SUPPORTING INFORMATION

Substituted 2-Azabicyclo[2.1.1]hexanes as Constrained Proline Analogs: Implications for Collagen Stability

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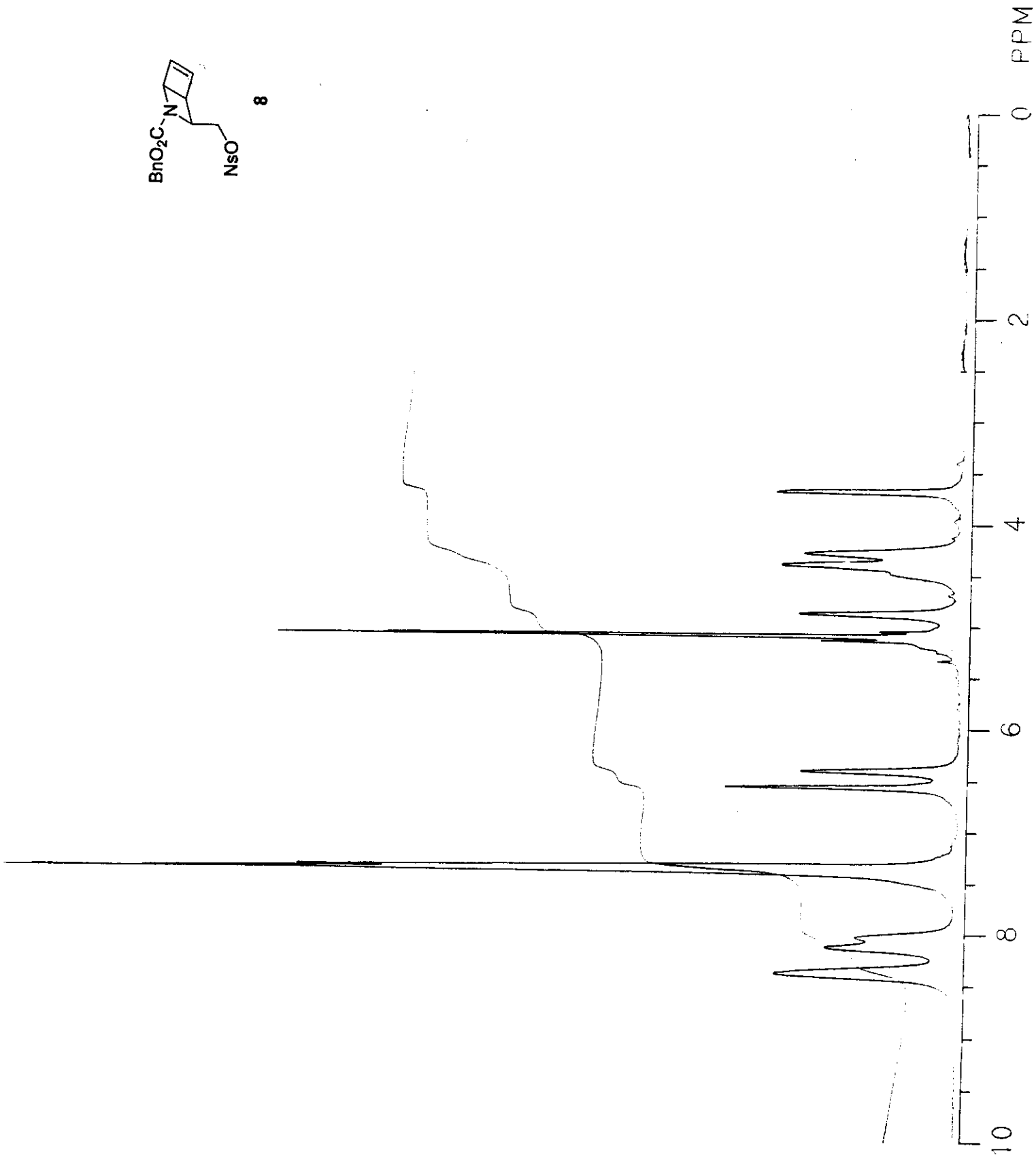
raines@biochem.wisc.edu; grantkrow@aol.com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N
NsO
8
PPM
0
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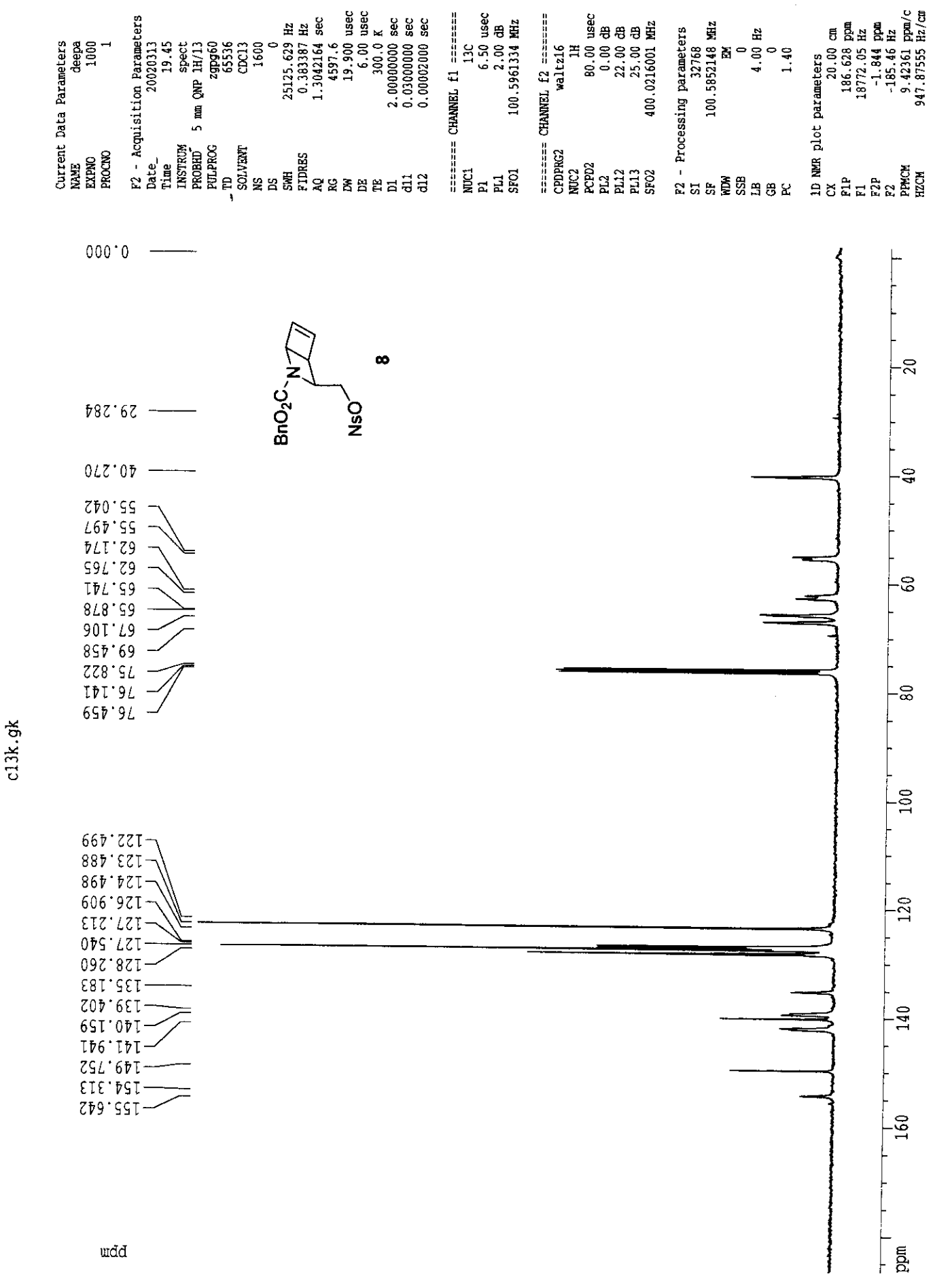
