Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supporting Information

Studies on the synthesis of sugar triazole based ligand for protein and DNA binding

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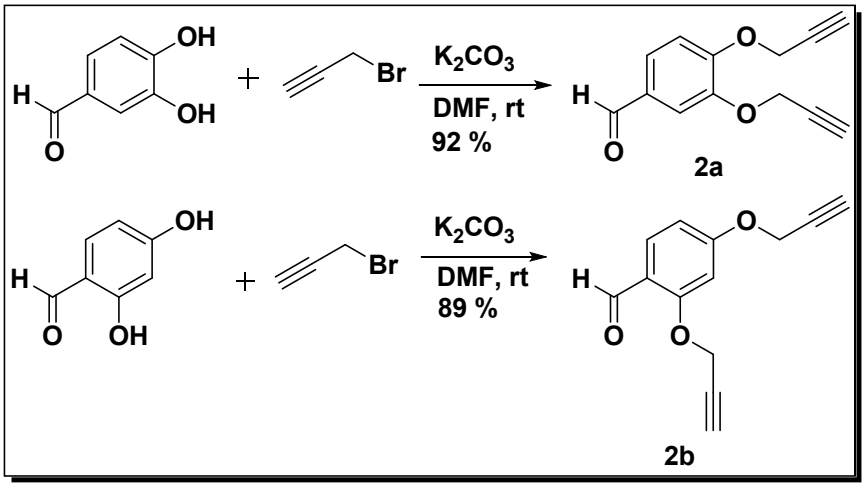
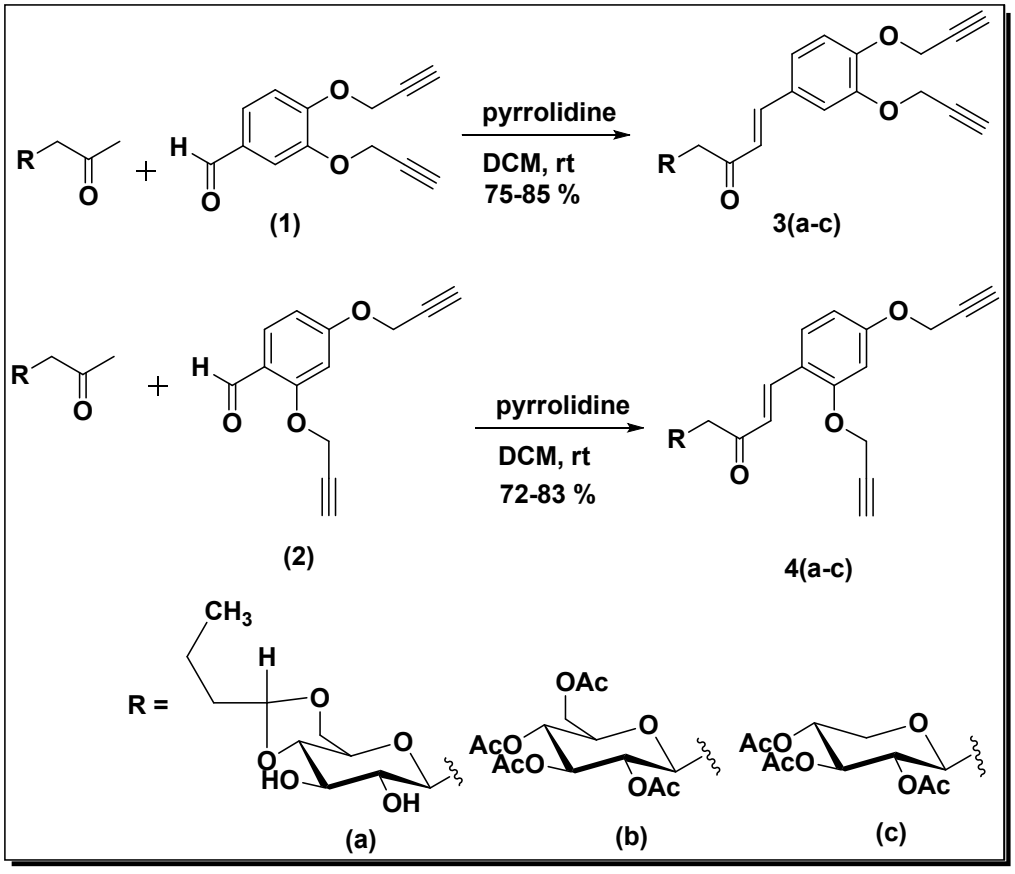


Scheme 1: Synthesis of bis propargylated aldehydes (**2a**) and (**2b**).



Scheme 2 Synthesis of sugar-chalcone based bis propargylated derivatives.

Table 1 Crystallographic data of compounds, **2a** & **2b**

Parameters	**2a**	**2b**
Formula	$C_{13}H_{10}O_3$	$C_{13}H_{10}O_3$
Formula Weight	216.19	216.19
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$
a (Å)	4.5734(4)	4.9212(6)
b (Å)	17.8195(13)	16.858(2)
c (Å)	13.2690(11)	13.4277(17)
α (deg)	90.00	90.00
β (deg)	91.727(4)	98.252(5)
γ (deg)	90.00	90.0090
V (A^3)	1080.88(15)	1102.4(2)
Z, Calculated density (Mg/m^3)	1.329	1.291
μ (mm^{-1})	0.099	0.092
T (K)	293(2)	293(2)
No. of unique reflections	3855	2171
No. of observed reflections	3680	10580
$R1$, Rw	0.0452, 0.135	0.0407, 0.1037
GOF	0.900	1.090
Crystal habit	Block, colorless	Block, colorless

Table 2 Hydrogen bonding interaction of compound, **2a** & **2b**

Compound No.	D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
2a	C(9)-H(9) ···O(3)#1	0.95(2)	2.28(2)	3.198(2)	162.5(15)
	C(13)-H(13) ···O(3)#2	0.94(3)	2.71(3)	3.525(2)	145(2)
2b	C(4)-H(4)...O(1)#1	0.93	2.48	3.364(2)	158.5
	C(8)-H(8A)...O(1)#2	0.97	2.63	3.446(2)	141.6
	C(10)-H(10)...O(1)#3	0.93	2.26	3.153(2)	159.7

Symmetry transformations: For compound **2a** #1 -x+3/2,y-1/2,-z+3/; #2 -x+1,-y+1,-z+1, For compound **2b**: #1 x-1/2,-y+1/2,z+1/2; #2 x+1/2,-y+1/2,z+1/2; #3 -x+5/2,y+1/2,-z+1/2.

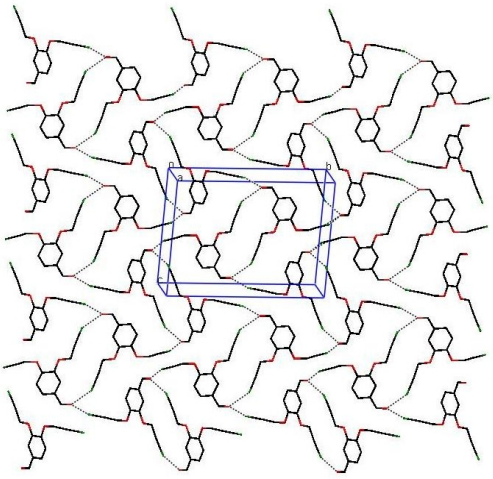


Figure 3 Hydrogen bonding interactions and crystal packing structure of the compound, **2a**.

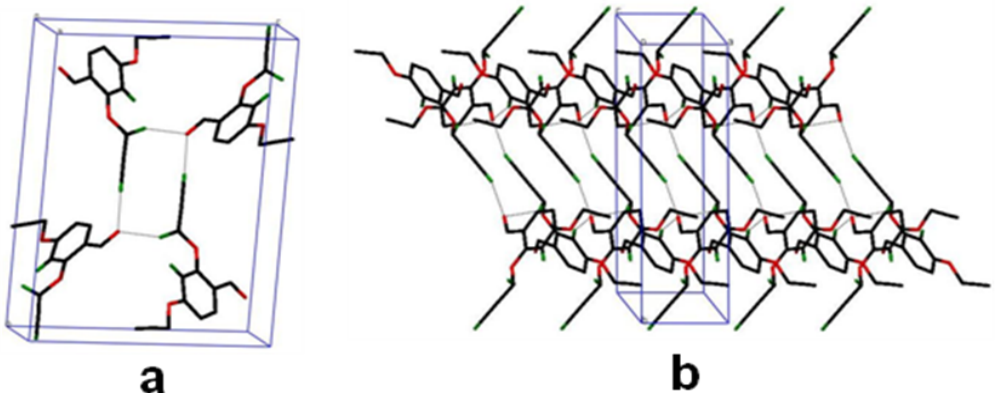
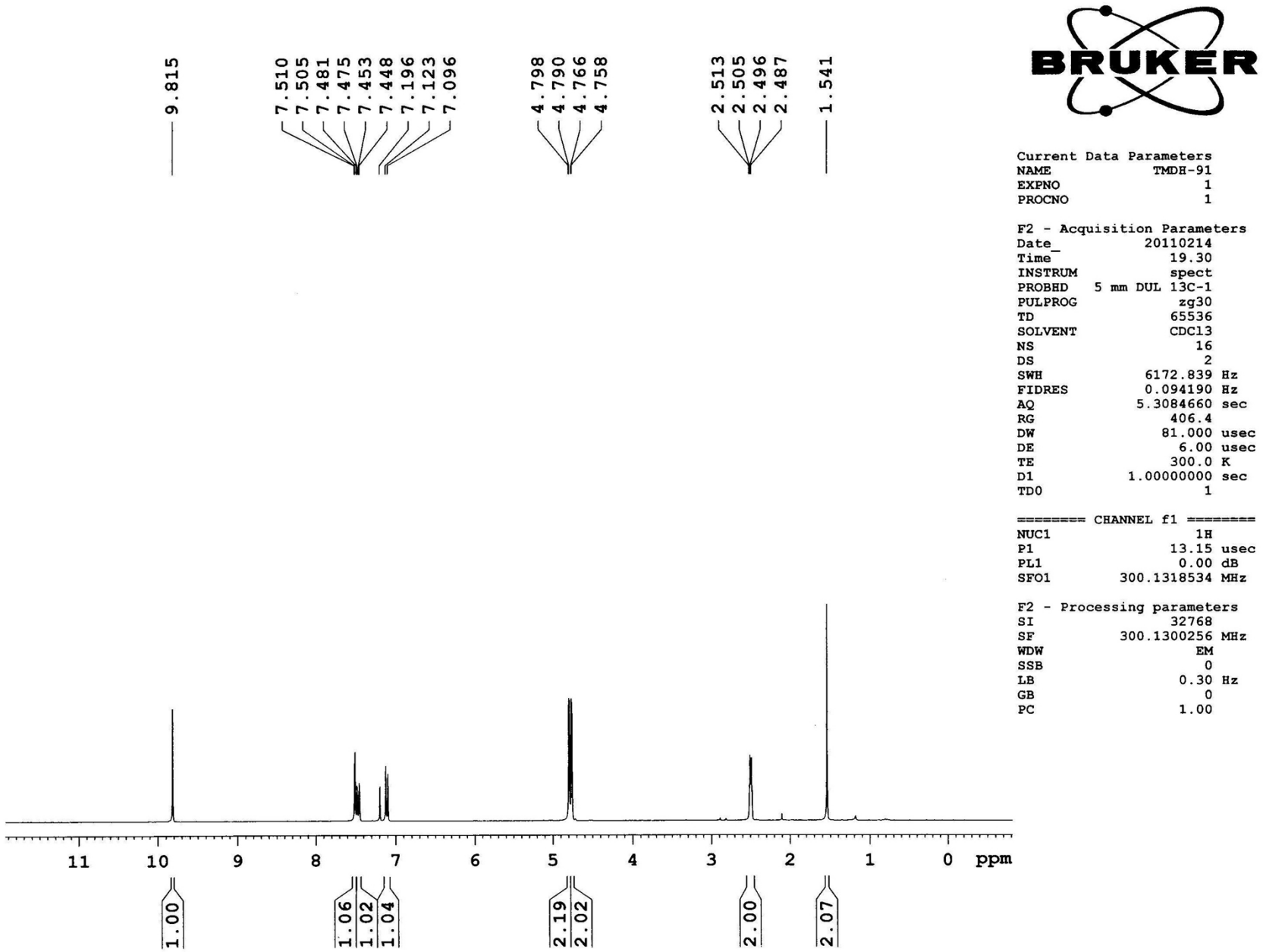


