

ELECTRONIC SUPPORTING INFORMATION (ESI)

Design and synthesis of sugar-triazole based uracil appended sugar-imine derivatives – An application in DNA binding studies

Arasappan Hemamalini^a, Ettayapuram Ramaprasad Azhagiya Singham^b, Sathish kumar Mudedla^b, Venkatesan Subramanian^b, Thangamuthu Mohan Das^{a,c,*}

^aDepartment of Organic Chemistry, University of Madras, Guindy Campus, Chennai – 600 025, INDIA.

^bChemical Laboratory, Central Leather Research Institute (CSIR) Adyar, Chennai- 600 020, INDIA

^cDepartment of Chemistry, School of Basic and Applied Sciences, Central University of Tamil Nadu, Thiruvarur -610 004; Ph. No. +919489054278; Fax 04366 – 225312; E-mail: tmohandas@cutn.ac.in

Table 1 Spectral data and optimization of reaction condition of sugar-triazole derivatives, **6-9**

Compound No.	R	Time (h)	Yield (%)	NMR data				
				δ Ano-H /ppm	δ Ald-H /ppm	δ Trz-H /ppm	δ Trz-C /ppm	Δ ($\delta_{C4}-\delta_{C5}$)
6	-H	24	85	5.91-5.88	10.48	7.92	121.5, 144.1	23
7	-OCH ₃	26	79	5.89-5.86	9.86	7.91	144.0, 121.7	22
8	-Cl	20	74	5.90-5.87	10.39	7.91	143.6, 121.6	22
9	-OH	24	83	5.91-5.88	9.98	7.88	144.4, 121.2	23

Table 2 Spectroscopic data and optimization of reaction condition of sugar-imine derivatives, **11-14**

Entry	R	Time (h)	Yield (%)	NMR data			
				δ Ano-H/ppm, J_{H1H2} Hz	δ Trz-H /ppm	δ Imin-H /ppm	δ Imin-C /ppm
11	-H	1	56	5.79, 9.0	7.27	7.61	165
12	-OCH ₃	3	58	5.58, 9.3	7.69	8.01	168
13	-Cl	3	35	5.60, ^a	7.67	7.93	167
14	-H	4	52	5.60-5.53, [*]	7.50	8.01	167

^{*}Peaks merged with saccharide proton, ^amerged with alkene proton

General procedure for the synthesis of *O*-propargylated derivative, 2-5

To the corresponding hydroxy benzaldehydes (1 mmol) in dry DMF, (5 mmol) anhydrous K_2CO_3 was added and stirred for 10 minutes. To the reaction mixture was added propargyl bromide (1.2 mmol) and stirred for 24 hours. After the completion of the reaction, work up was done using chloroform. The organic layer was evaporated and the product was purified using silica gel column chromatography.

Spectral data of 2-(prop-2-ynyloxy)-1-benzaldehyde (2):

Pale yellow solid; Mp: 64-66 °C; Yield: 0.12 g (75%); 1H NMR (300 MHz, $CDCl_3$): δ 10.49 (s, 1H, -CHO), 7.87 (d, J = 7.8 Hz, 1H, Ar-H), 7.61-7.55 (m, 1H, Ar-H), 7.14-7.07 (m, 2H, Ar-H), 4.9 (s, 2H, -OCH₂), 2.57 (t, J = 2.4 Hz, 1H, -C $\equiv$ CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 189.5, 159.8, 135.7, 128.6, 125.5, 121.7, 113.2, 77.7, 76.5, 56.4.

Spectral data of 2-methoxy-4-(prop-2-ynyloxy)-1-benzaldehyde (3):

Pale yellow solid; Mp: 86-88 °C; Yield: 0.16 g (84%); 1H NMR (300 MHz, $CDCl_3$): δ 9.88 (s, 1H, -CHO), 7.49-7.45 (m, 2H, Ar-H), 7.15 (d, J = 8.1 Hz, 1H, Ar-H), 4.87 (d, J = 2.4 Hz, 2H, -OCH₂), 3.95 (s, 3H, -OCH₃), 2.57 (t, J = 2.3 Hz, 1H, -C $\equiv$ CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 190.8, 152.2, 150.1, 131.0, 126.2, 112.7, 109.6, 77.0, 76.6, 56.6, 56.0.

Spectral data of 5-chloro-2-(prop-2-ynyloxy)-1-benzaldehyde (4):

Yellow solid; Mp: 60-62 °C; Yield: 0.14 g (74%); 1H NMR (300 MHz, $CDCl_3$): δ 10.41 (s, 1H, -CHO), 7.81 (s, 1H, Ar-H), 7.51 (d, J = 9.0 Hz, 1H, Ar-H), 7.09 (d, J = 9.0 Hz, 1H, Ar-H), 4.83 (d, J = 2.4 Hz, 2H, -OCH₂), 2.59 (t, J = 2.4 Hz, 1H, -C $\equiv$ CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 188.2, 158.1, 135.2, 128.1, 127.5, 126.5, 115.0, 77.2, 76.9, 56.8.

Spectral data of 3-(prop-2-ynyloxy)-1-benzaldehyde (5):

Yield 0.13 g, (81%); 1H NMR (300 MHz, $CDCl_3$): δ 9.97 (s, 1H, -CHO), 7.52-7.44 (m, 3H, Ar-H), 7.28-7.23 (m, 1H, Ar-H), 4.76 (d, J = 2.4 Hz, 2H, -OCH₂), 2.57 (t, J = 2.4 Hz, 1H, -C $\equiv$ CH); ^{13}C NMR (75 MHz, $CDCl_3$): δ 192.0, 158.1, 137.8, 130.2, 124.1, 122.1, 113.6, 77.9, 76.2, 56.0.

1H NMR, ^{13}C NMR, DEPT-135, Mass spectrum are available in the ESI

Contents

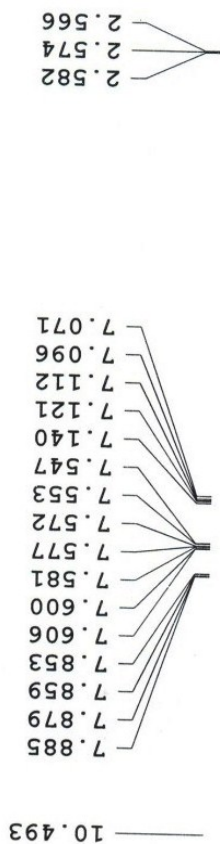
- Figure 1: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 2.
- Figure 2: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 2.
- Figure 3: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 3.
- Figure 4: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 3.
- Figure 5: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 4.
- Figure 6: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 4.
- Figure 7: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 5.
- Figure 8: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 5.
- Figure 9: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 6.
- Figure 10: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 6.
- Figure 11: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 7.
- Figure 12: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 7.
- Figure 13: DEPT-135 spectrum (75 MHz, CDCl_3) of compound 7.
- Figure 14: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 8.
- Figure 15: ^1H NMR expansion spectrum (300 MHz, CDCl_3) of compound 8.
- Figure 16: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 8.
- Figure 17: ^1H - ^{13}C COSY spectrum (CDCl_3) of compound 8.
- Figure 18: ^1H - ^{13}C COSY spectrum expansion (CDCl_3) of compound 8.
- Figure 19: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 9.
- Figure 20: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 9.
- Figure 21: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 11.
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- Figure 25 Mass spectrum of compound, 12.
- Figure 26: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 13.

Figure 27: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 13.

Figure 28: ^1H NMR spectrum (300 MHz, CDCl_3) of compound 14.

Figure 29: ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound 14.

Figure 30: Hydrogen bonding interaction of compounds (a) 6, (b) 11, (c) 7 (d) 12, (e) 8 (f) 13.



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 TD 65536
 SOLVENT CDC13
 NS 17
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 322.5
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

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 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
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 WDW EM
 SSB 0
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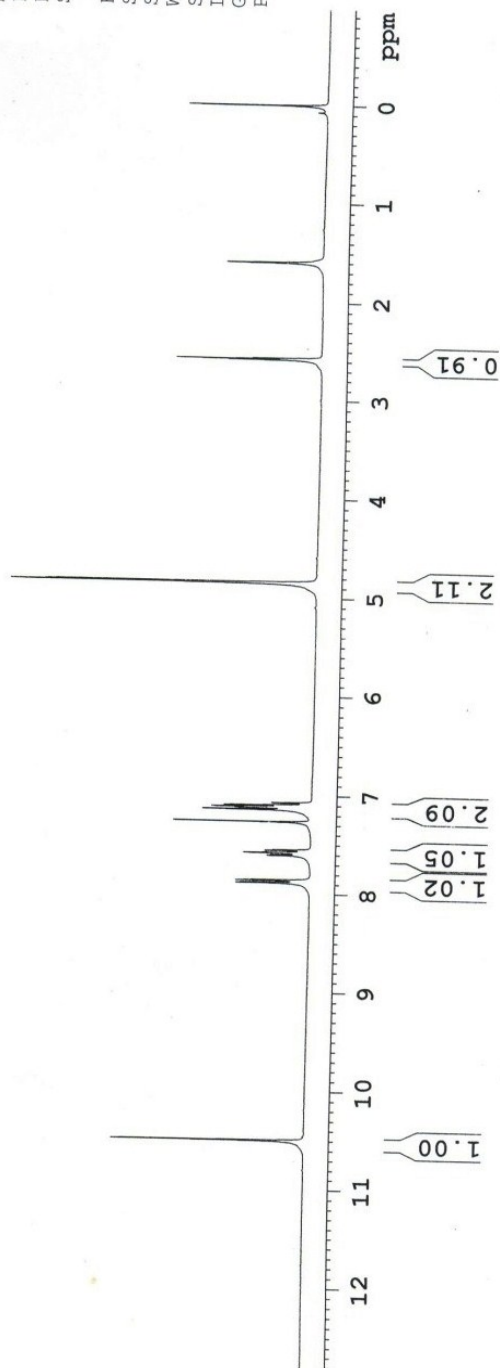
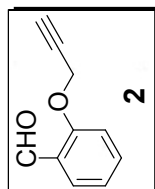
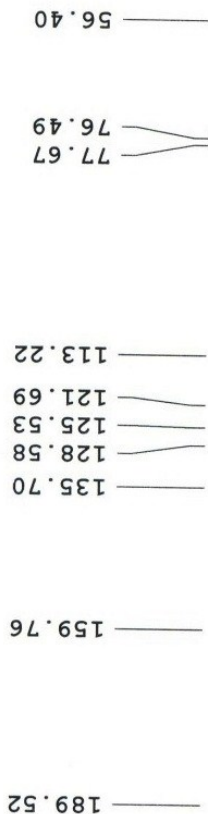


Figure 1 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 2.



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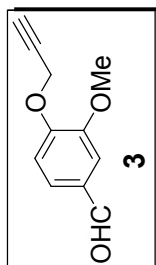
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 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 213
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 1448.2
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
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 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 2 ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound, 2



Current Data Parameters
NAME TMDH-333
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130327
Time 16.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
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TE 300.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
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PL1 0.00 dB
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F2 - Processing parameters
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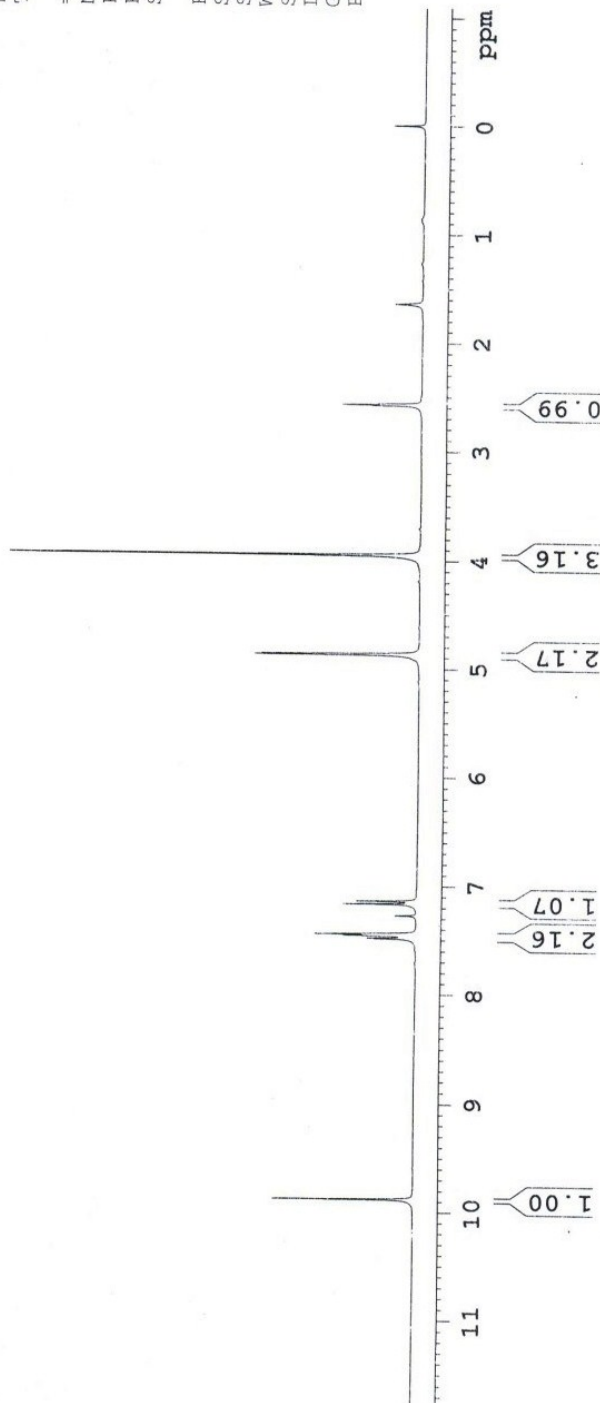


Figure 3 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 3.



