

Supplementary Material

Synthesis of cyclic and acyclic pyrimidine nucleosides analogues with anticipated antiviral activity

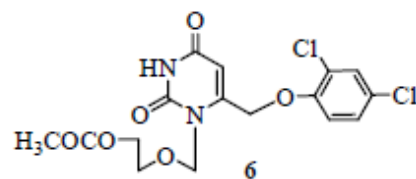
Mohamed F. Elshehry

Pesticides Chemistry Department, National Research Centre, Dokki, 12622, Giza, Egypt

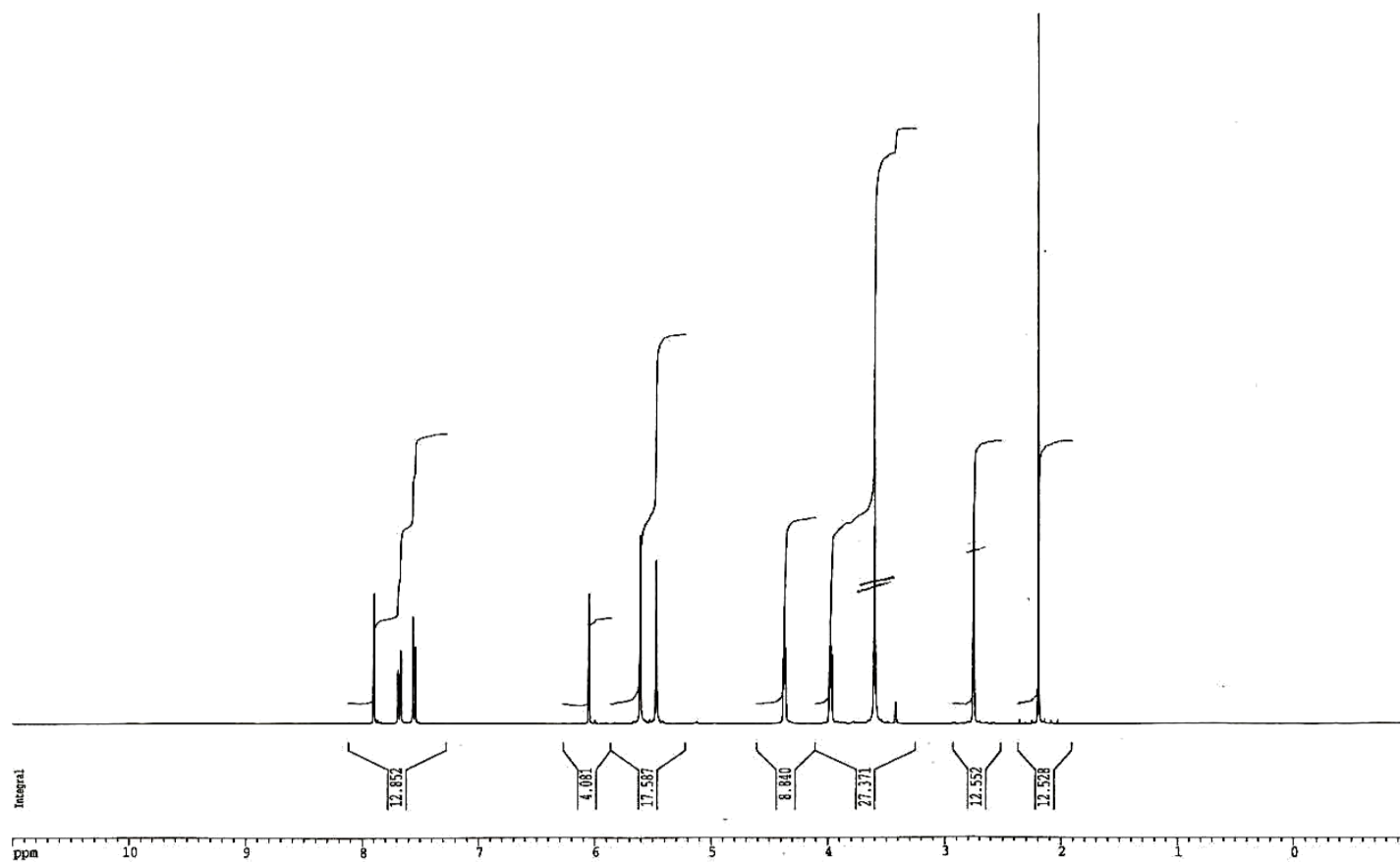
E-mail: moh_elshehry2000@yahoo.com

Table of Contents

¹H NMR and ¹³C NMR spectra copies



El-shehry Mg
PROTON DMSO x guest 31



Current AMX400 Data

DU /x
NAME 20070511
EXPNO 310
PROCNO 1

F2 - Acquisition Parameters

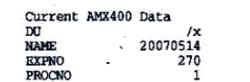
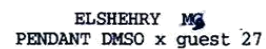
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RG 256
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DE 85.71 usec
TE 300.0 K
HL1 1 dB
DI 1.00000000 sec
PI 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters

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PC 1.00

1D NMR plot parameters

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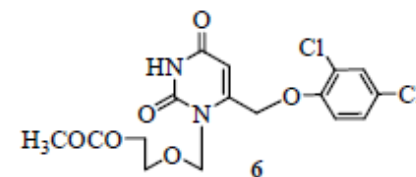
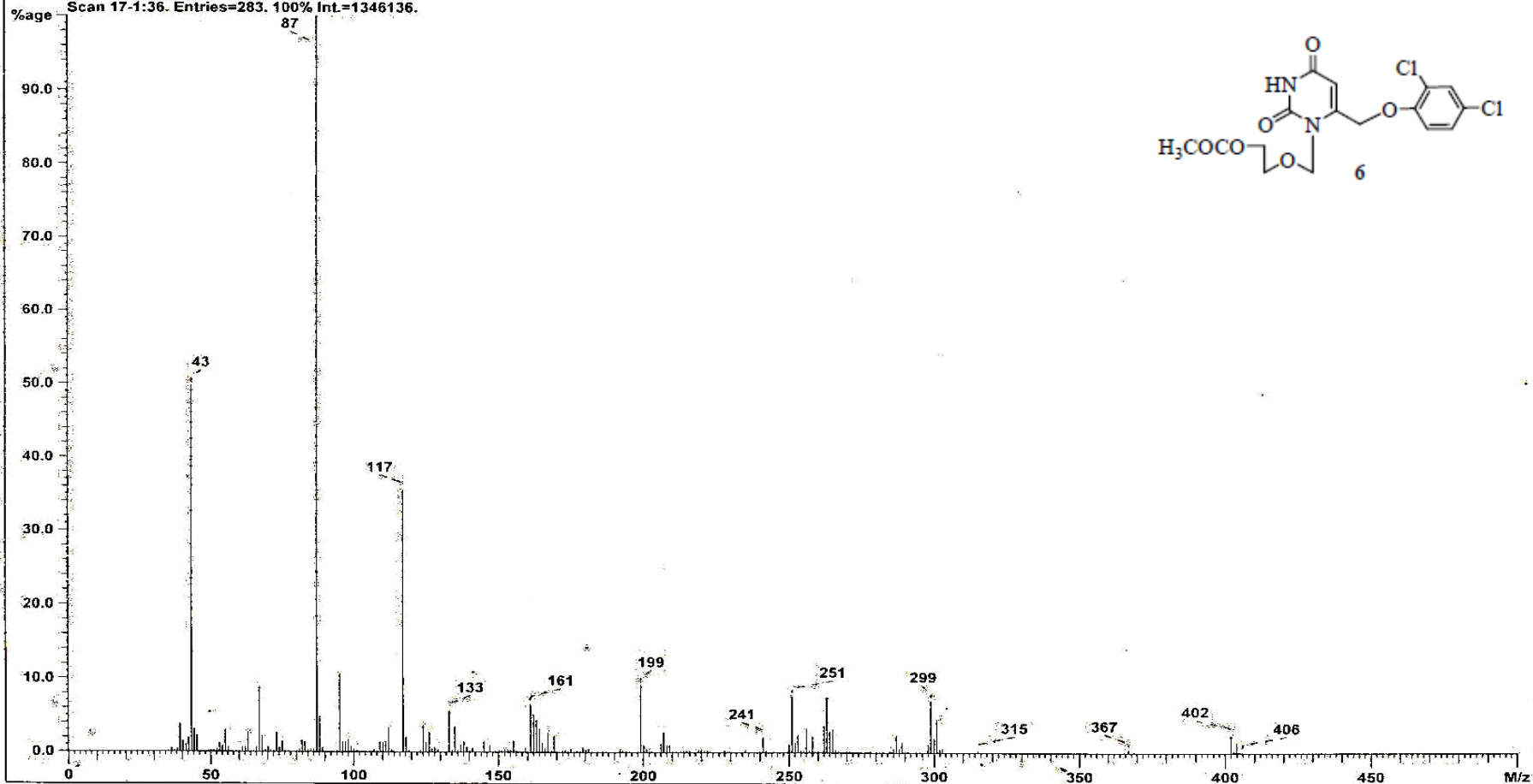
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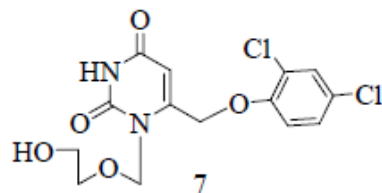
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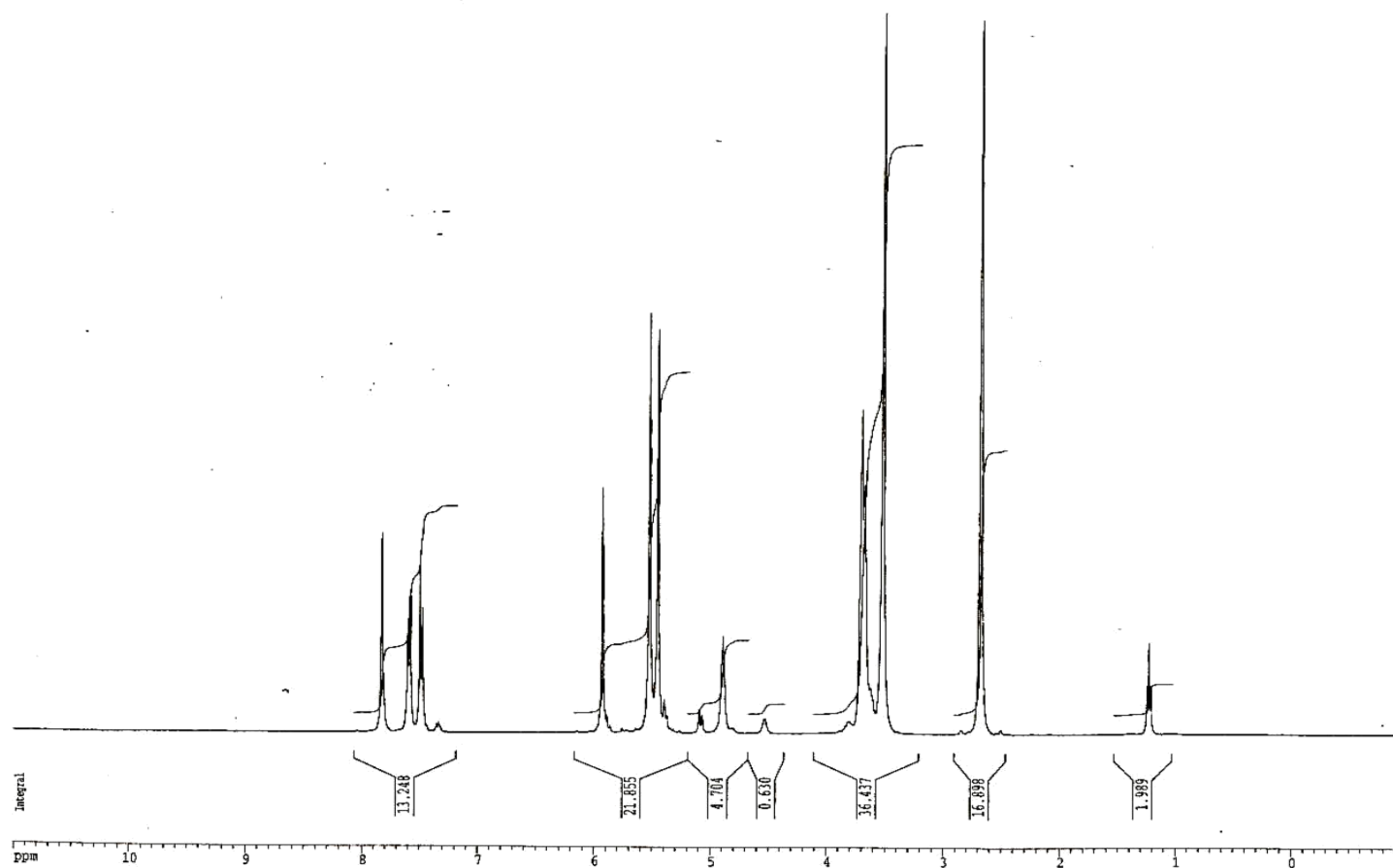
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el-shehry m13
PROTON DMSO x guest 9

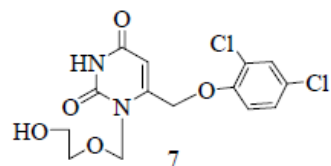


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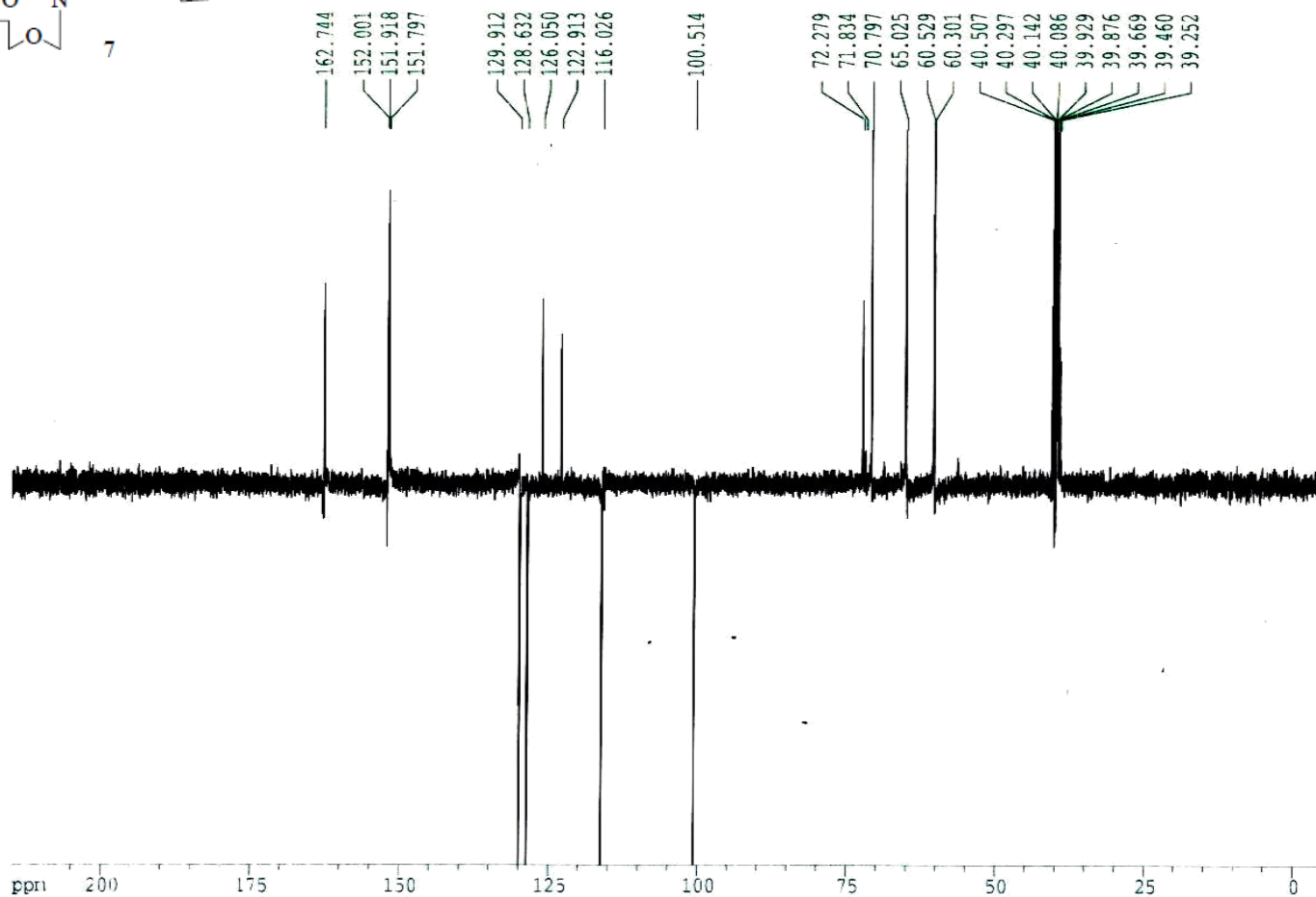
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NUCLEUS 1H