Figure 4 Crystal packing of compound, **2b**, (a), with four molecules; (b), one dimensional network.



BRUKER

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PROCNO 1

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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 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
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SSB 0
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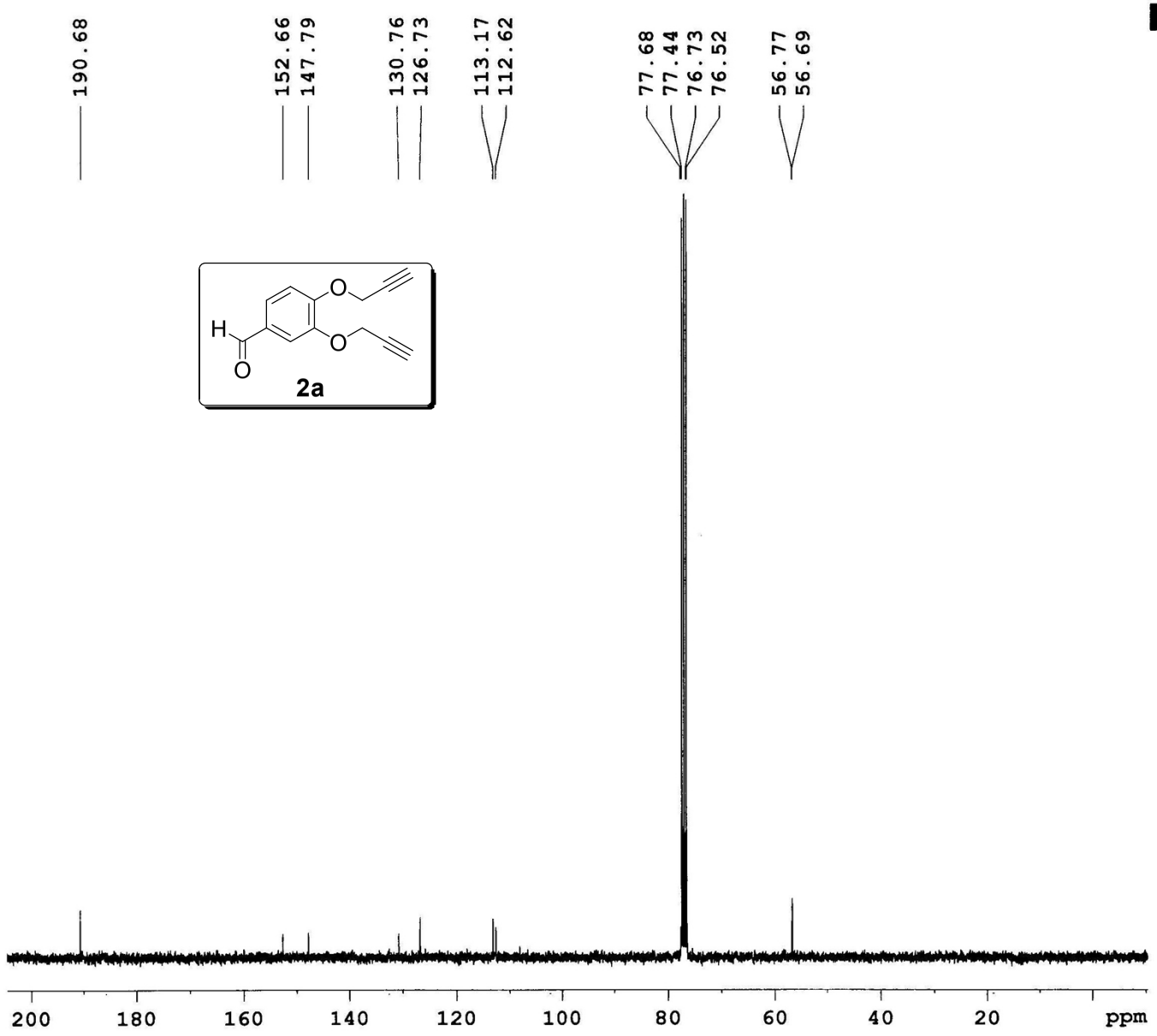
PC 1.00

Figure 1 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 2a.



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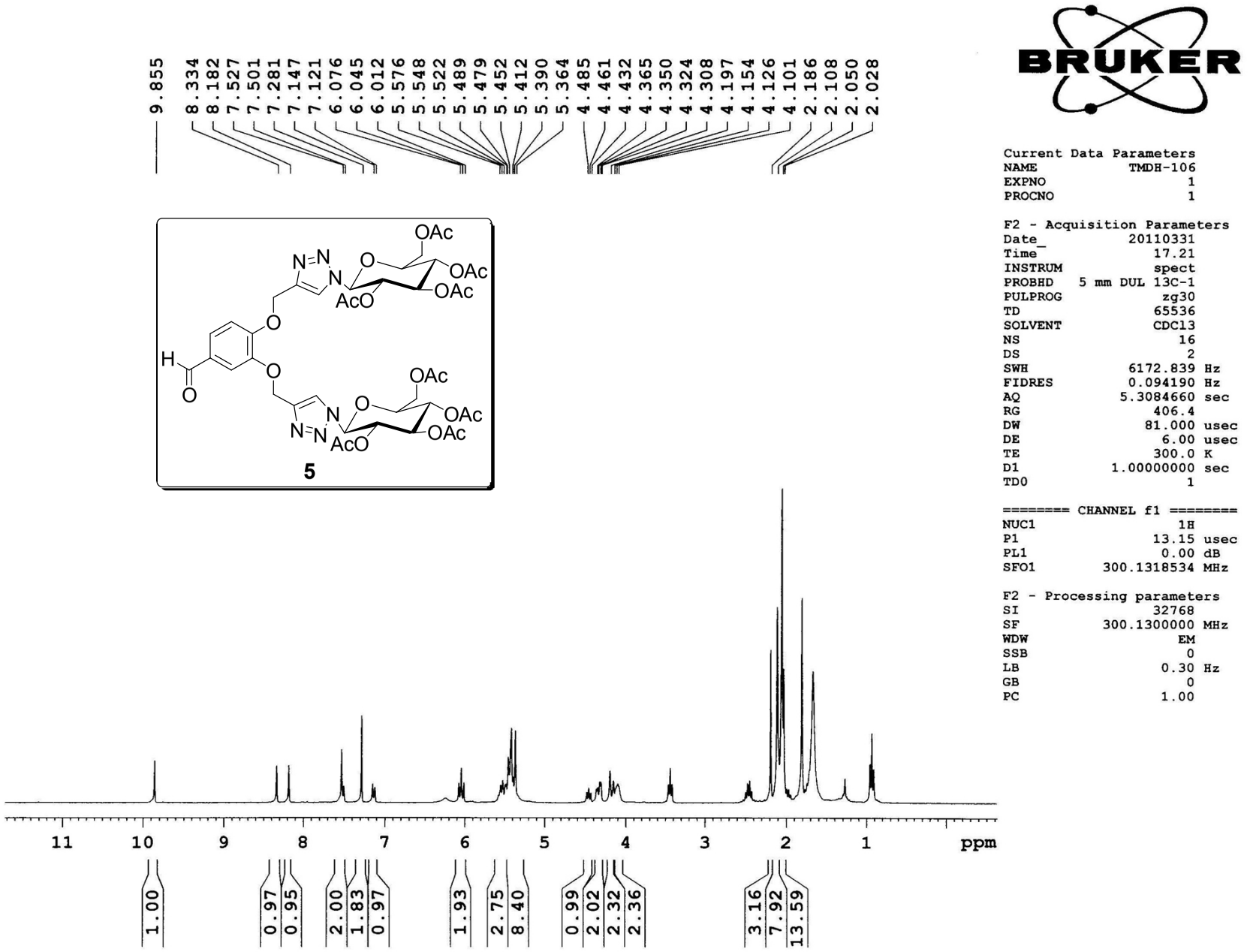
SOLVENT CDCl3
NS 433
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 362
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
PL1 -2.00 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, 2a.