Current Data Parameters
 NAME TMDH-333
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130327
 Time_ 16.58
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 417
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 2298.8
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

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 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

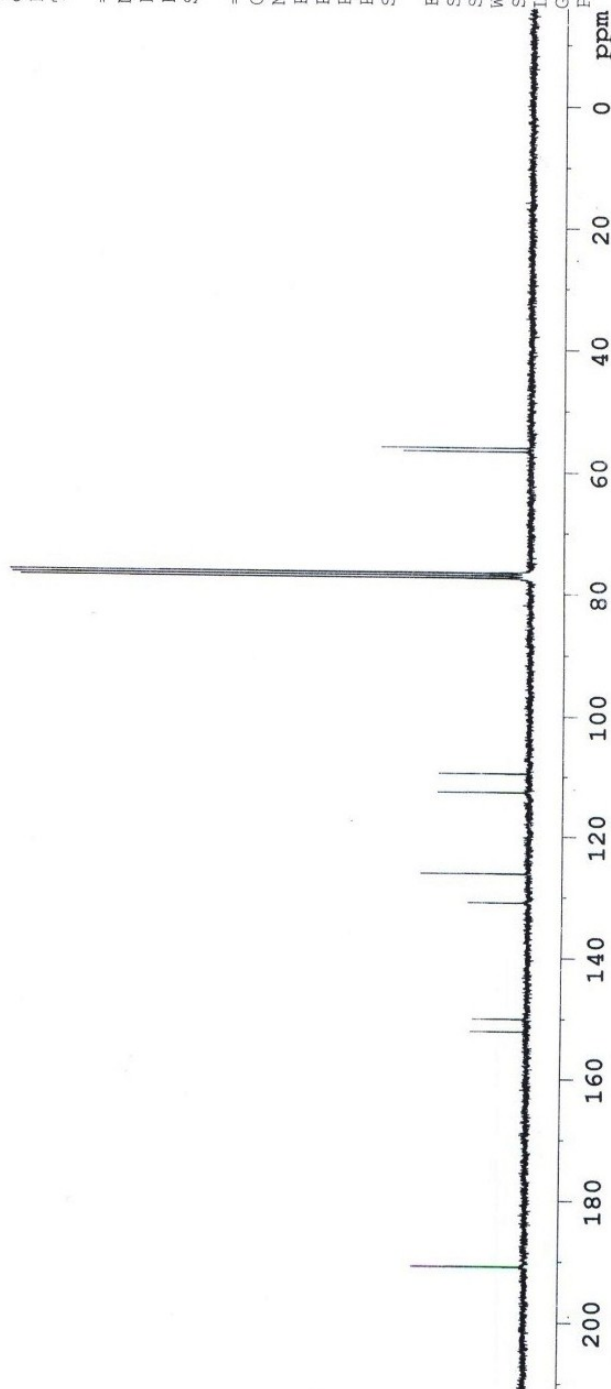
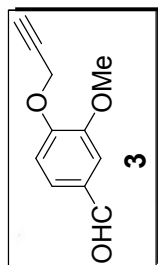
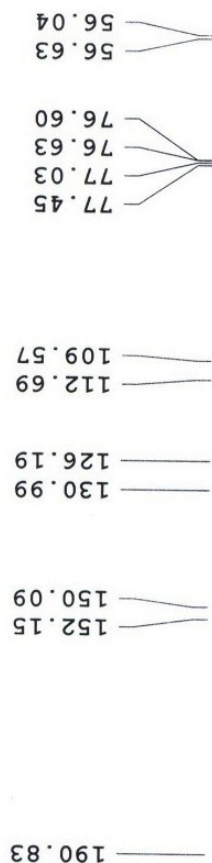
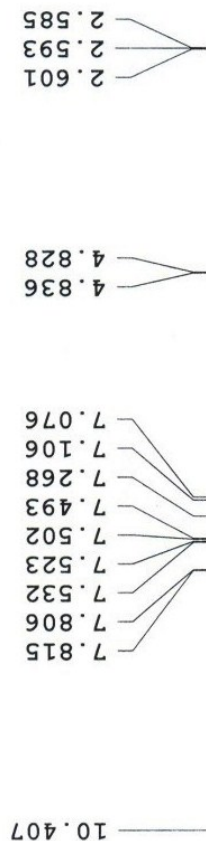


Figure 4 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 3



Current Data Parameters
NAME TMDH-321
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130216
Time 10.32
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

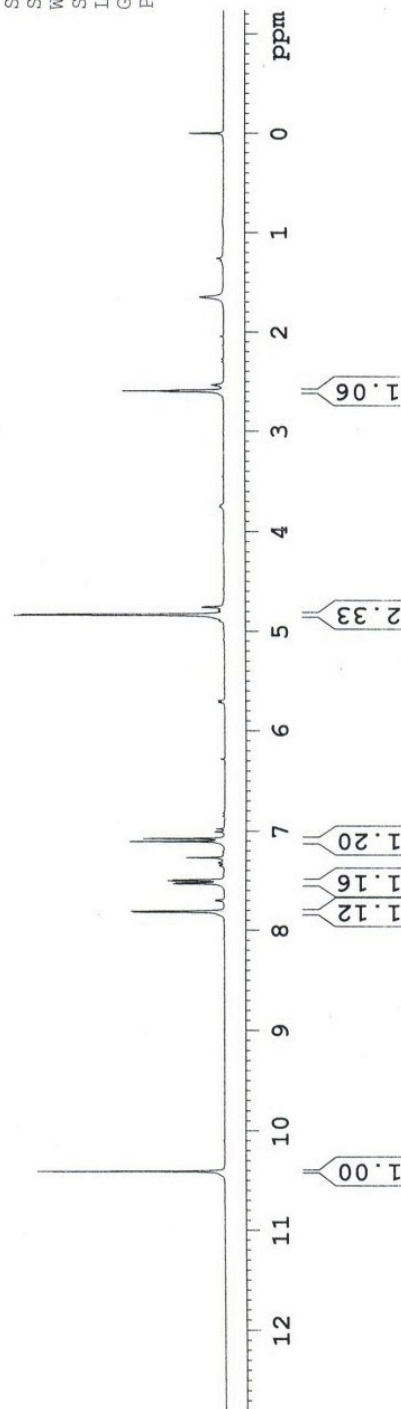


Figure 5 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 4.



Current Data Parameters
 NAME TMDH-321
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130216
 Time 14.05
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 724.1
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

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

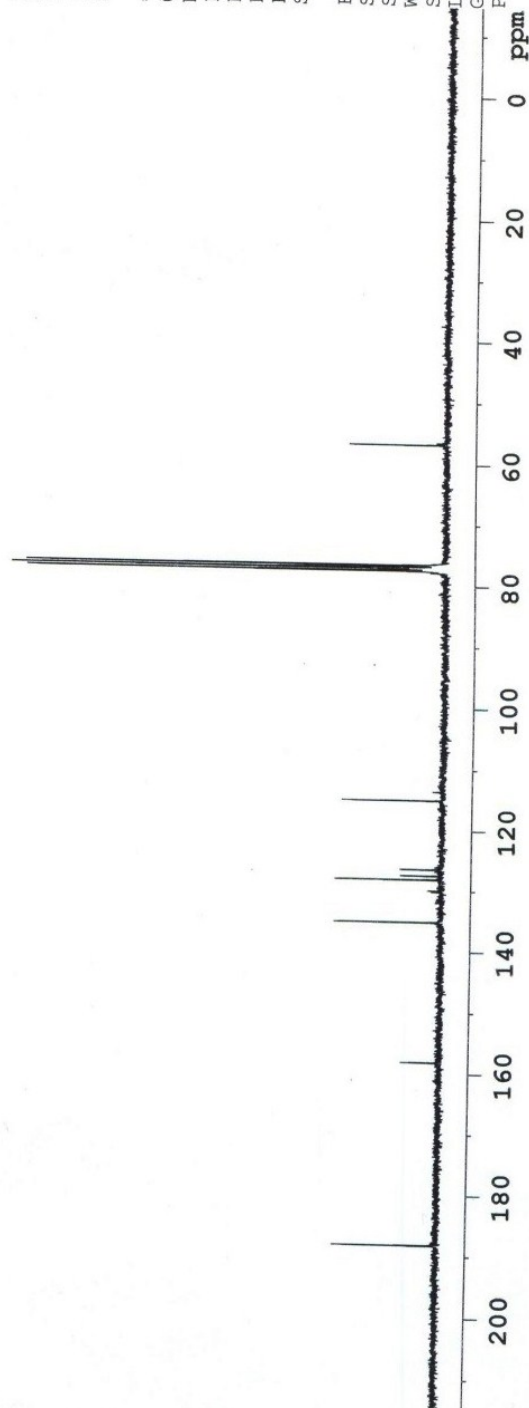
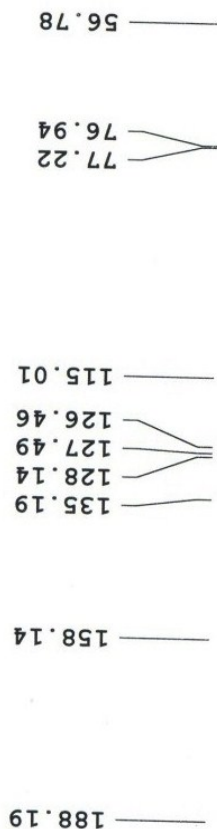


Figure 6 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 4.



