

**Supplementary Information**  
**for**  
**Synthesis of  $\beta$ -Analogues of C-Mannosyltryptophan, a Novel**  
**C-Glycosylamino acid Found in Proteins**

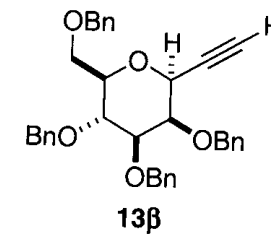
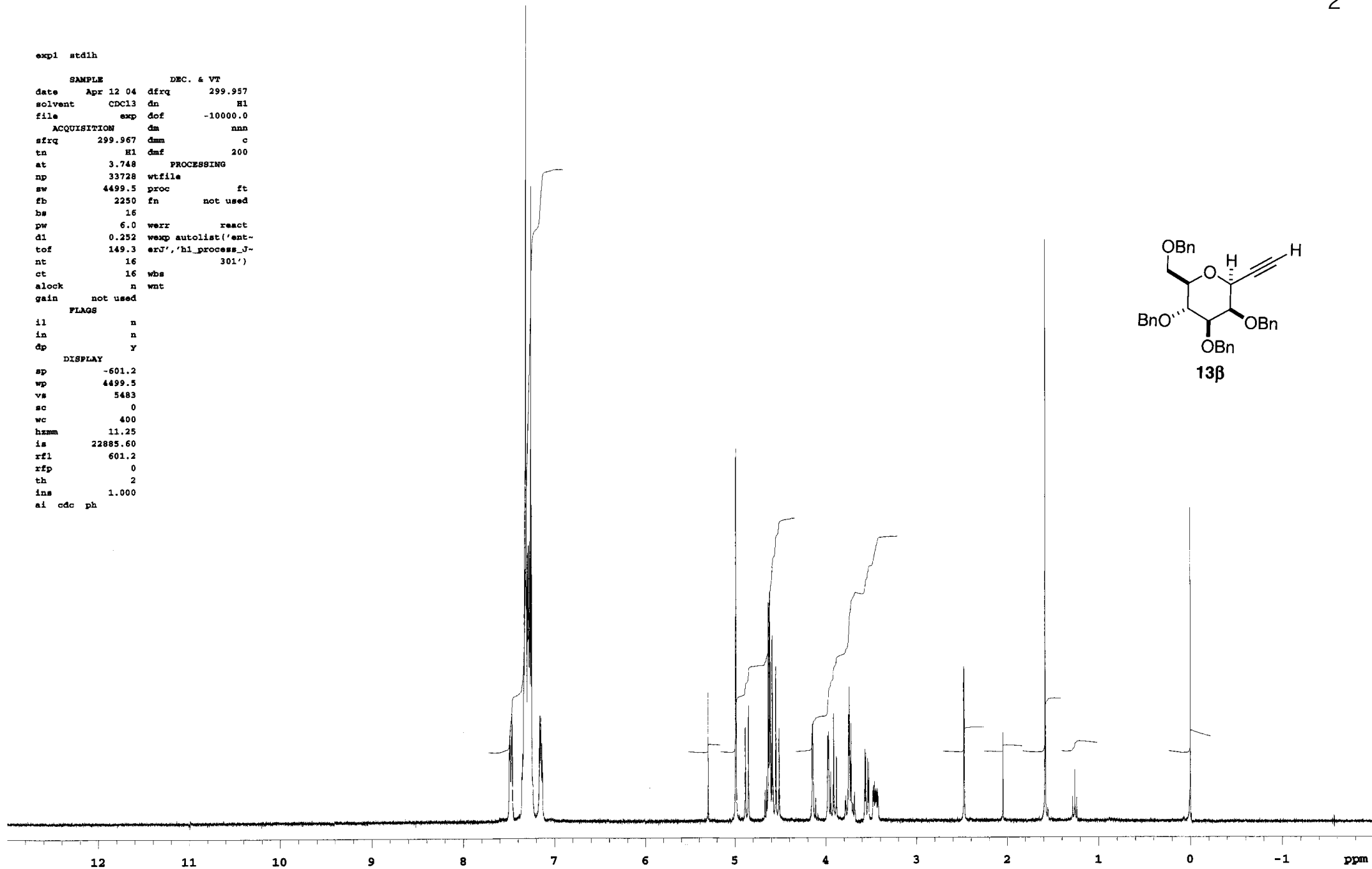
Toshio Nishikawa,<sup>a,b,\*</sup> Yuya Koide,<sup>a</sup> Akira Kanakubo,<sup>a</sup> Hiroshi Yoshimura,<sup>a</sup> and Minoru Isobe<sup>a,\*</sup>

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Nagoya University, Chikusa, Nagoya 464-8601, Japan*

*<sup>b</sup>PRESTO, Japan Science and Technology Agency*

expi stdlh

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date	Apr 12 04	dfrq	299.957
solvent	CDCl3	dn	H1
file	exp	dof	-10000.0
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at	3.748	dmf	200
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tof	149.3	erJ', 'hl_process_J-	
nt	16		301')
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alock	n	wnt	
gain	not used		
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il	n		
in	n		
dp	y		
DISPLAY			
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va	5483		
sc	0		
wc	400		
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ai	cdc ph		

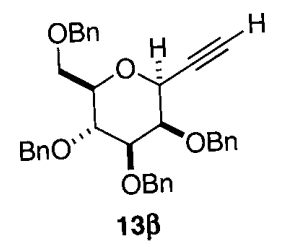
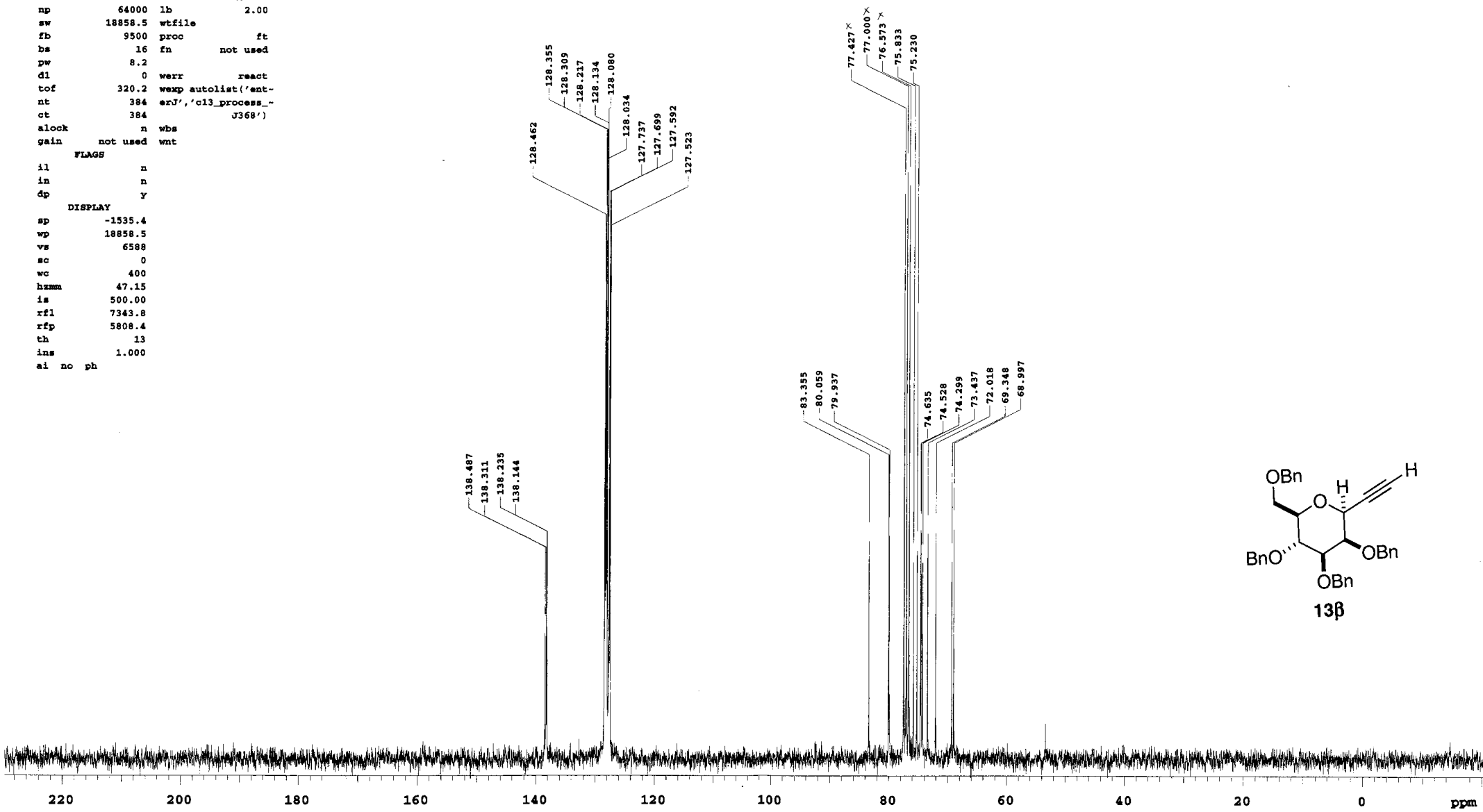


expl std13c

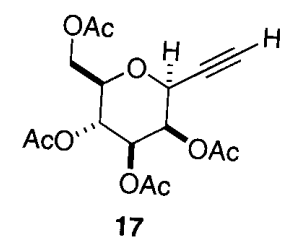
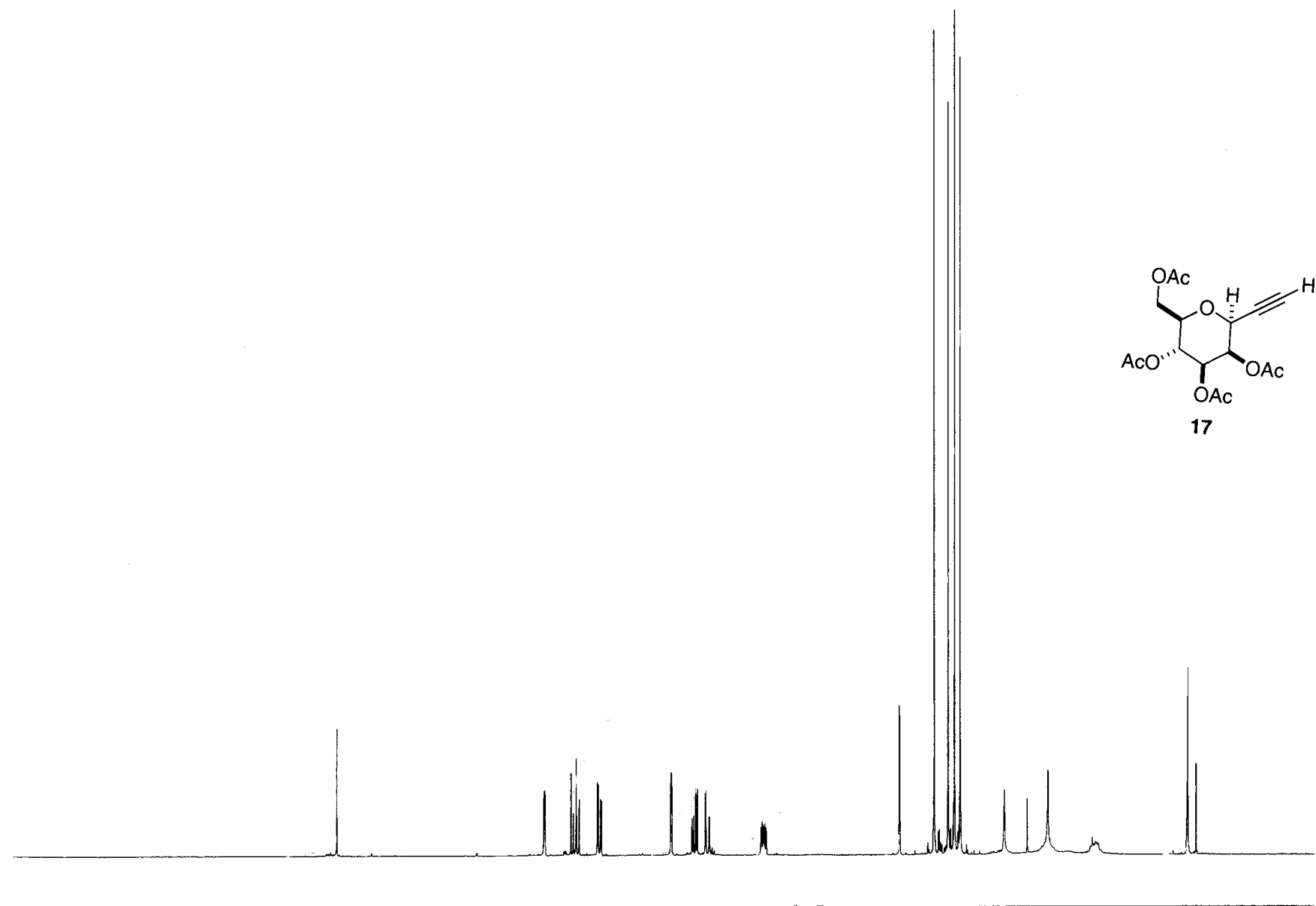
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ct 384 J368')
alock n wbs
gain not used vnt