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PROCNO                       1

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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                       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                  300.1300000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
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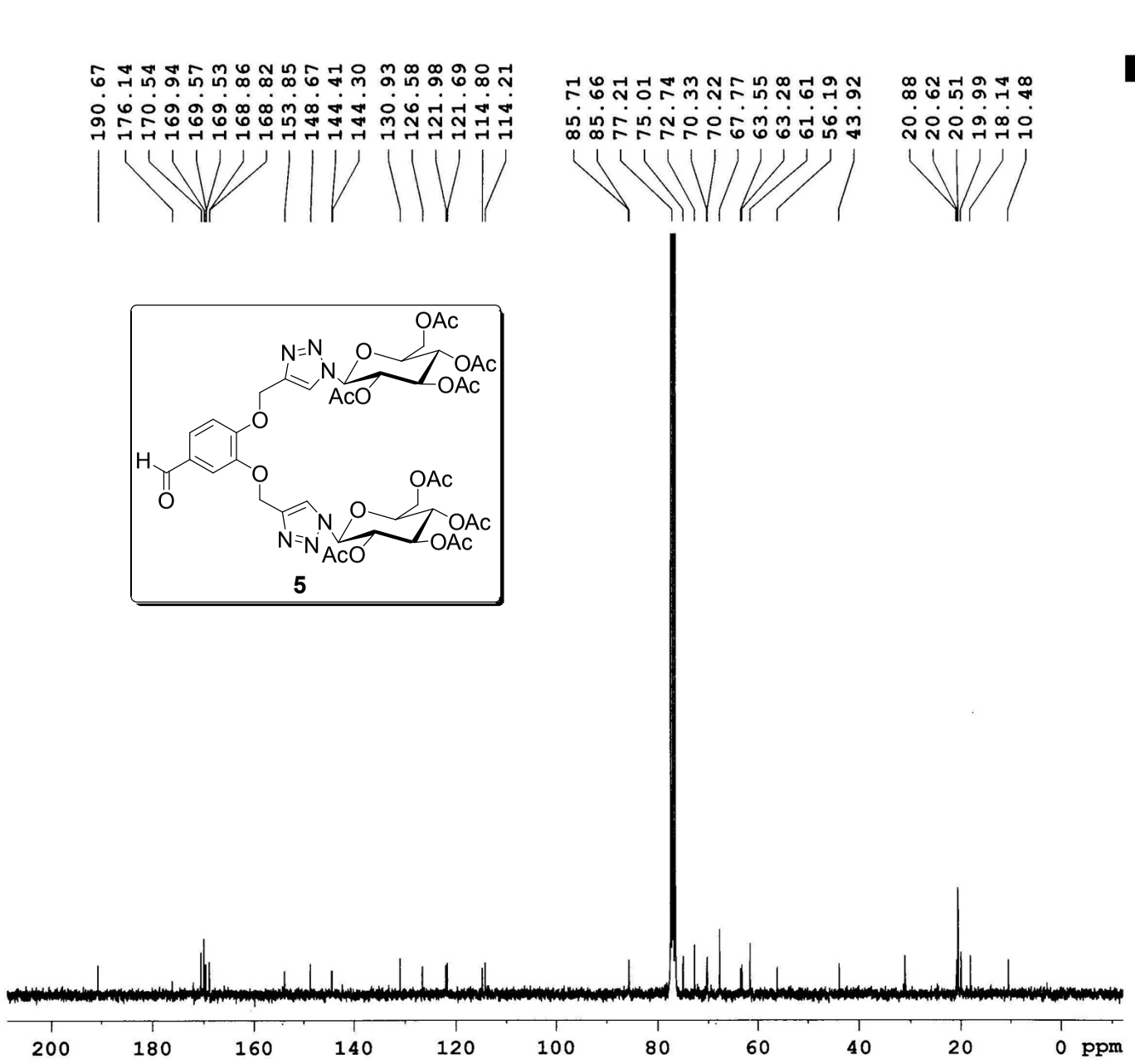
Figure 3 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 5.



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PROCNO                       1

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PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       5000
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 ========
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 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 5.

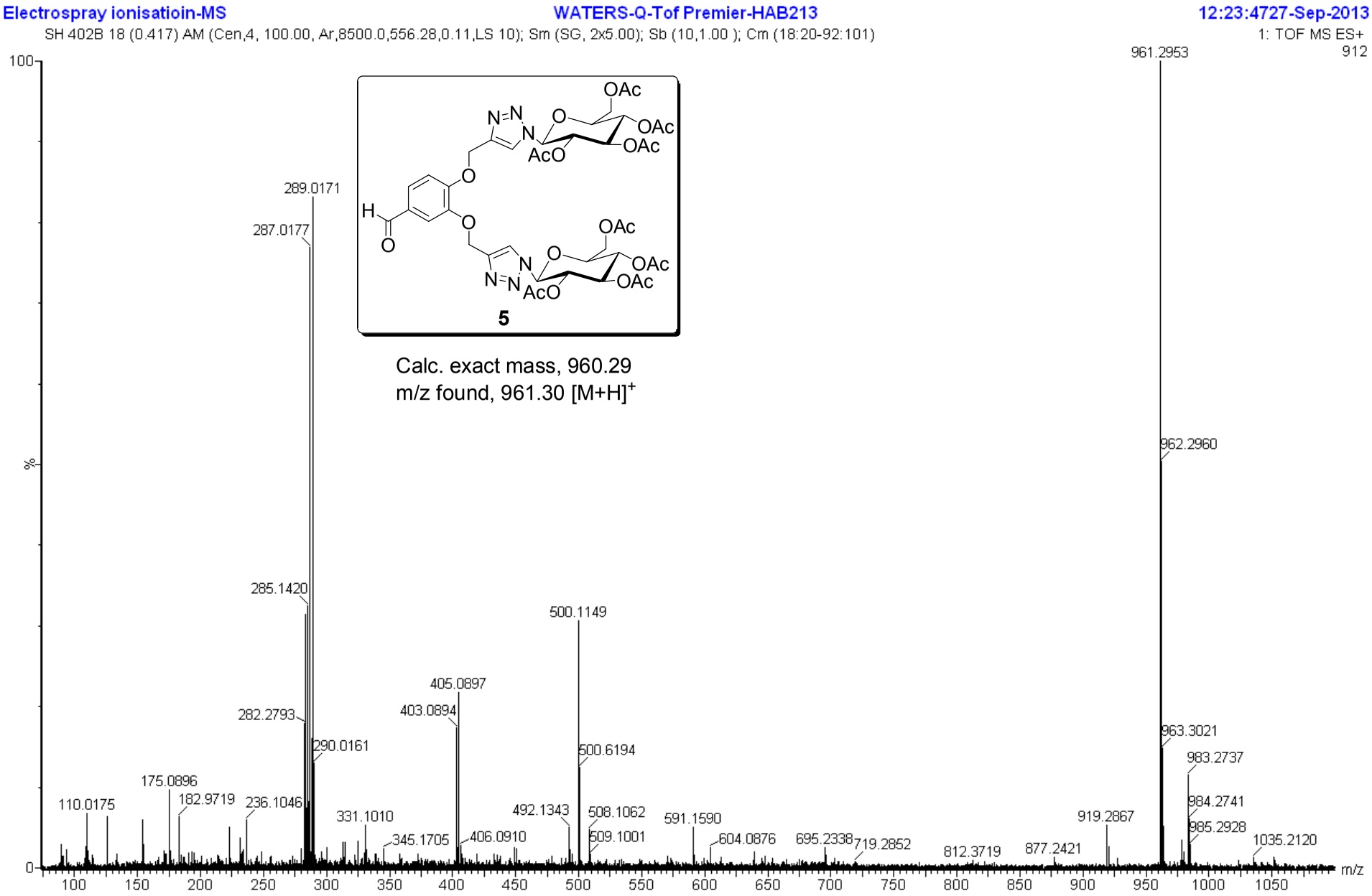


Figure 5 Mass spectrum of compound, 5.