Current Data Parameters
 NAME TMDH-339
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130423
 Time_ 19.23
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 57
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299999 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

2.578
2.570
2.562

4.759
4.751

7.524
7.500
7.494
7.491
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7.234
7.228

9.973

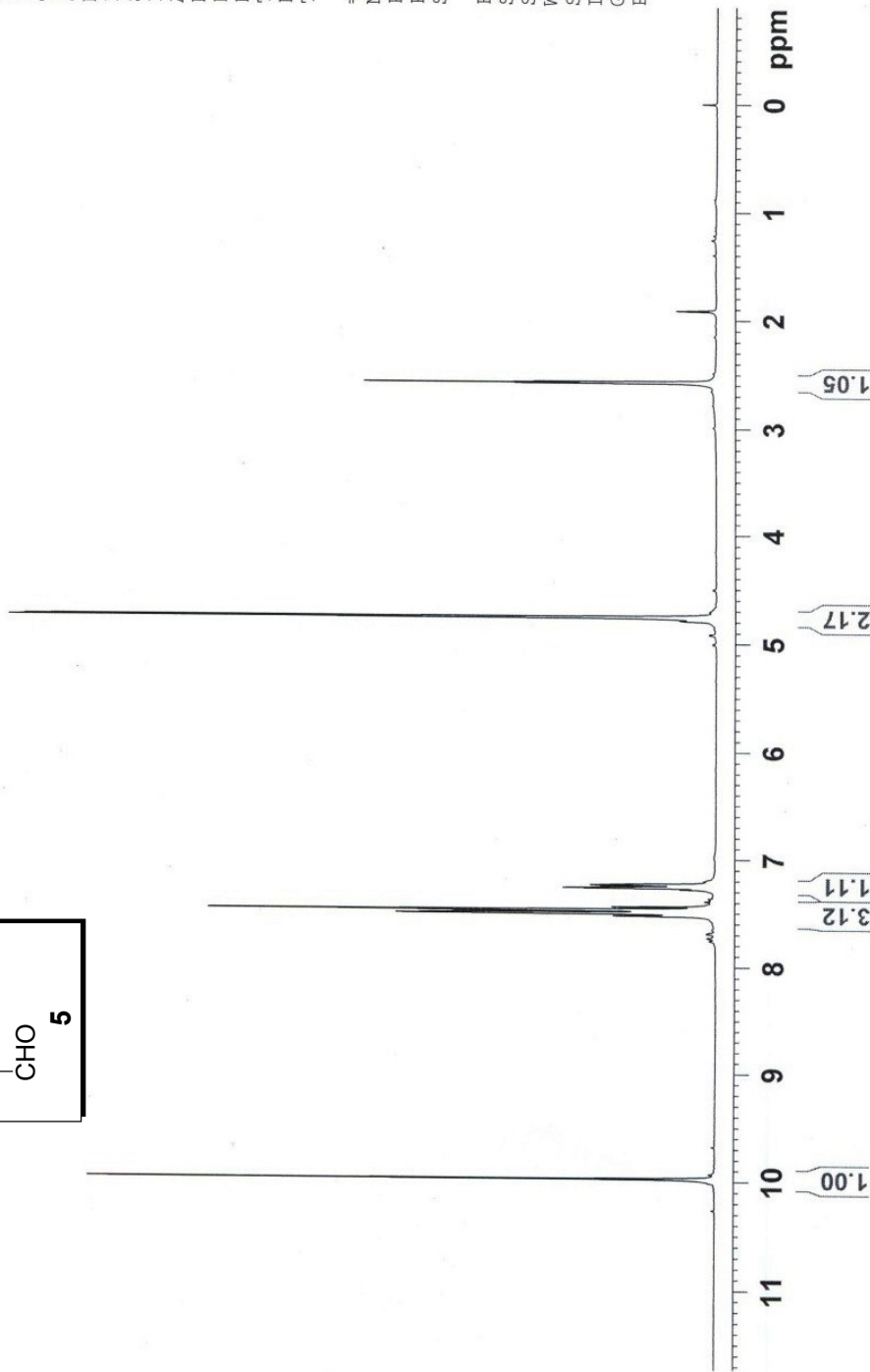
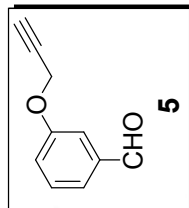
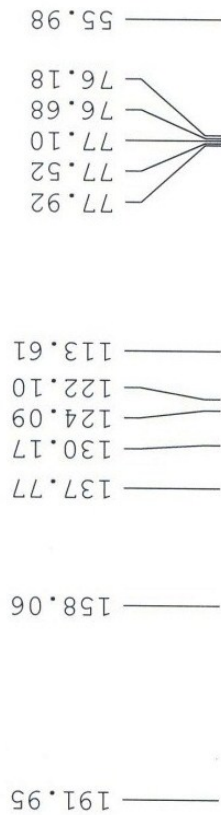


Figure 7 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 5.



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 PROCNO 1

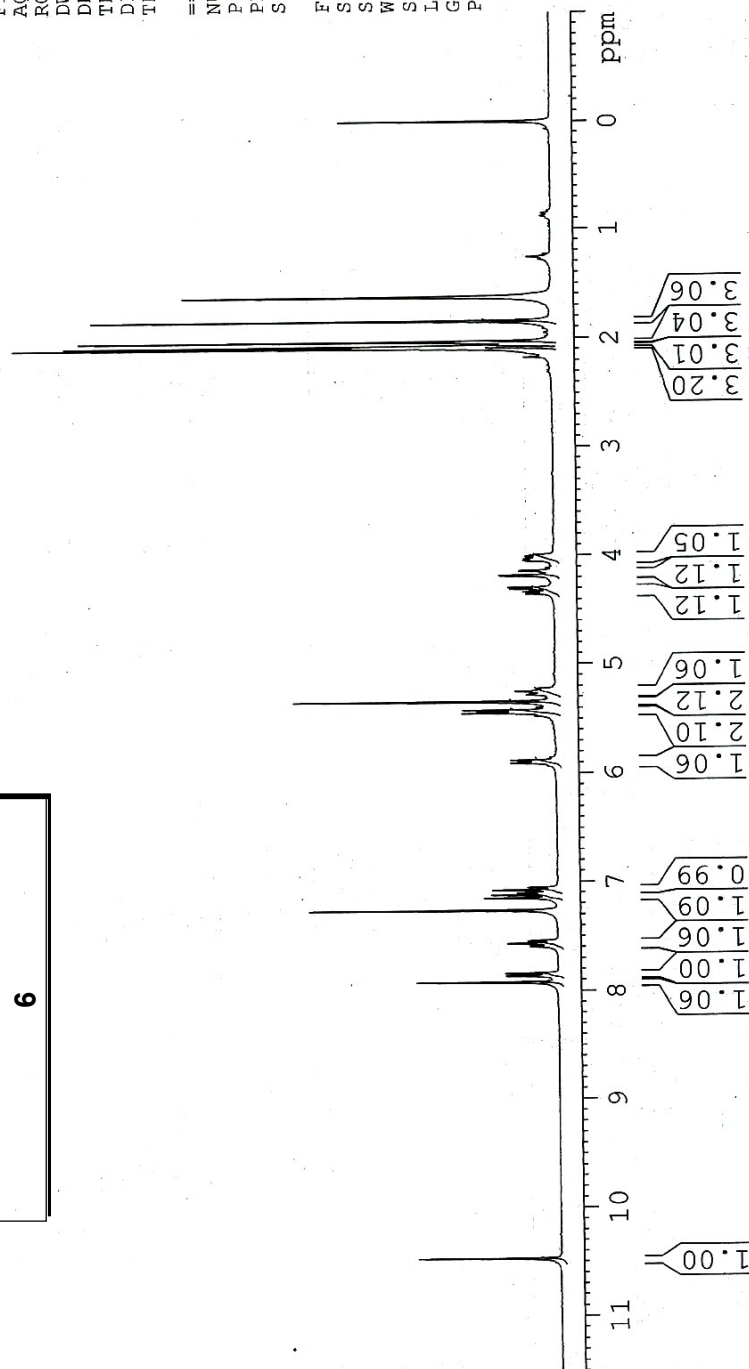
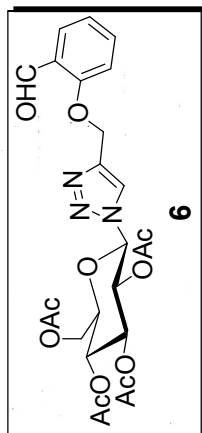
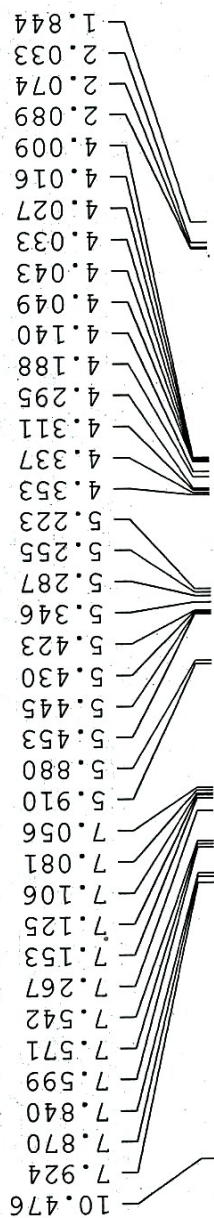
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 TD 65536
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 NS 34
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 1024
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SF01 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SF02 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 8 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 5.



Current Data Parameters	
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EXPNO	1
PROCNO	1

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Time_ 19.57

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PULPROG			zg30
TD			65536
SOLVENT			CDCl3

NS DS 44 2

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FTDRES	0.094190

AQ 5.3084660
PG 322 5

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DW	6.00
DE	

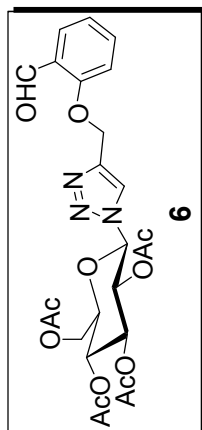
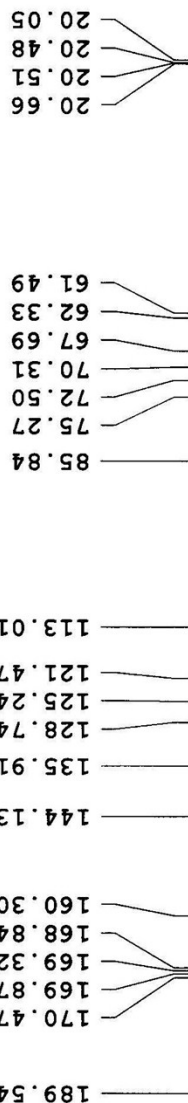
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F2 - Processing parameters	
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SF	300.1300047 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

Figure 9 ^1H NMR spectrum (300 MHz, CDCl_3) of compound, 6.



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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TD 65536
SOLVENT CDCl3
NS 973
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 574.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

==== CHANNEL f2 =====
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NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 10 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 6



Current Data Parameters
 NAME TMDH-334
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 Time_ 13.53
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 322.5
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
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 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
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 SF 300.1300048 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

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5.862
5.432
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4.311
4.286
4.269
4.164
4.128
4.031
4.024
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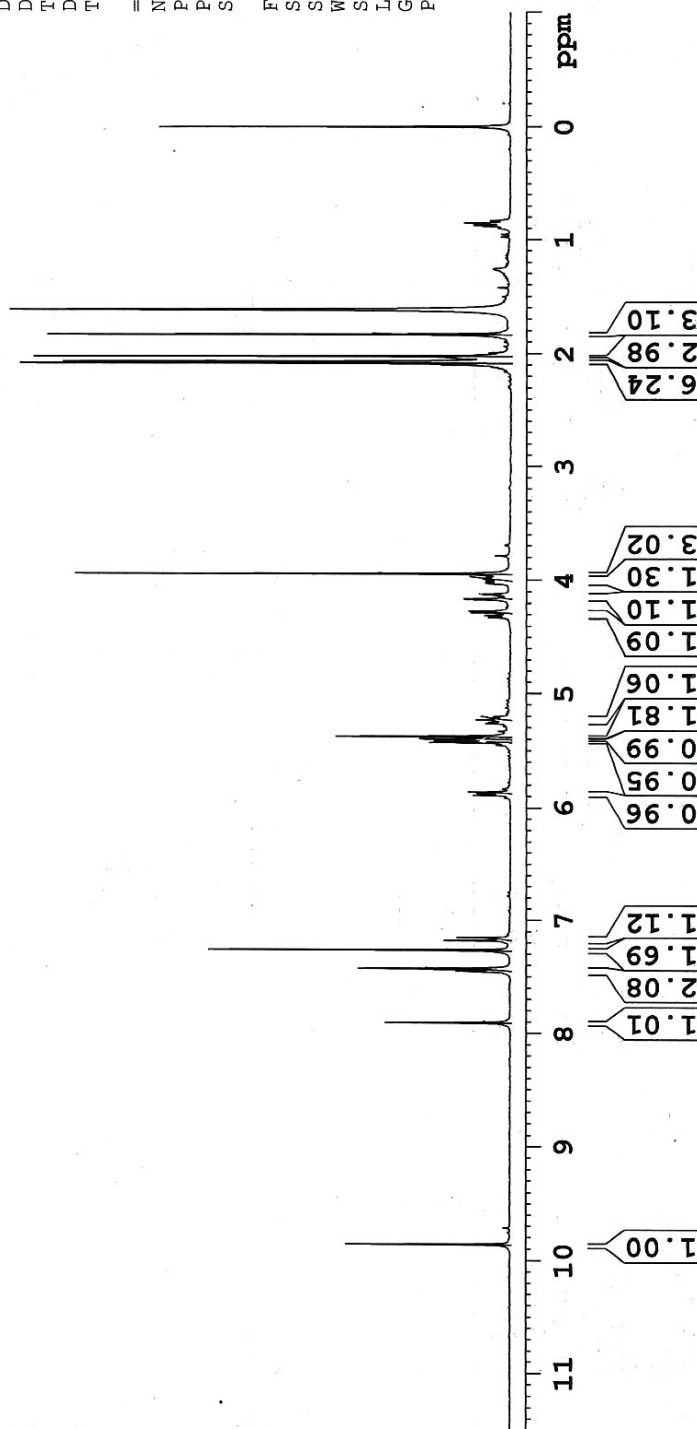
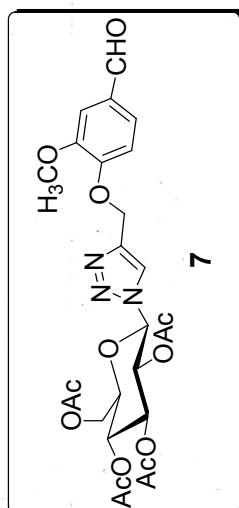


Figure 11 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 7.