FLAGS
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in n
dp Y

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Ac-III



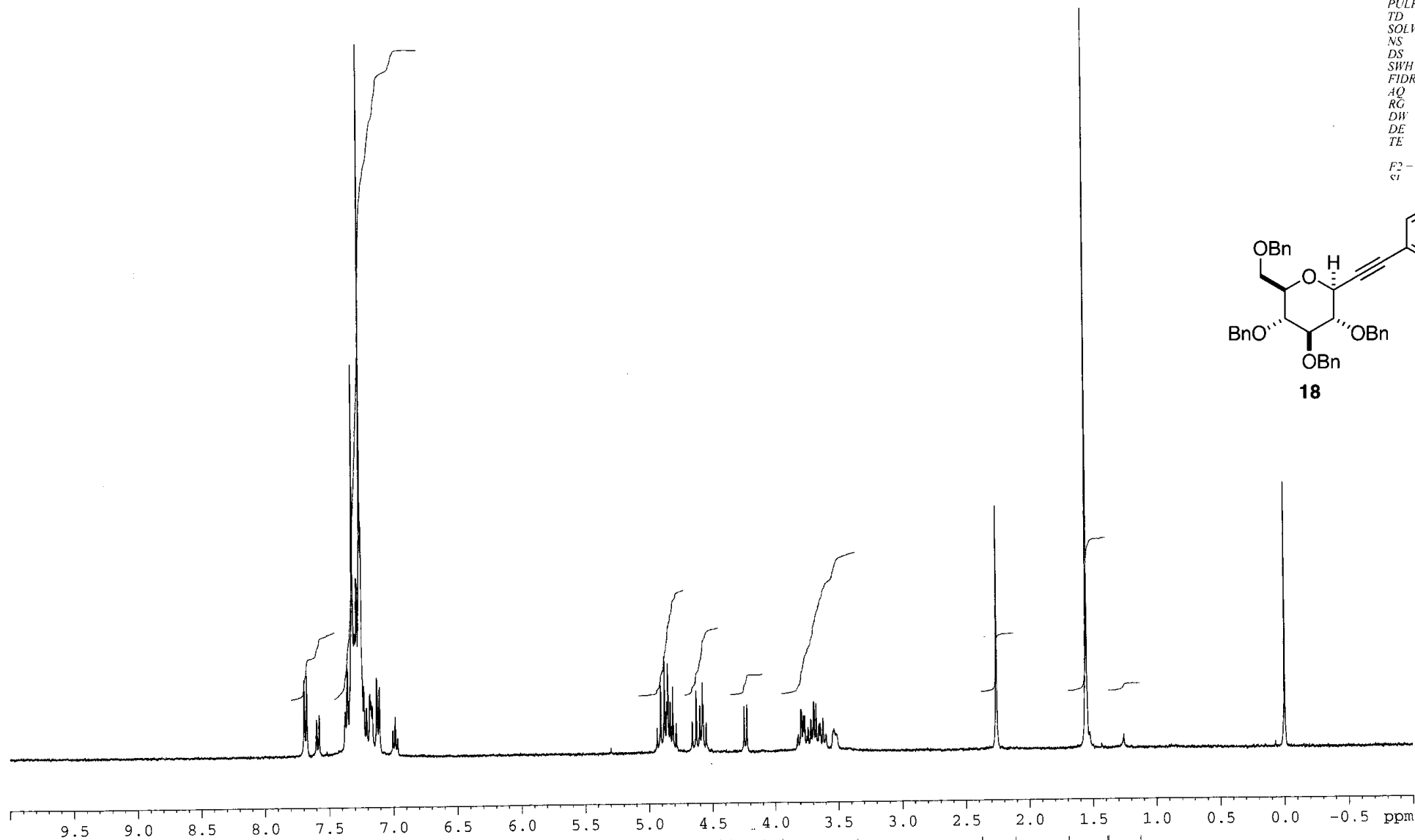
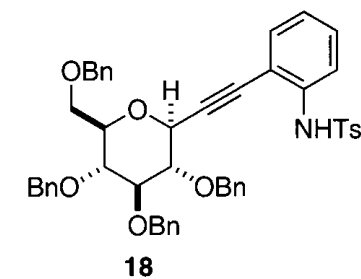
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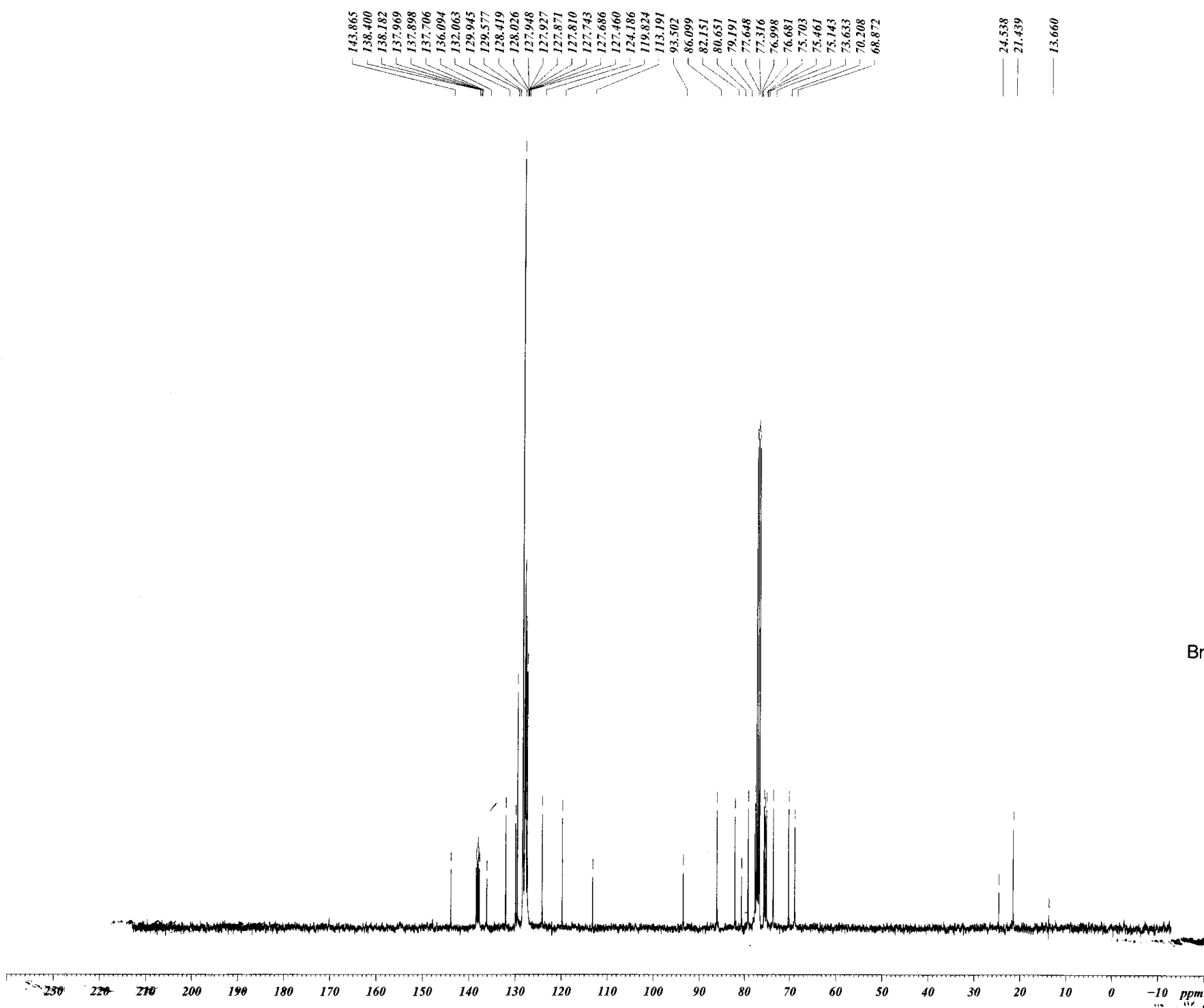
M1



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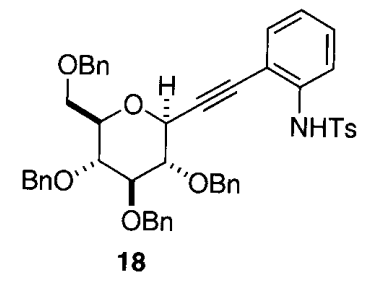
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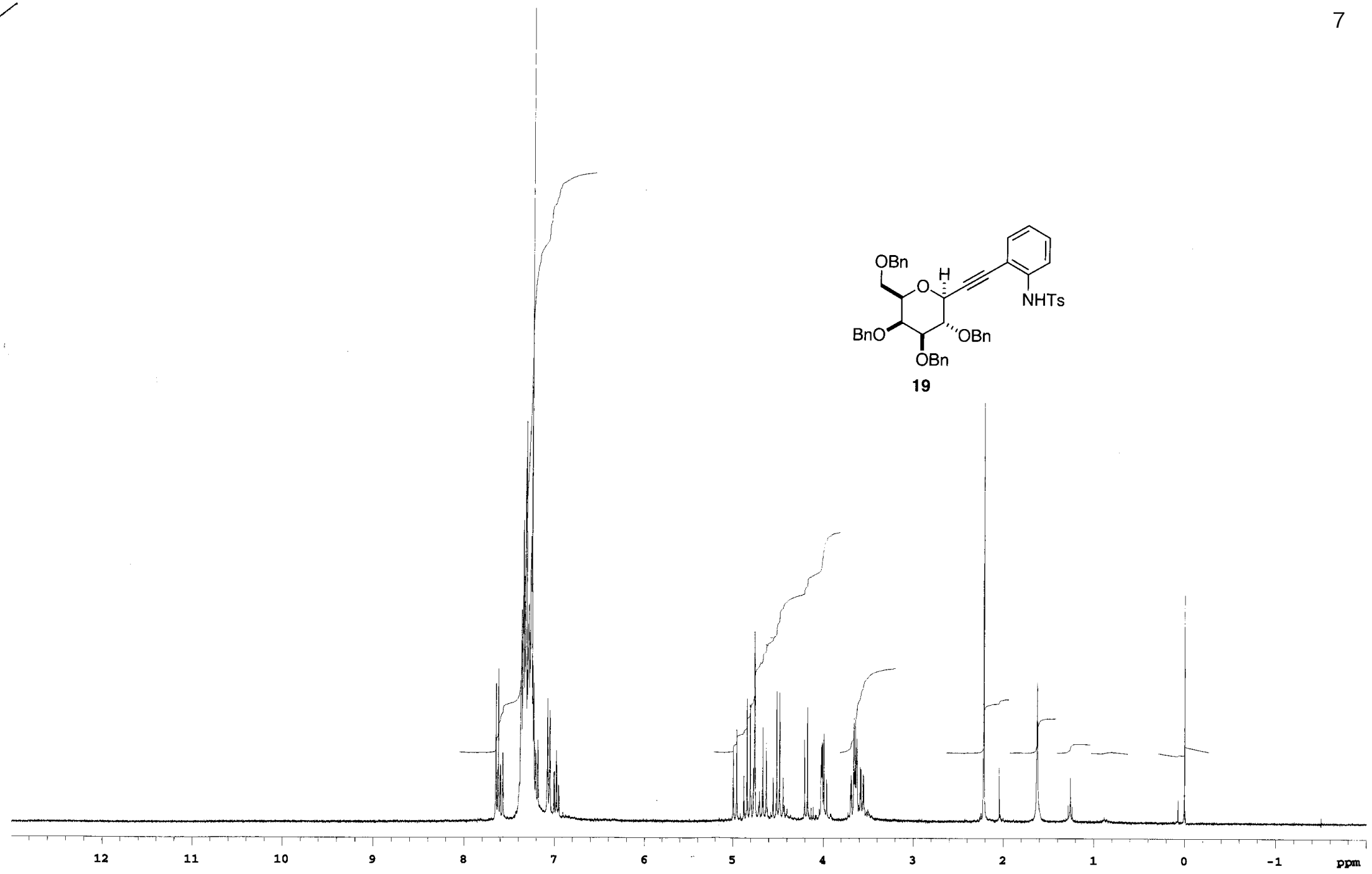
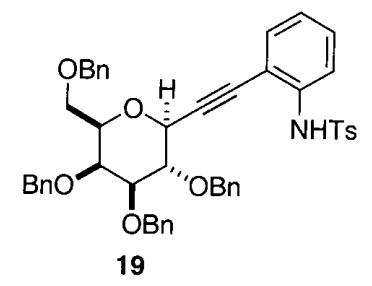


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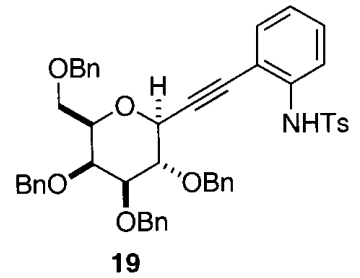
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F2 - Processing parameters  
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*1H NMR spectrum*