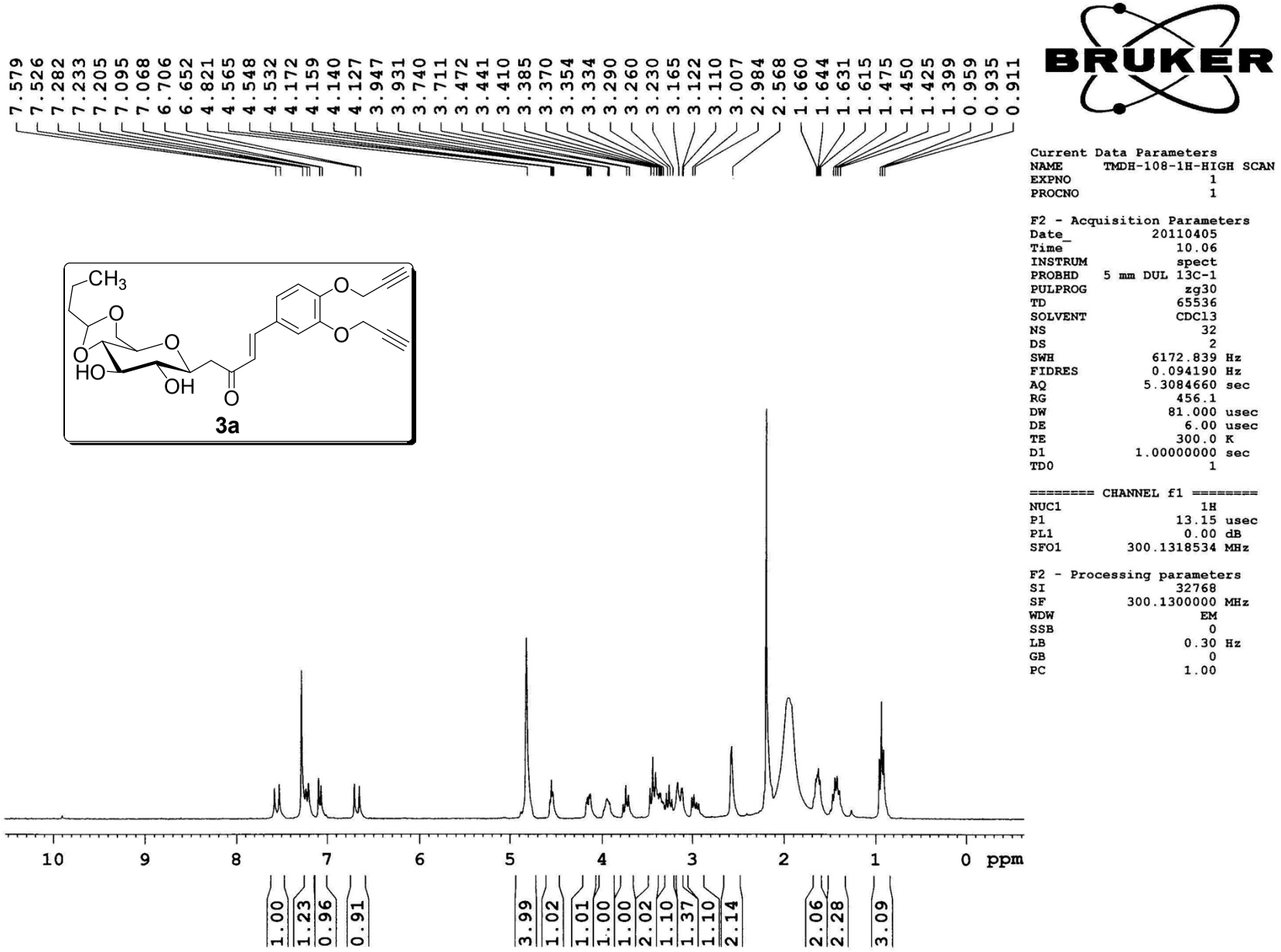
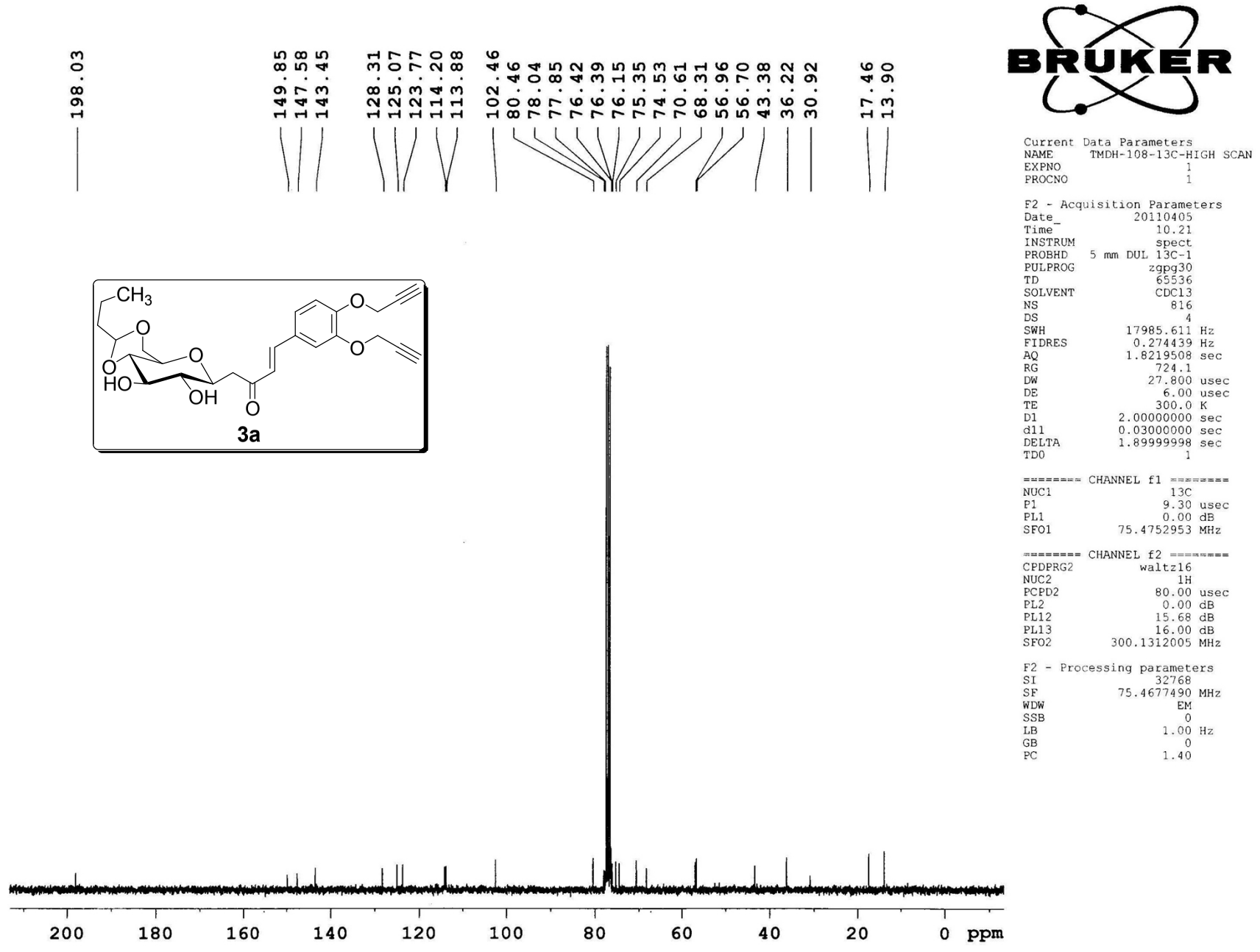


Figure 6 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 3a.



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Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

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PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	816
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
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Figure 7 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 3a.

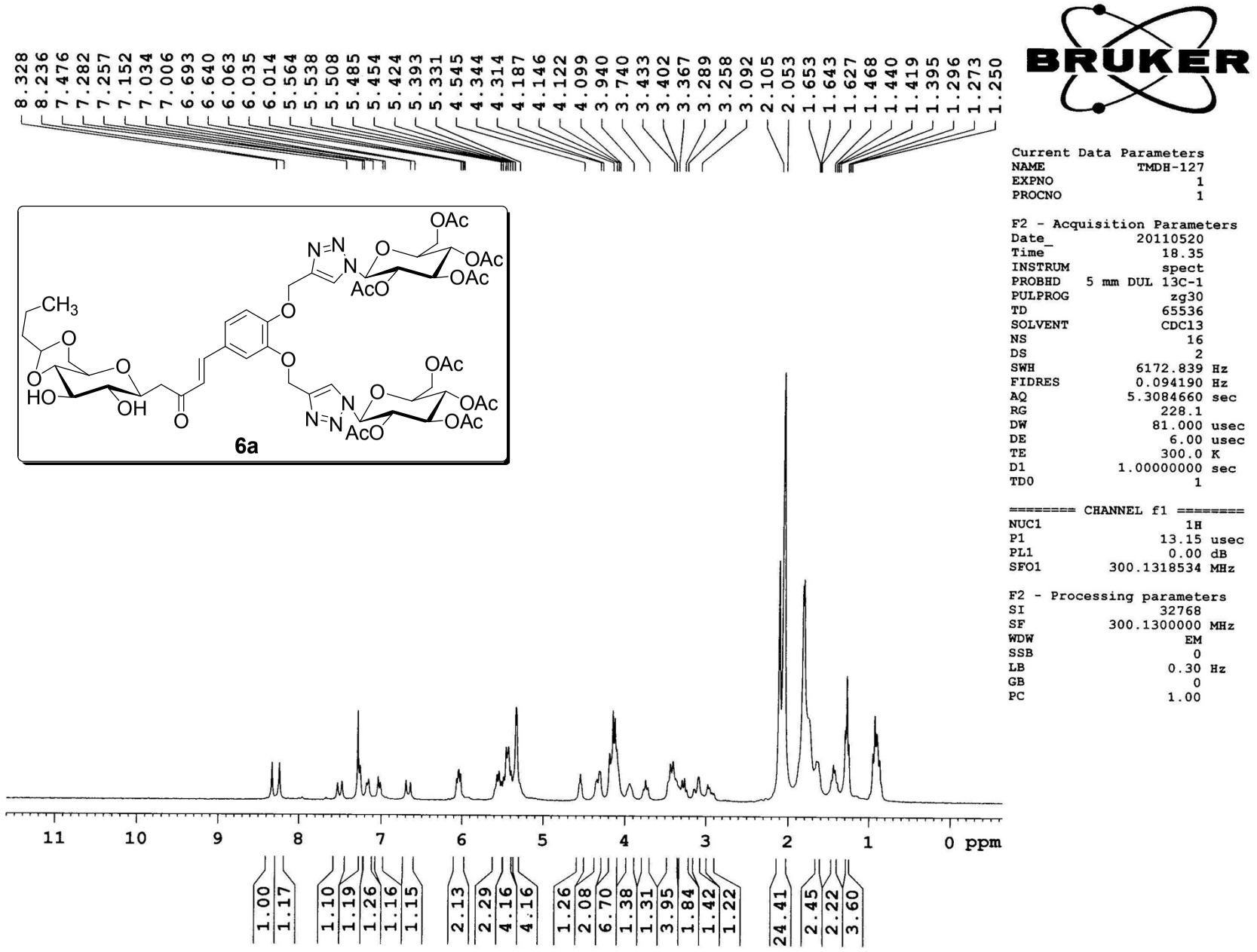
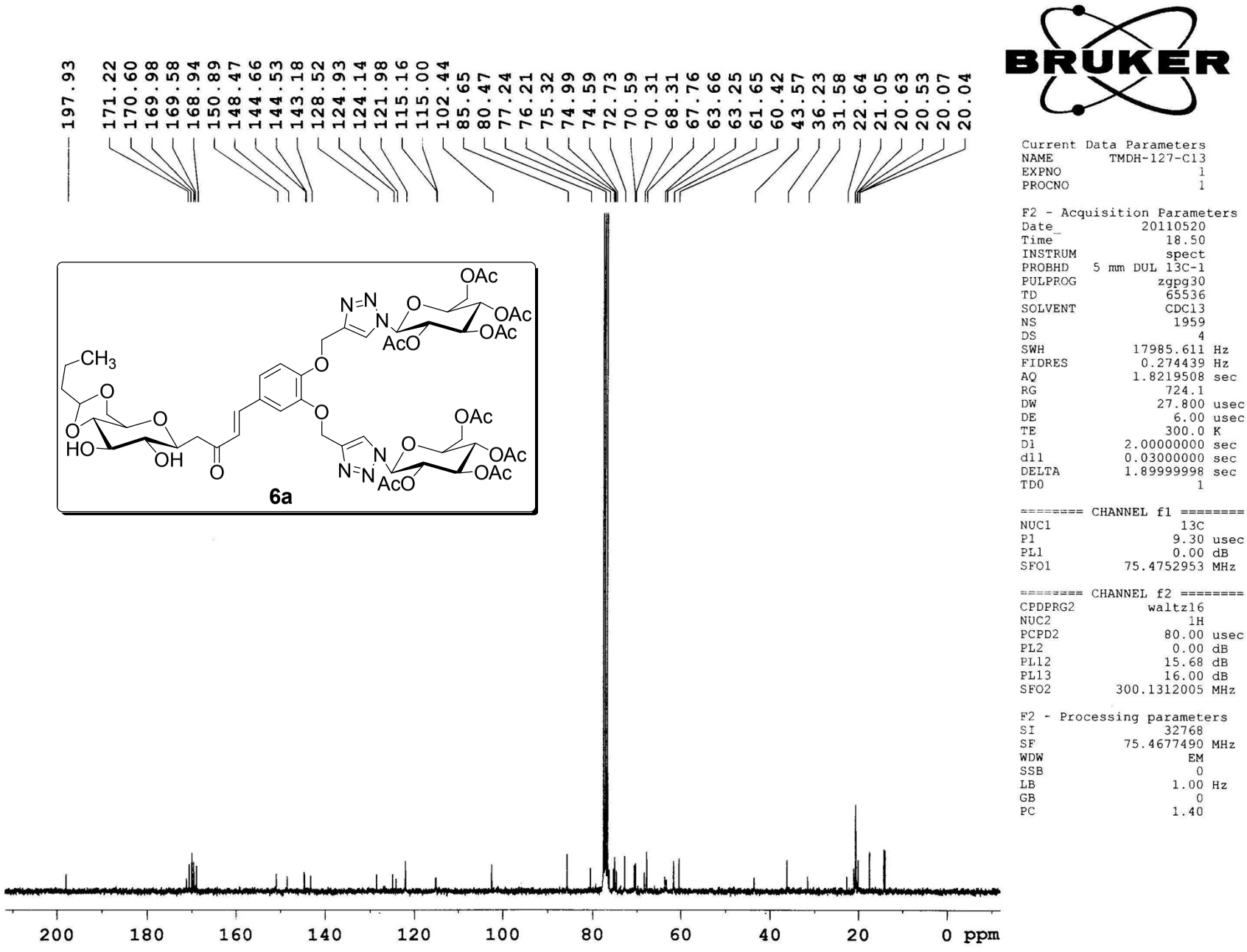


Figure 8 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound, 6a.