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1D NMR plot parameters
CX 30.00 cm
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F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
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El-shehry M13
PENDANT DMSO x guest 20



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EXPNO 200
PROCNO 1

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FIDRES 0.381472 Hz
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RG 32768
DN 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNUC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
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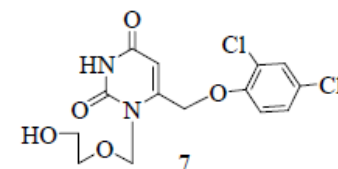
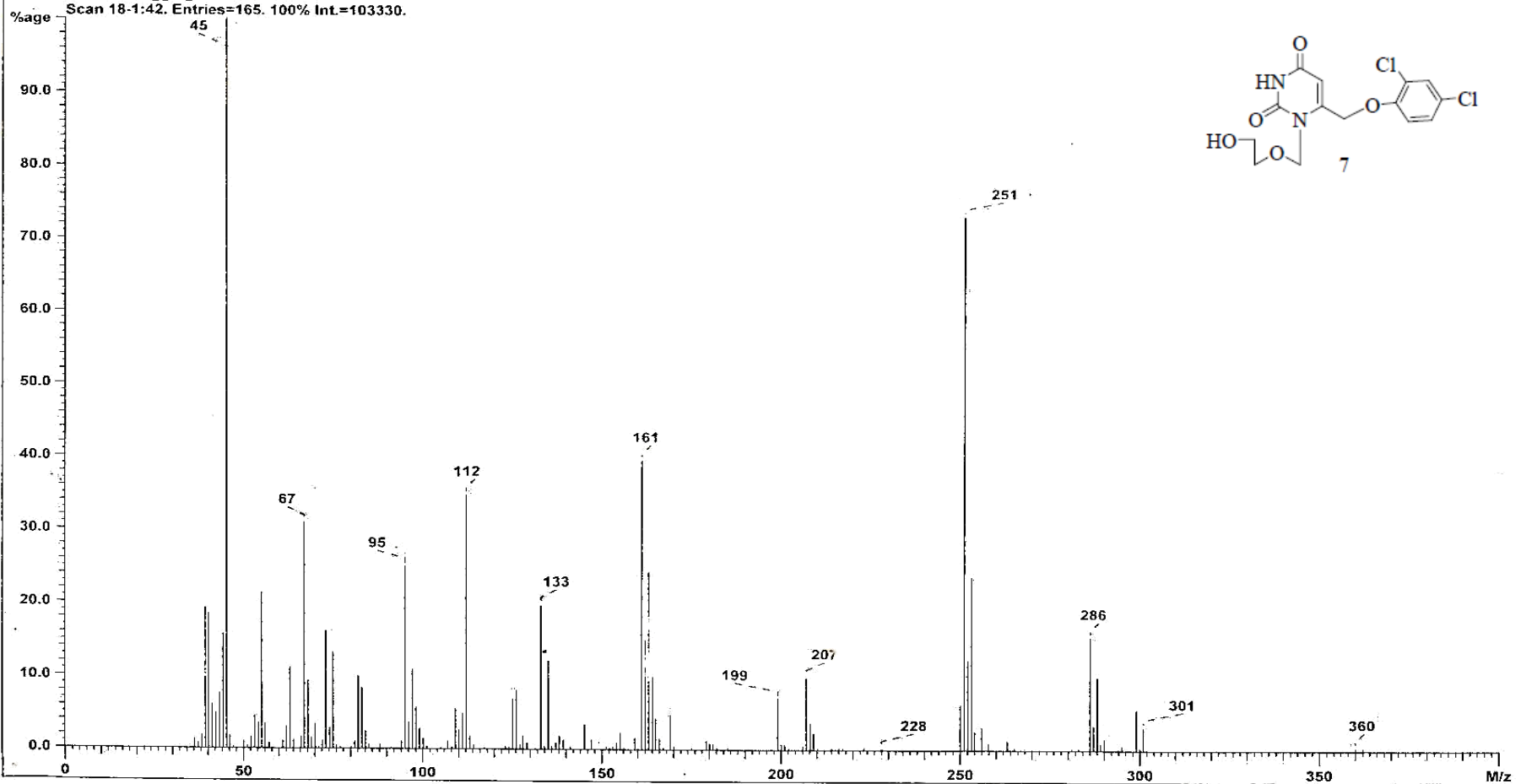
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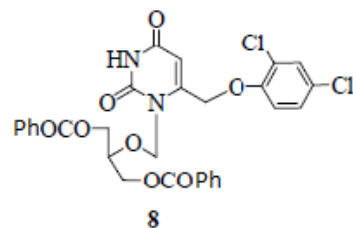
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F2P -5.000 ppm
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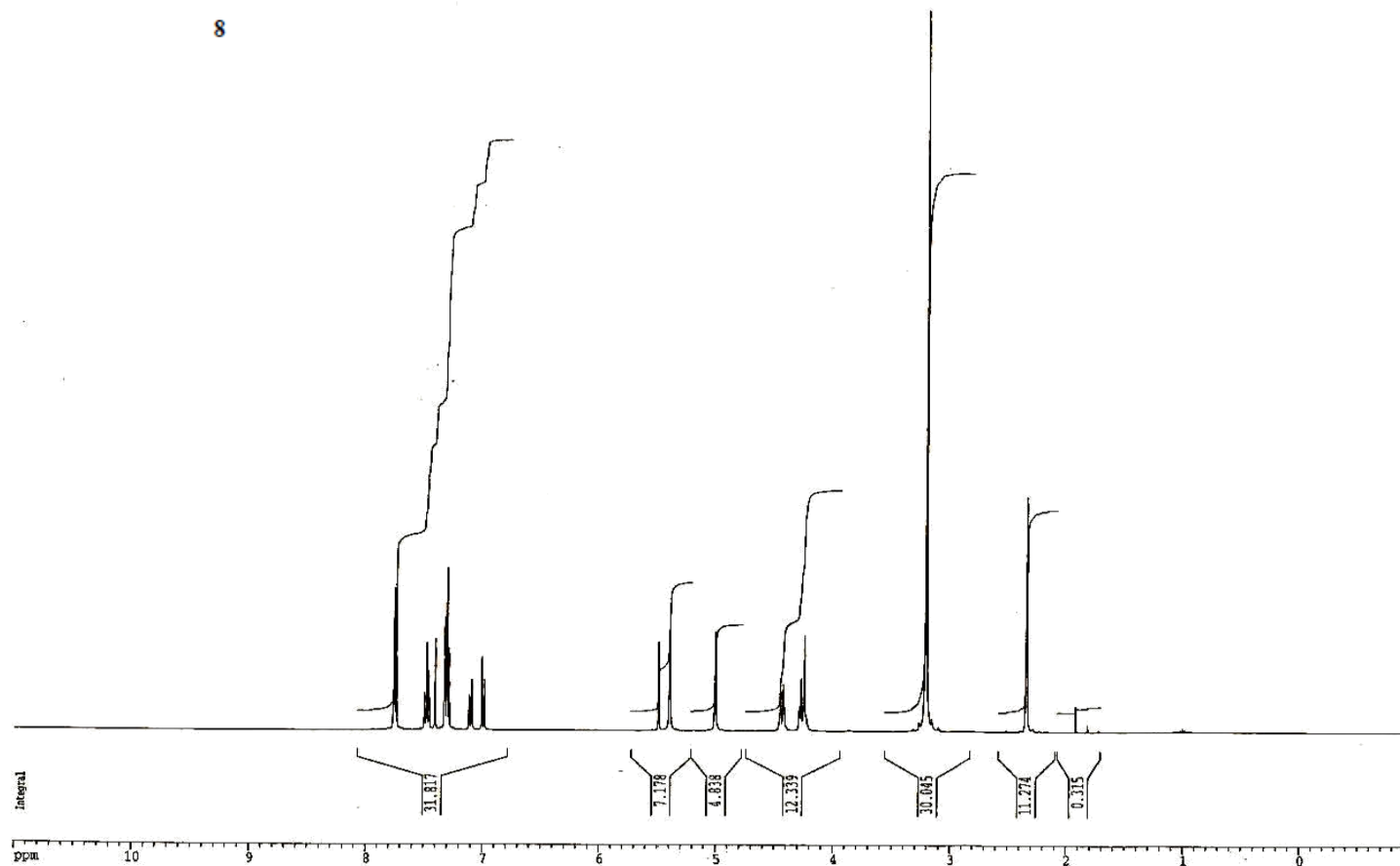
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Cl El-shehry, M10
PROTON DMSO x guest 20



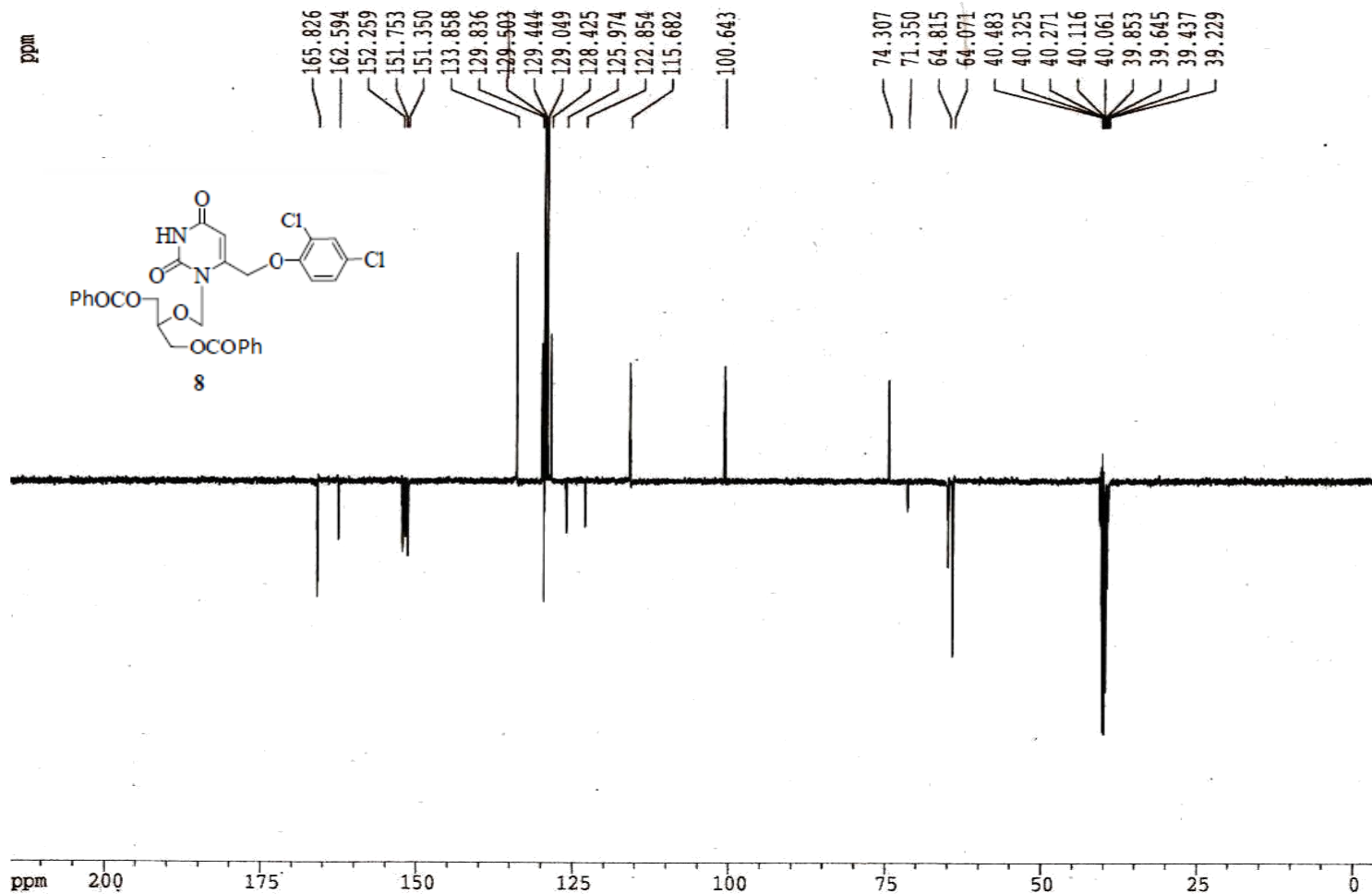
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FIDRES 0.127157 Hz
AQ 3.9322100 sec
RG 256
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.00000000 sec
F1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters
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PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
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HZCM 160.05453 Hz/cm

el-shehry m10
PENDANT DMSO x guest 20



Current AMX400 Data

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EXPNO 200
PROCNO 1

F2 - Acquisition Parameters

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TD 65536
SOLVENT DMSO
NS 800
DS 4
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FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNUC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
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SFO1 100.6245885 MHz
NUCLEUS 13C
CPDPRG waltz16
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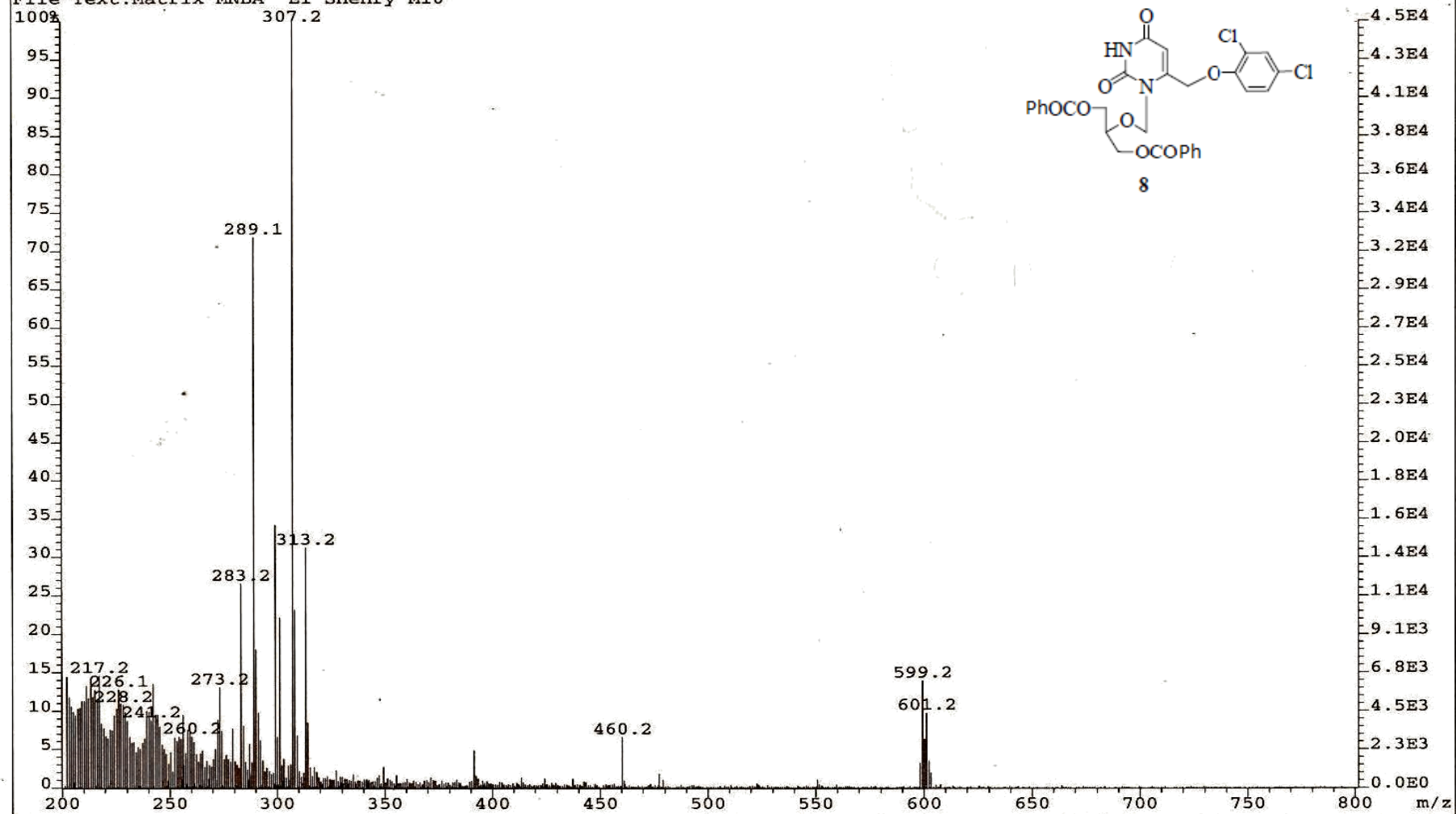
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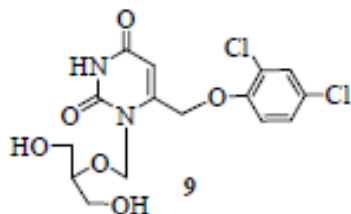
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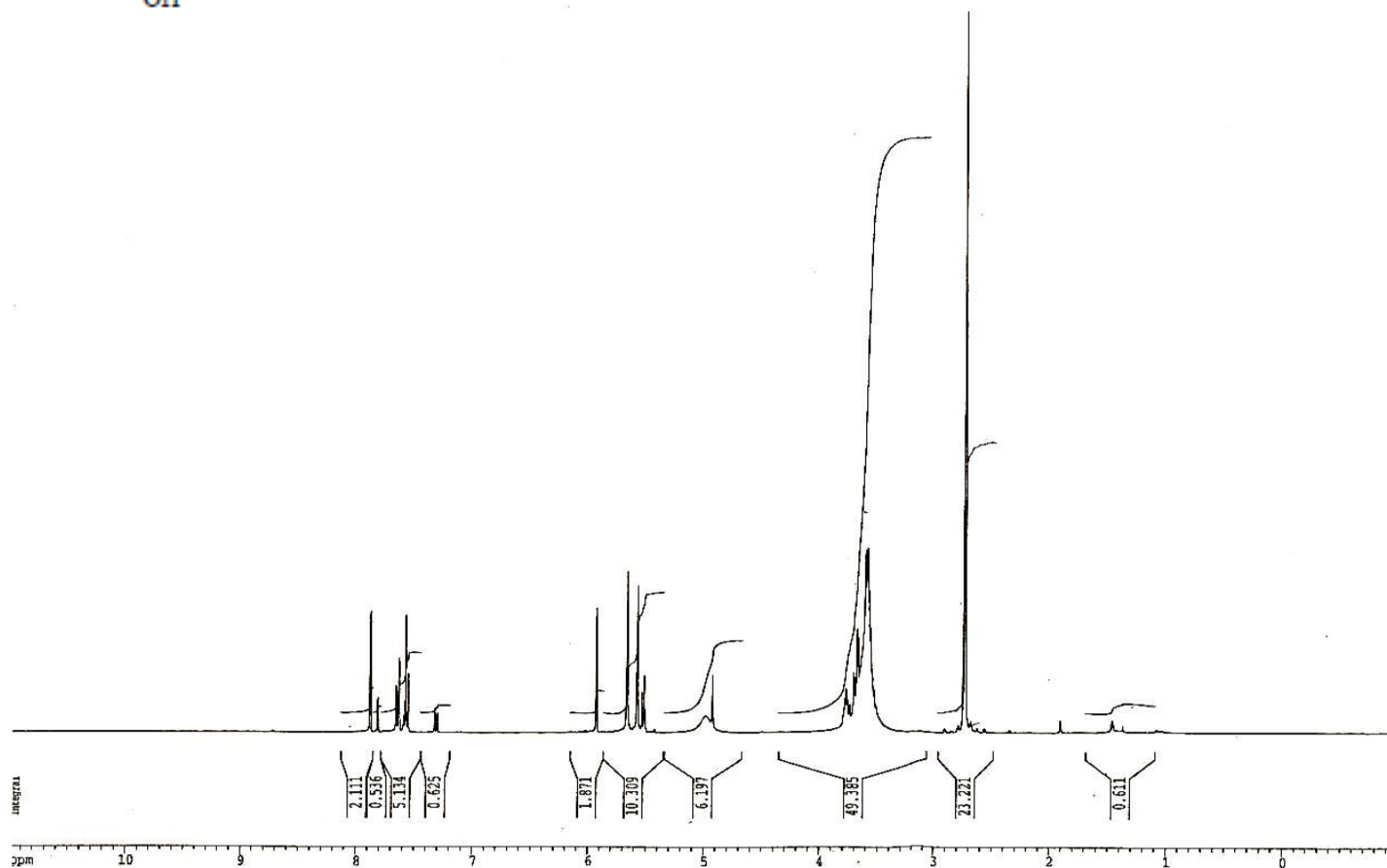
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EL-SHEHRY M600
PROTON DMSO x guest 17