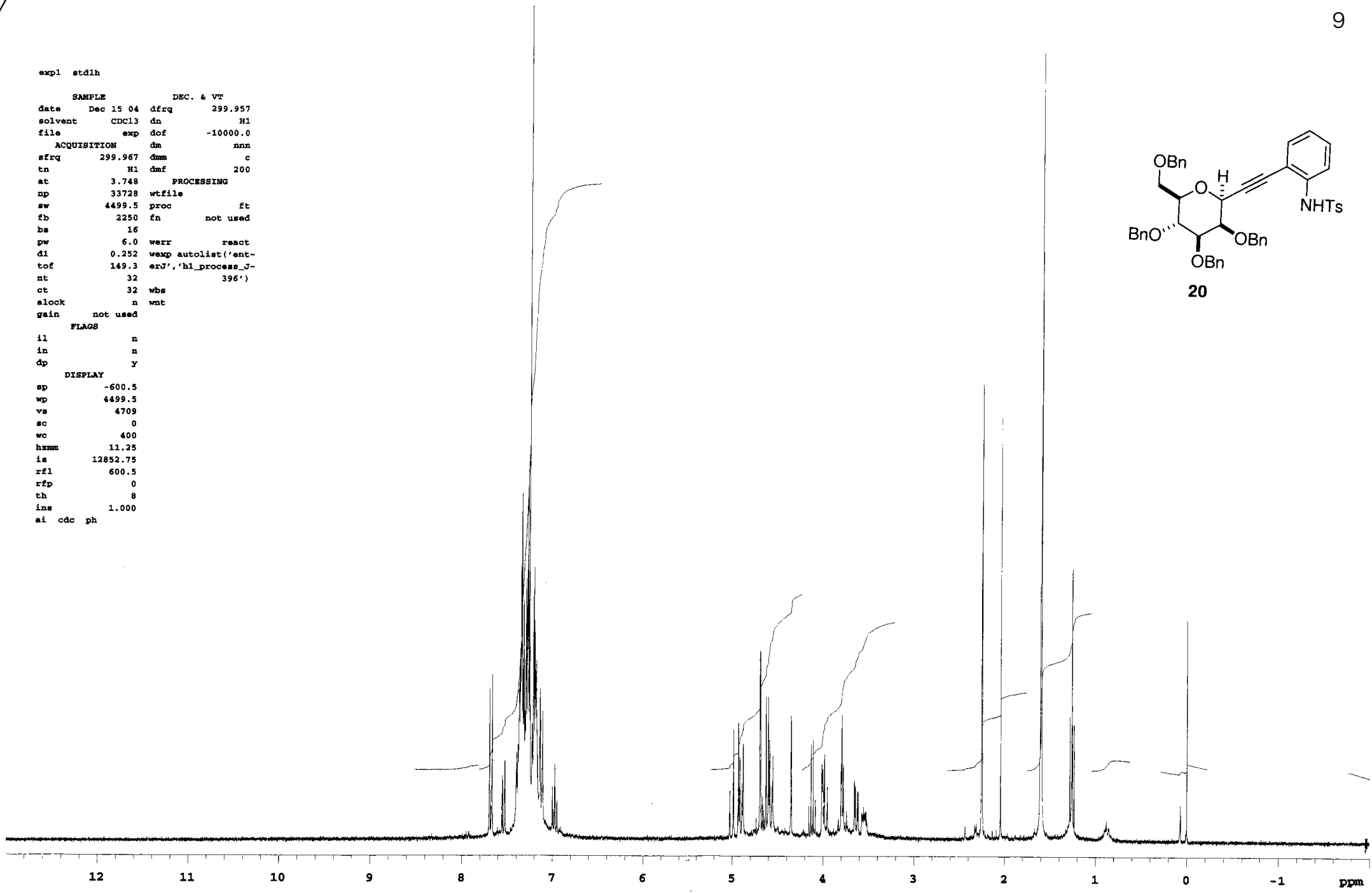
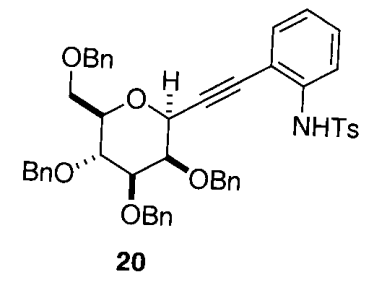
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 H26: 34  
 N2: 2  
 O5: 5

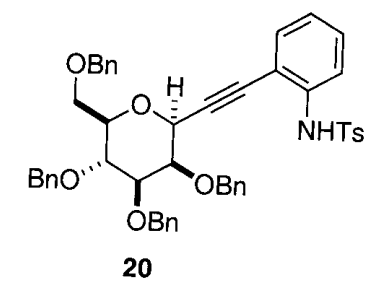
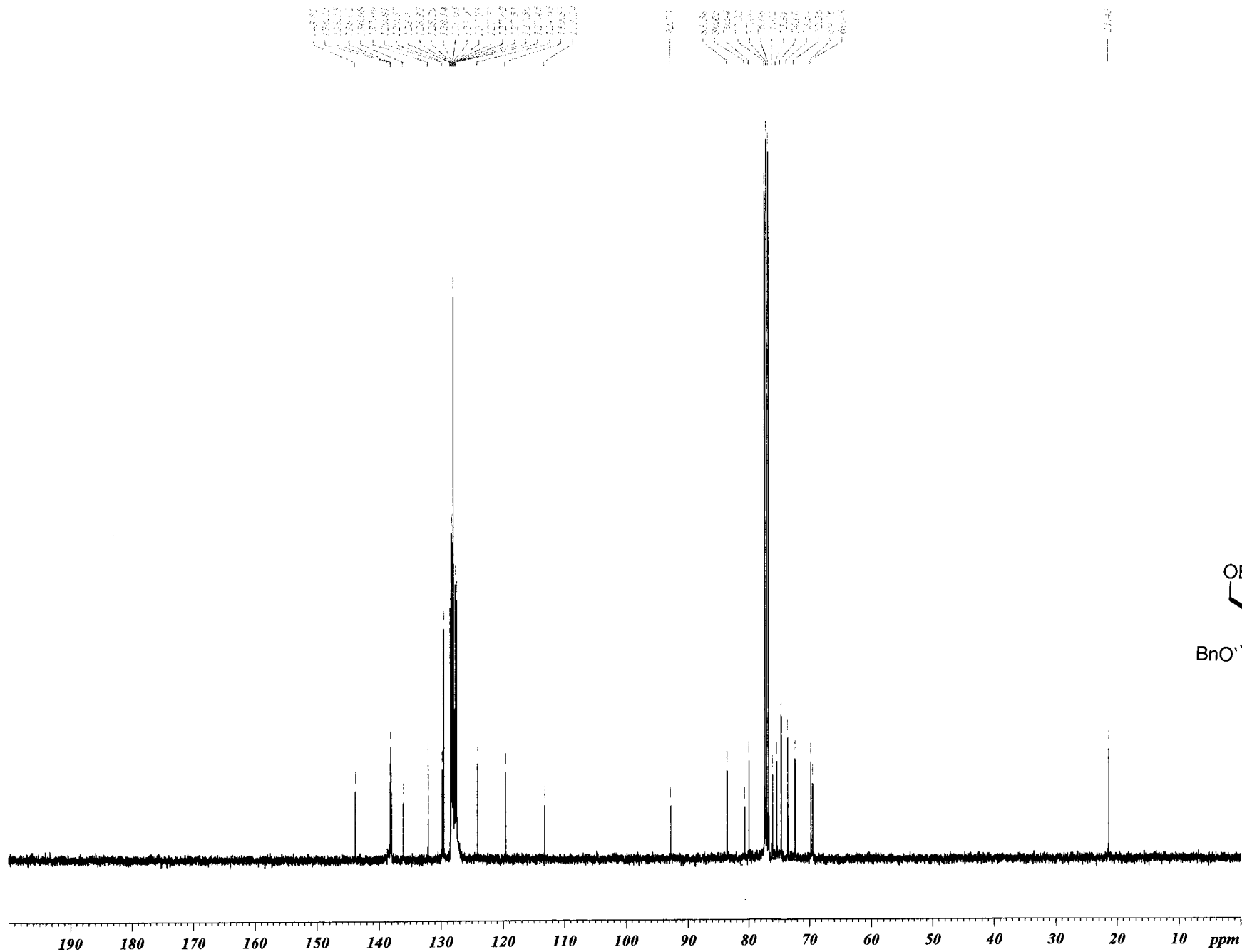
*13C NMR (CDCl3) parameters*