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PROCNO 1

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Time 18.50
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1959
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
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 9 ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound, 6a.

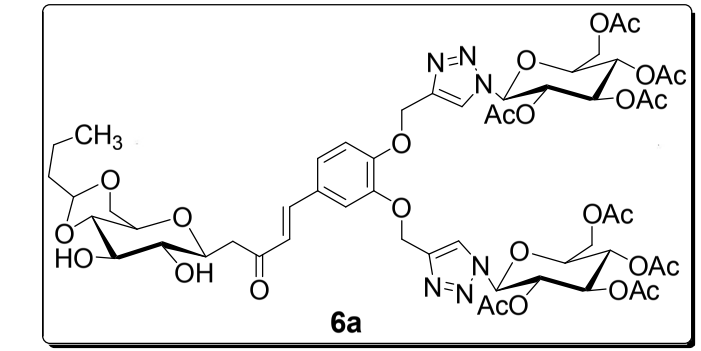
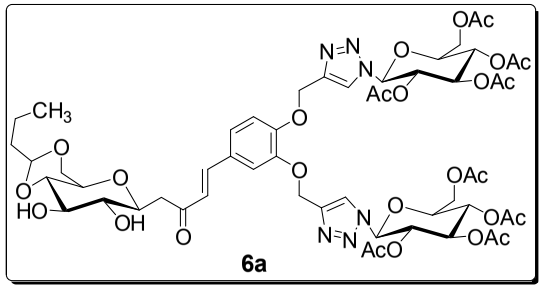
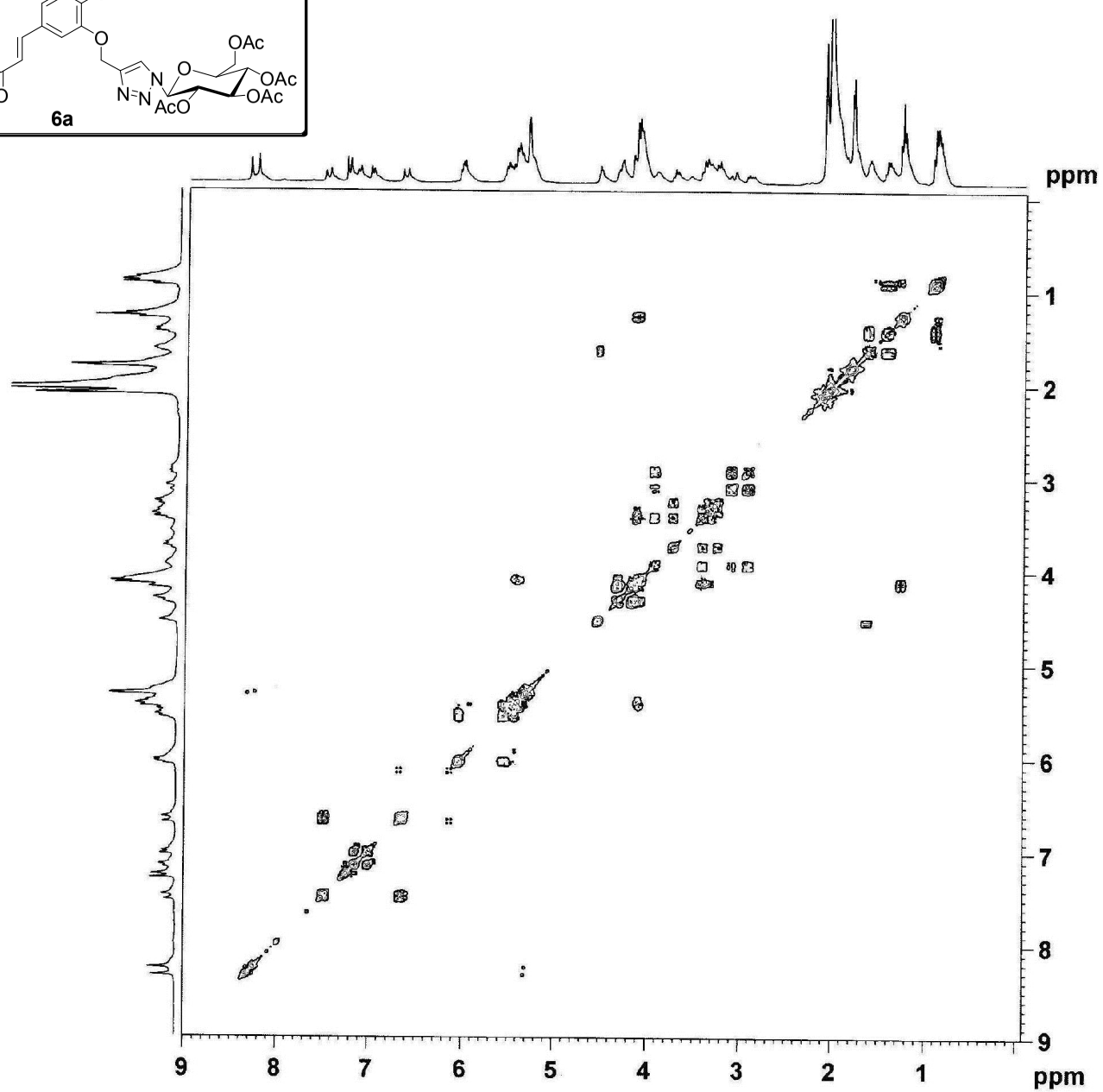


Figure 10 DEPT-135 spectrum (75 MHz, $CDCl_3$) of compound, 6a.





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PROCNO                      1

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Time                     0.44
INSTRUM                 spect
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PULPROG             cosyqf90
TD                      2048
SOLVENT                CDCl3
NS                        10
DS                         4
SWH                2723.312 Hz
FIDRES             1.329742 Hz
AQ                 0.3760628 sec
RG                        57
DW                  183.600 usec
DE                    6.00 usec
TE                   300.0 K
d0                0.00000300 sec
D1                1.95494401 sec
IN0               0.00036720 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                   13.15 usec
PL1                   0.00 dB
SFO1          300.1313400 MHz

F1 - Acquisition parameters
ND0                        1
TD                       256
SFO1           300.1313 MHz
FIDRES        10.637936 Hz
SW                 9.074 ppm
FnMODE                    QF