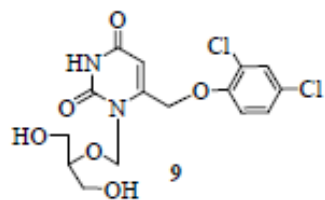


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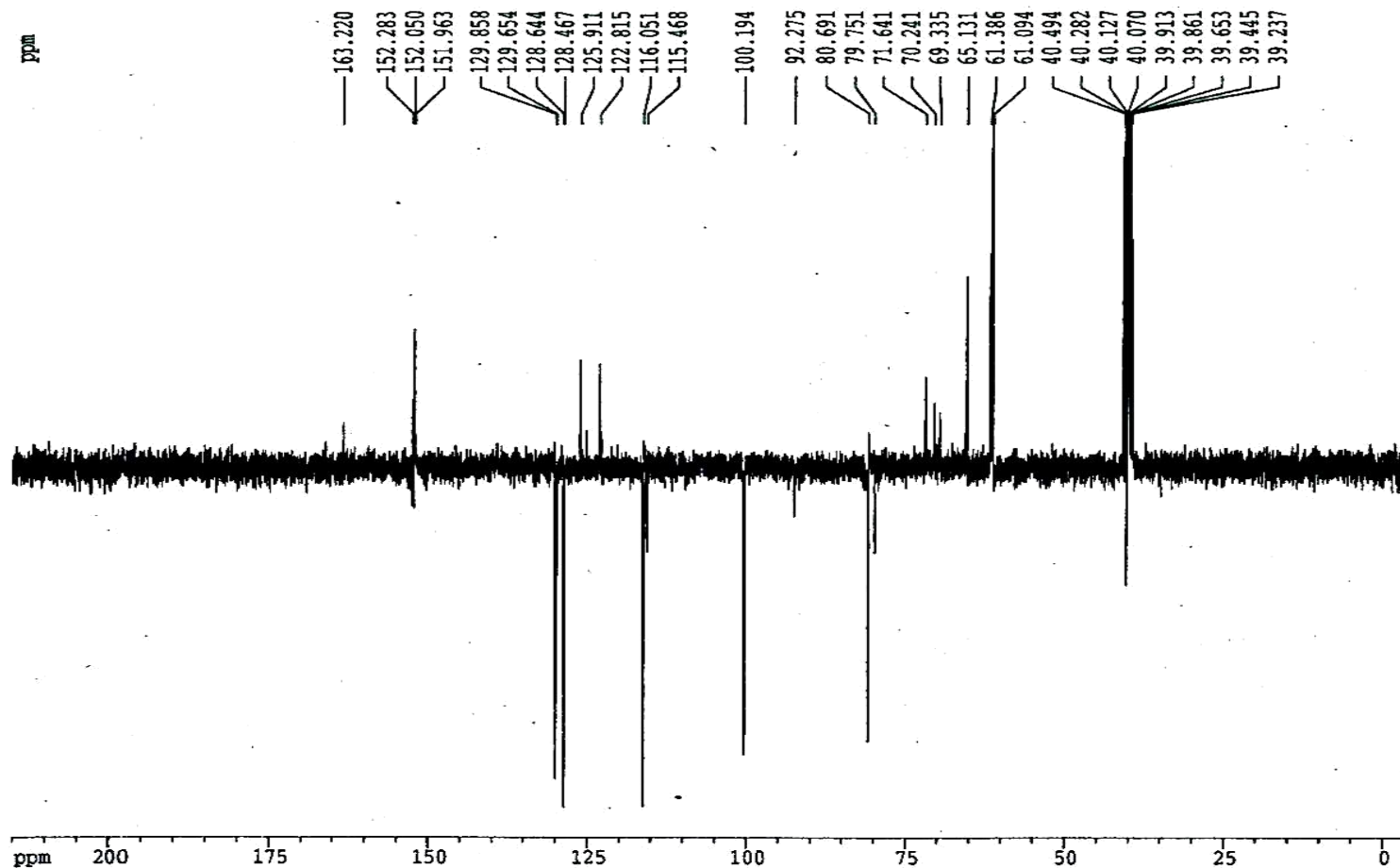
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FIDRES 0.127157 Hz
AQ 3.9322100 sec
RG 512
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.00000000 sec
P1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters
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SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
FLP 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
PPMCM 0.40000 ppm/cm
HZCM 160.05447 Hz/cm



EL-SHEHRY M600
PENDANT DMSO x guest 8



Current AMX400 Data
DU /x
NAME 20071004
EXPNO 80
PROCNO 1

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Date_ 20071004
Time 14.29
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PULPROG pendant.amx
TD 65536
SOLVENT DMSO
NS 800
DS 4
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FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNOC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
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SFO1 100.6245885 MHz
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CPDPRG waltz16
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D2 0.00357143 sec

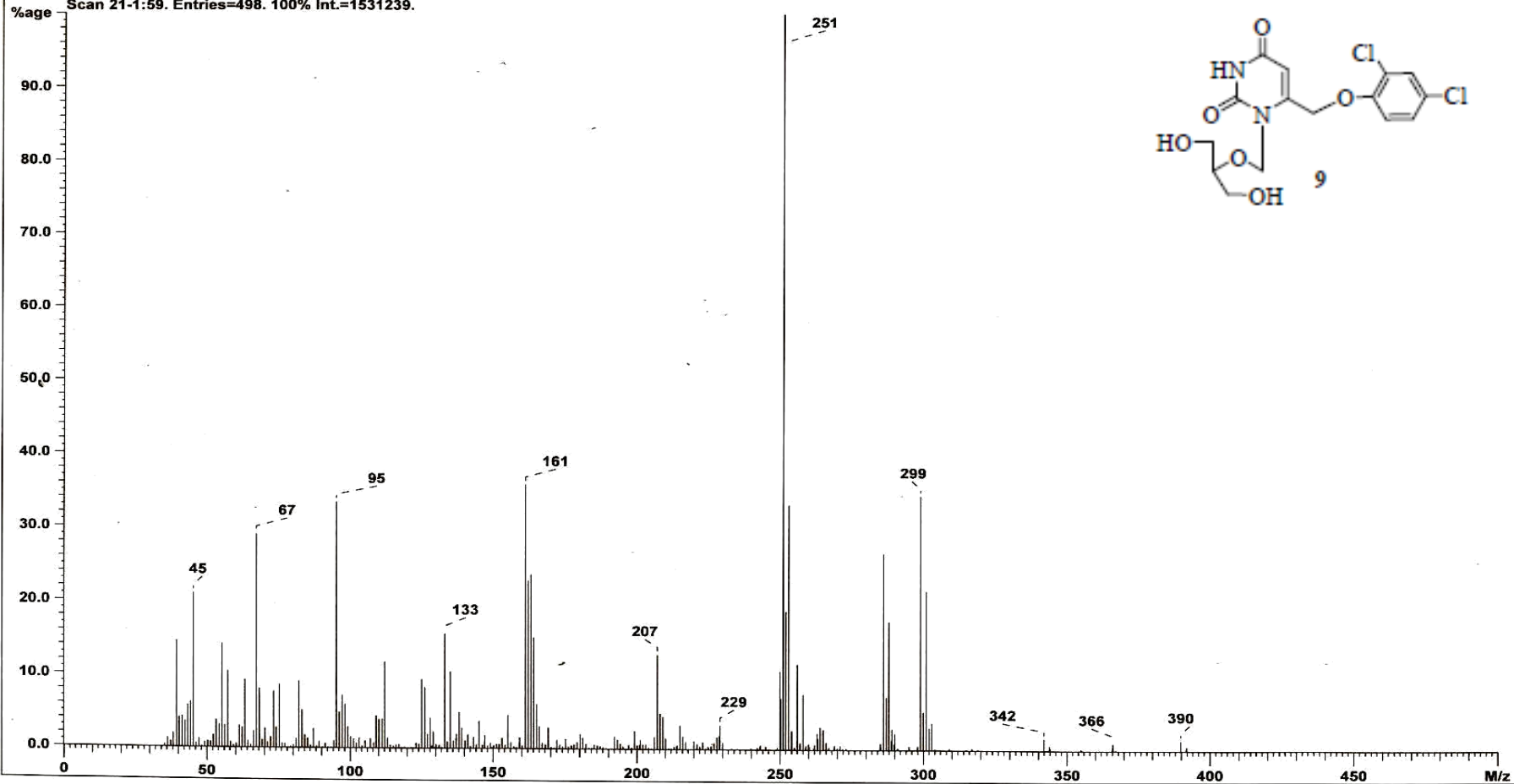
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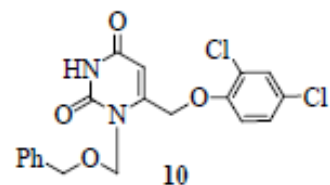
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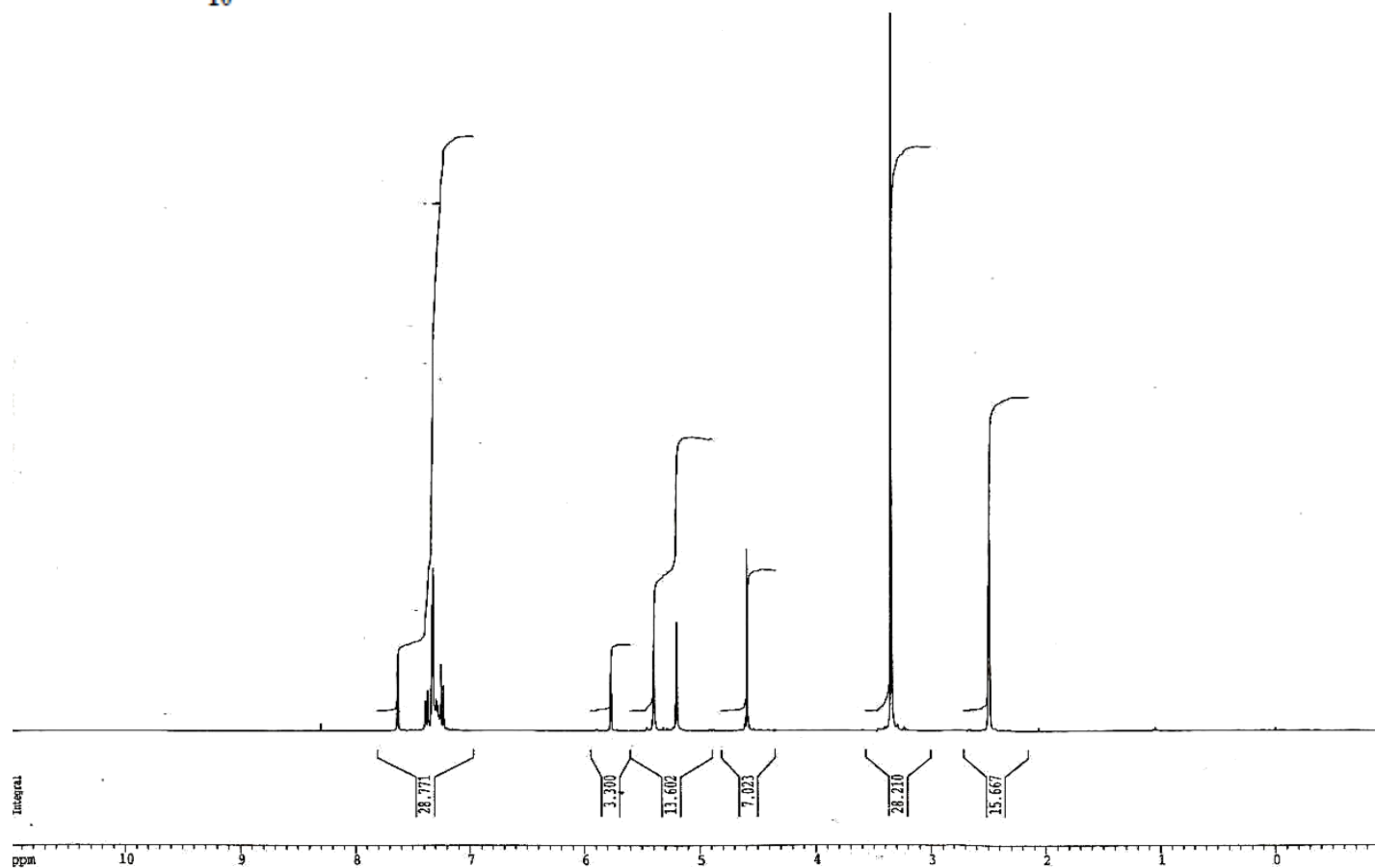
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PROTON DMSO x guest 21