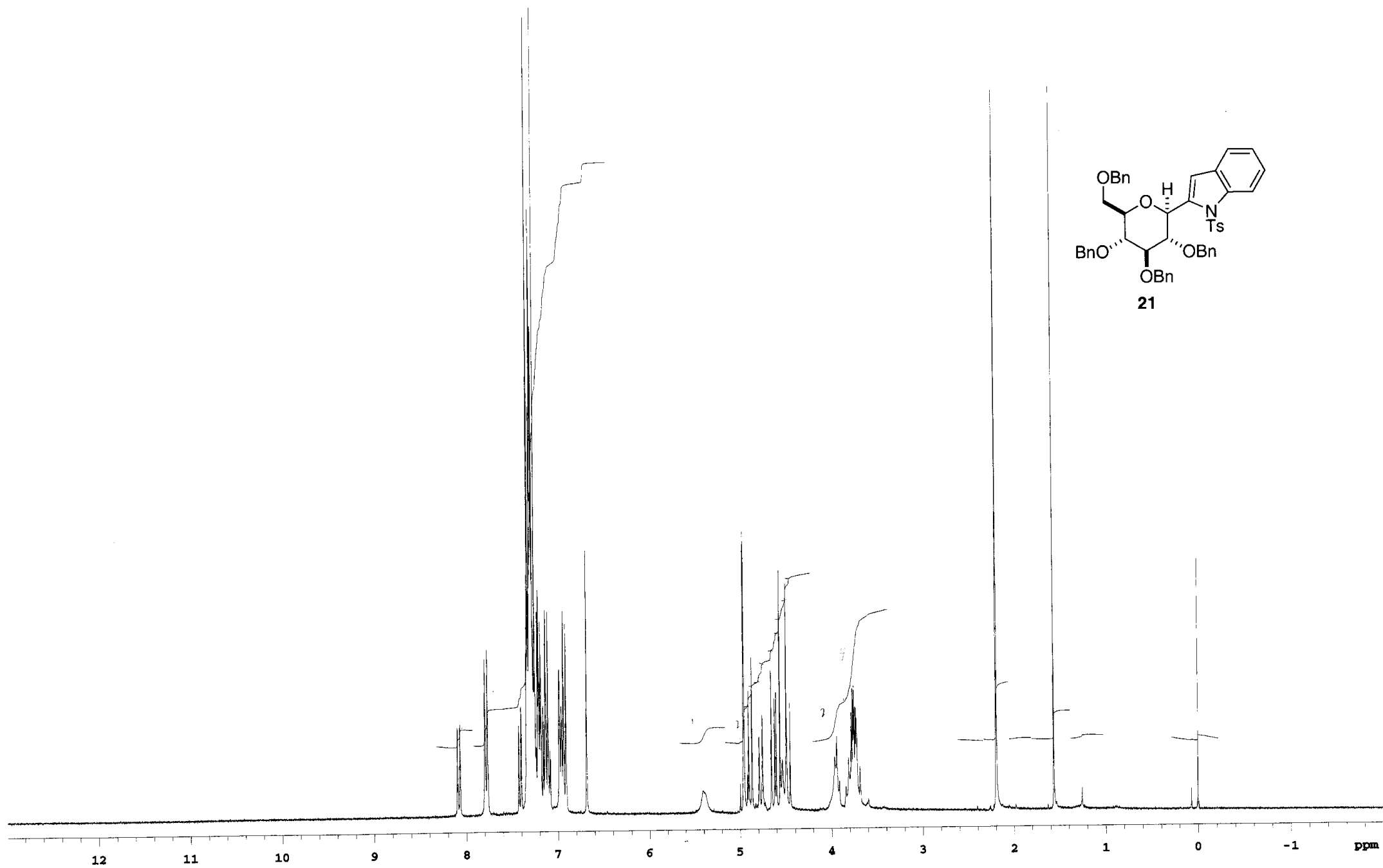
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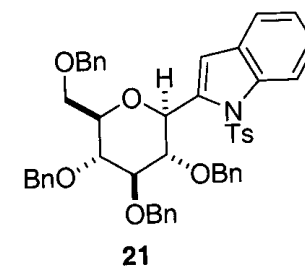
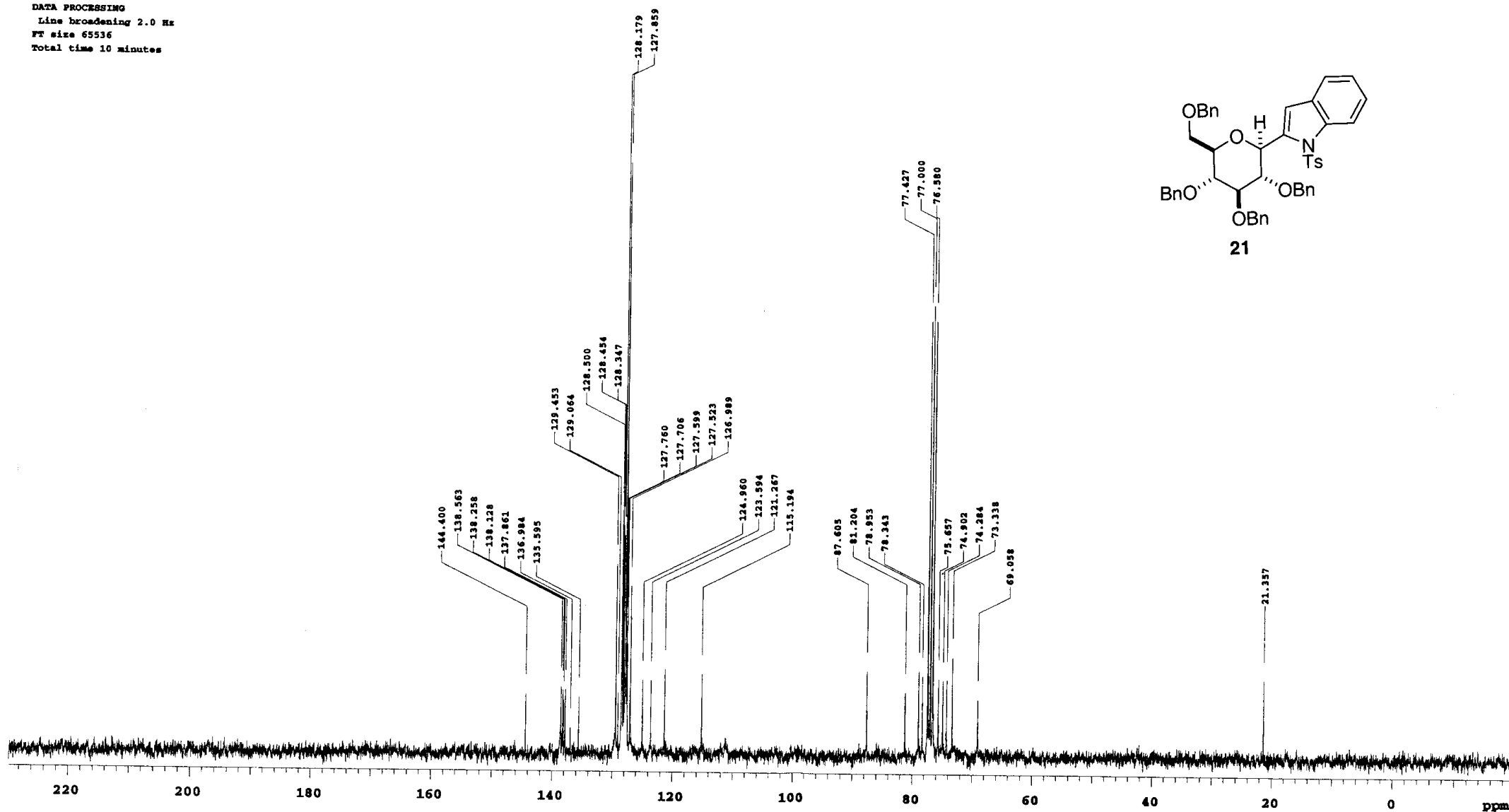
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solvent  CDCl3    dn      H1
file     exp     dof     -10000.0
ACQUISITION    dm      nnn
sfrq     299.967 dmm     c
tn       H1     dmf     200
at       3.748   PROCESSING
np       33728  wtfile
sw       4499.5 proc     ft
fb       2250  fn      not used
bs       16
pw       6.0   werr     react
dl       0.252 wexp autolist('ent-
tof      149.3  erJ', 'hl_process_J-
nt       32    396')
ct       32   wbs
alock    n     wat
gain     not used
FLAGS
il        n
in        n
dp        y
DISPLAY
sp        -600.5
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vs        4709
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ai cdc ph
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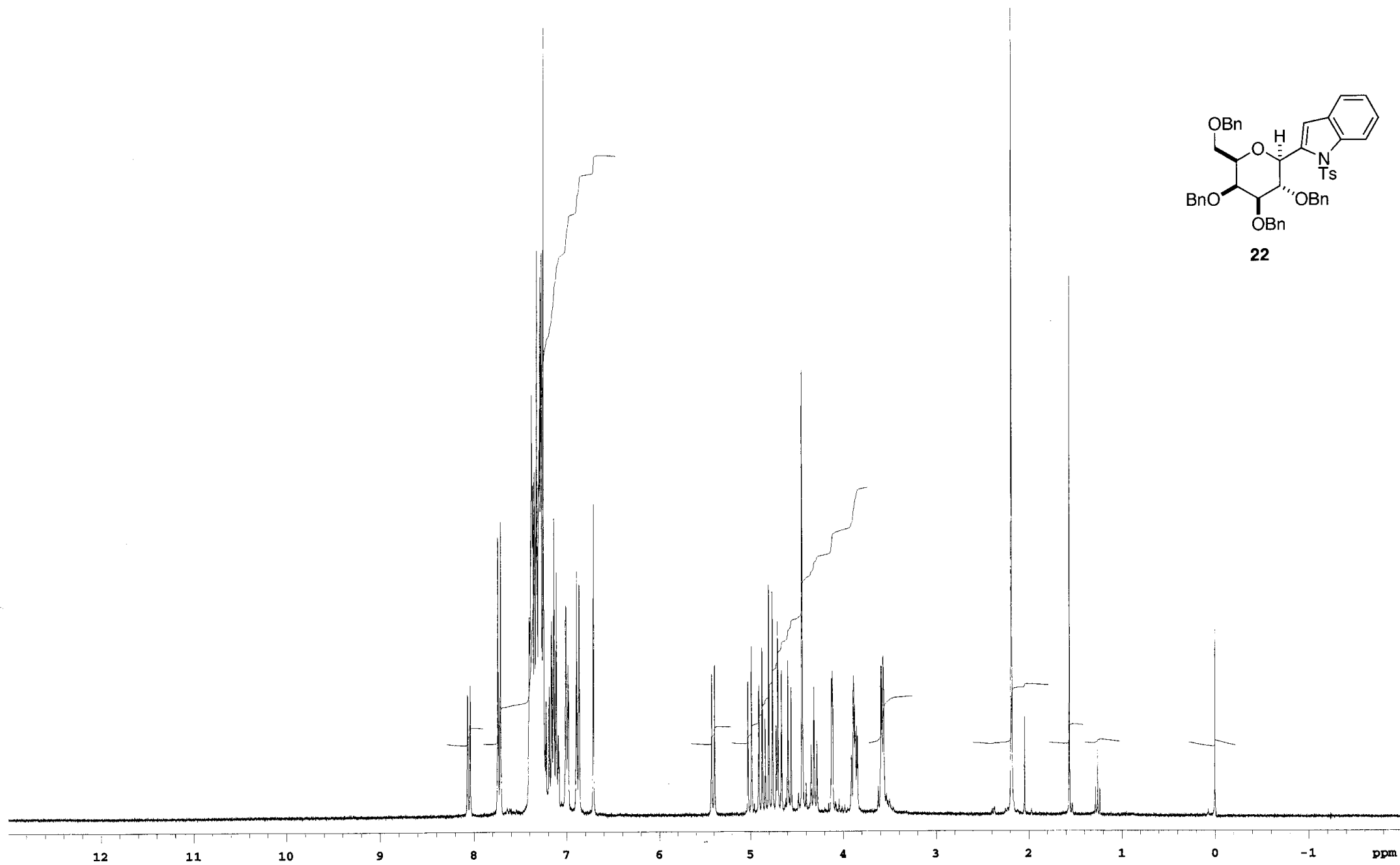
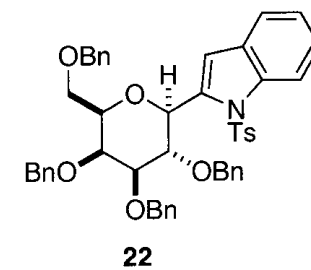






Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 GEMINI-300 "varian"  
 PULSE SEQUENCE  
 Pulse 35.0 degrees  
 Acq. time 1.697 sec  
 Width 18858.5 Hz  
 384 repetitions  
 OBSERVE C13, 75.4264075 MHz  
 DECOUPLE H1, 299.9672195 MHz  
 Power 30 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 2.0 Hz  
 FT size 65536  
 Total time 10 minutes



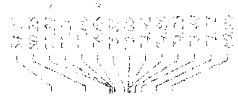


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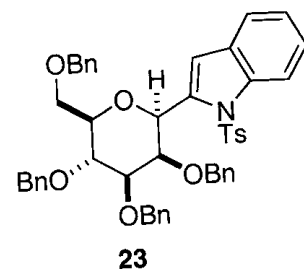


10/10

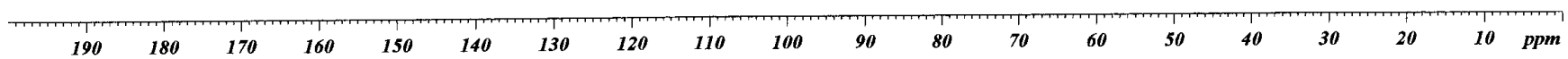


4.23  
X  
2.2  
2.1

X  
2.2  
2.1



13C NMR (101 MHz, CDCl<sub>3</sub>)  
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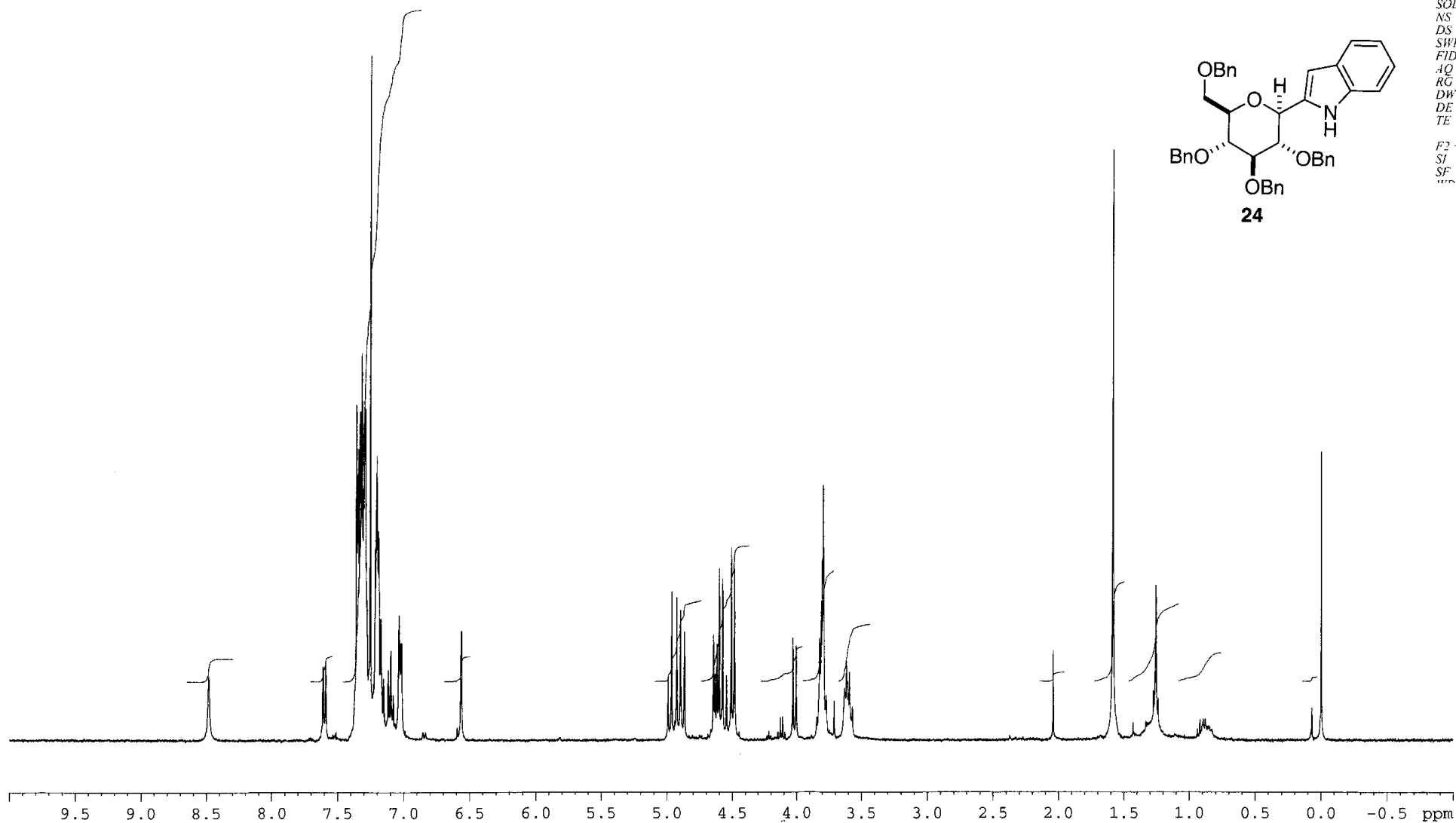
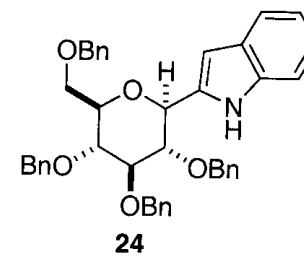