Current Data Parameters
 NAME AT-55F-13
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130406
 Time_ 13.31
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 568
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 2298.8
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

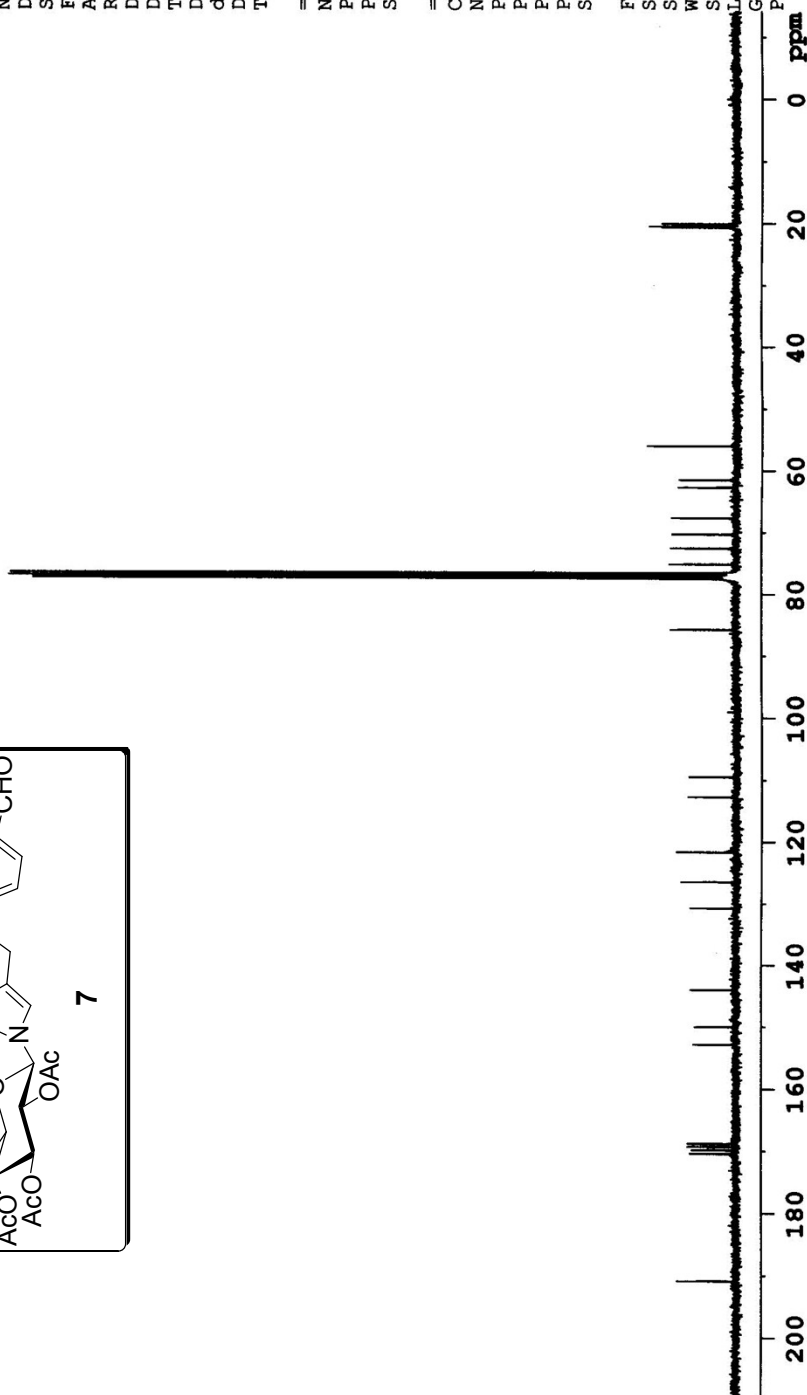
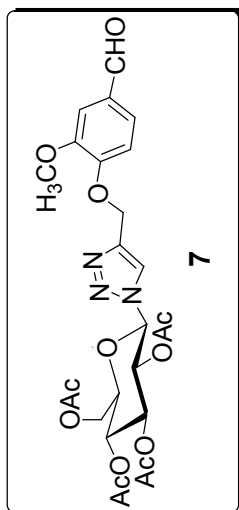
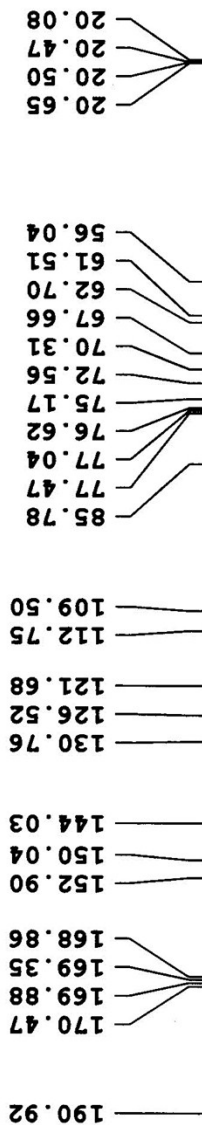


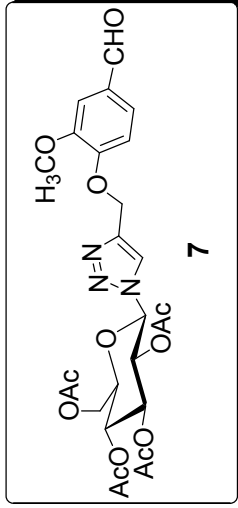
Figure 12 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 7.



Experiment Data Parameters
 Experiment: TMDH-334
 Date: 1
 Time: 1

Acquisition Parameters

File: 20130408
 Name: 23.43
 Spectrum: spect
 P1: 5 mm DUL 13C-1
 P2: dept135
 P3: 65536
 P4: CDCL3
 P5: 350
 P6: 4
 F1: 17985.611 Hz
 F2: 0.274439 Hz
 SFO: 1.8219508 sec
 AQ: 16384
 SC: 27.800 usec
 PC: 6.00 usec
 K: 300.0 K
 P7: 145.0000000
 P8: 2.000000000 sec
 P9: 0.00344828 sec
 P10: 0.00002000 sec
 P11: 0.00001184 sec
 P12: 1
 P13: 1



===== CHANNEL f1 =====
 13C
 9.30 usec
 18.60 usec
 0.00 dB
 75.4752953 MHz

===== CHANNEL f2 =====
 waltz16
 1H
 13.15 usec
 26.30 usec
 80.00 usec
 0.00 dB
 15.68 dB
 300.1312005 MHz

Processing parameters
 32768
 75.4677490 MHz
 EM
 0
 1.00 Hz
 0
 1.40

Figure 13 DEPT-135 spectrum (75 MHz, CDCl₃) of compound, 7.

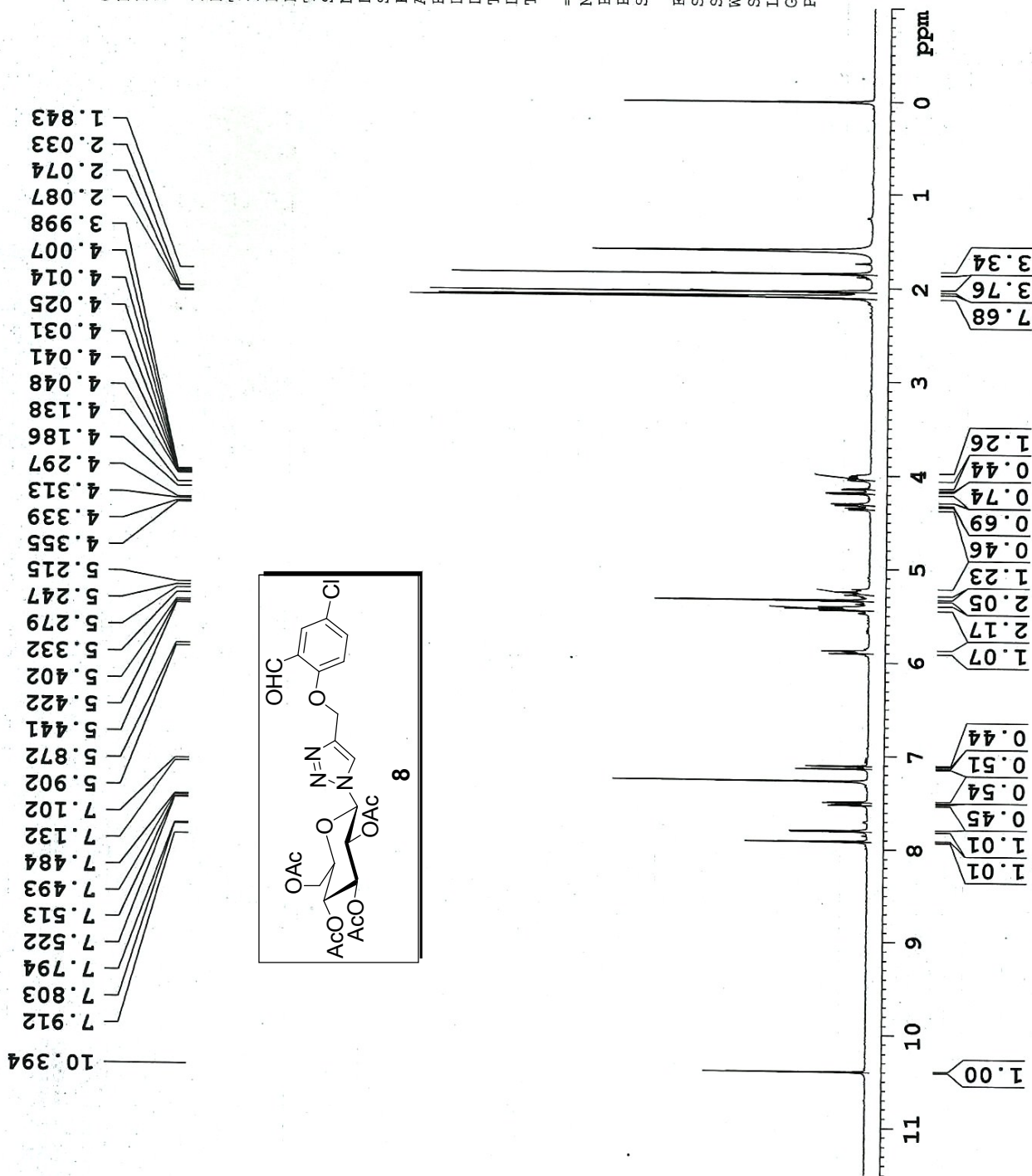


Current Data Parameters
 NAME TMDH-335
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130408
 Time_ 20.10
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 362
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 14 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 8.