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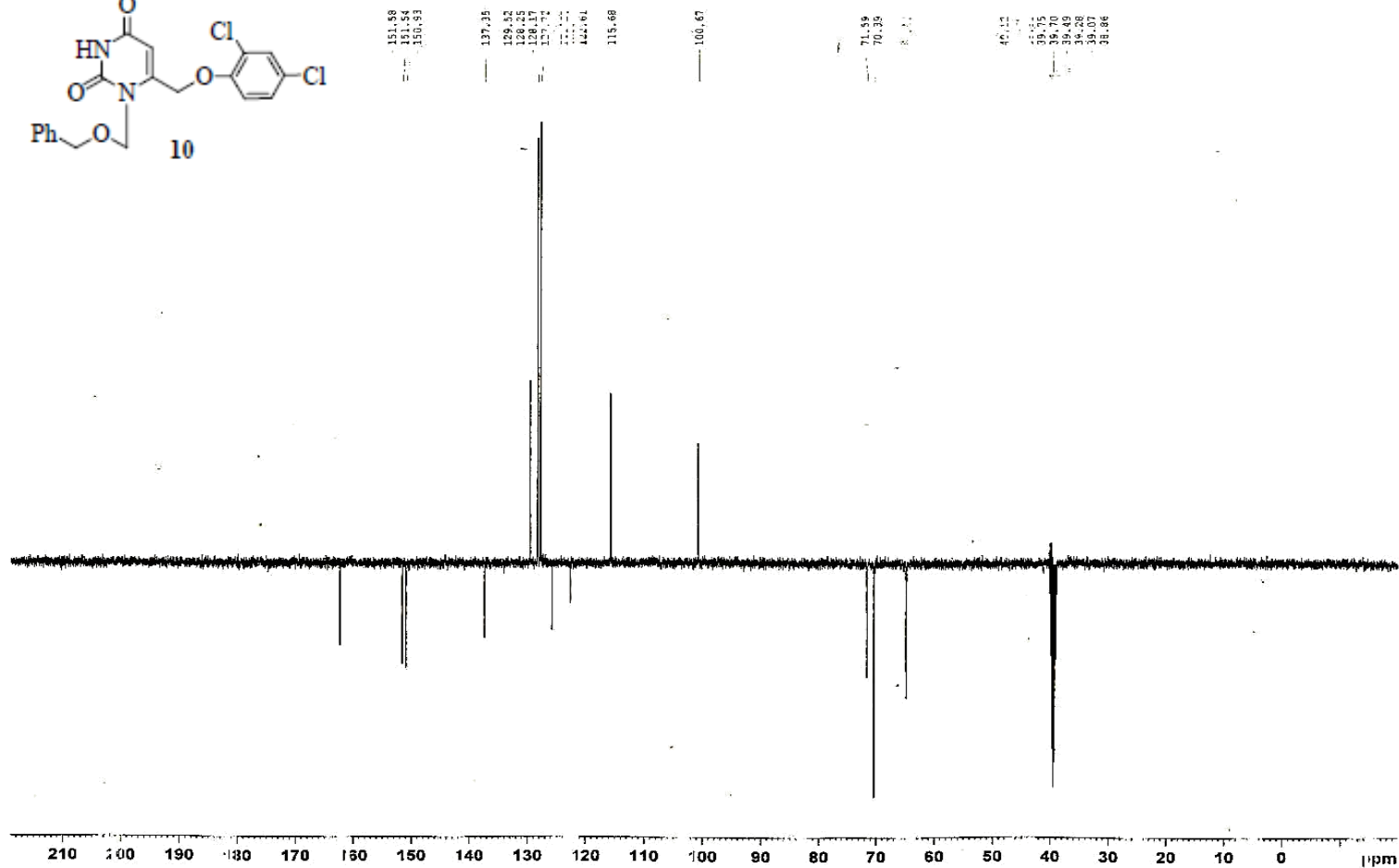
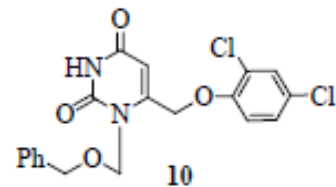
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RG 512
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.00000000 sec
P1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters
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GB 0
PC 1.00

1D NMR plot parameters
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F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
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HZCM 160.05452 Hz/cm



EL-SHEHRY M8R



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PROCNO 1

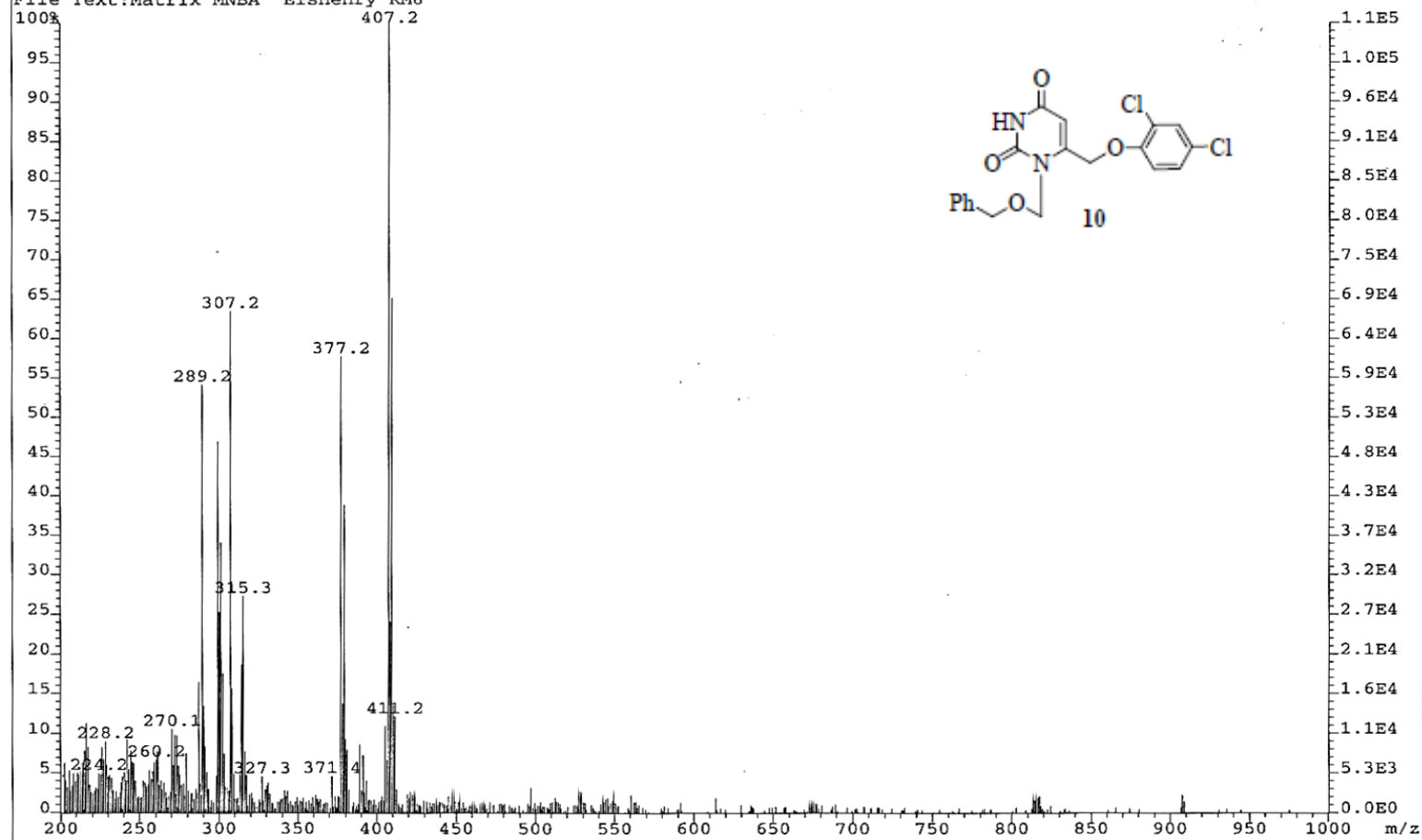
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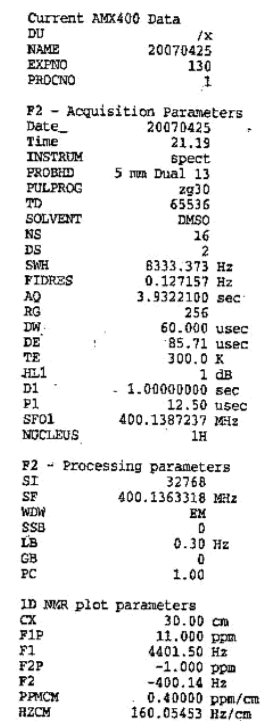
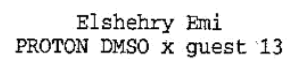
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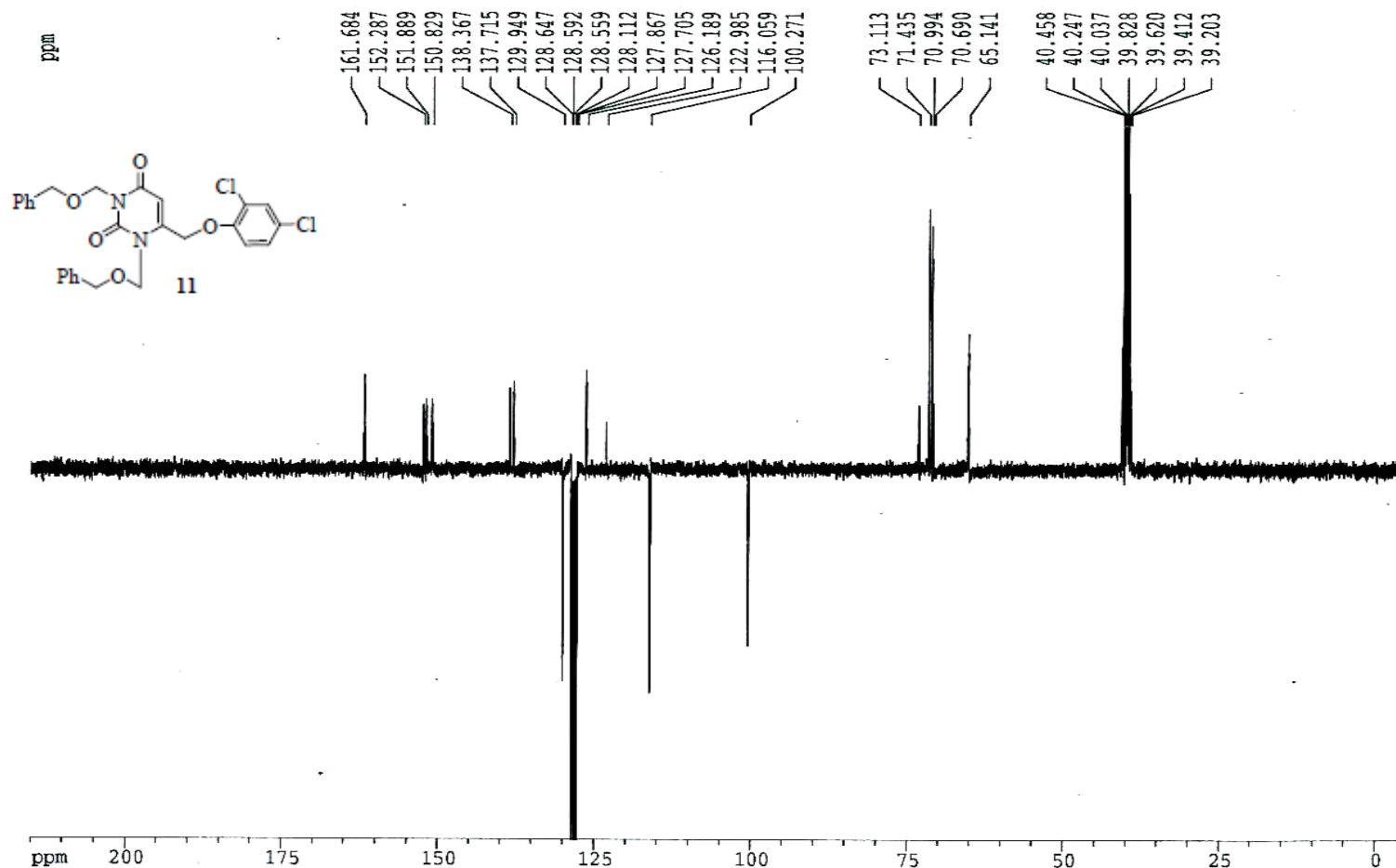
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Elshehry, EMI
PENDANT DMSO x guest 43



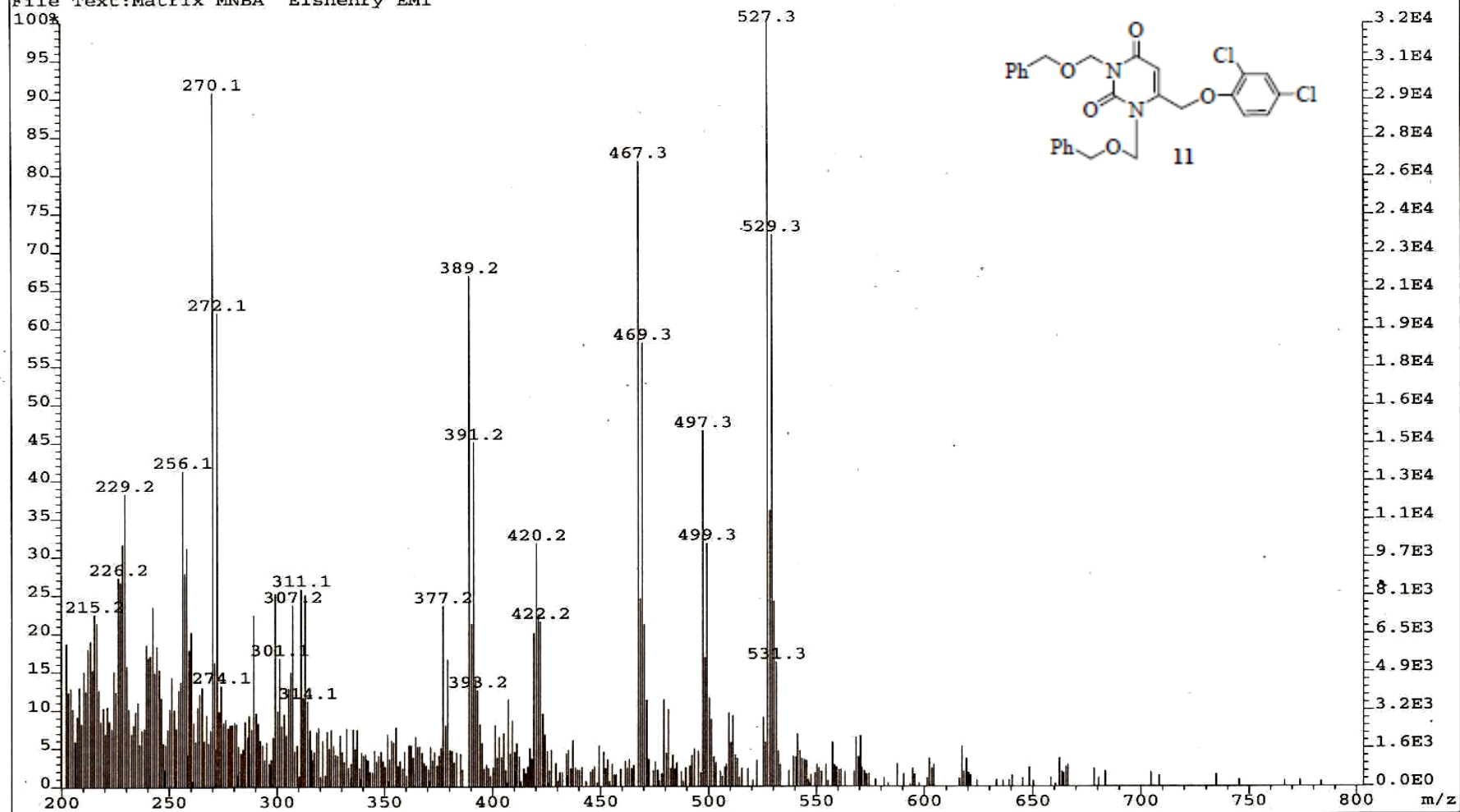
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PROCNO 1