Current Data Parameters  
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 EXPNO 21  
 PROCNO 1

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 Time 2.47  
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 PROBHD 5 mm QNP  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCL3  
 NS 8  
 DS 2  
 SWH 6410.256 Hz  
 FIDRES 0.195625 Hz  
 AQ 2.5559540 sec  
 RG 1430  
 DW 78.000 usec  
 DE 97.50 usec  
 TE 300.0 K

F2 - Processing parameters  
 SI 16384  
 SF 400.1343969 MHz



Solvent: CDCl<sub>3</sub>  
 Ambient temperature  
 GEMINI-300 "varian"

## PULSE SEQUENCE

Pulse 35.0 degrees  
 Acq. time 1.697 sec  
 Width 18858.5 Hz  
 384 repetitions

OBSERVE C13, 75.4264086 MHz

DECOUPLE H1, 299.9672195 MHz

Power 30 dB

continuously on

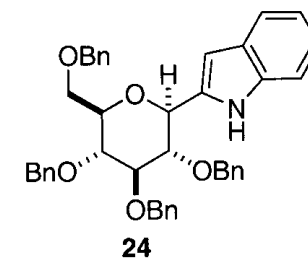
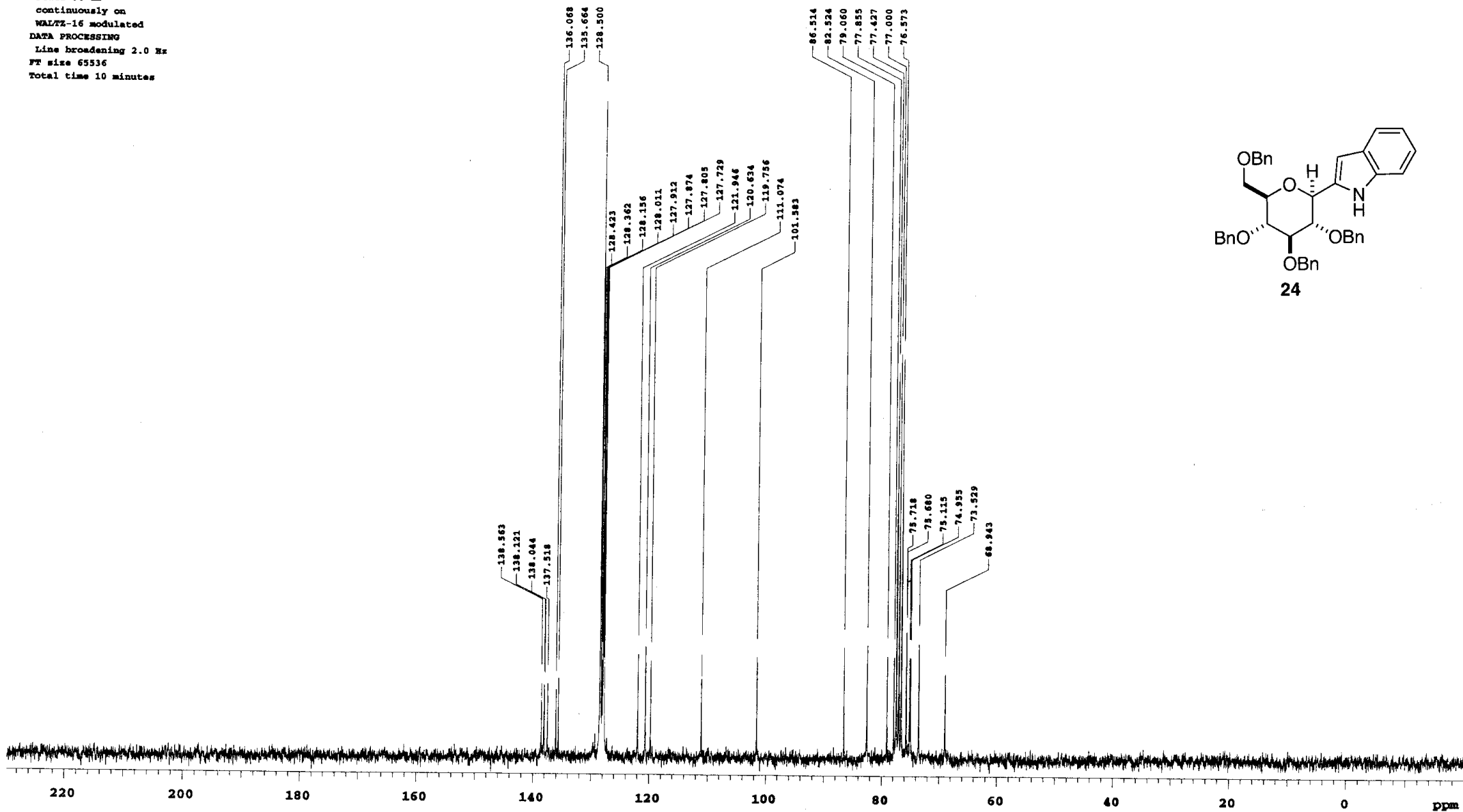
WALTZ-16 modulated