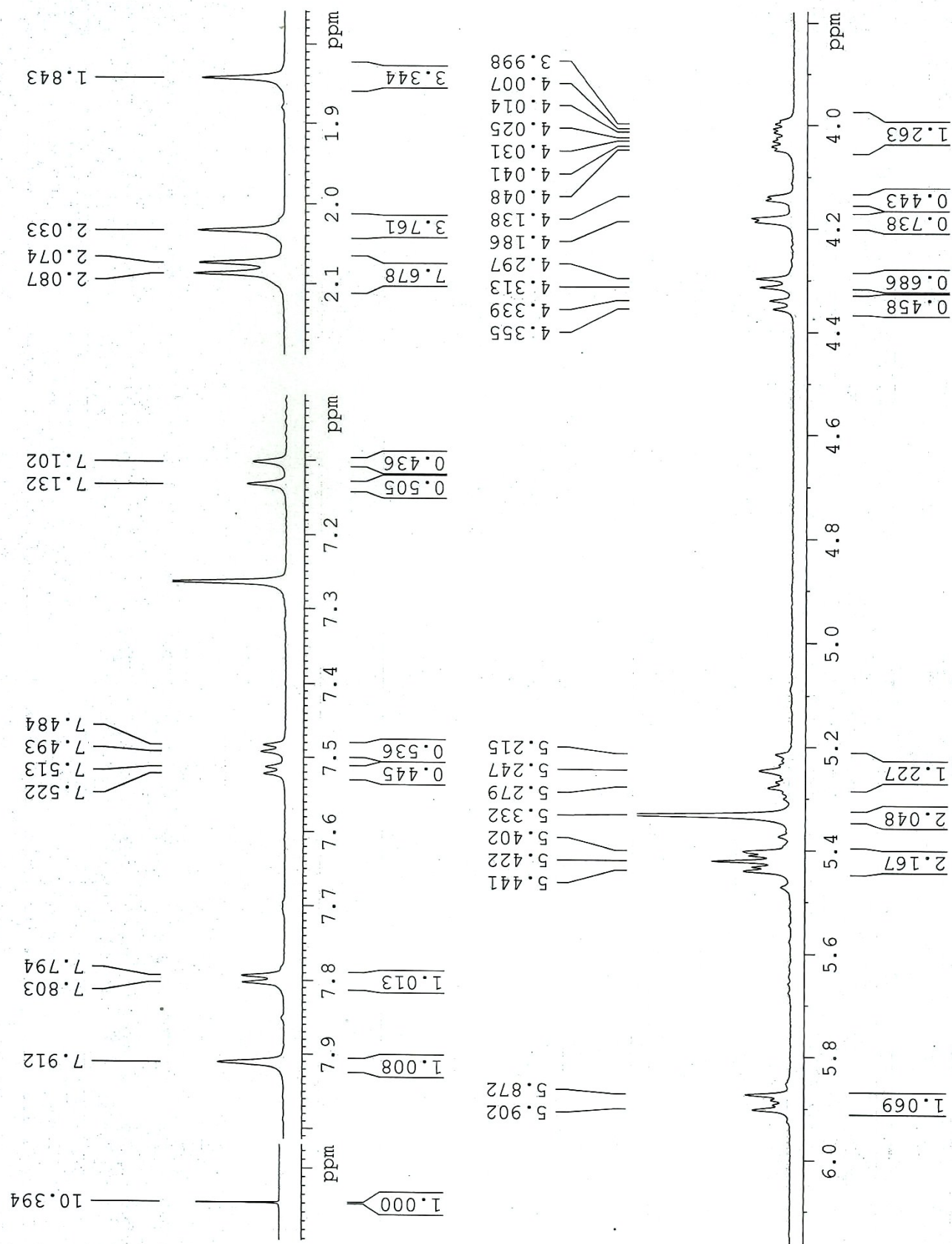


Figure 15 ^1H NMR expansion spectrum (300 MHz, CDCl_3) of compound, 8.



Current Data Parameters
NAME TMDH-335
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130429
Time 23.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 237
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DE 27.800 usec
TE 300.0 K
CNST2 2.0000000 sec
CNST11 0.03000000 sec
d0 1.89999998 sec
d1 1.89999998 sec
d2 1.89999998 sec
d3 1.89999998 sec
d11 1.89999998 sec
d12 1.89999998 sec
INO 1.89999998 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
NUC2 1H
P2 13.15 usec
PL2 80.00 dB
SFO2 300.1312005 MHz

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 300.1317 MHz
FIDRES 26.251680
SW 11.196 ppr
FnMODE QF

F2 - Processing parameters
EM 0
1.00 Hz
1.40

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
NUC2 1H
P2 13.15 usec
PL2 80.00 dB
SFO2 300.1312005 MHz

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 300.1317 MHz
FIDRES 26.251680
SW 11.196 ppr
FnMODE QF

F2 - Processing parameters
EM 0
1.00 Hz
1.40

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
NUC2 1H
P2 13.15 usec
PL2 80.00 dB
SFO2 300.1312005 MHz

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 300.1317 MHz
FIDRES 26.251680
SW 11.196 ppr
FnMODE QF

F2 - Processing parameters
EM 0
1.00 Hz
1.40

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
NUC2 1H
P2 13.15 usec
PL2 80.00 dB
SFO2 300.1312005 MHz

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 300.1317 MHz
FIDRES 26.251680
SW 11.196 ppr
FnMODE QF

F2 - Processing parameters
EM 0
1.00 Hz
1.40

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
NUC2 1H
P2 13.15 usec
PL2 80.00 dB
SFO2 300.1312005 MHz

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 300.1317 MHz
FIDRES 26.251680
SW 11.196 ppr
FnMODE QF

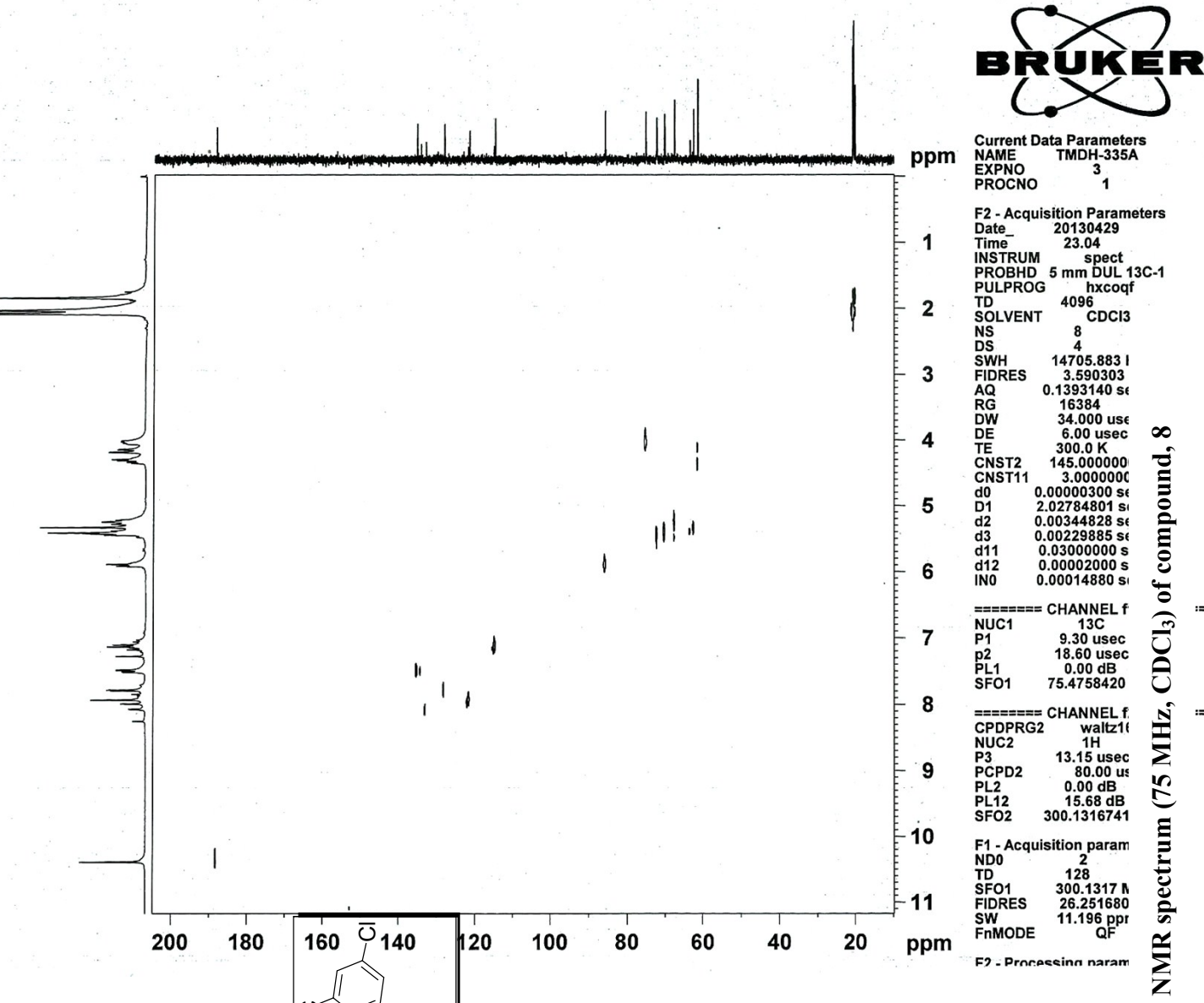


Figure 17 ¹H - ¹³C COSY spectrum (CDCl₃) of compound, 8

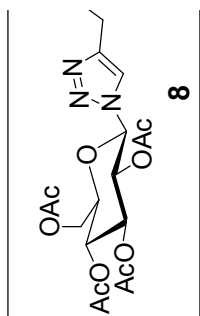


Figure 16 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 8

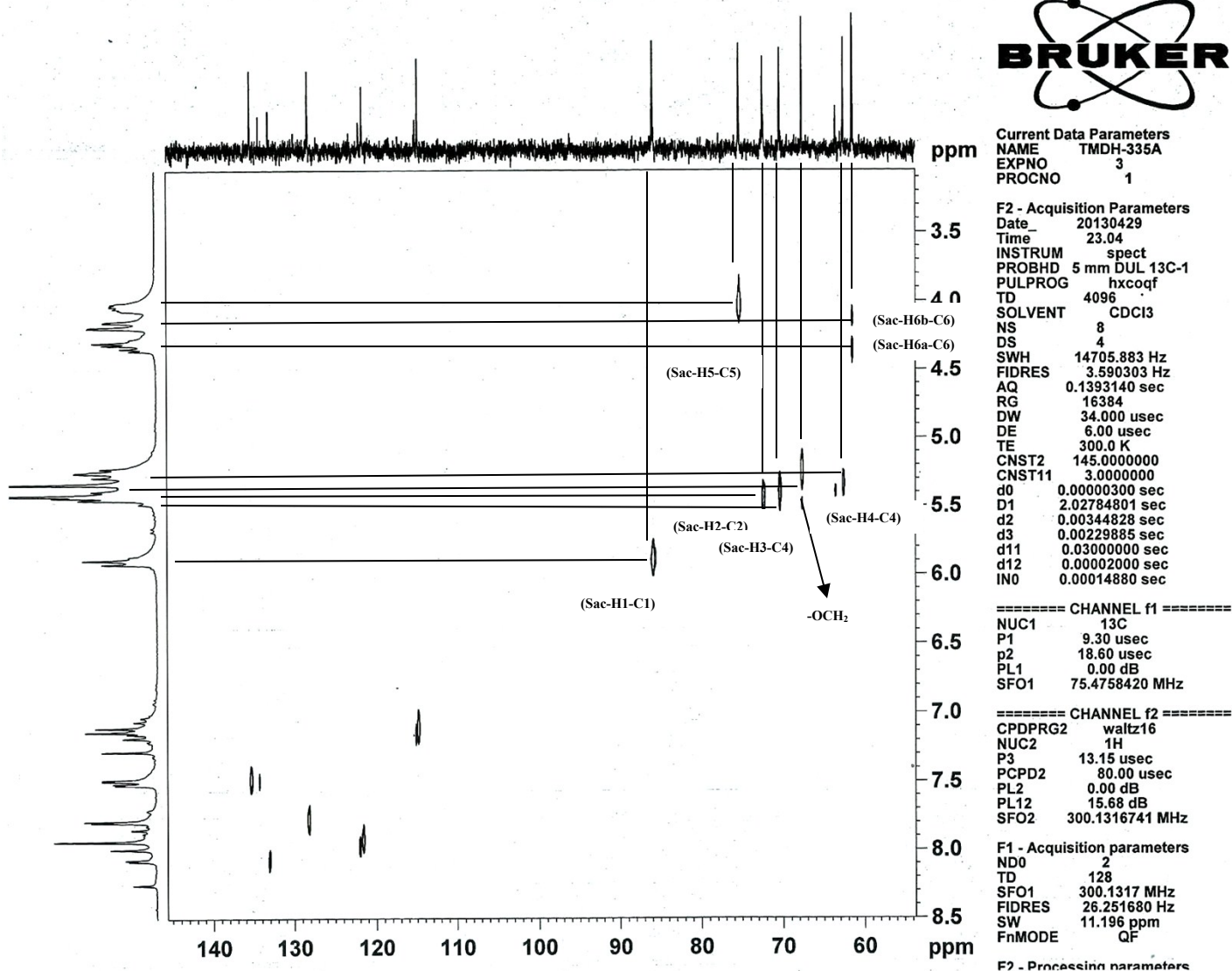


Figure 18 ^1H - ^{13}C COSY expansion spectrum (CDCl_3) of compound, 8



Current Data Parameters
 NAME TMDH-341
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130430
 Time 19.08
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 25
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 362
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300050 MHz
 EM
 WDW 0
 SSB 0.30 Hz
 LB 0
 GB 0
 PC 1.00