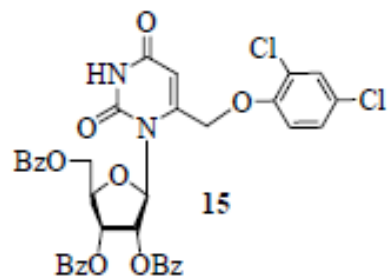
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FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.000000
HL1 1 dB
D1 1.5000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNOC 1H
D4 0.0017241 sec
P4 21.2 usec
F2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
S2 26 dB
SFO1 100.6245885 MHz
NUCLEUS 13C
CPDPRG waltz16
P31 90.00 usec
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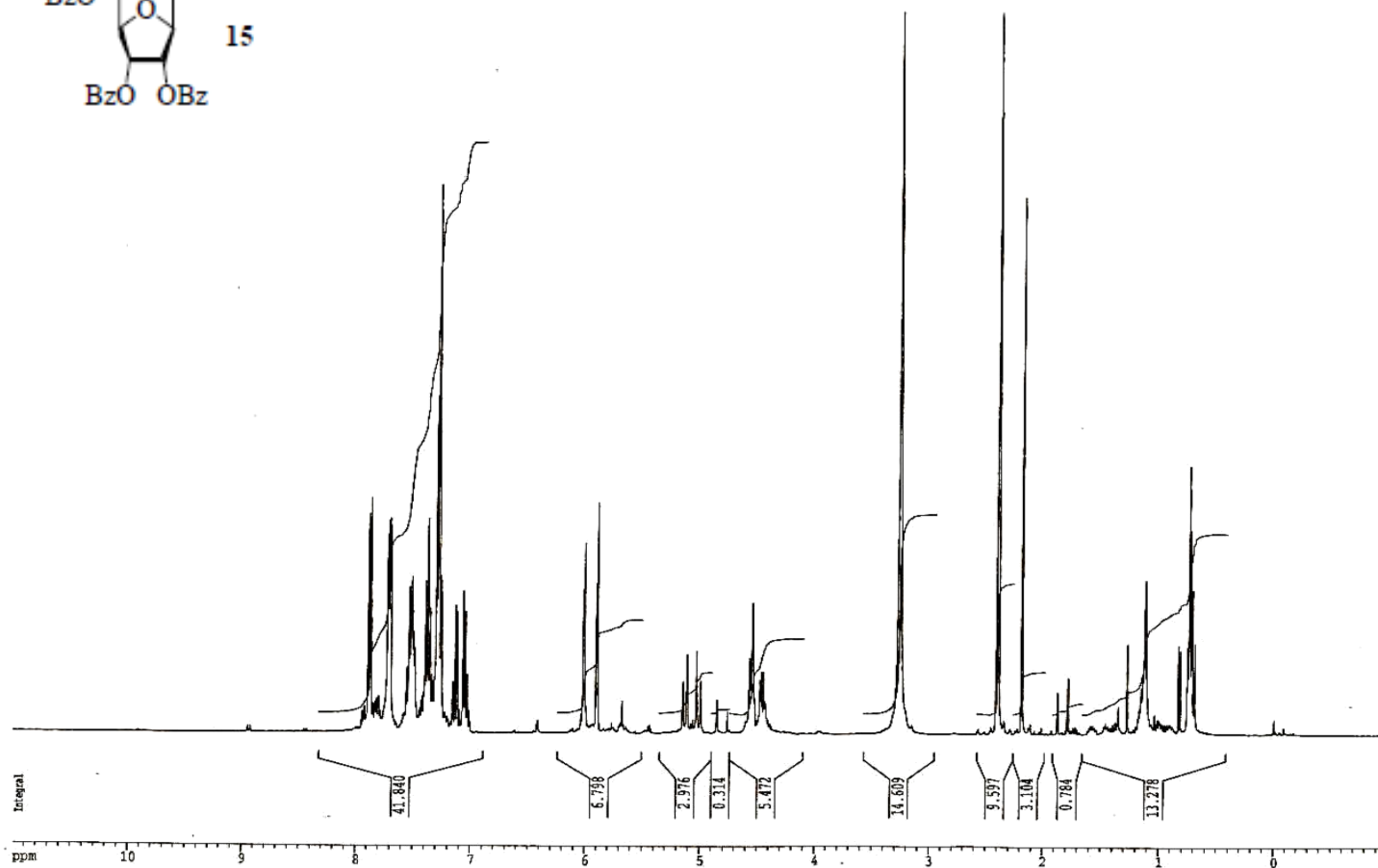
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FLP 215.000 ppm
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F2P -5.000 ppm
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PPMCM 11.00000 ppm/cm
HZCM 1106.75793 Hz/cm

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El-shehry M7b
PROTON DMSO x guest 41



Current AMX400 Data

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EXPNO 410
PROCNO 1

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FIDRES 0.127157 Hz
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RG 256
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
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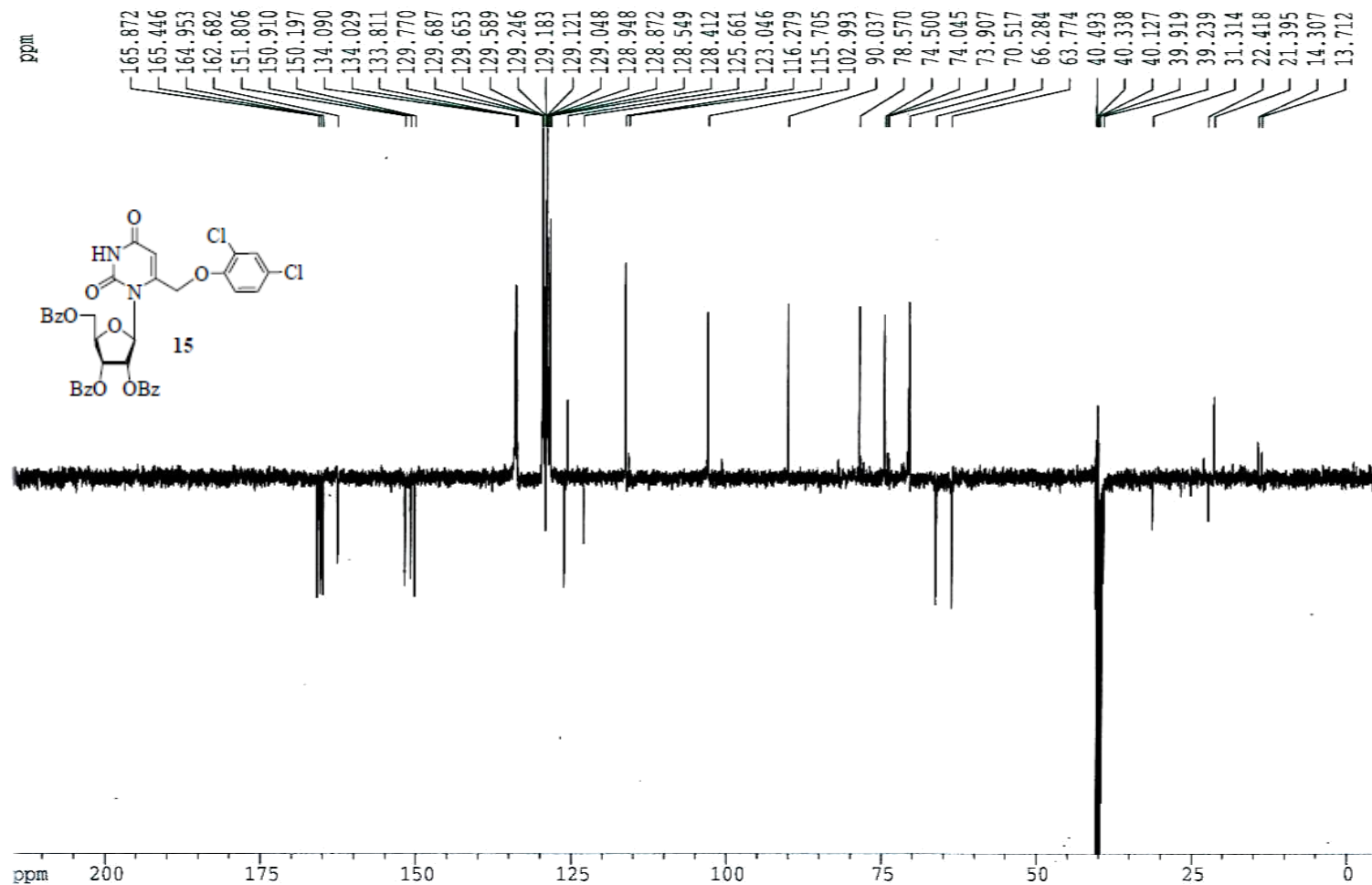
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SF 400.1363282 MHz
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LB 0.30 Hz
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PC 1.00

1D NMR plot parameters

CX 30.00 cm
F1P 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
PPMCM 0.40000 ppm/cm
HZCM 160.05453 Hz/cm

ELSHEHRY M7B
PENDANT DMSO x guest 18



Current AMX400 Data

DU /x
NAME 20070514
EXPNO 180
PROCNO 1

F2 - Acquisition Parameters

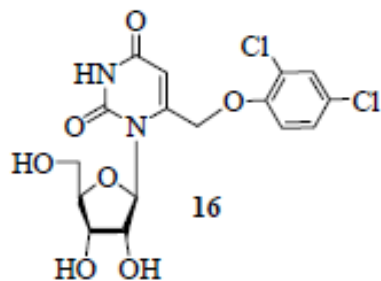
Date_ 20070514
Time 18.08
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG pendant.amx
TD 65536
SOLVENT DMSO
NS 800
DS 4
SWH 25000.119 Hz
FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNUG 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
S2 26 dB
SFO1 100.6245885 MHz
NUCLEUS 13C
CPDPRG waltz16
P31 90.00 usec
D2 0.00357143 sec

F2 - Processing parameters

SI 32768
SF 100.6143589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 215.000 ppm
F1 21632.09 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.75793 Hz/cm



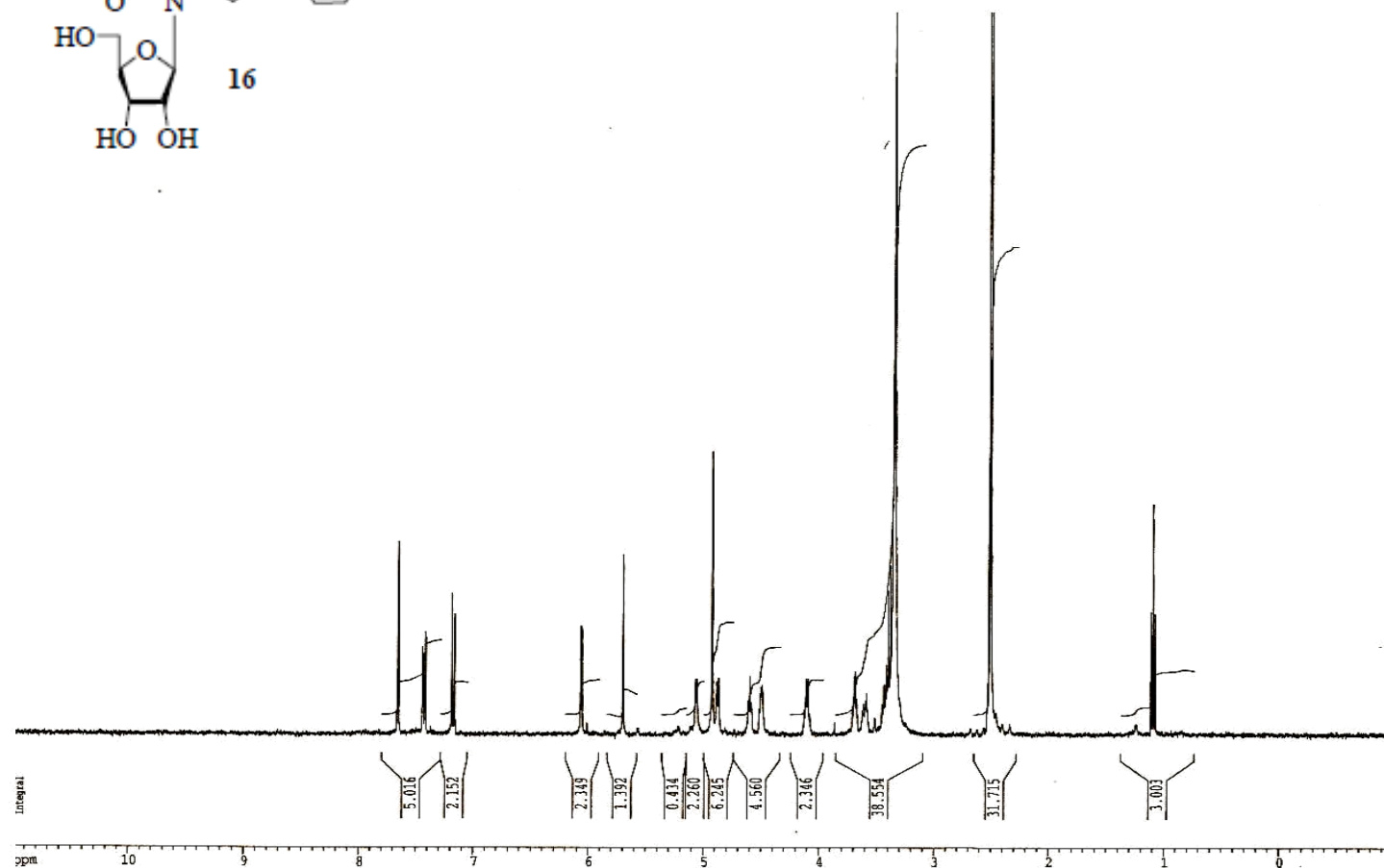
EL-SHEHRY M 350
PROTON DMSO x guest 10

Current AMX400 Data
DU /x
NAME 20071017
EXPNO 100
PROCNO 1

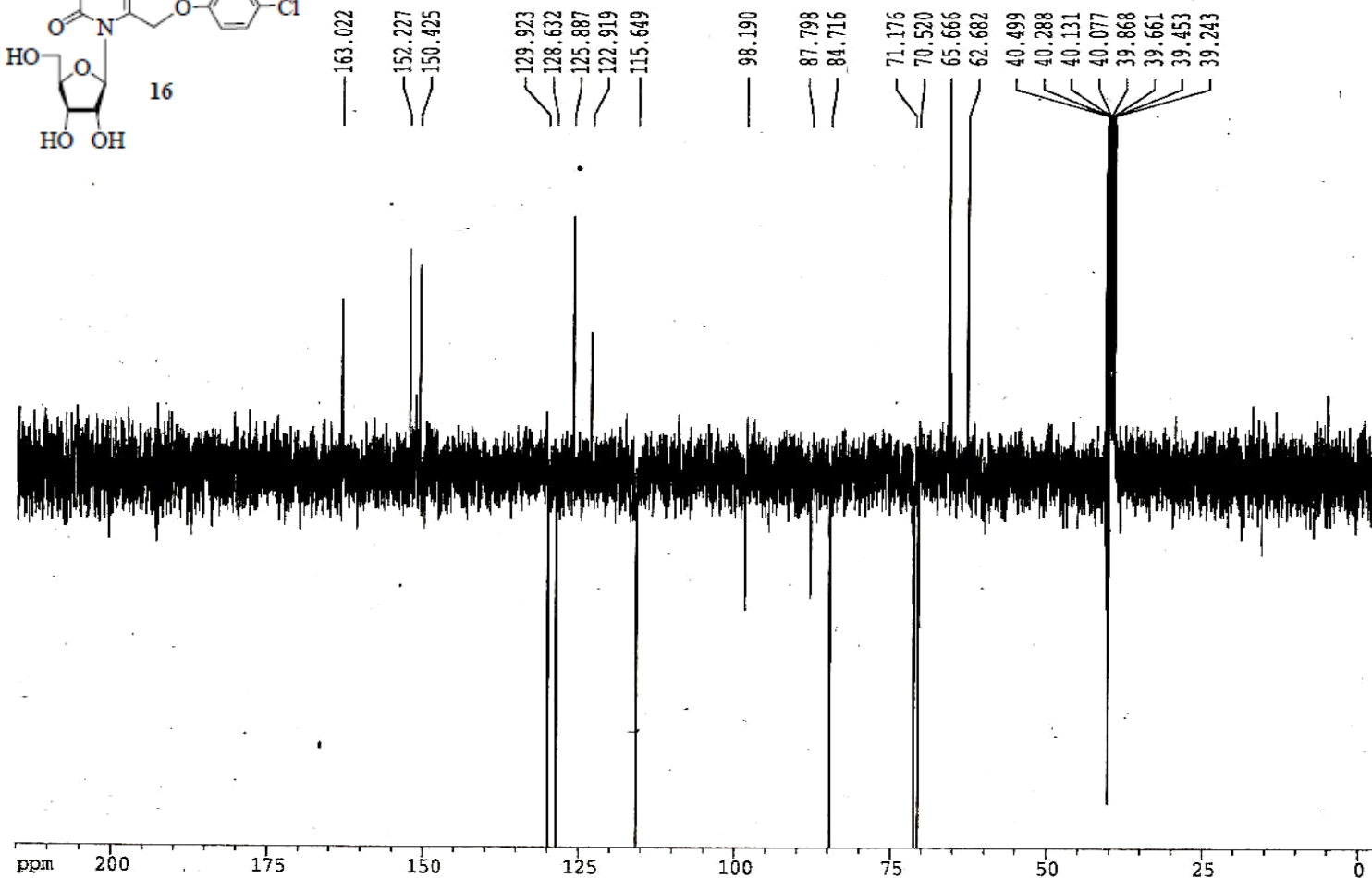
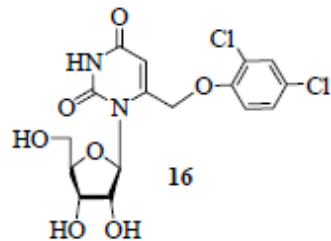
F2 - Acquisition Parameters
Date_ 20071017
Time 23.00
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8333.373 Hz
FIDRES 0.127157 Hz
AQ 3.9322100 sec
RG 512
DN 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.00000000 sec
P1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 32768
SF 400.1362838 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
PEMCM 0.40000 ppm/cm
HZCM 160.05452 Hz/cm



el-fshehrym 350
PENDANT DMSO x guest 23



Current AMX400 Data

DJ /x
NAME 20071019
EXPNO 230
PROCNO 1

F2 - Acquisition Parameters

Date_ 20071019
Time 18.36
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG pendant.amx
TD 65536
SOLVENT DMSO
NS 800
DS 4
SWH 25000.119 Hz
FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNOC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
S2 26 dB
SFO1 100.6245885 MHz
NUCLEUS 13C
CPDPRG waltz16
P31 90.00 usec
D2 0.00357143 sec