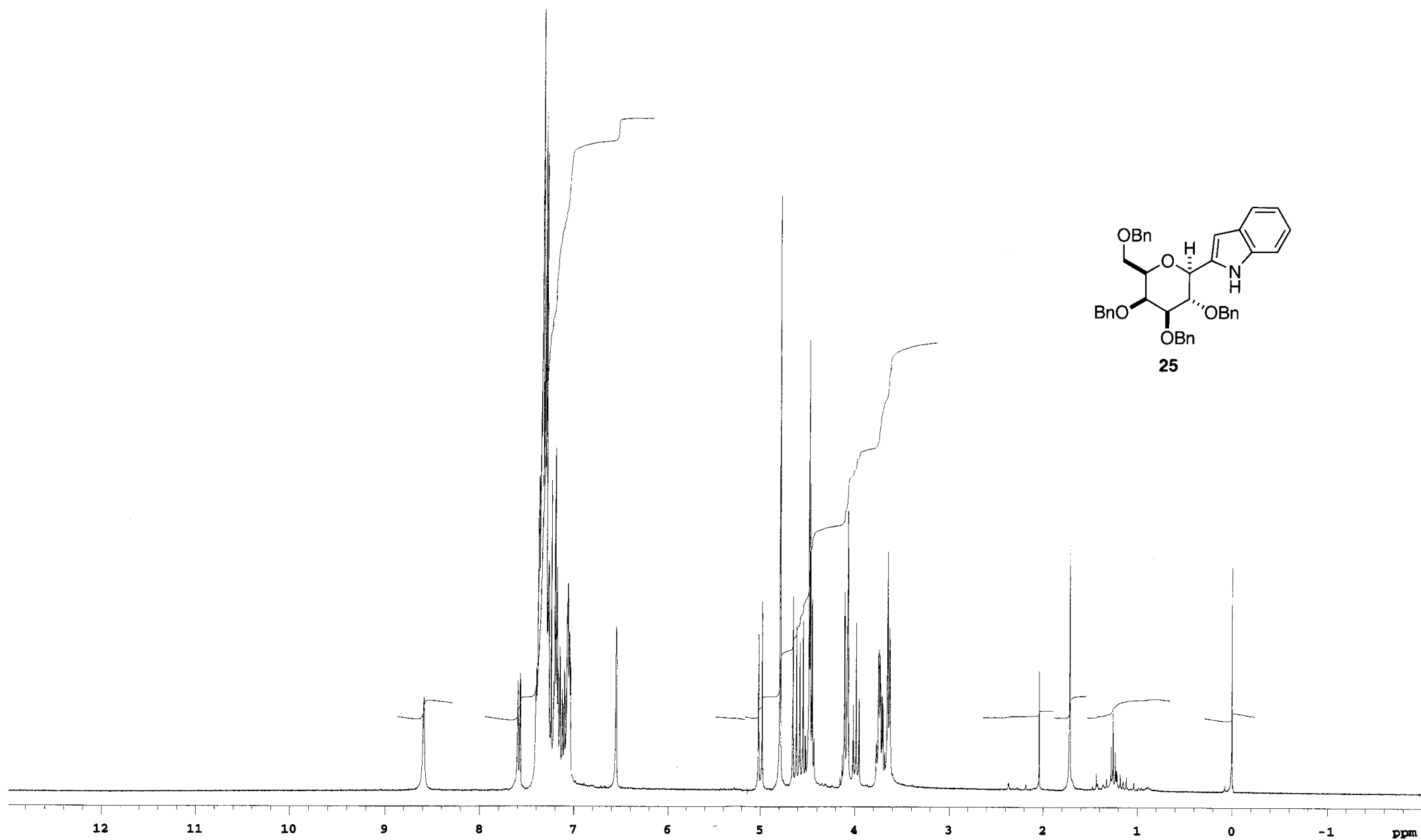
DATA PROCESSING

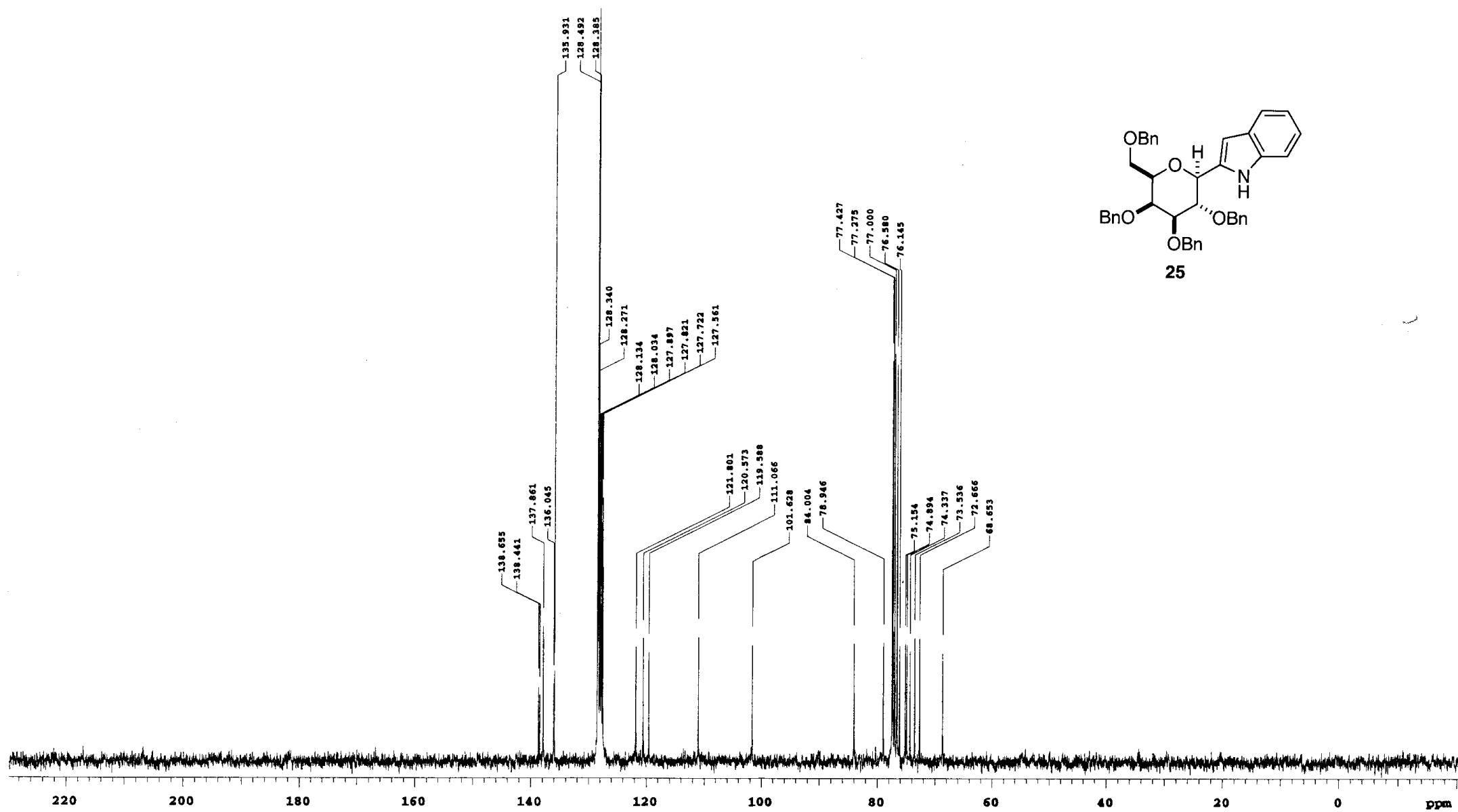
Line broadening 2.0 Hz

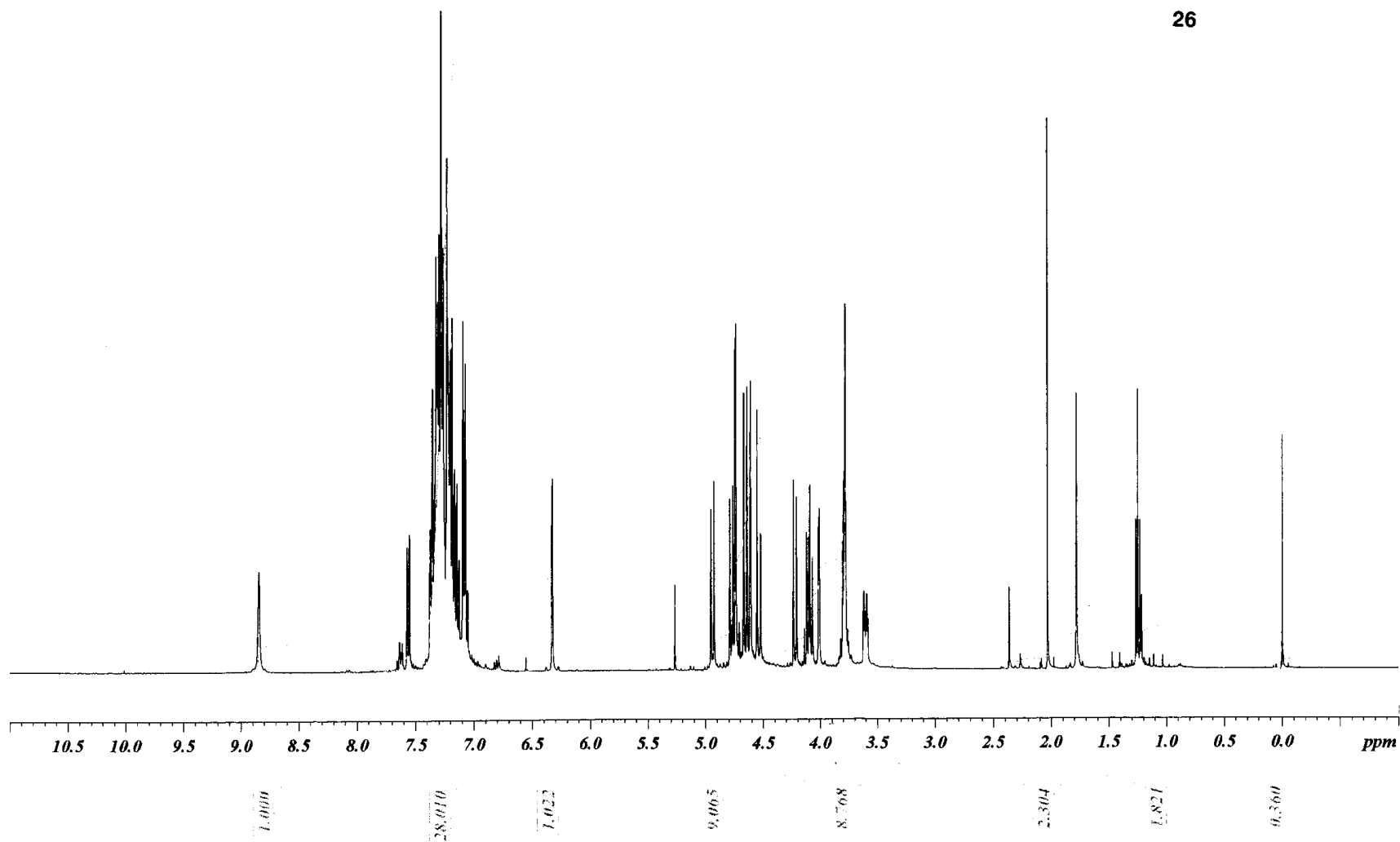
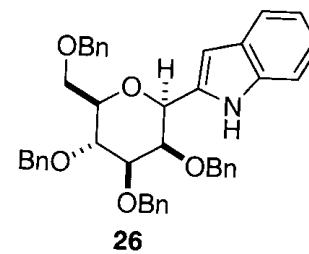
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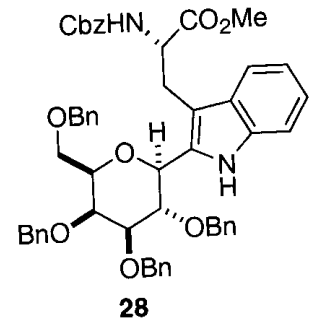
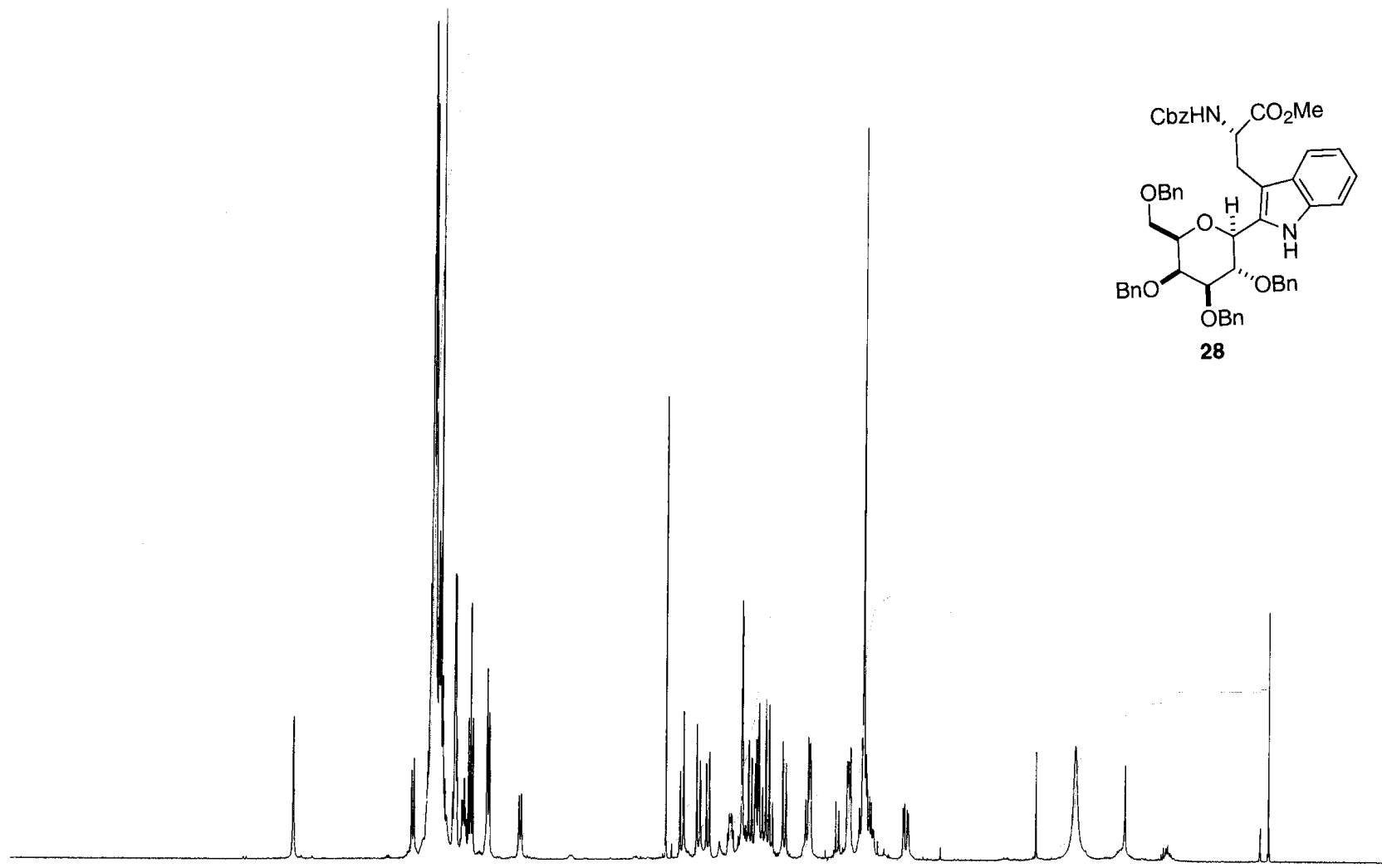






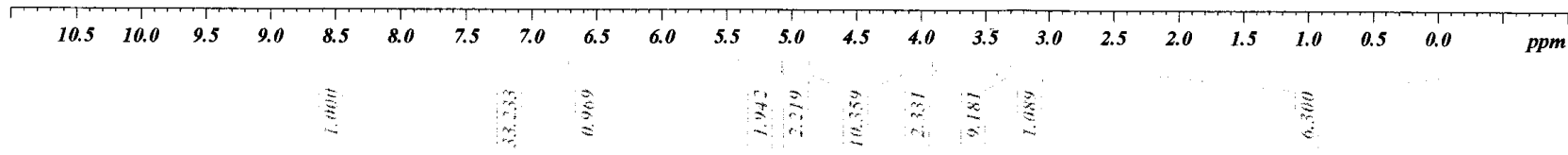




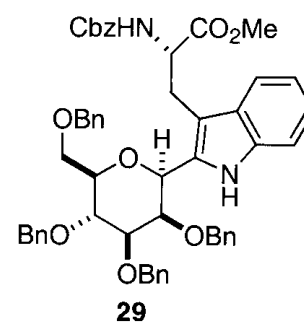


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 MW: 514.54  
 C<sub>28</sub>H<sub>36</sub>N<sub>2</sub>O<sub>7</sub>  
 Formula: COC(=O)C[C@@H](c1ccccc1)C[C@H]2O[C@@H](COC(=O)c3ccccc3)[C@H](OC(=O)c4ccccc4)[C@@H](OC(=O)c5ccccc5)[C@H]2OC(=O)c6ccccc6  
 SMILES: COC(=O)C[C@@H](c1ccccc1)C[C@H]2O[C@@H](COC(=O)c3ccccc3)[C@H](OC(=O)c4ccccc4)[C@@H](OC(=O)c5ccccc5)[C@H]2OC(=O)c6ccccc6  
 InChI: COC(=O)C[C@@H](c1ccccc1)C[C@H]2O[C@@H](COC(=O)c3ccccc3)[C@H](OC(=O)c4ccccc4)[C@@H](OC(=O)c5ccccc5)[C@H]2OC(=O)c6ccccc6  
 InChIKey: COC(=O)C[C@@H](c1ccccc1)C[C@H]2O[C@@H](COC(=O)c3ccccc3)[C@H](OC(=O)c4ccccc4)[C@@H](OC(=O)c5ccccc5)[C@H]2OC(=O)c6ccccc6

