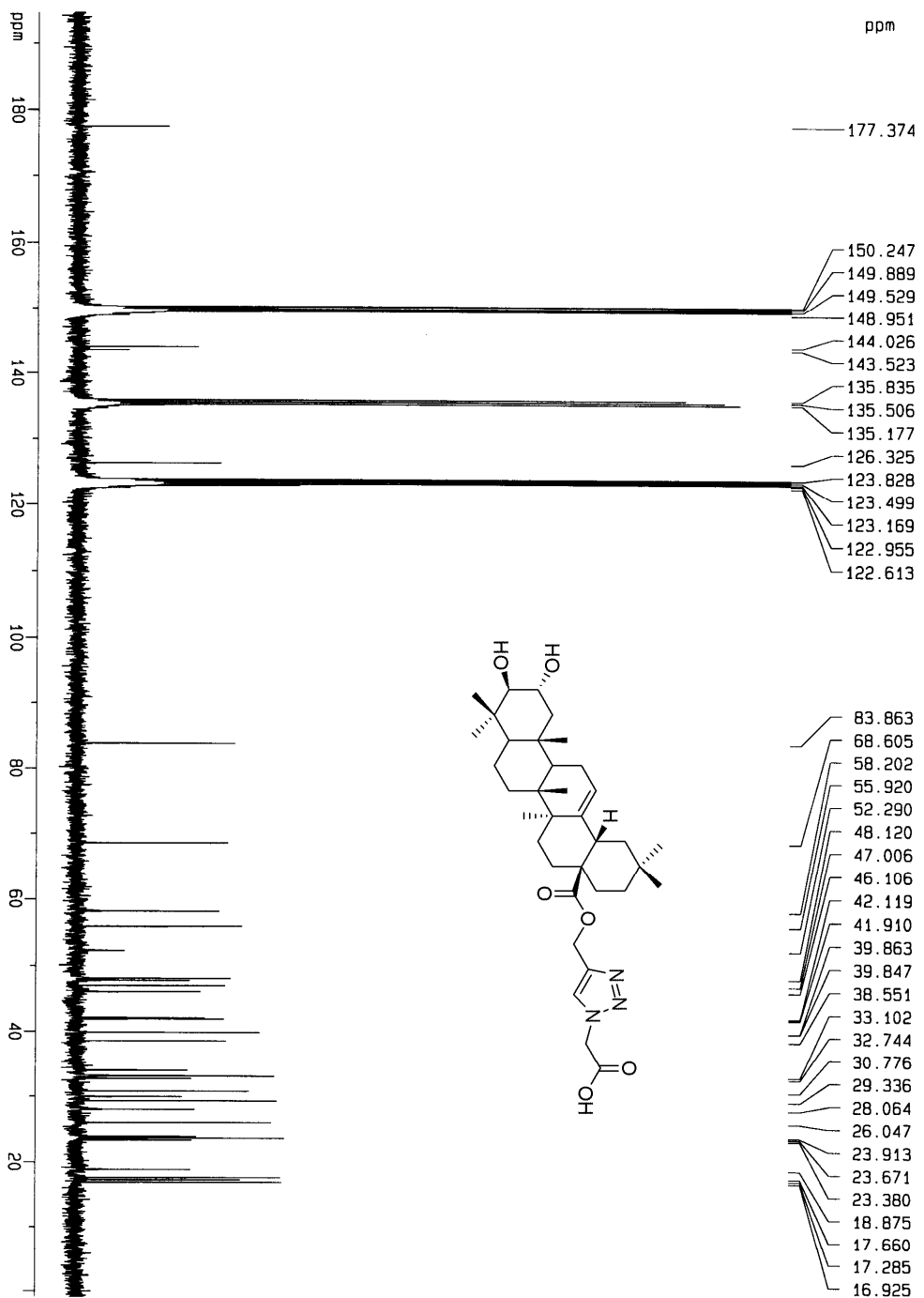
F2 - Acquisition Parameters
 Date_ 20080429
 Time 17.58
 INSTRUM spect
 PROCNO 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 32768
 SOLVENT Pyr
 NS 1876
 DS 8
 SMH 18115.941 Hz
 FIDRES 0.552855 Hz
 AQ 0.9044468 sec
 RG 102400
 DM 27.600 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec

***** CHANNEL f1 *****
 NUC1 13C
 P1 8.00 usec
 PL1 -2.00 dB
 SFO1 75.4763978 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -4.00 dB
 PL12 19.25 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.467277 MHz
 KDN EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.00

1D NMR pilot parameters
 CX 22.50 cm
 CY 20.00 cm
 F1P 194.760 ppm
 F1 14698.08 Hz
 F2P -0.898 ppm
 F2 -67.79 Hz
 PPRGN 8.65982 ppm/cm
 HZCM 656.26129 Hz/cm



- 177.374
- 150.247
- 149.889
- 149.529
- 148.951
- 144.026
- 143.523
- 135.835
- 135.506
- 135.177
- 126.325
- 123.828
- 123.499
- 123.169
- 122.955
- 122.613
- 83.863
- 68.605
- 58.202
- 55.920
- 52.290
- 48.120
- 47.006
- 46.106
- 42.119
- 41.910
- 39.863
- 39.847
- 38.551
- 33.102
- 32.744
- 30.776
- 29.336
- 28.064
- 26.047
- 23.913
- 23.671
- 23.380
- 18.875
- 17.660
- 17.285
- 16.925