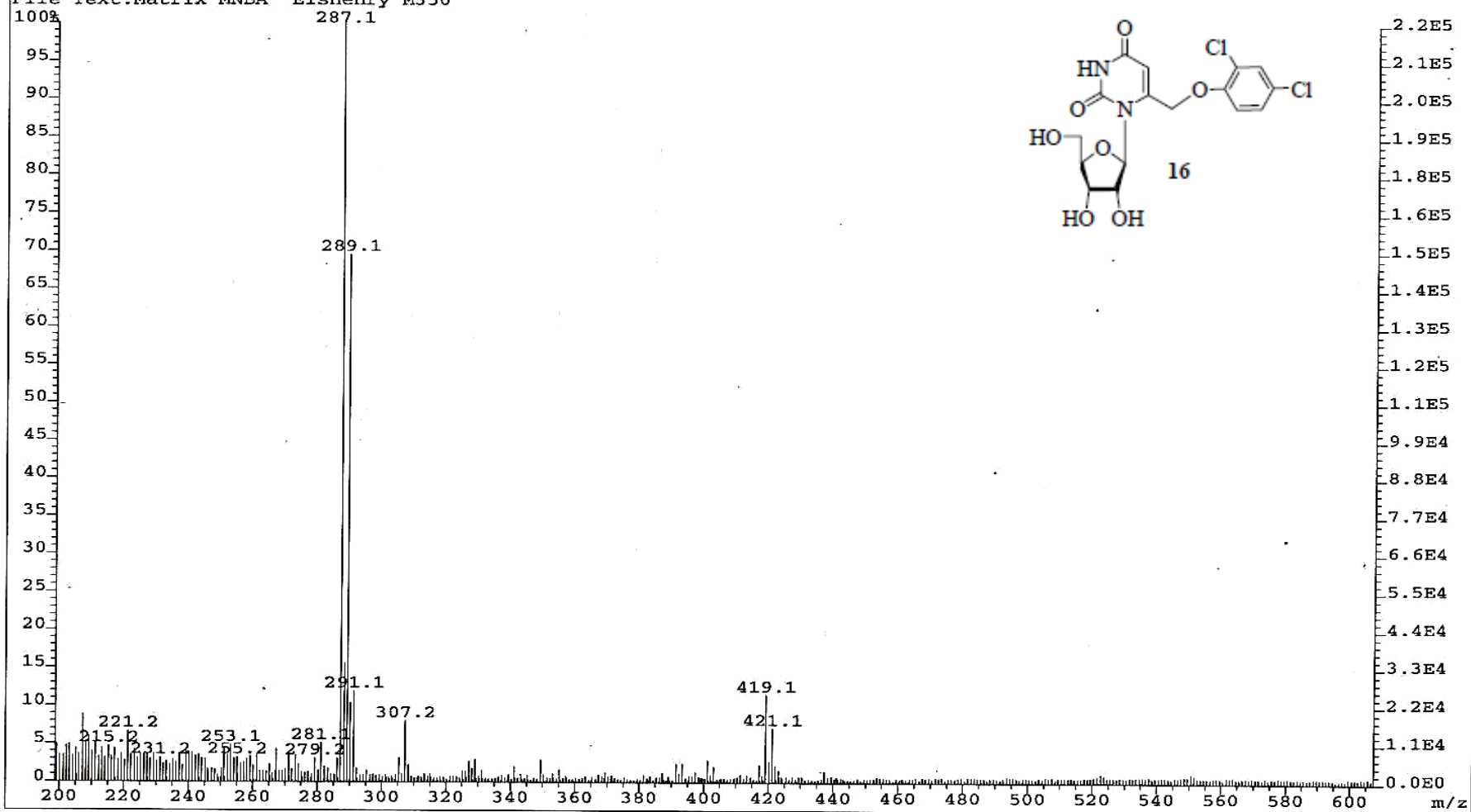
F2 - Processing parameters

SI 32768
SF 100.6143589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

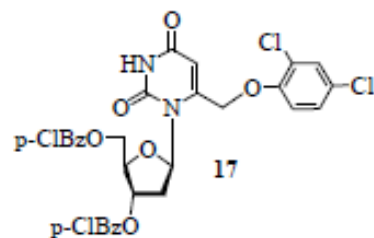
1D NMR plot parameters

CX 20.00 cm
F1P 215.000 ppm
F1 21632.09 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.75793 Hz/cm

File:M350 Ident:2_35 Win 500PPM Acq: 9-OCT-2007 15:18:21 +0:40 Cal:PG8107D
70S FAB+ Magnet BpM:154 BpI:257775 TIC:4608086 Flags:HALL
File Text:Matrix MNBA Elskehry M350



ELSHEHERY M27b
PROTON DMSO x guest 22



Current AMX400 Data

DU /x
NAME 20070703
EXPNO 220
PROCNO 1

F2 - Acquisition Parameters

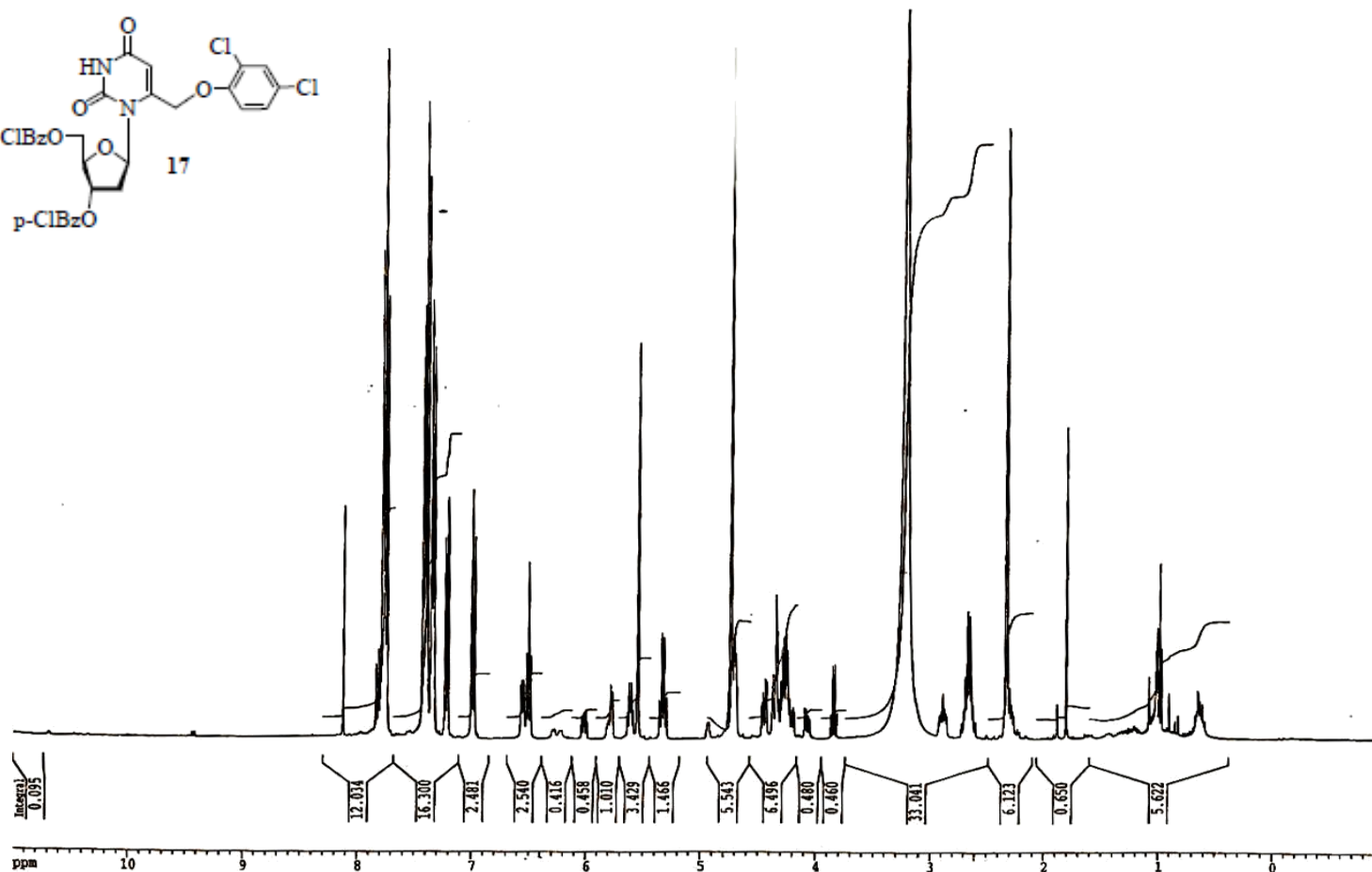
Date_ 20070703
Time 23.05
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8333.373 Hz
FIDRES 0.127157 Hz
AQ 3.9322100 sec
RG 256
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.00000000 sec
P1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters

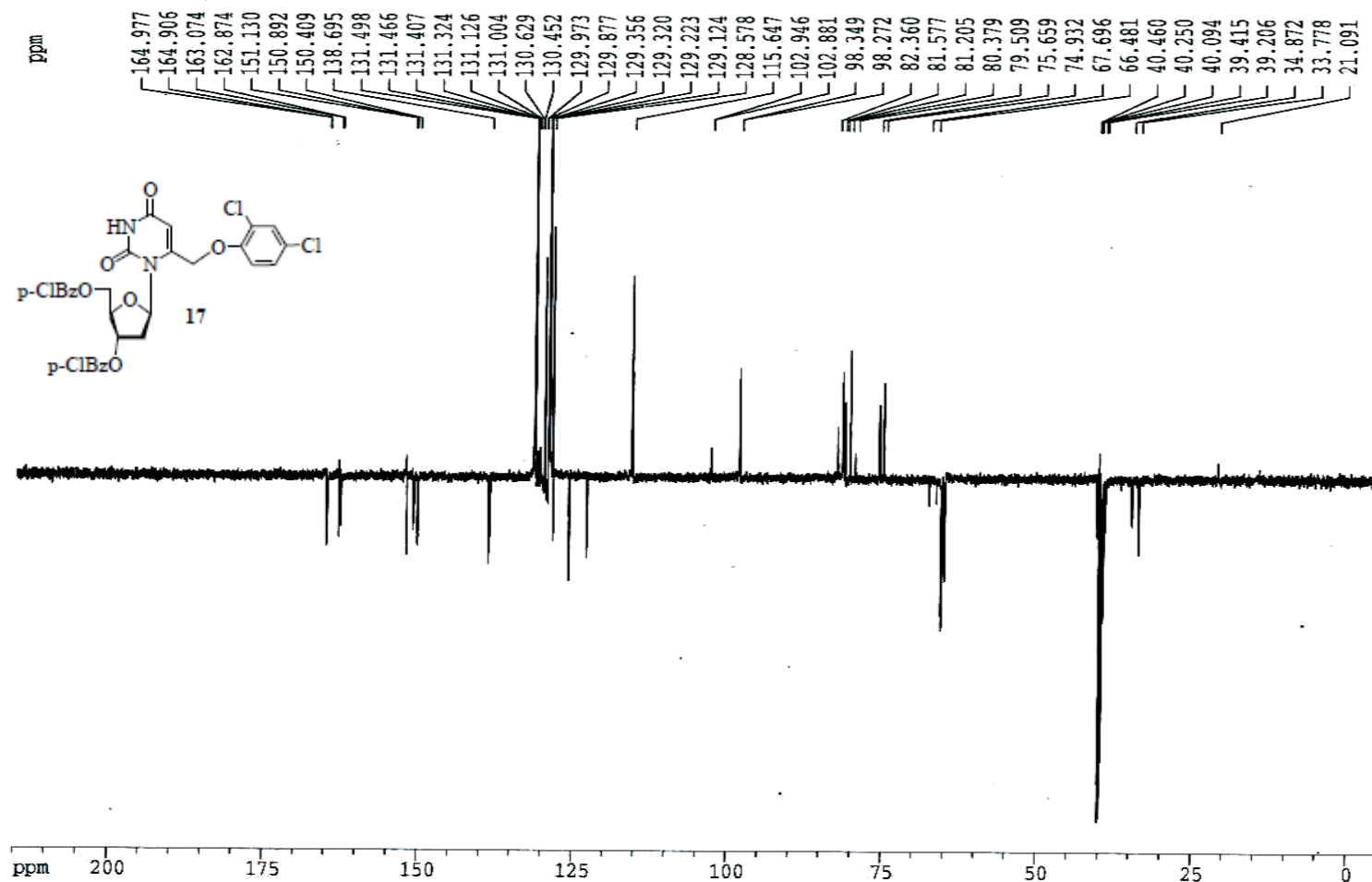
SI 32768
SF 400.1363549 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters

CX 30.00 cm
F1P 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
PPMCM 0.40000 ppm/cm
HZCM 160.05453 Hz/cm



El-Shehry M27b
PENDANT DMSO x guest 5



Current AMX400 Data

DU /x
NAME 20070709
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters

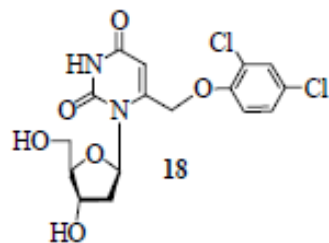
Date_ 20070709
Time 17.32
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG pendant.amx
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 25000.119 Hz
FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNOC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
S2 26 dB
SFO1 100.6245885 MHz
NUCLEUS 13C
CEDPRG waltz16
P31 90.00 usec
D2 0.00357143 sec

F2 - Processing parameters

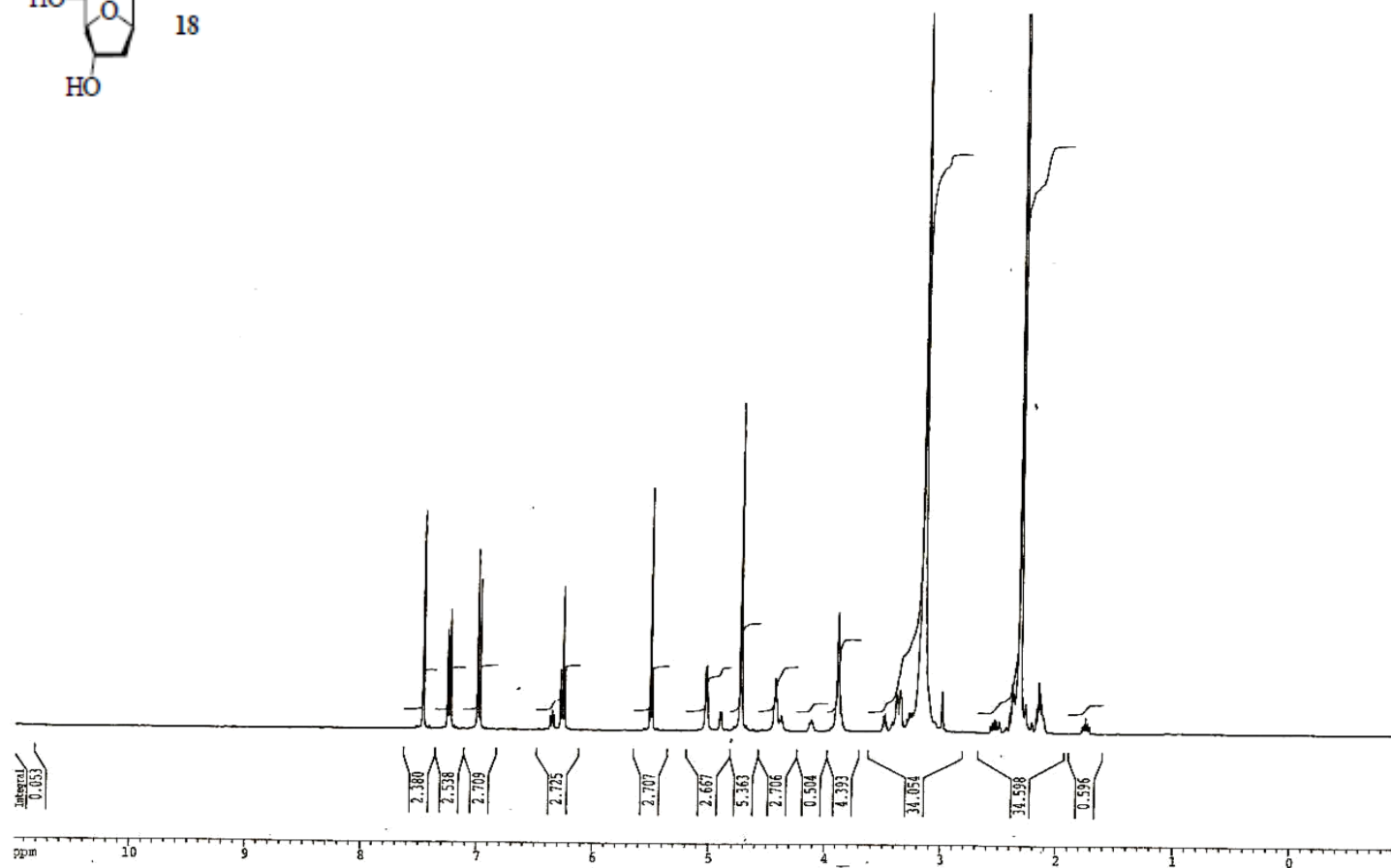
SI 32768
SF 100.6143589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters

CX 20.00 cm
F1P 215.000 ppm
F1 21632.09 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.75793 Hz/cm



El Shehry, M71
PROTON DMSO x guest 28



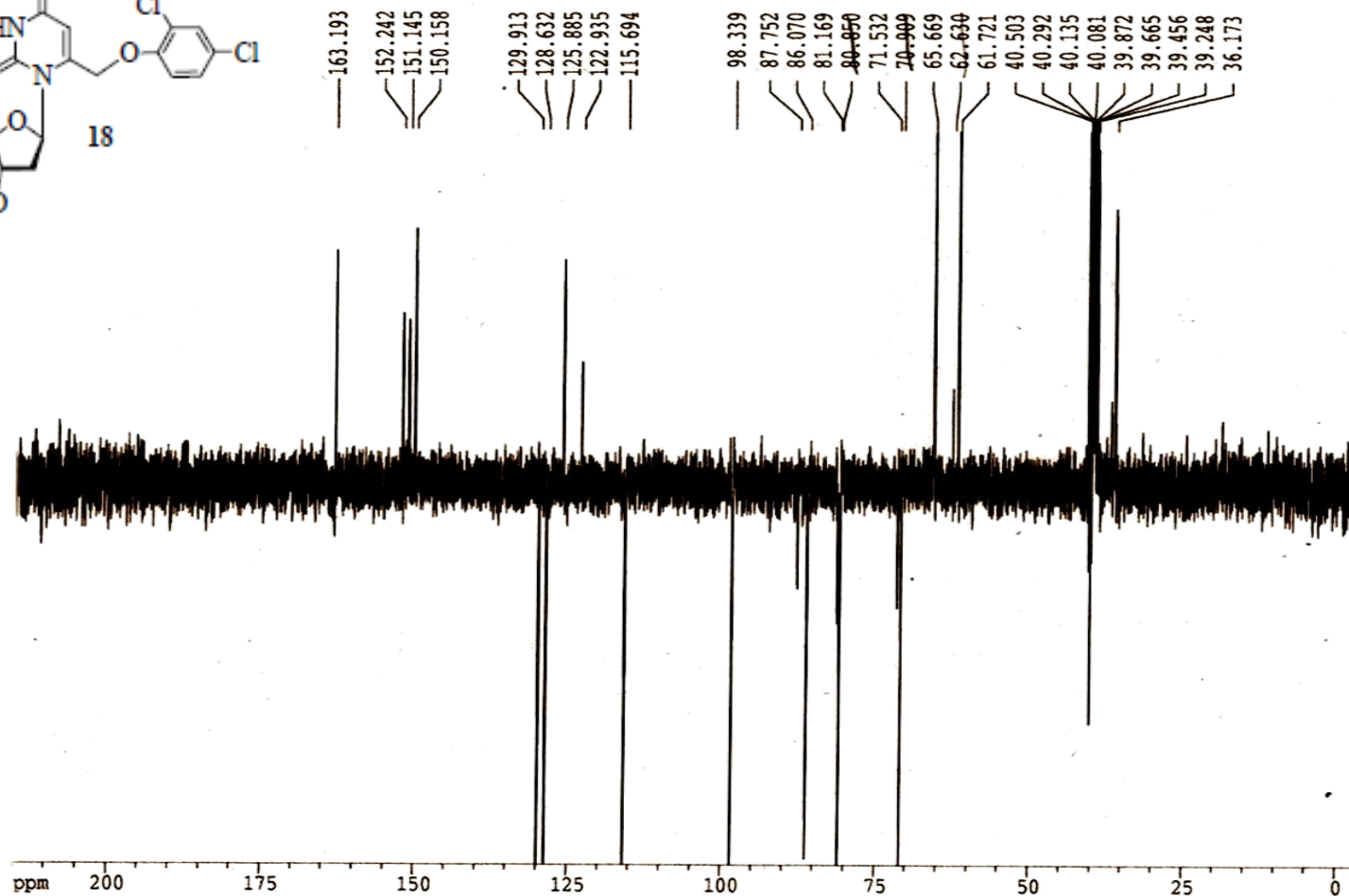
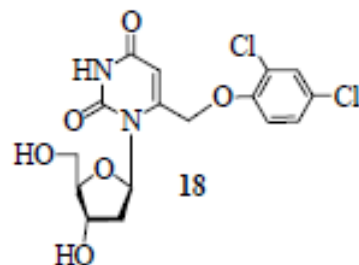
Current AMX400 Data
DU /x
NAME 20071004
EXPNO 280
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071005
Time 6.02
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8333.373 Hz
FIDRES 0.127157 Hz
AQ 3.9322100 sec
RG 512
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.00000000 sec
P1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 32768
SF 400.1363574 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
PPMCM 0.40000 ppm/cm
HZCM 160.05453 Hz/cm

El-shehry M71
PENDANT DMSO x guest 7



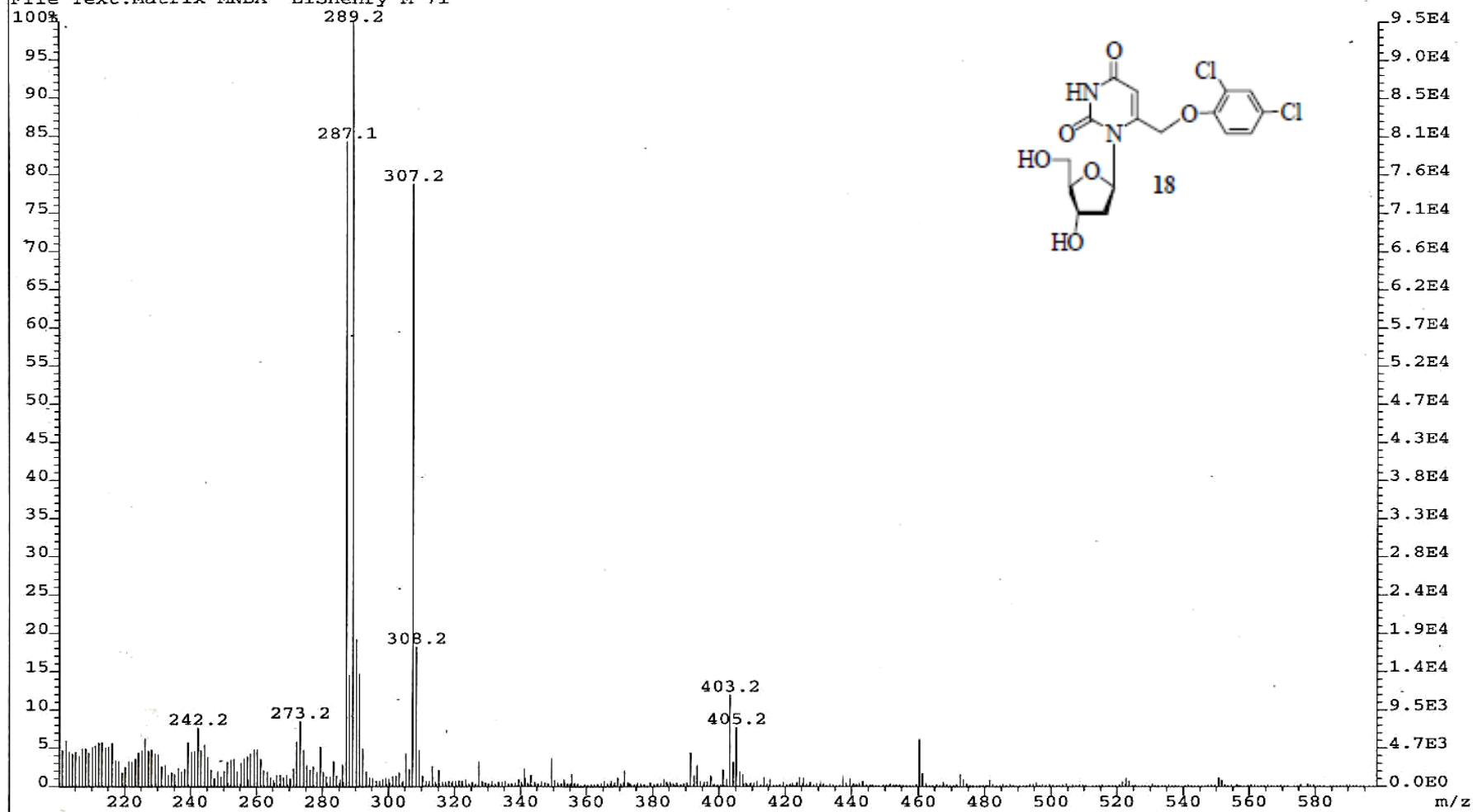
Current AMX400 Data
DU /x
NAME 20071005
EXPNO 70
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071005
Time 15.19
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG pendant.amx
TD 65536
SOLVENT DMSO
NS 800
DS 4
SWH 25000.119 Hz
FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECMUC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
S2 26 dB
SFO1 100.6245885 MHz
NUCLEUS 13C
CPDPRG waltz16
P31 90.00 usec
D2 0.00357143 sec

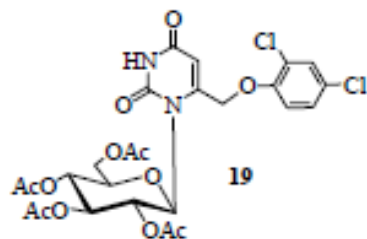
F2 - Processing parameters
SI 32768
SF 100.6143589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 215.000 ppm
F1 21632.09 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.00000 ppm/
HZCM 1106.75793 Hz/cm

File:M71 Ident:3_22 Win 500PPM Acq: 4-OCT-2007 14:26:09 +0:29 Cal:PG2107D
70S FAB+ Magnet BpM:154 BpI:502074 TIC:3269956 Flags:HALL
File Text:Matrix MNBA ElShehry M 71



El Shehry, M70
PROTON DMSO x guest 27

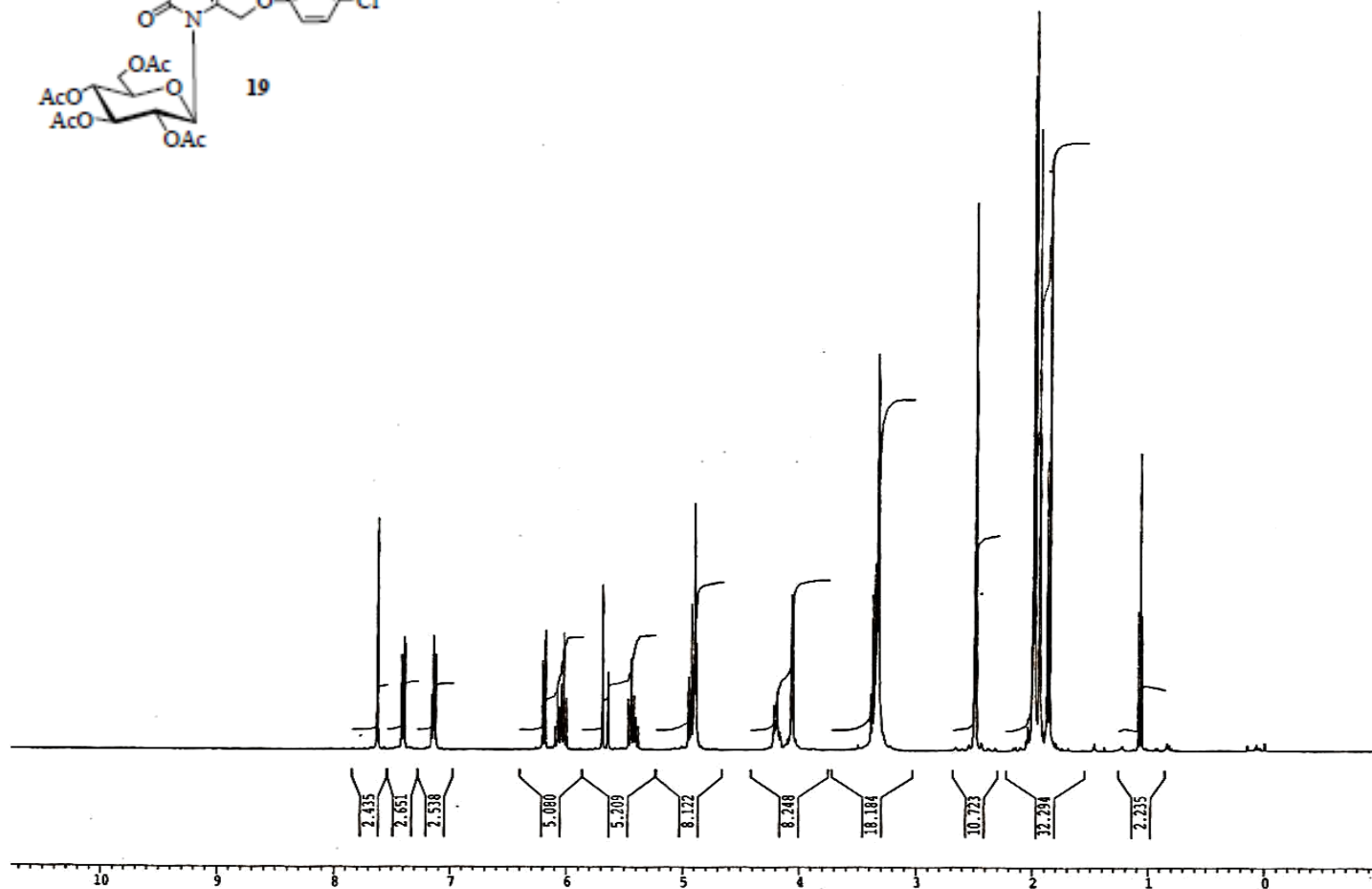


Current AMX400 Data
DU /x
NAME 20071004
EXPNO 270
PROCNO 1

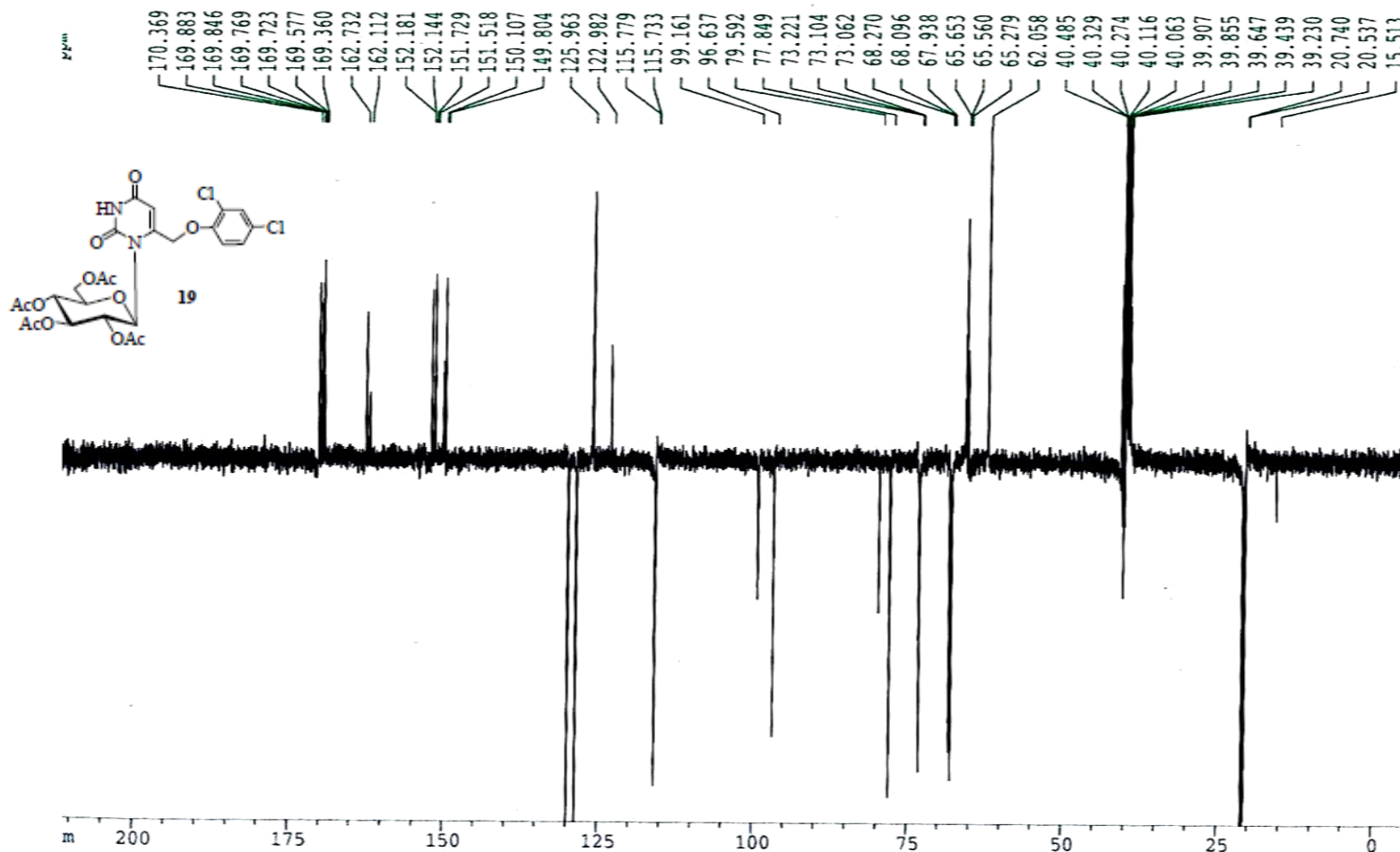
F2 - Acquisition Parameters
Date_ 20071005
Time 5.51
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8333.373 Hz
FIDRES 0.127157 Hz
AQ 3.9322100 sec
RG 256
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.0000000 sec
P1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 32768
SF 400.1362915 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
PPMCM 0.40000 ppm/cm
HZCM 160.05452 Hz/cm