F2 - Processing parameters
SI                      1024
SF            300.1300000 MHz
WDW                     SINE
SSB                        0
LB                    0.00 Hz
GB                         0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                       QF
SF            300.1300000 MHz
WDW                     SINE
SSB                        0
LB                    0.00 Hz
GB                         0
```

Figure 11 ^{1}H-^{1}H [COSY] spectrum (300 MHz, $CDCl_3$) of compound, 6a.

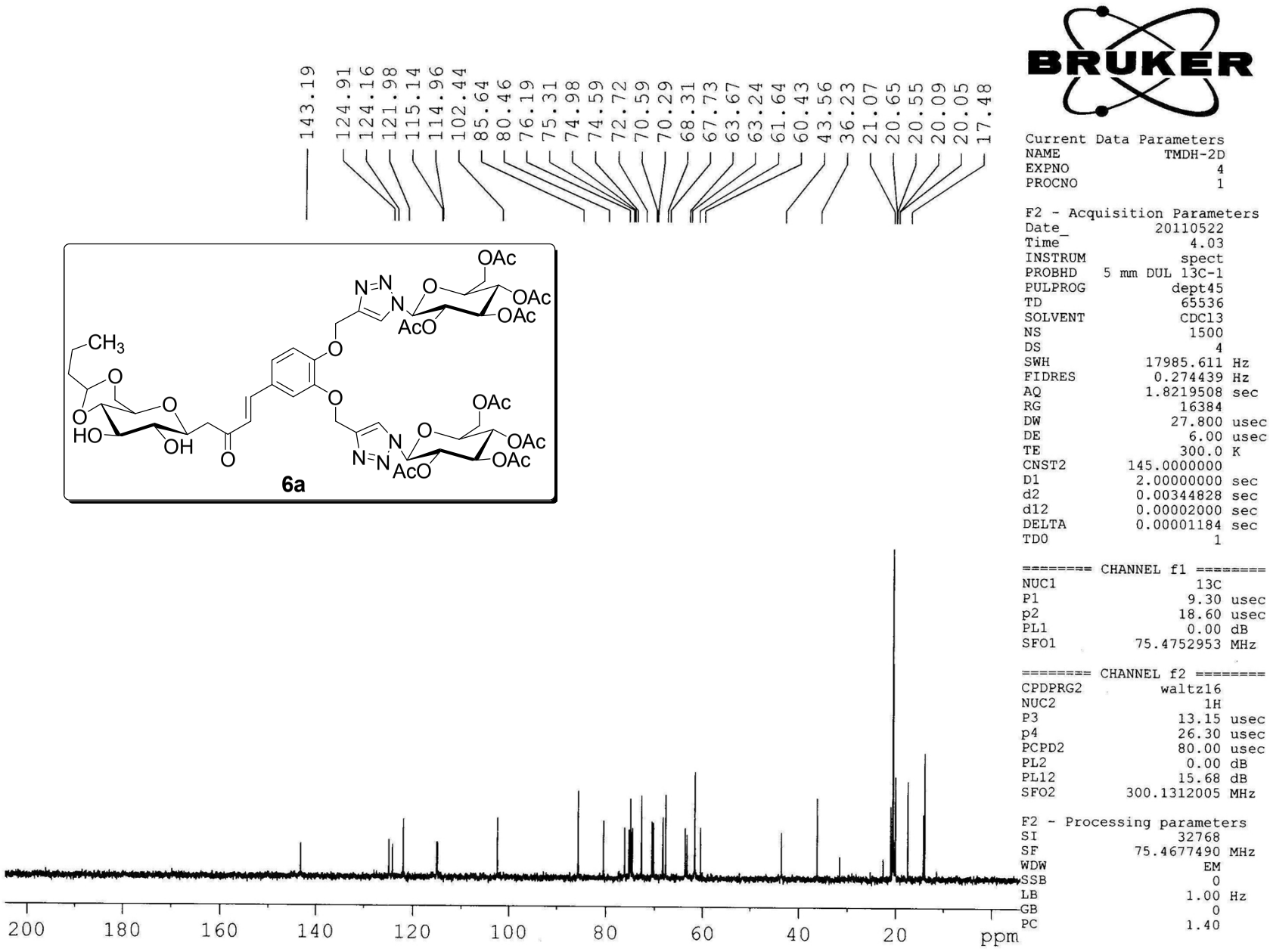
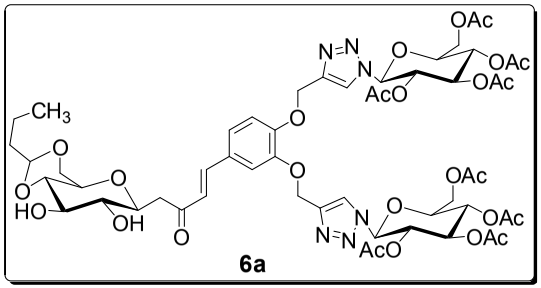
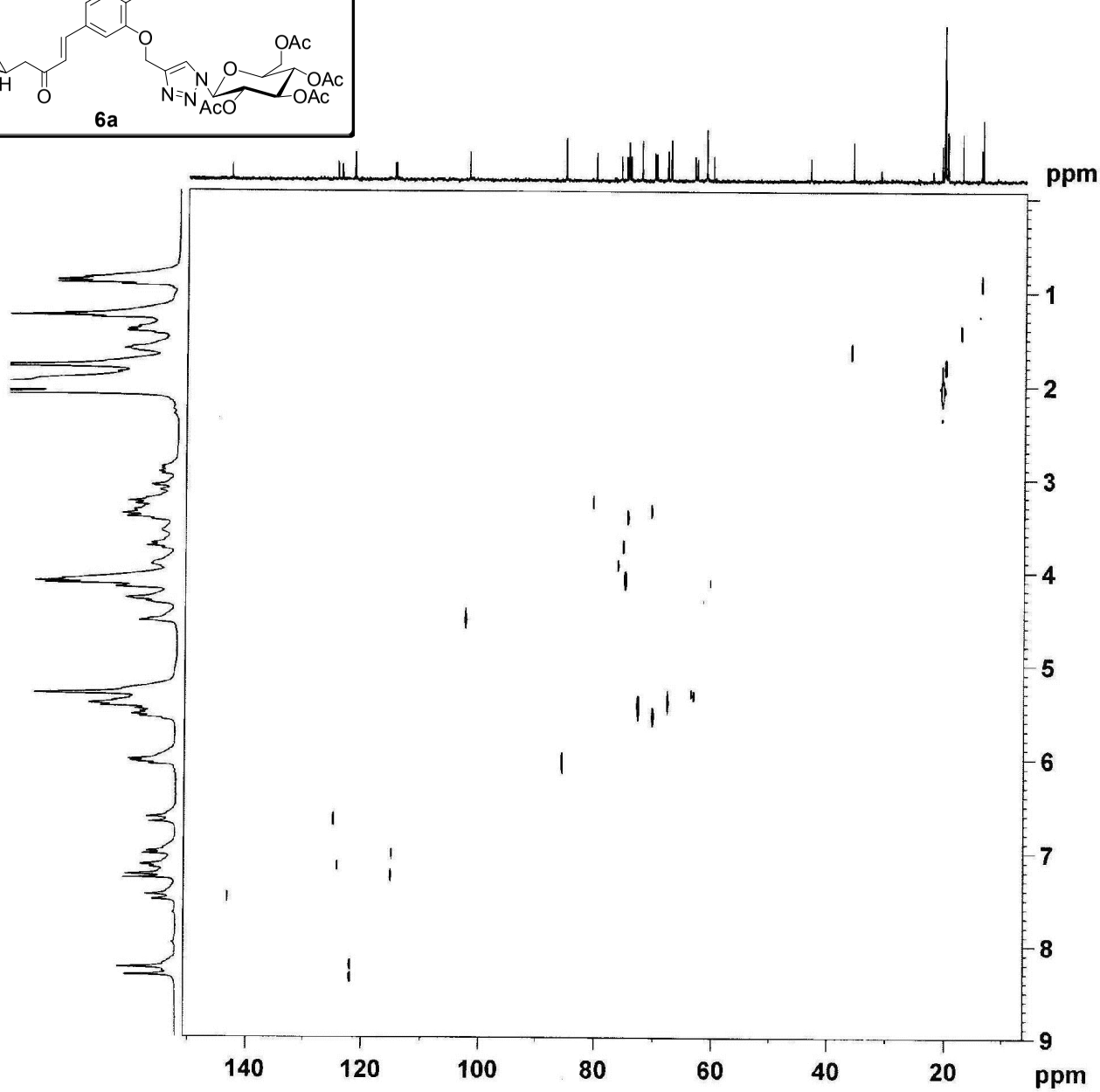
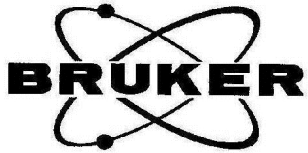


Figure 12 DEPT-45 spectrum (75 MHz, $CDCl_3$) of compound, 6a.





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PROCNO                      1

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PULPROG              hxcogf
TD                     4096
SOLVENT               CDCl3
NS                       10
DS                        4
SWH               10893.246 Hz
FIDRES             2.659484 Hz
AQ                 0.1880564 sec
RG                     16384
DW                  45.900 usec
DE                   6.00 usec
TE                   300.0 K
CNST2            145.0000000
CNST11             3.0000000
d0                 0.00000300 sec
D1                 1.97869599 sec
d2                 0.00344828 sec
d3                 0.00229885 sec
d11                0.03000000 sec
d12                0.00002000 sec
IN0                0.00018360 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                   9.30 usec
p2                  18.60 usec
PL1                   0.00 dB
SFO1           75.4736775 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
P3                  13.15 usec
PCPD2               80.00 usec
PL2                   0.00 dB
PL12                 15.68 dB
SFO2           300.1313400 MHz

F1 - Acquisition parameters
ND0                        2
TD                       128
SFO1             300.1313 MHz
FIDRES          21.275871 Hz
SW                   9.074 ppm
FnMODE                    QF

F2 - Processing parameters
SI                      2048
SF             75.4677490 MHz
WDW                    QSINE
SSB                        2
LB                    0.00 Hz
GB                         0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2                       QF
SF            300.1300000 MHz
WDW                    QSINE
SSB                        2
LB                    0.00 Hz
GB                         0
```

Figure 13 ^{1}H-^{13}C [COSY] spectrum (75 MHz, $CDCl_3$) of compound, 6a.

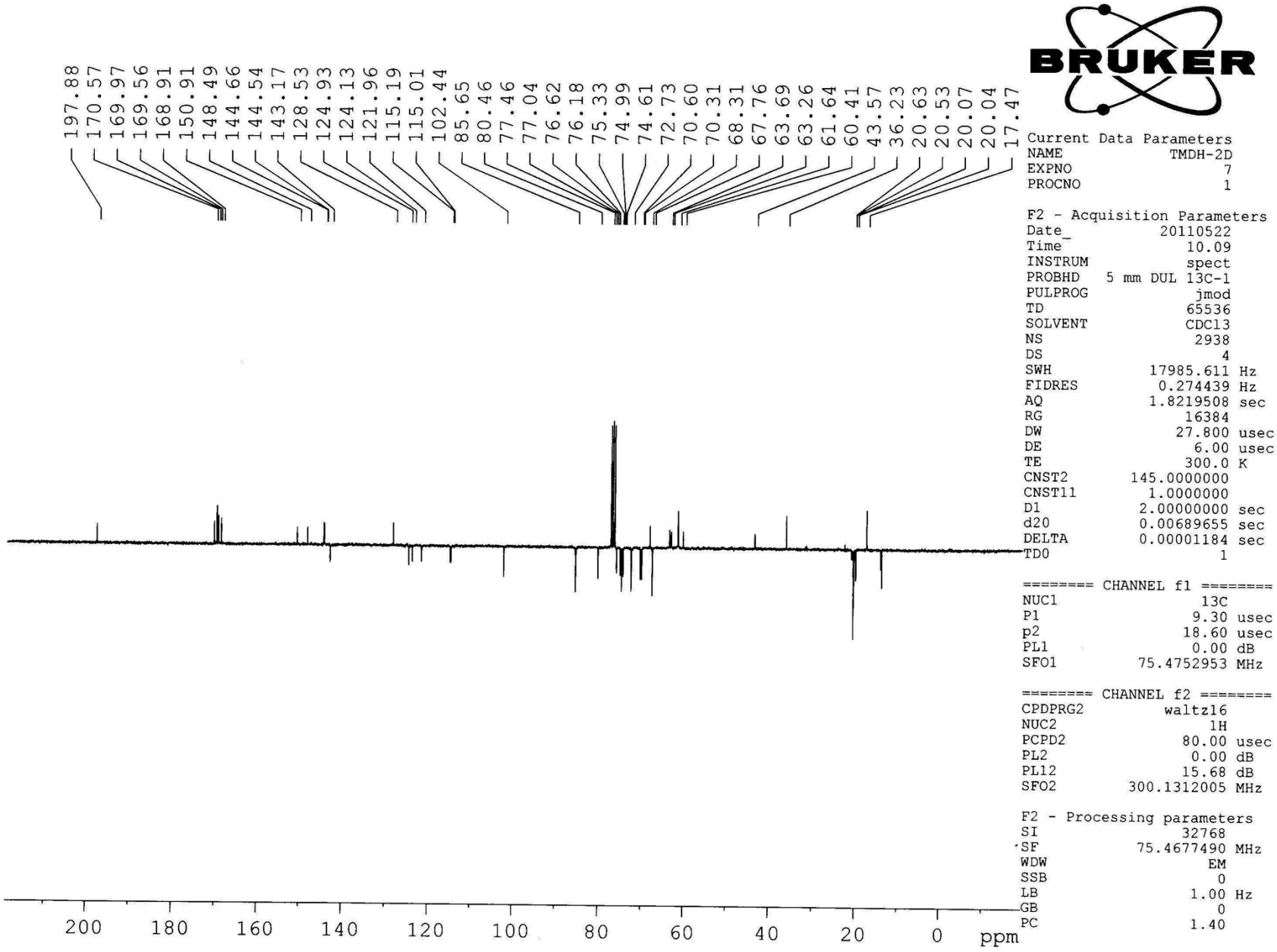


Figure 14 APT spectrum (75 MHz, $CDCl_3$) of compound, 6a.