*Handwritten signature*





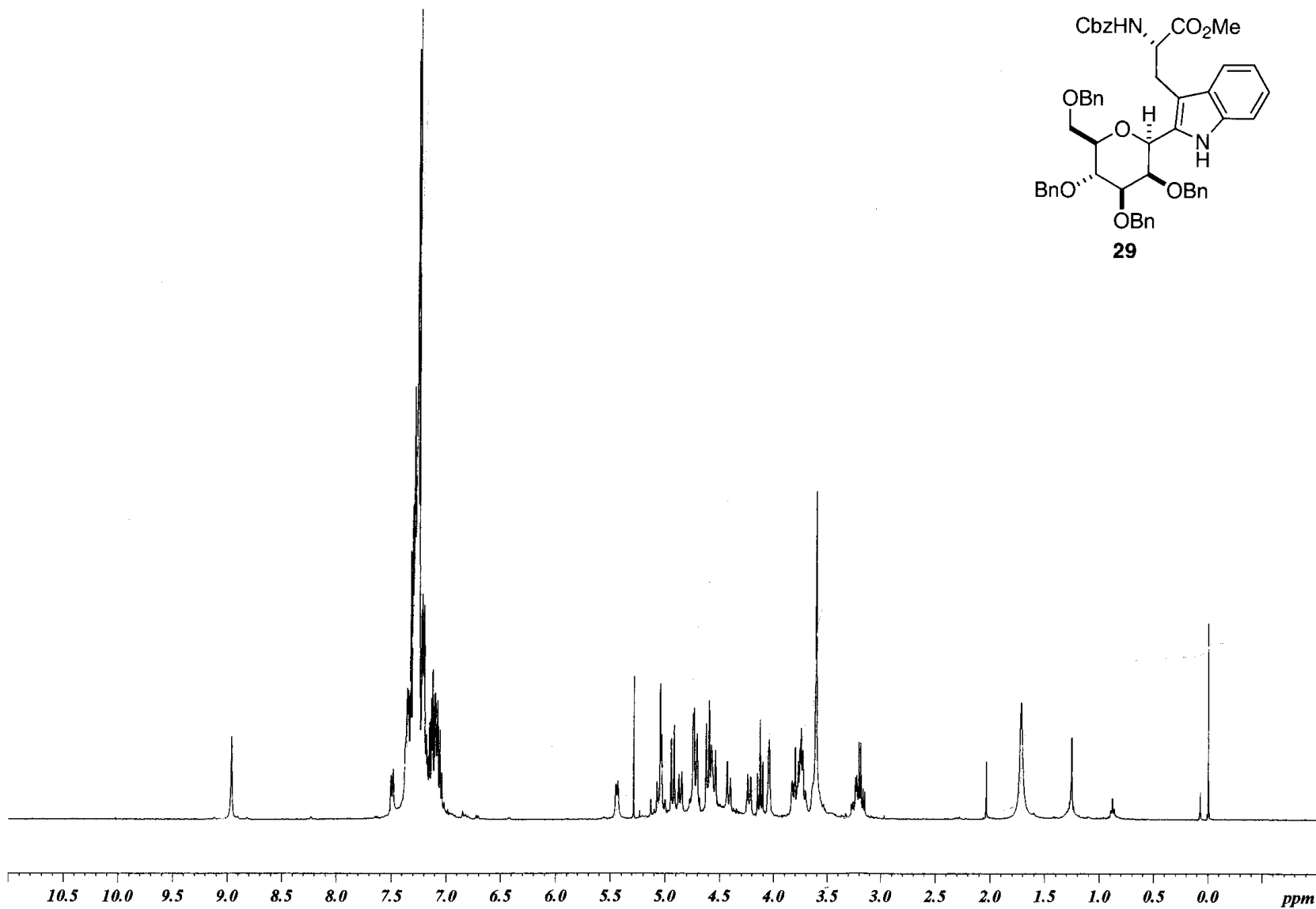


*1H*-NMR (400 MHz, CDCl<sub>3</sub>) δ: 7.40 (d, 1H), 7.35 (d, 1H), 7.25 (d, 1H), 7.15 (d, 1H), 7.05 (d, 1H), 6.95 (d, 1H), 6.85 (d, 1H), 6.75 (d, 1H), 6.65 (d, 1H), 6.55 (d, 1H), 6.45 (d, 1H), 6.35 (d, 1H), 6.25 (d, 1H), 6.15 (d, 1H), 6.05 (d, 1H), 5.95 (d, 1H), 5.85 (d, 1H), 5.75 (d, 1H), 5.65 (d, 1H), 5.55 (d, 1H), 5.45 (d, 1H), 5.35 (d, 1H), 5.25 (d, 1H), 5.15 (d, 1H), 5.05 (d, 1H), 4.95 (d, 1H), 4.85 (d, 1H), 4.75 (d, 1H), 4.65 (d, 1H), 4.55 (d, 1H), 4.45 (d, 1H), 4.35 (d, 1H), 4.25 (d, 1H), 4.15 (d, 1H), 4.05 (d, 1H), 3.95 (d, 1H), 3.85 (d, 1H), 3.75 (d, 1H), 3.65 (d, 1H), 3.55 (d, 1H), 3.45 (d, 1H), 3.35 (d, 1H), 3.25 (d, 1H), 3.15 (d, 1H), 3.05 (d, 1H), 2.95 (d, 1H), 2.85 (d, 1H), 2.75 (d, 1H), 2.65 (d, 1H), 2.55 (d, 1H), 2.45 (d, 1H), 2.35 (d, 1H), 2.25 (d, 1H), 2.15 (d, 1H), 2.05 (d, 1H), 1.95 (d, 1H), 1.85 (d, 1H), 1.75 (d, 1H), 1.65 (d, 1H), 1.55 (d, 1H), 1.45 (d, 1H), 1.35 (d, 1H), 1.25 (d, 1H), 1.15 (d, 1H), 1.05 (d, 1H), 1.95 (d, 1H), 1.85 (d, 1H), 1.75 (d, 1H), 1.65 (d, 1H), 1.55 (d, 1H), 1.45 (d, 1H), 1.35 (d, 1H), 1.25 (d, 1H), 1.15 (d, 1H), 1.05 (d, 1H), 0.95 (d, 1H), 0.85 (d, 1H), 0.75 (d, 1H), 0.65 (d, 1H), 0.55 (d, 1H), 0.45 (d, 1H), 0.35 (d, 1H), 0.25 (d, 1H), 0.15 (d, 1H).

*13C*-NMR (100 MHz, CDCl<sub>3</sub>) δ: 175.0, 170.0, 165.0, 160.0, 155.0, 150.0, 145.0, 140.0, 135.0, 130.0, 125.0, 120.0, 115.0, 110.0, 105.0, 100.0, 95.0, 90.0, 85.0, 80.0, 75.0, 70.0, 65.0, 60.0, 55.0, 50.0, 45.0, 40.0, 35.0, 30.0, 25.0, 20.0, 15.0, 10.0, 5.0, 0.0.

*13C*-NMR (100 MHz, CDCl<sub>3</sub>) δ: 175.0, 170.0, 165.0, 160.0, 155.0, 150.0, 145.0, 140.0, 135.0, 130.0, 125.0, 120.0, 115.0, 110.0, 105.0, 100.0, 95.0, 90.0, 85.0, 80.0, 75.0, 70.0, 65.0, 60.0, 55.0, 50.0, 45.0, 40.0, 35.0, 30.0, 25.0, 20.0, 15.0, 10.0, 5.0, 0.0.

*13C*-NMR (100 MHz, CDCl<sub>3</sub>) δ: 175.0, 170.0, 165.0, 160.0, 155.0, 150.0, 145.0, 140.0, 135.0, 130.0, 125.0, 120.0, 115.0, 110.0, 105.0, 100.0, 95.0, 90.0, 85.0, 80.0, 75.0, 70.0, 65.0, 60.0, 55.0, 50.0, 45.0, 40.0, 35.0, 30.0, 25.0, 20.0, 15.0, 10.0, 5.0, 0.0.



1.000

3.2586

0.868

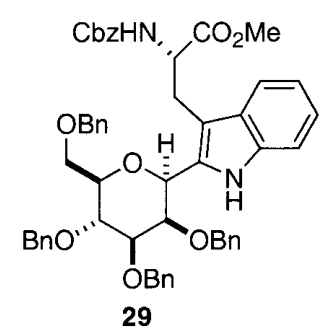
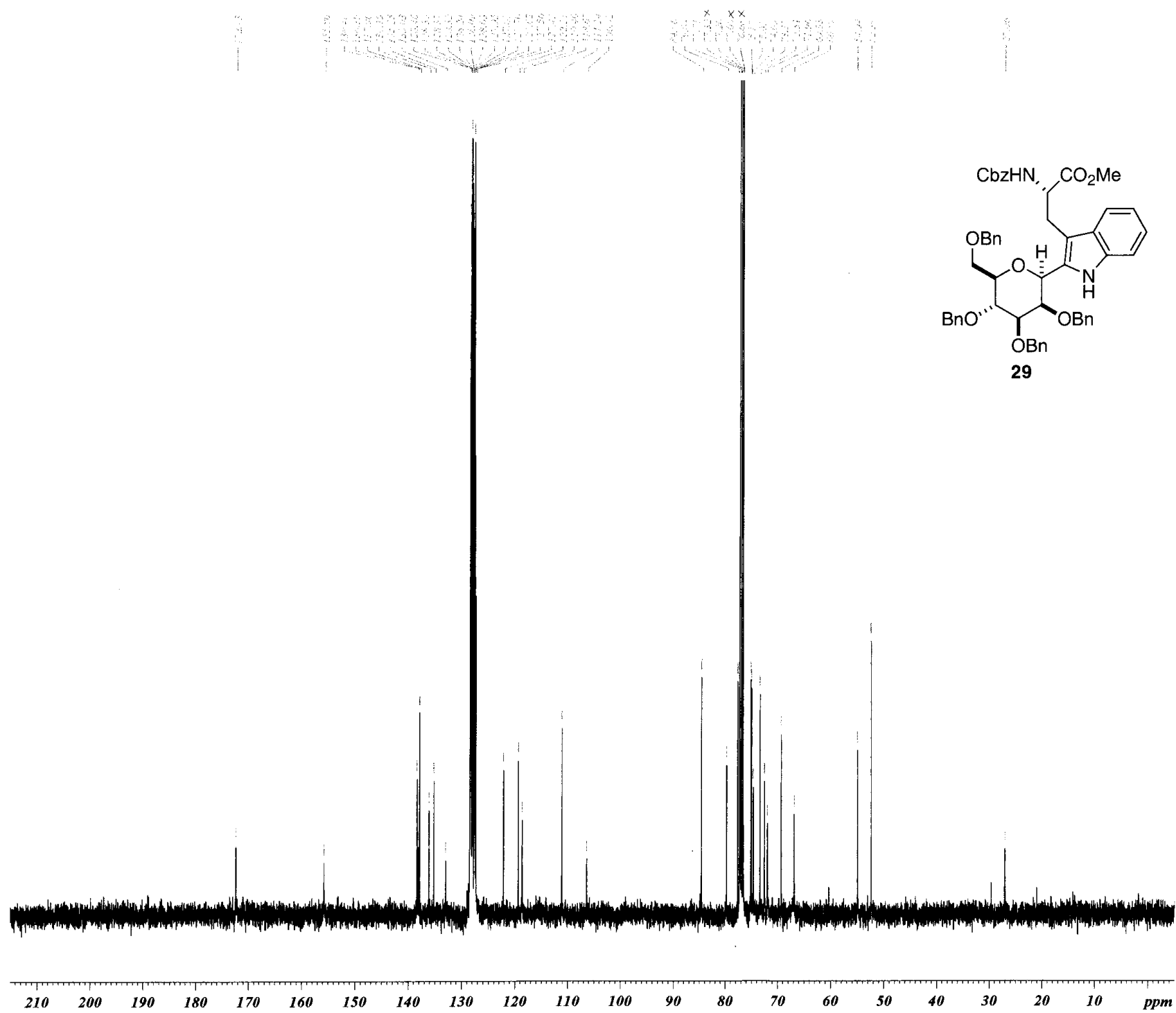
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3.436

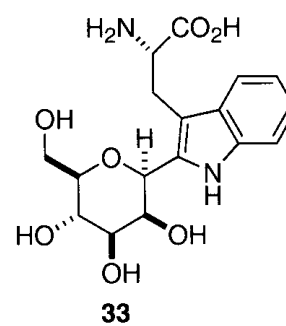
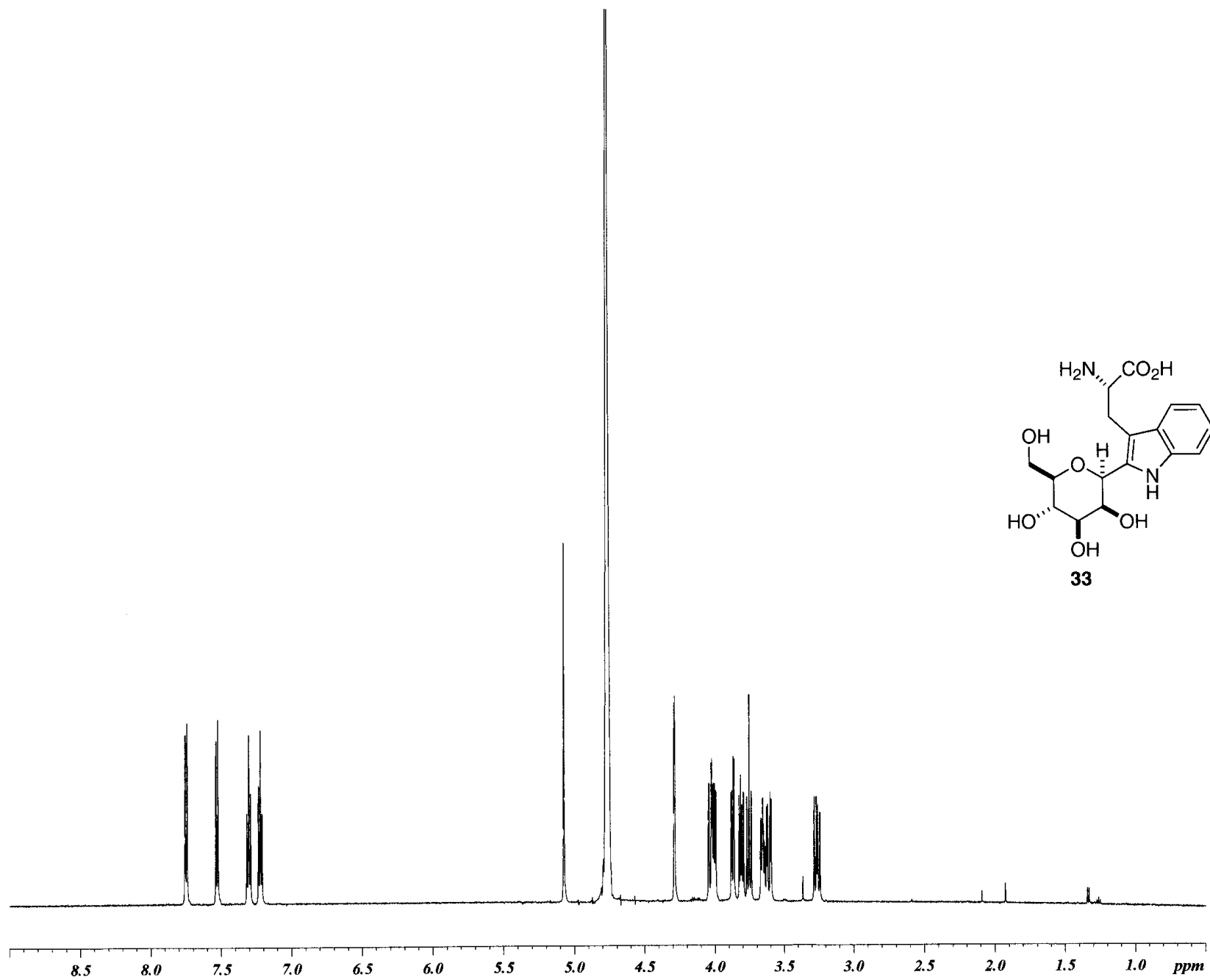
8.125