El-shehry M70
PENDANT DMSO x guest 8



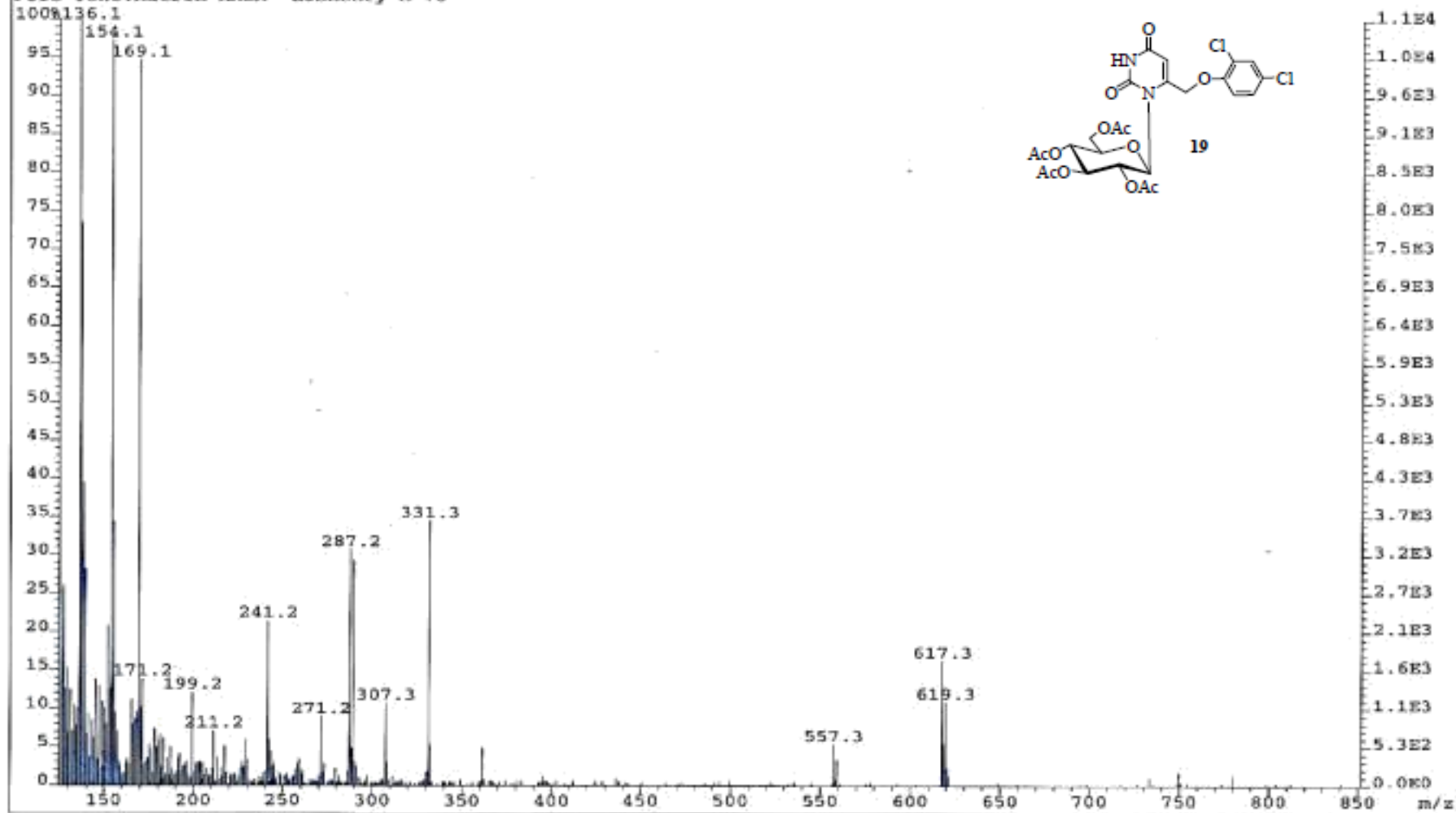
Current AMX400 Data
DU /x
NAME 20071005
EXFNO 80
PROCNO 1

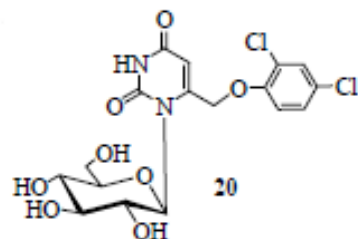
F2 - Acquisition Parameters
Date_ 20071005
Time 16.06
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG pendant.amx
TD 65536
SOLVENT DMSO
NS 800
DS 4
SWH 25000.119 Hz
FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 29.57 usec
TE 300.0 K
P1 5.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNUC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
S2 26 dB
SFO1 100.6245885 MHz
NUCLEUS 13C
CFDPRG waltz16
P31 90.00 usec
D2 0.00357143 sec

F2 - Processing parameters
SI 32768
SF 100.6143589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

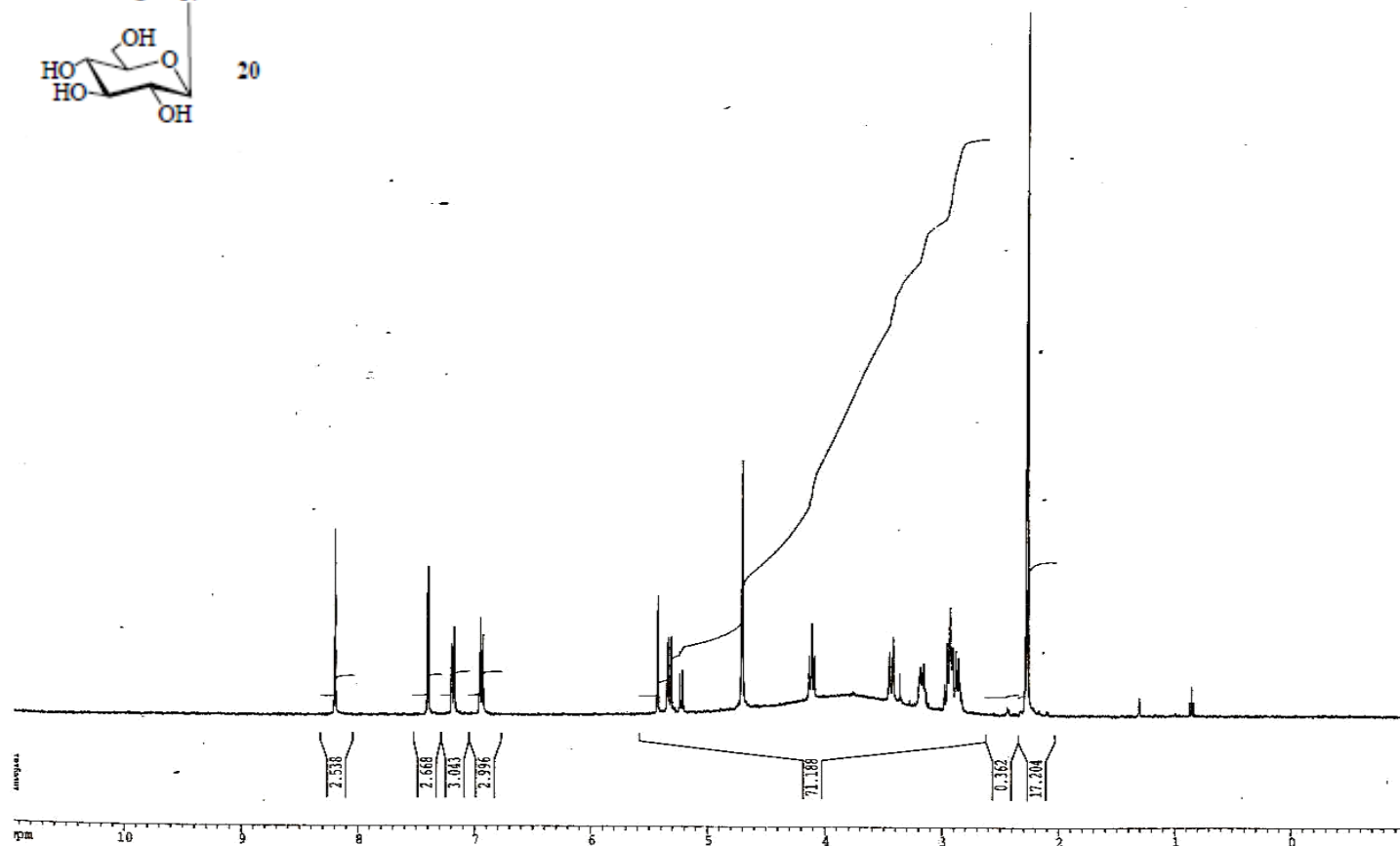
1D NMR plot parameters
CX 20.00 cm
F1P 215.000 ppm
F1 21632.09 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.75793 Hz/cm

File:M70 Ident:1_11 Win 500PPM Acq: 4-OCT-2007 10:28:01 +0:14 Cal:PG2107D
70S FAB+ Magnet BpM:136 BpI:10670 TIC:147750 Flags:NULL
File Text:Matrix MNBA ElShehry M 70
100%136.1





El-shehry N73
PROTON DMSO x guest 18



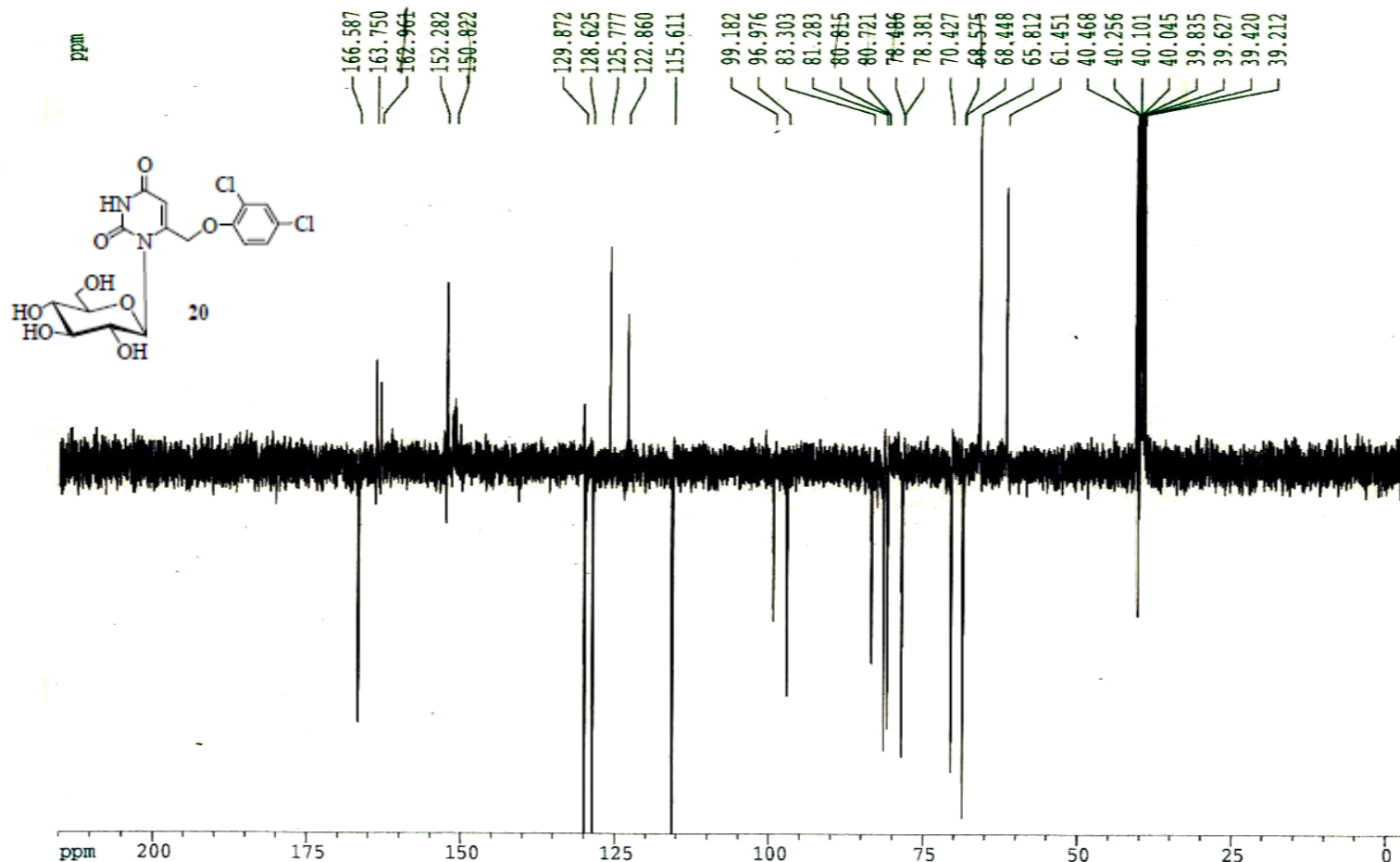
Current AMX400 Data
DU /x
NAME 20071102
EXPNO 180
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071102
Time 17.15
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8333.373 Hz
FIDRES 0.127157 Hz
AQ 3.9322100 sec
RG 512
DW 60.000 usec
DE 85.71 usec
TE 300.0 K
HL1 1 dB
D1 1.60060000 sec
P1 12.50 usec
SFO1 400.1387237 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 32768
SF 400.1363785 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 30.00 cm
F1P 11.000 ppm
F1 4401.50 Hz
F2P -1.000 ppm
F2 -400.14 Hz
PPMCM 0.40000 ppm/cm
HZCM 160.05455 Hz/cm

el-shehry n 73
PENDANT DMSO x guest 26



Current AMX400 Data
DU /x
NAME 20071105
EXPNO 260
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071105
Time 21.03
INSTRUM spect
PROBHD 5 mm Dual 13
PULPROG pendant.amx
TD 65536
SOLVENT DMSO
NS 800
DS 4
SWH 25000.119 Hz
FIDRES 0.381472 Hz
AQ 1.3107700 sec
RG 32768
DW 20.000 usec
DE 28.57 usec
TE 300.0 K
P1 6.50 usec
P3 10.60 usec
CNST2 145.0000000
HL1 1 dB
D1 1.50000000 sec
S1 1 dB
SFO2 400.1379006 MHz
DECNOC 1H
D4 0.0017241 sec
P4 21.2 usec
P2 13.0 usec
D15 0.0043103 sec
D13 0.0000040 sec
S2 26 dB
SFO1 100.6245885 MHz
NUCLEUS 13C
CPDPRG waltz16
P31 90.00 usec
D2 3.00357143 sec

F2 - Processing parameters
SI 32768
SF 100.6143589 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
F1P 215.900 ppm
F1 21632.09 Hz
F2P -5.000 ppm
F2 -503.07 Hz
PPMCM 11.00000 ppm/cm
HZCM 1106.75793 Hz/cm

File:N74B Ident:2_29 Win 500PPM Acq: 7-NOV-2007 10:29:44 +0:34 Cal:PG5117E
70S FAB+ Magnet BpM:136 BpI:118587 TIC:2375537 Flags:HALL
File Text:Matrix MNBA Elshehry N74B
100%169.1