9.984
7.883
7.527
7.523
7.503
7.496
7.489
7.479
7.470
7.445
7.266
7.247
7.247
5.913
5.882
5.444
5.435
5.421
5.413
5.277
5.266
5.241
5.218
4.342
4.326
4.300
4.284
4.178
4.130
4.042
4.036
4.026
4.019
4.008
4.002
3.992
2.088
2.074
2.031
1.852

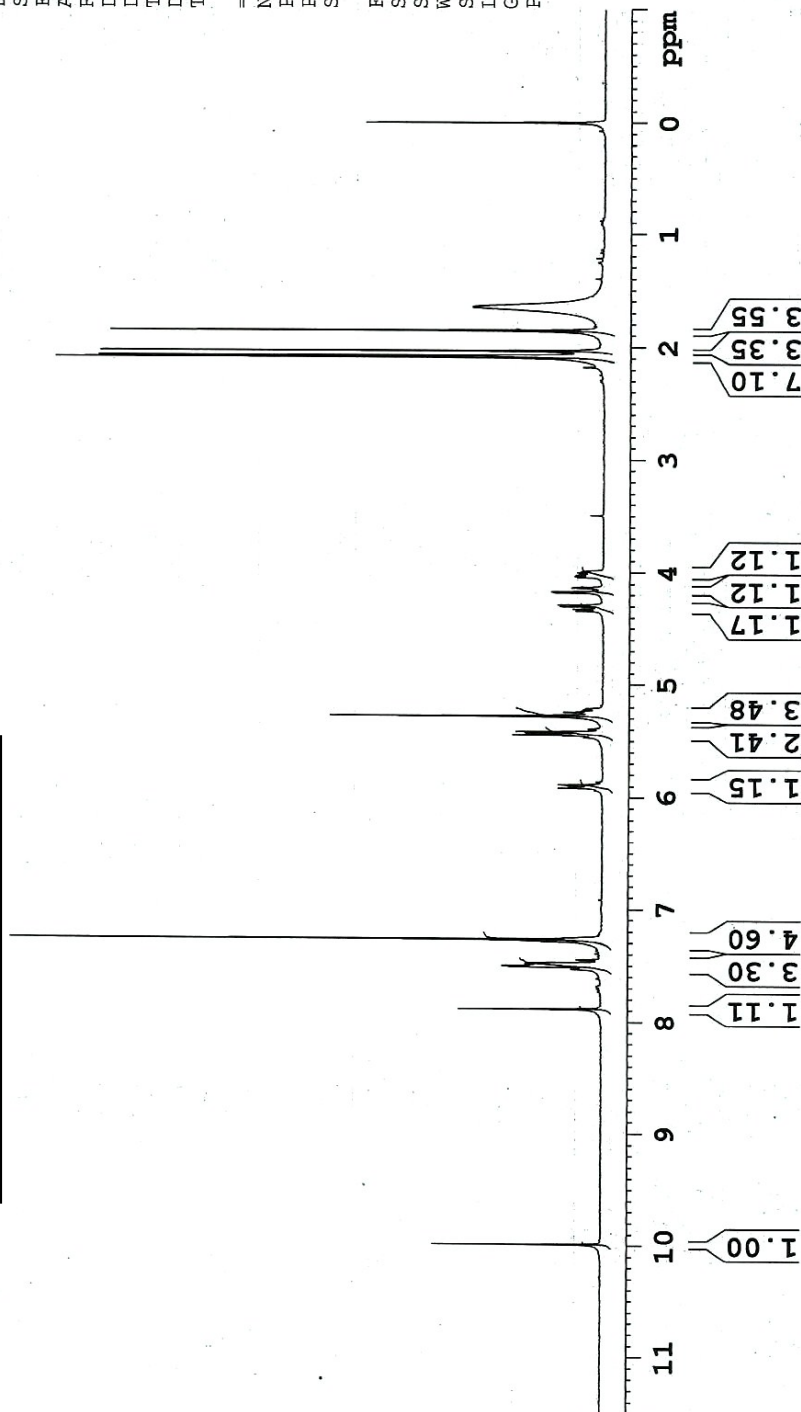
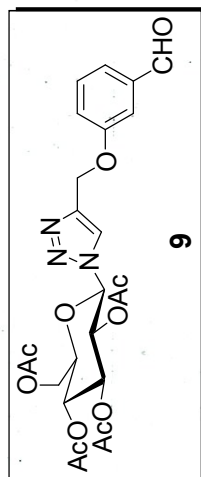
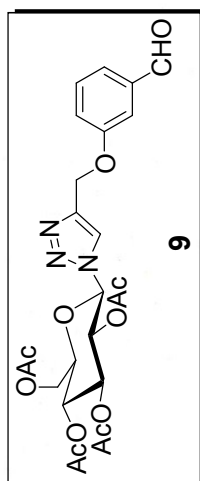
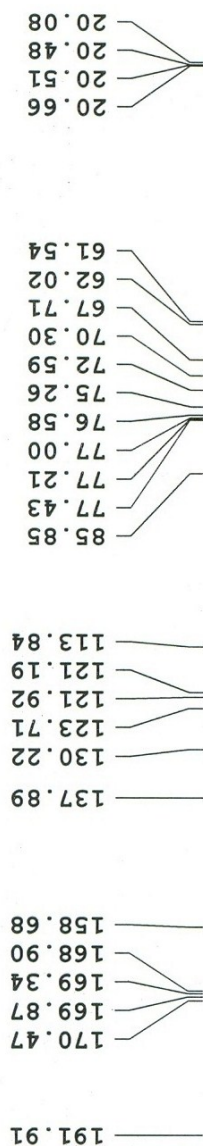


Figure 19 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 9.



Current Data Parameters
 NAME TMDH-341
 EXPNO 1
 PROCNO 1

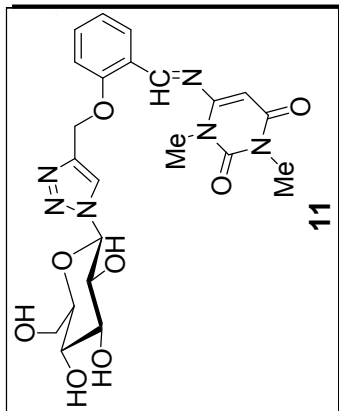
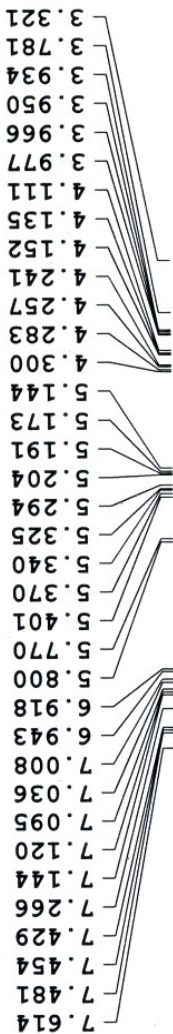
F2 - Acquisition Parameters
 Date_ 20130625
 Time_ 8.02
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 6000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 1024
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 20 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 9.



Current Data Parameters
 NAME TMDH-331
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130318
 Time_ 19.42
 INSTRUM spect
 PROBD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 50
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 256
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300049 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

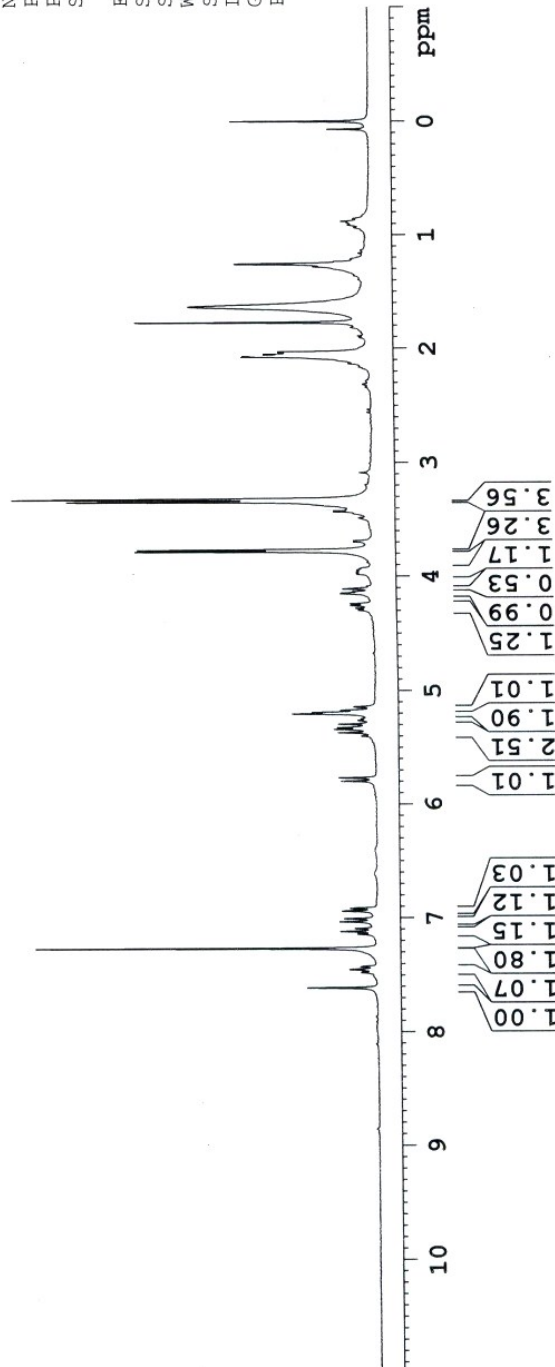


Figure 21 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 11.

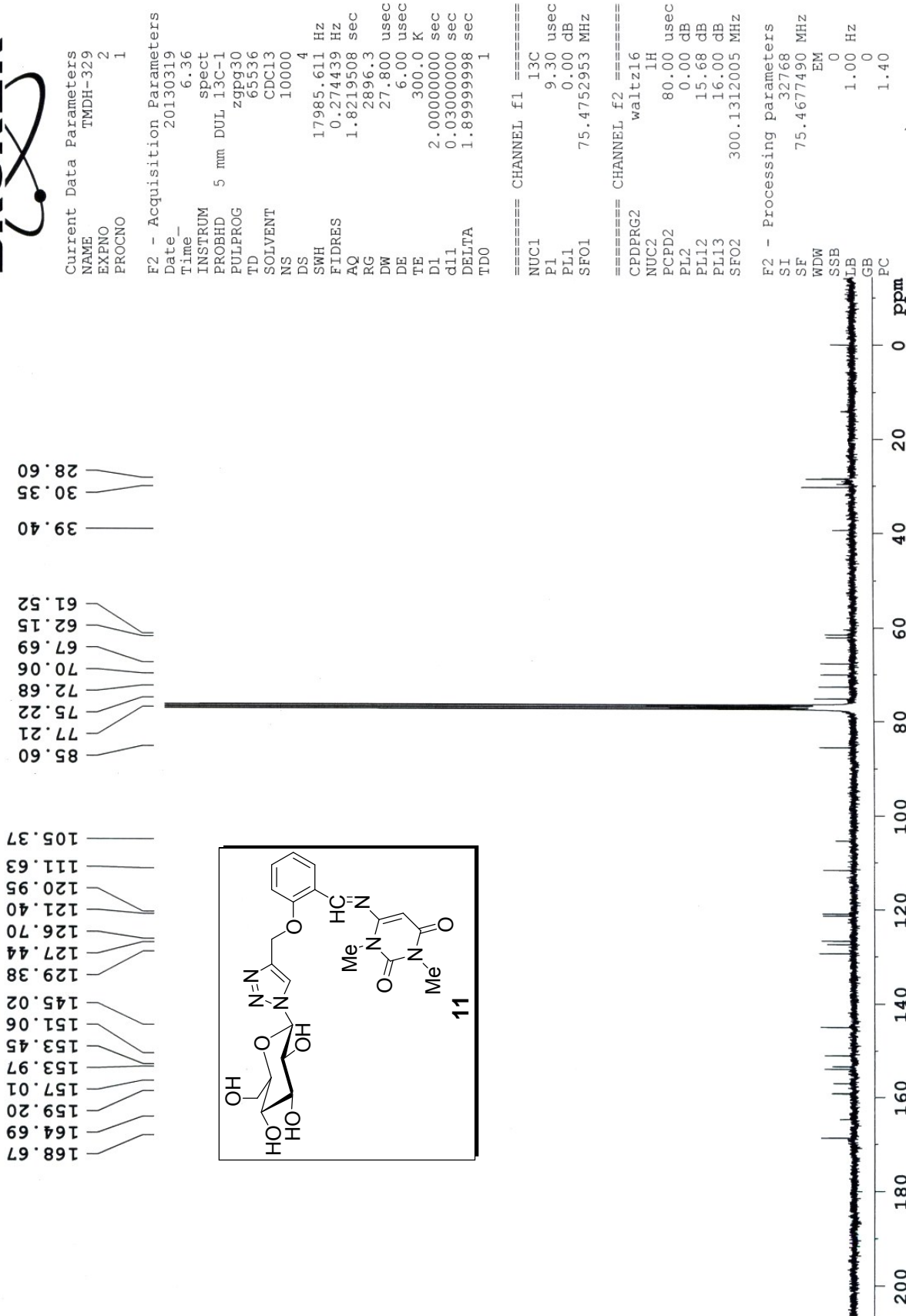


Figure 22 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 11.