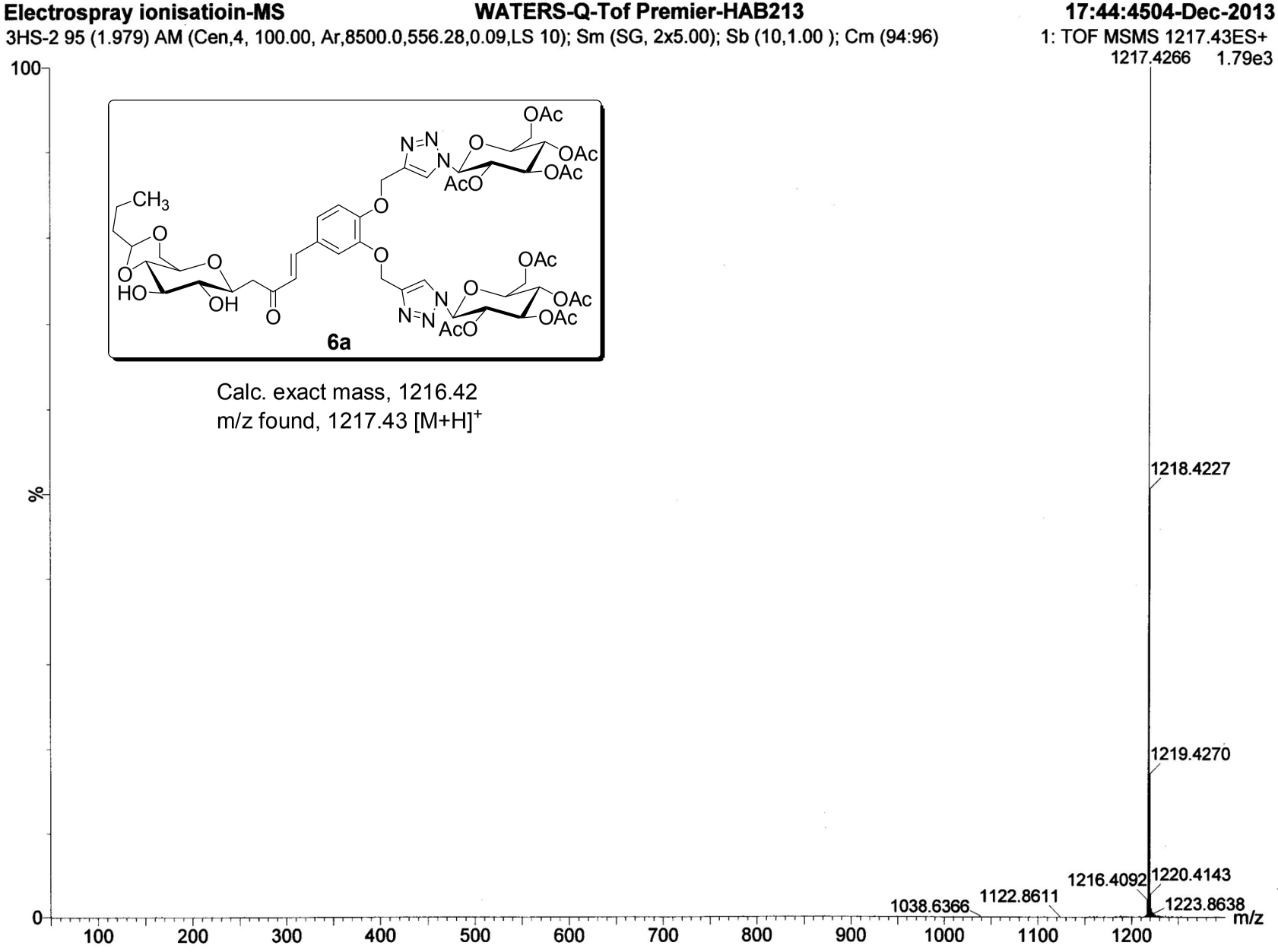


Figure 15 Mass spectrum of compound, 6a.

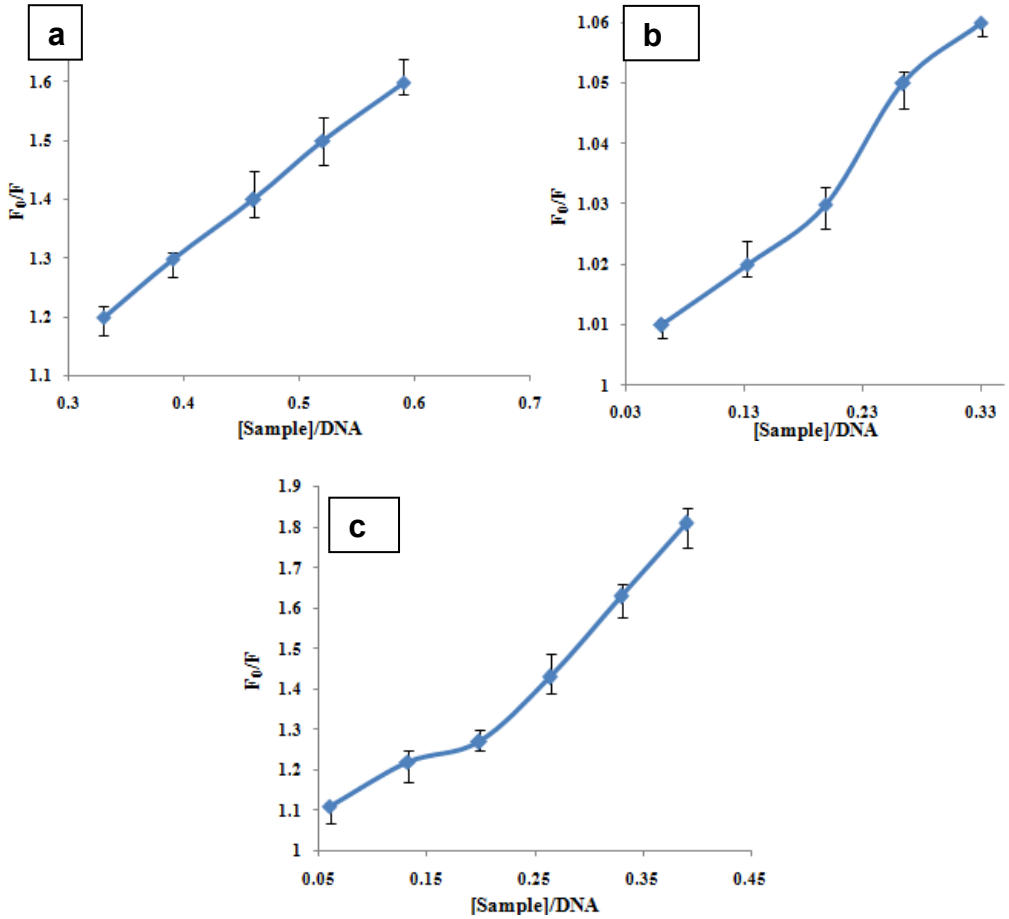


Figure 16 K_{sv} graph for compound, (a) **5**, (b) **6a** and (c) **6c** with protein (BSA)

Stern-Volmer equation $F_0/F=1+ K_{sv}[Q]$, where F_0 and F are the steady-state fluorescence intensities in the absence and presence of quencher respectively. [Q] is the concentration of quencher and K_{sv} is the Stern-Volmer quenching constant which in turn was obtained by plotting F_0/F vs [Q]. According to the equation, $KSV=Kq.\tau_0$, where Kq is the quenching rate constant and τ_0 is the fluorescence lifetime of protein in the absence of quencher, the value of τ_0 is considered to be 10^{-8} s.

Cyclic Voltammetric studies

The electrochemical behaviour of the ligand 6c without and with CT-DNA has been studied by cyclic voltammetry (CV) in acetonitrile containing 0.1 TBAP. In cyclic voltammetric study, the changes in the current of compound, **6c** with and without CT-DNA and BSA are depicted in **Figure 17**.

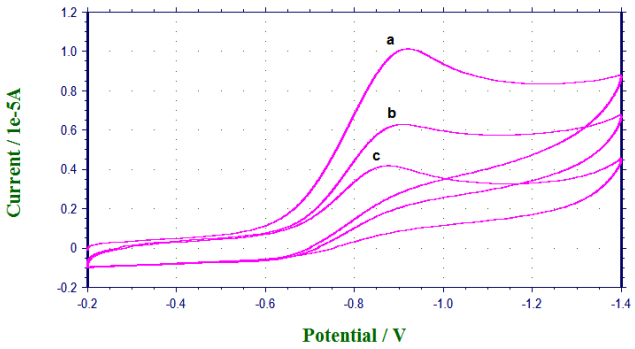


Figure 17 Cyclic voltammogram of compound, **6c** (a) without CT-DNA, (b) with CT-DNA, (c) with BSA; Scan rate: 0.1 Vs^{-1}

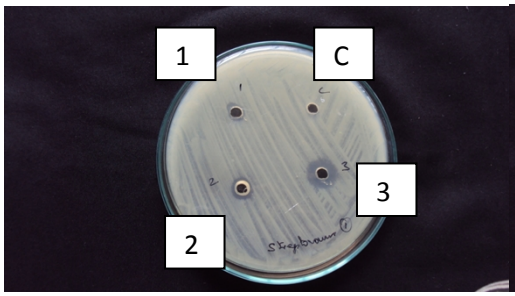
It was observed while recording CV for compound, **6c** in the forward scan, a single cathodic peak was observed at a potential of -0.92V with a current of $1x10^{-5}$A, which corresponds to the reduction of **6c** whereas in the reverse scan, no anodic peak was observed which indicates that the process is irreversible. When CT-DNA was added to the solution of **6c**, marked decrease in the peak current heights to $6.29x10^{-6}$A and shift in the peak potential to a slight positive value of -0.90V were observed. Similarly, addition of BSA to the ligand, **6c** clearly depresses the peak current height to $4.1x10^{-6}$A accompanied with the shift in the potential to -0.87V which is of higher extent compared to that of CT-DNA. These results not only provides an information about the interaction of compound, **6c** with both BSA and DNA but also an evident for the change in the electrochemical properties. Since the change with BSA observed is higher compared to that of CT-DNA, it means that the change in the electrochemical property of the compound, **6c** with BSA is higher compared to that of CT-DNA.