2.271

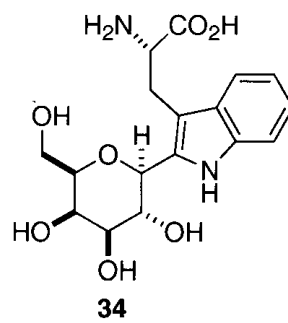
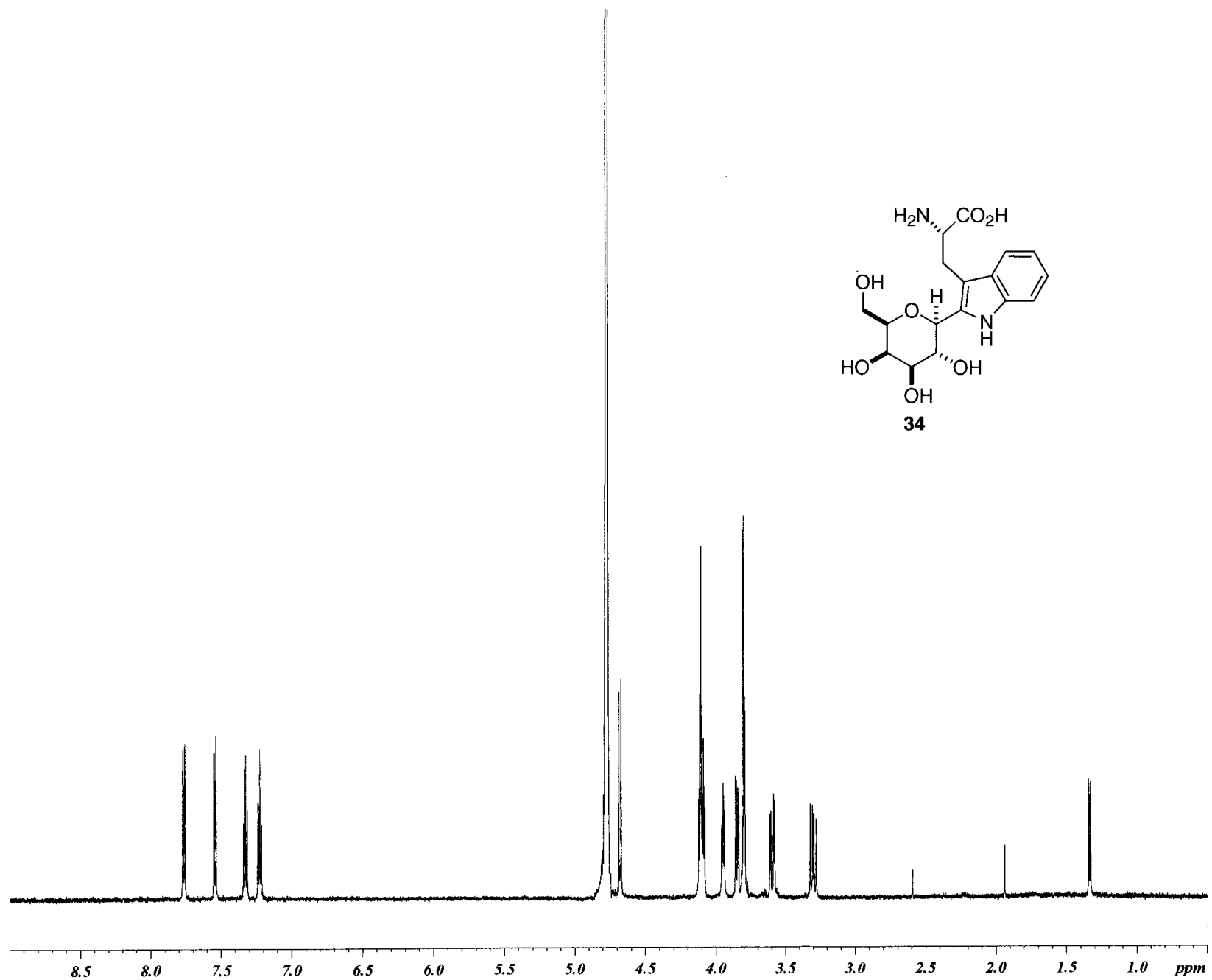
6.328



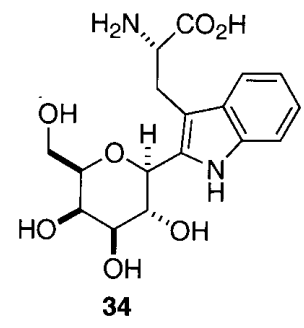
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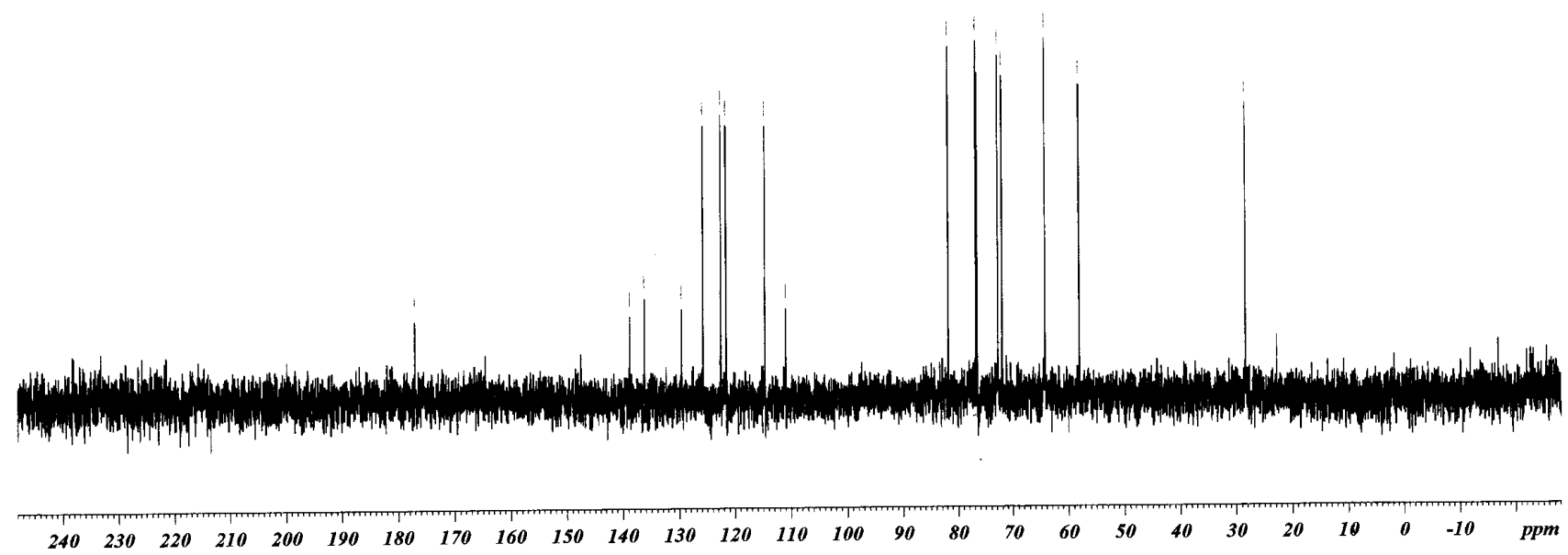


100-100-600



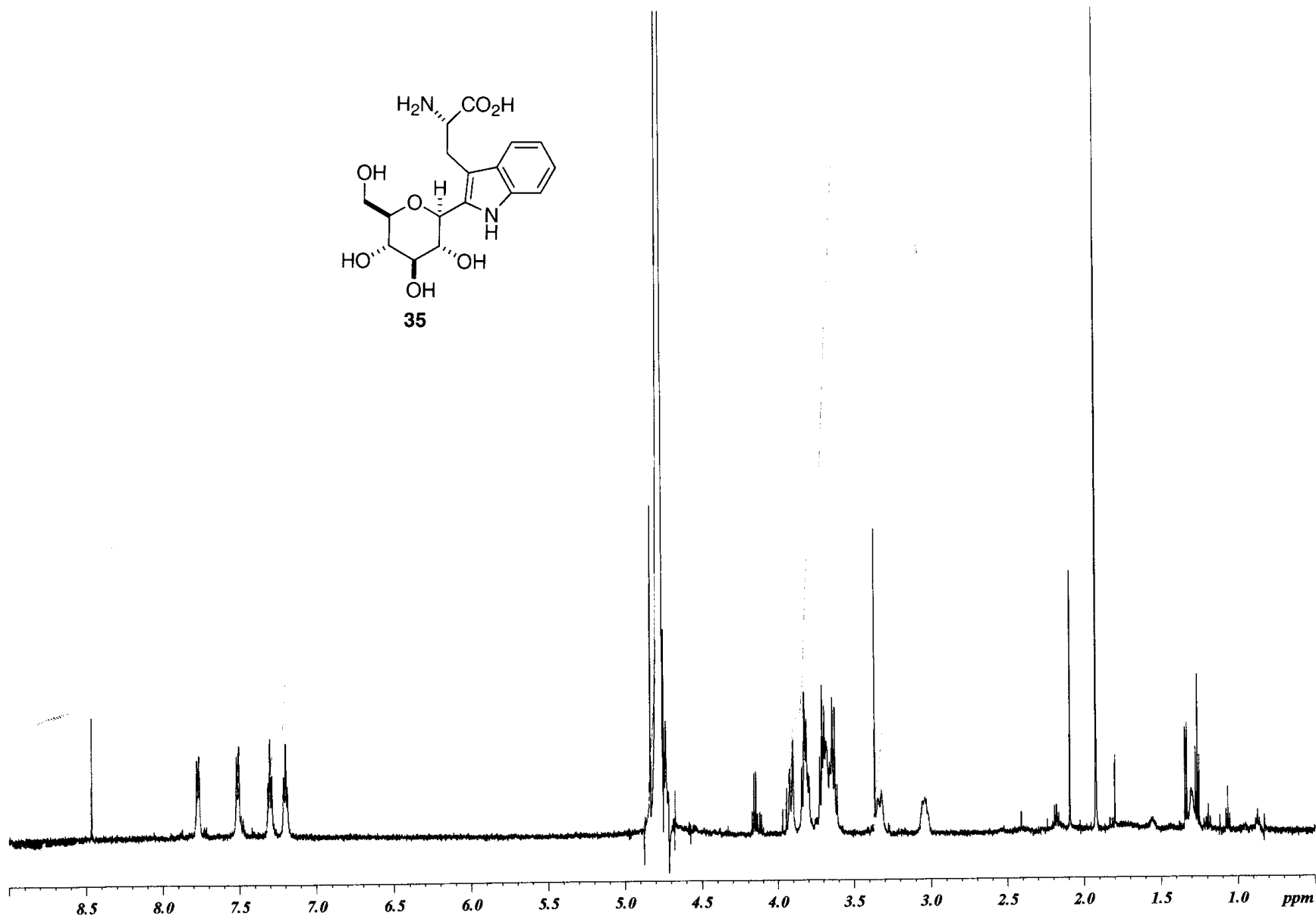
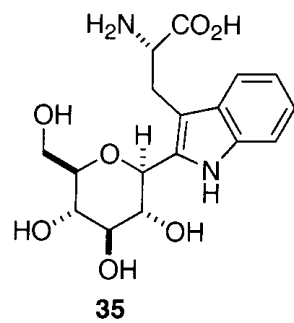
*13*C NMR (CDCl<sub>3</sub>) δ

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No title



1.000

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1.136

0.671

## Current Data Parameters

NAME koide  
EXPNO 21  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 720119  
Time 14.19  
INSTRUM AMX2600  
PROBHD 5 mm Dual 19  
PULPROG zg0dc  
TD 65536  
SOLVENT water  
NS 40000  
DS 2  
SWH 41666.668 Hz  
FIDRES 0.635783 Hz  
AQ 0.7864820 sec  
RG 32768  
DW 12.000 usec  
DE 15.00 usec  
TE 300.0 K

## F2 - Processing parameters

SI 65536  
SF 150.9043853 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