Current Data Parameters
 NAME TMDH-336
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130415
 Time 13.23
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 50
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 143.7
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1314026 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

8.014
7.692
7.687
6.942
6.912
6.681
6.659
5.686
5.595
5.564
5.324
5.309
5.168
5.032
4.969
4.471
3.935
3.906
3.889
3.860
3.837
3.818
3.799
3.710
3.542
3.437

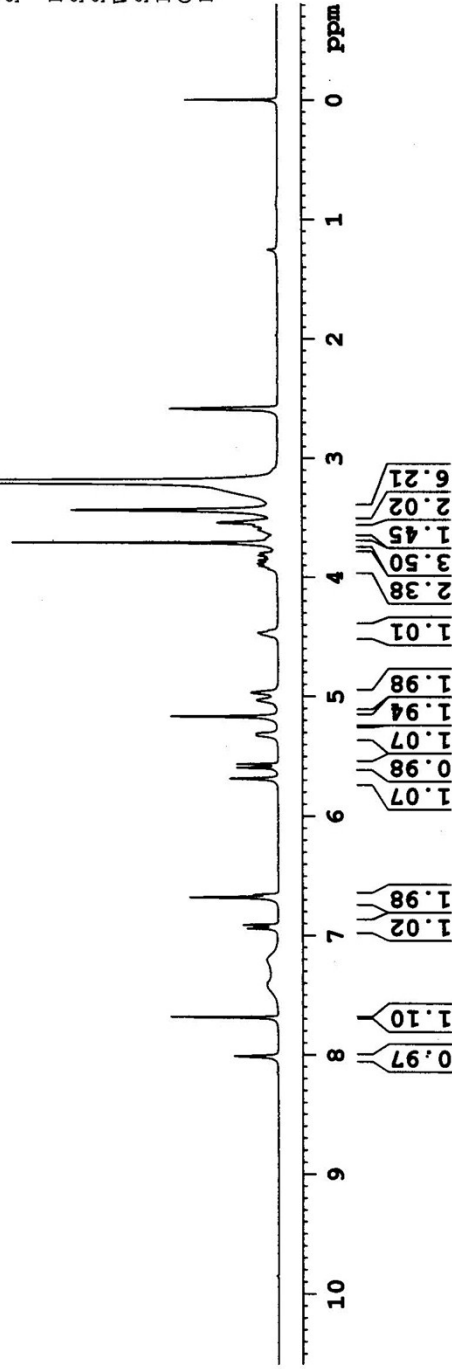
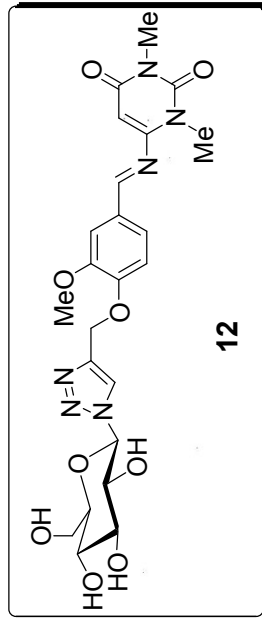


Figure 23 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 12.



Current Data Parameters
NAME TMDH-336
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130415
Time 23.46
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9479
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

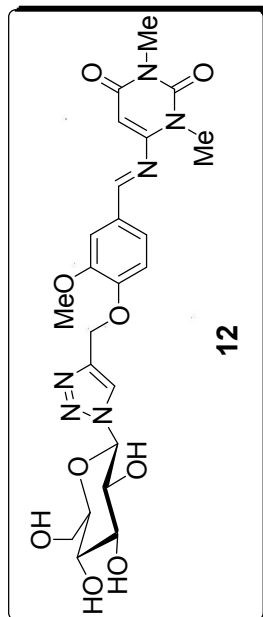
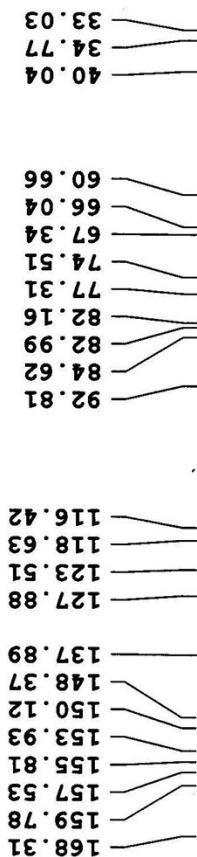
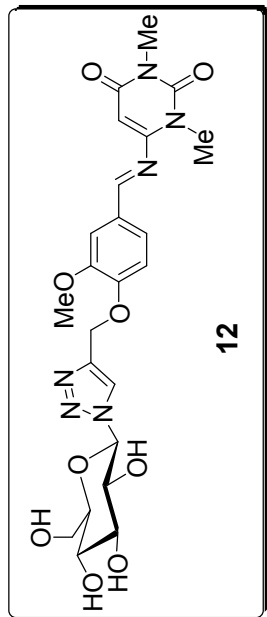
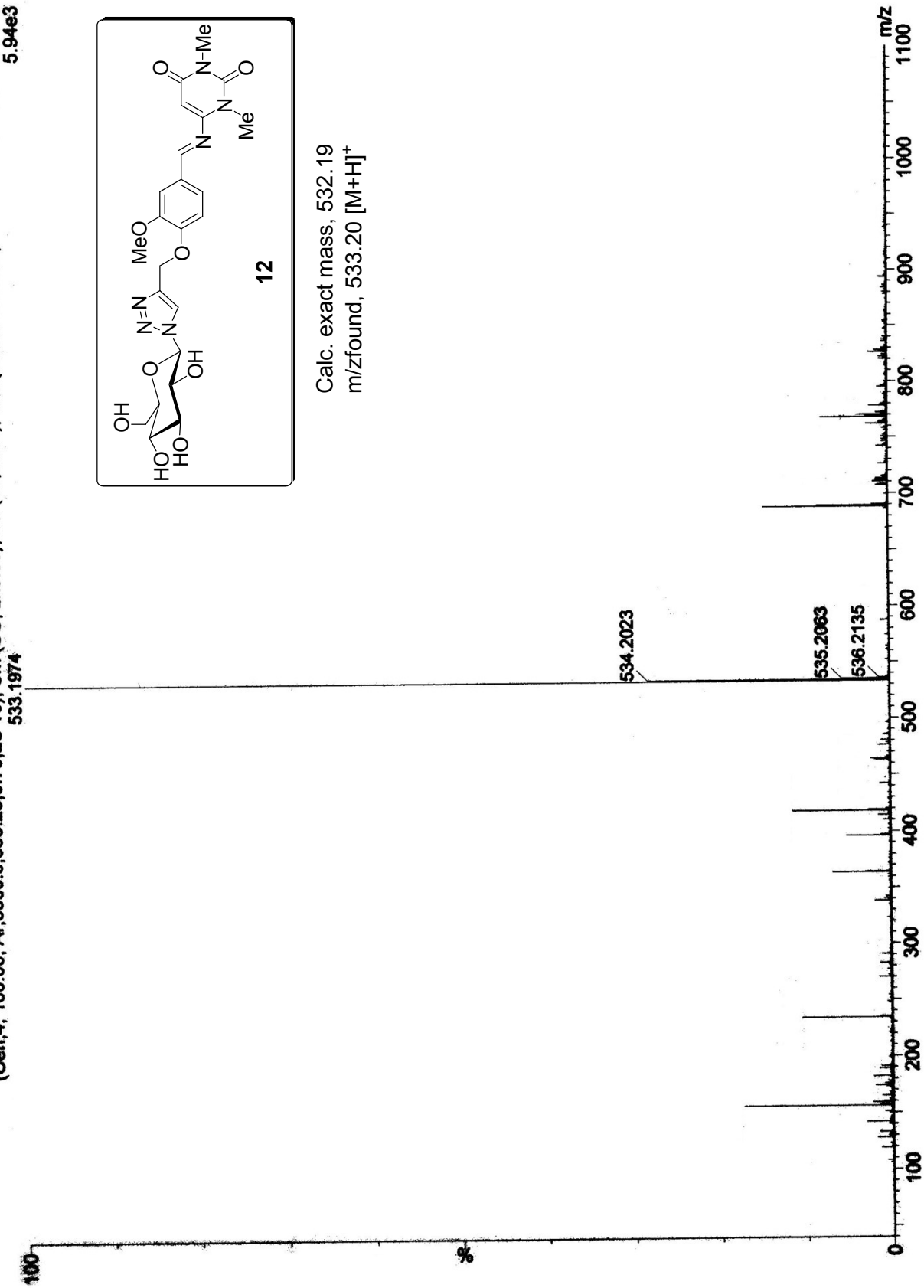


Figure 24 ¹³C NMR spectrum (75 MHz, CDCl₃) of compound, 12.

Electrospray Ionisation-MS
(Cen.4, 100.00, Ar.8500.0,556.28,0.75,LS 10; Sm (SG, 2x5.00); Sb (10,1.00); Cm (16:22-180:192)

WATERS-Q-ToF Premier-HAB213

1: TOF MS ES+
5.94e3



Calc. exact mass, 532.19
 m/z found, 533.20 $[M+H]^+$

Figure 25 Mass spectrum of compound, 12.



Current Data Parameters
 NAME TMDH-338
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20130422
 Time 19.55
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 50
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 203.2
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters

SI 32768
 SF 300.1314005 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ppm