Antibacterial studies:

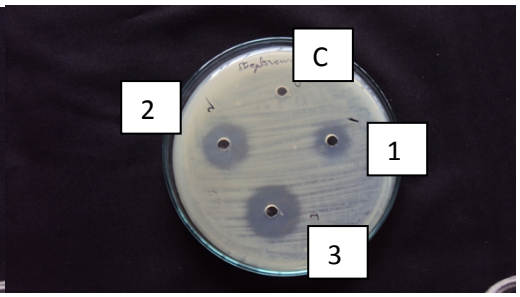
Figure 17. Zone of inhibition of compounds **5**, **6a** and **6c** by agar diffusion method

Streptococcus pyogenes

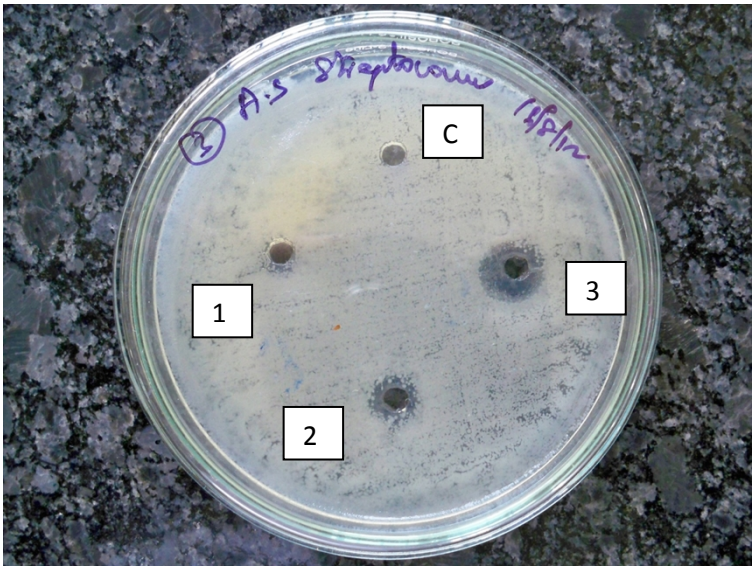
Compound 5



Compound 6a

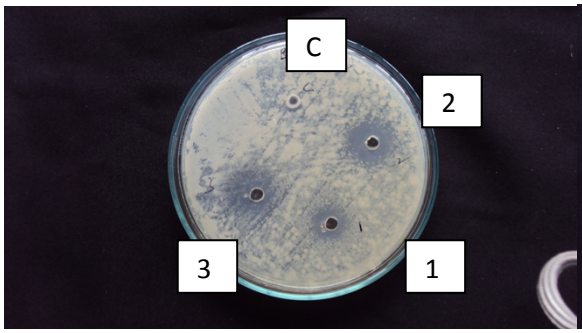


Compound 6c

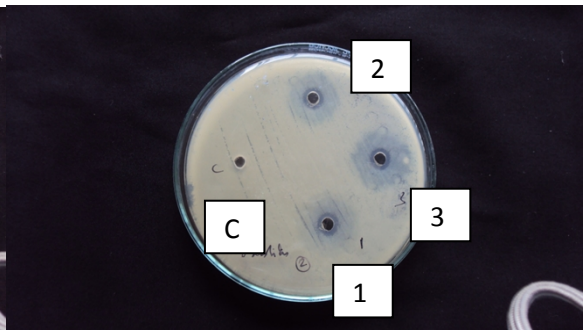


Bacillus subtilis

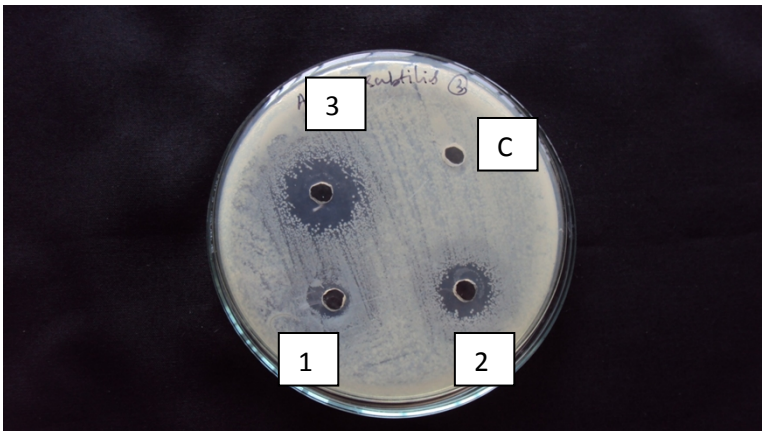
Compound 5



Compound 6a

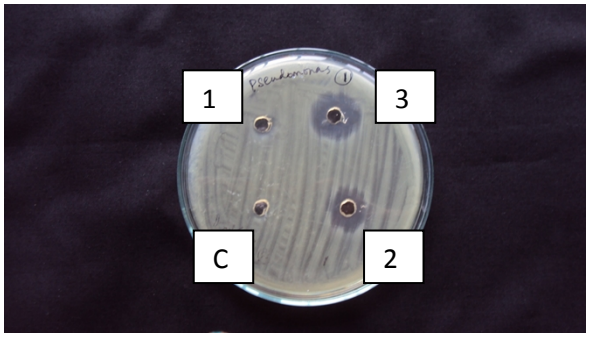


Compound 6c

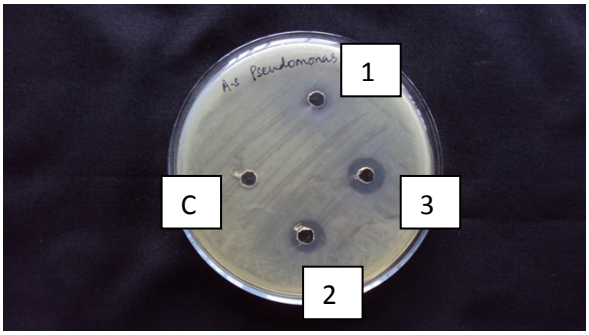


Pseudomonas aeruginosa

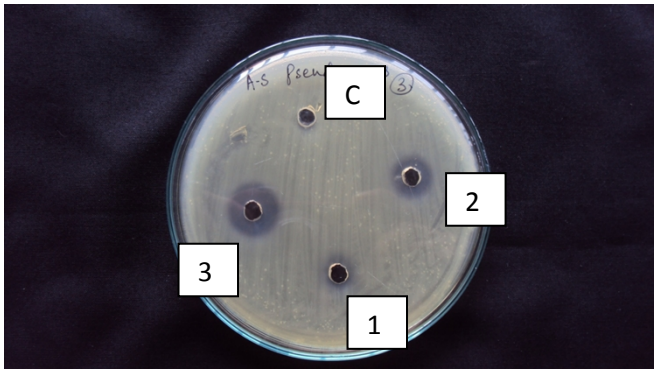
Compound 6a



Compound 5

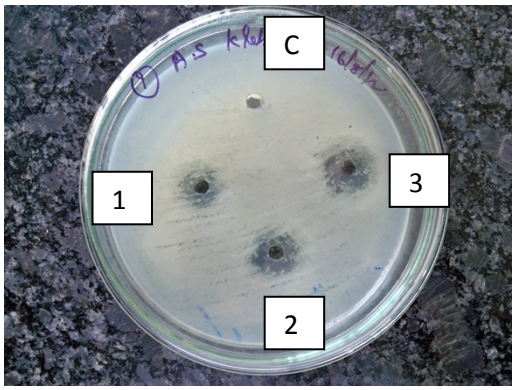


Compound 6c

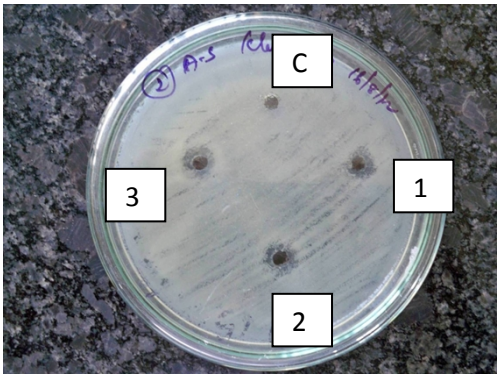


Klebsiella pneumoniae

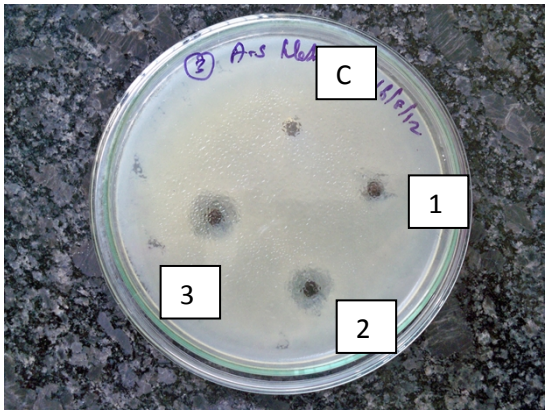
Compound 6a



Compound 5



Compound 6c



C – Control

1 - 25µL

2 - 50µL

3 - 75µL

Table 1. Inhibition effect of compounds **5**, **6a** and **6c** on growth of *Streptococcus pyogenes*.

S. No	Compounds	Zone of inhibition (diameter in mm)		
		25 µL (1%)	**50 µL (1%)**	**75 µL (1%)**
1	1	1	3	5
2	2	6	11	13
3	3	1	4	11
4	**Control**	NI	NI	NI

NI: No Inhibition

Table 2. Inhibition effect of compounds **5**, **6a** and **6c** on growth of *Bacillus subtilis*

S. No	Compounds	Zone of inhibition (diameter in mm)		
		25 µL (1%)	**50 µL (1%)**	**75 µL (1%)**
1	1	3	11	12
2	2	4	12	13
3	3	3	6	13
4	**Control**	NI	NI	NI

NI: No Inhibition

Table 3. Inhibition effect of compounds **5**, **6a** and **6c** on growth of *Pseudomonas aeruginosa*

S. No	Compounds	Zone of inhibition (diameter in mm)		
		25 µL (1%)	**50 µL (1%)**	**75 µL (1%)**
1	1	-	4	11
2	2	1	3	6
3	3	1	6	11

4	**Control**	NI	NI	NI

NI: No Inhibition

Table 4. Inhibition effect of compounds **5**, **6a** and **6c** on growth of *Klebsiella pneumoniae*

S. No	**Compounds**	**Zone of inhibition (diameter in mm)**		
		25 µL (1%)	**50 µL (1%)**	**75 µL (1%)**
1	1	5	6	8
2	2	1	2	3
3	3	1	3	5
4	**Control**	NI	NI	NI

NI: No Inhibition