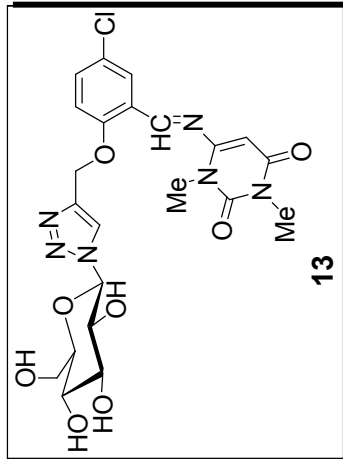
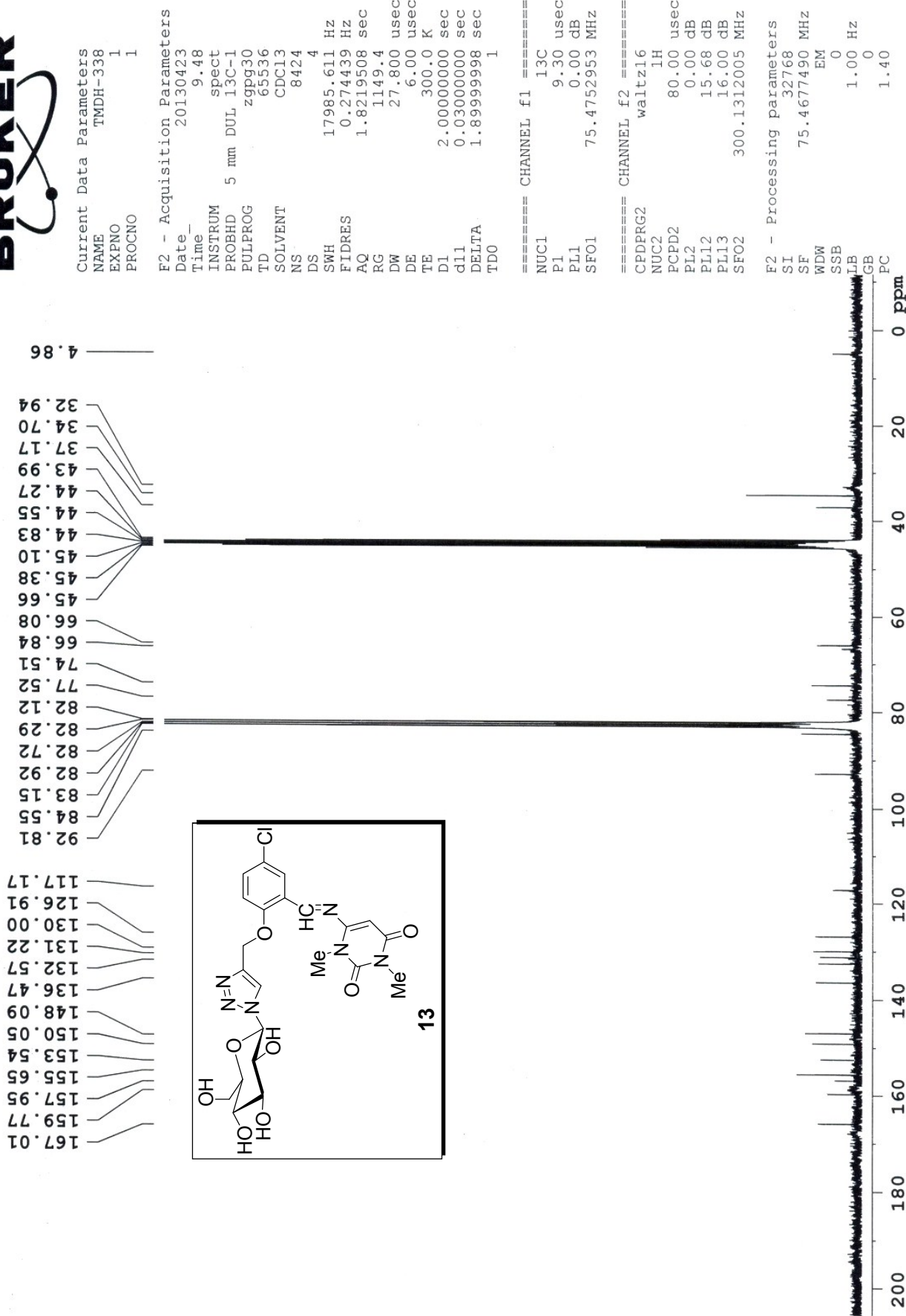
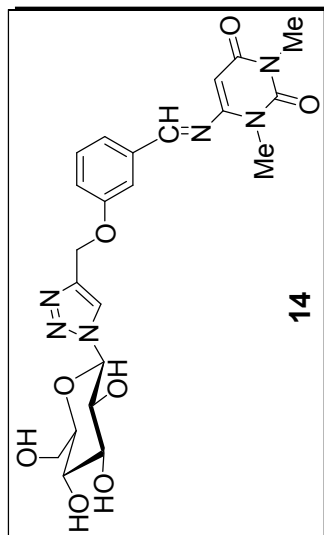


Figure 26 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 13.

Figure 27 ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound, 13.



8.063
7.919
7.497
7.162
7.136
7.111
6.781
6.755
6.721
5.691
5.595
5.563
5.531
5.239
5.144
4.838
4.241
4.221
3.890
3.870
3.831
3.809
3.757
3.716
3.532
3.418
2.576



Current Data Parameters
NAME TMDH-344
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130514
Time 19.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 406.4
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1314066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

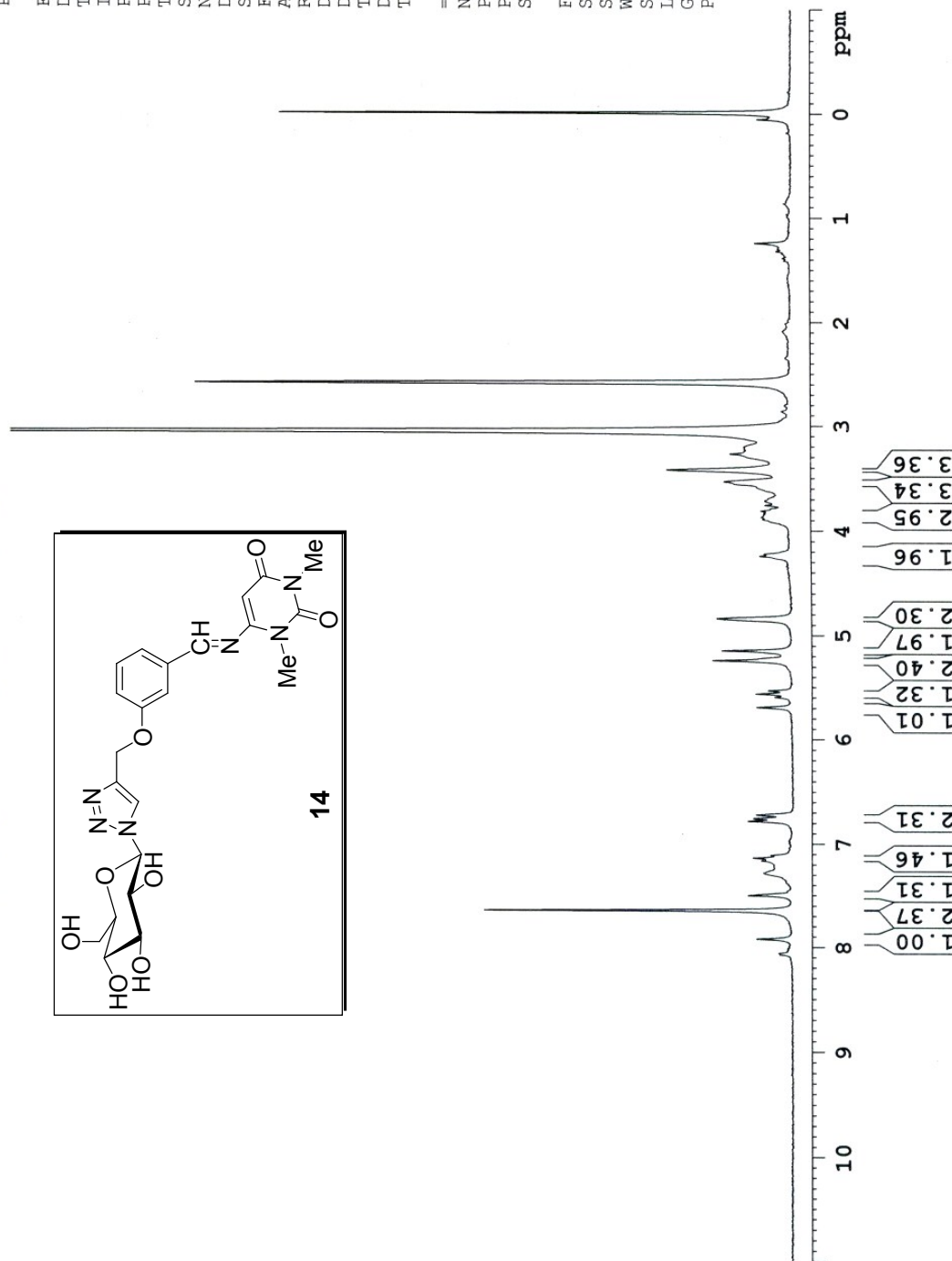
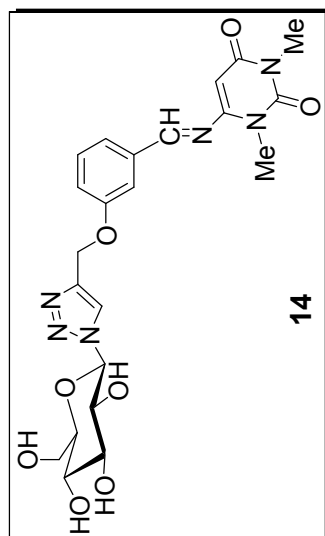
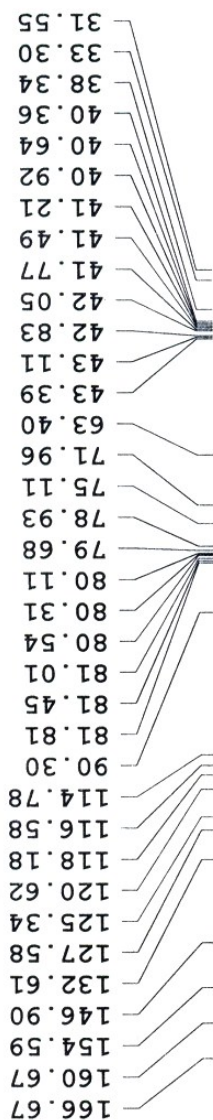


Figure 28 ¹H NMR spectrum (300 MHz, CDCl₃) of compound, 14.



Current Data Parameters
 NAME AT-MRS-7-13
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130817
 Time 22.43
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 13000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 1290.2
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 29 ^{13}C NMR spectrum (75 MHz, CDCl_3) of compound, 14.

Docking Studies:

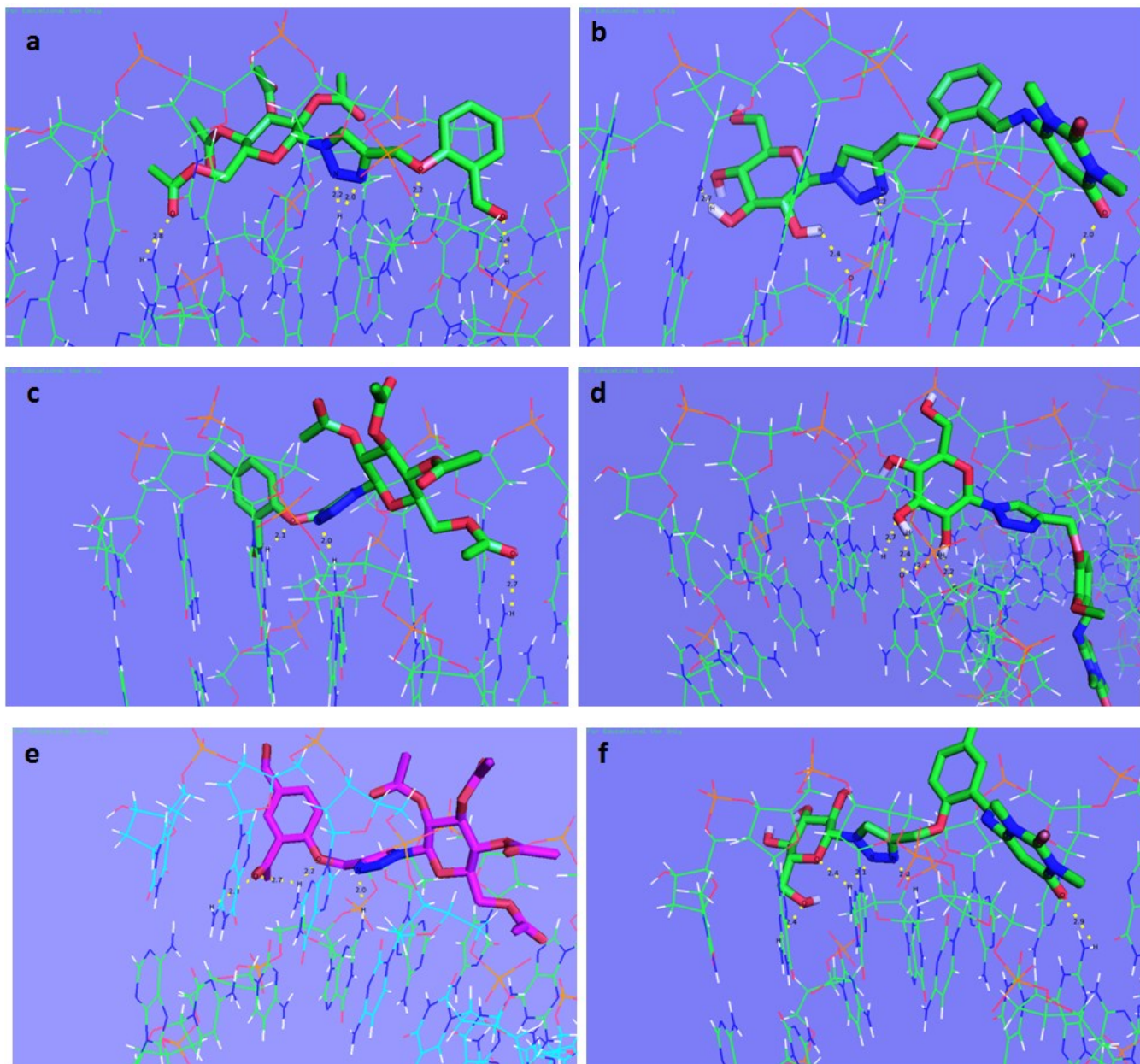


Figure 30 Hydrogen bonding interaction of compounds (a) 6, (b) 11, (c) 7, (d) 12, (e) 8, (f) 13.