4
6
8
10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F1 18772.05 Hz
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c13k.gk
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76.459
122.499
123.488
124.498
126.909
127.213
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128.260
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139.402
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BnO2C
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NsO
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ppm
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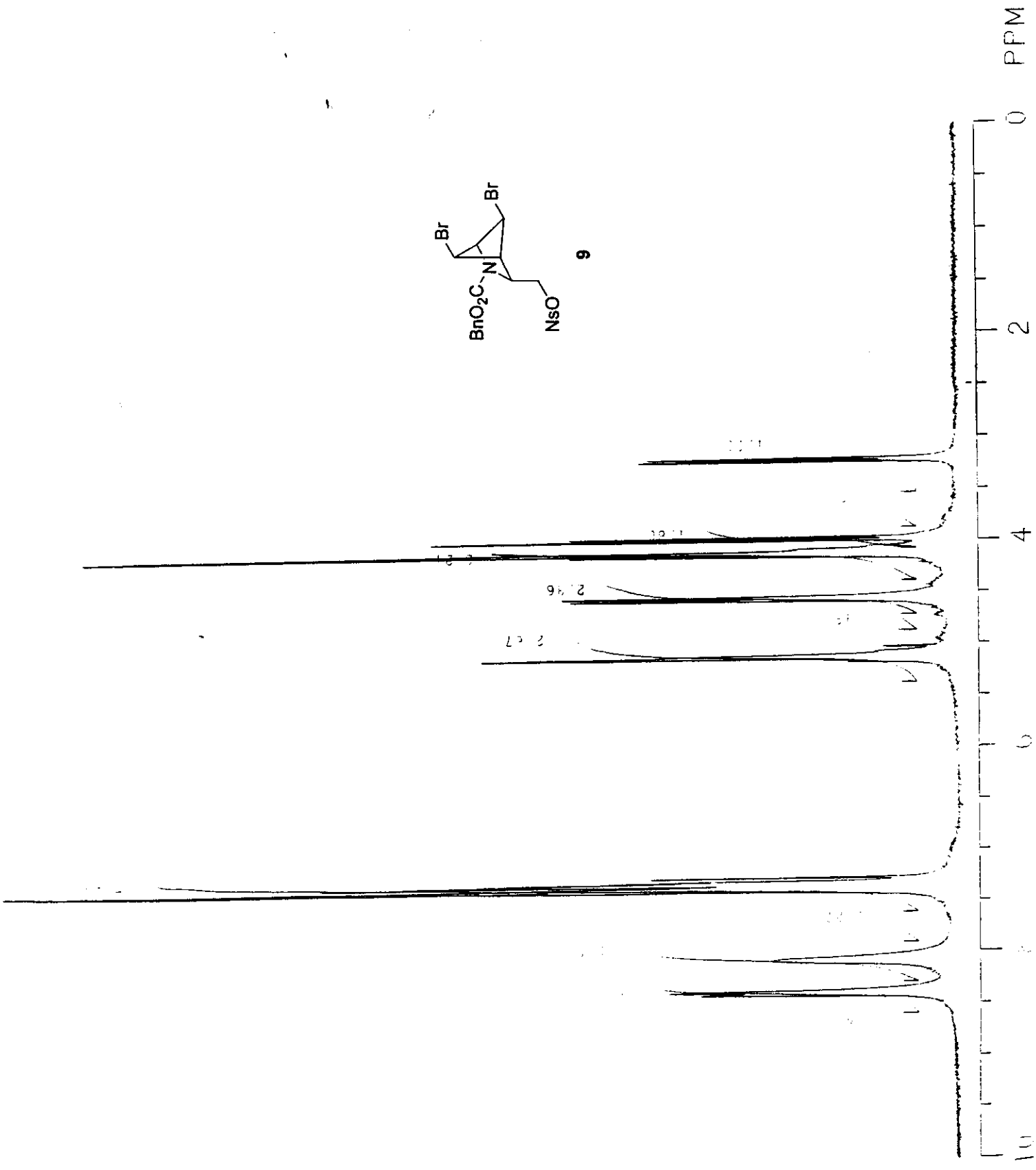
40
60
80
100
120
140
160
ppm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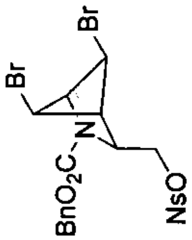
N
BnO2C
NsO
9
PPM
0
2
4
6
10



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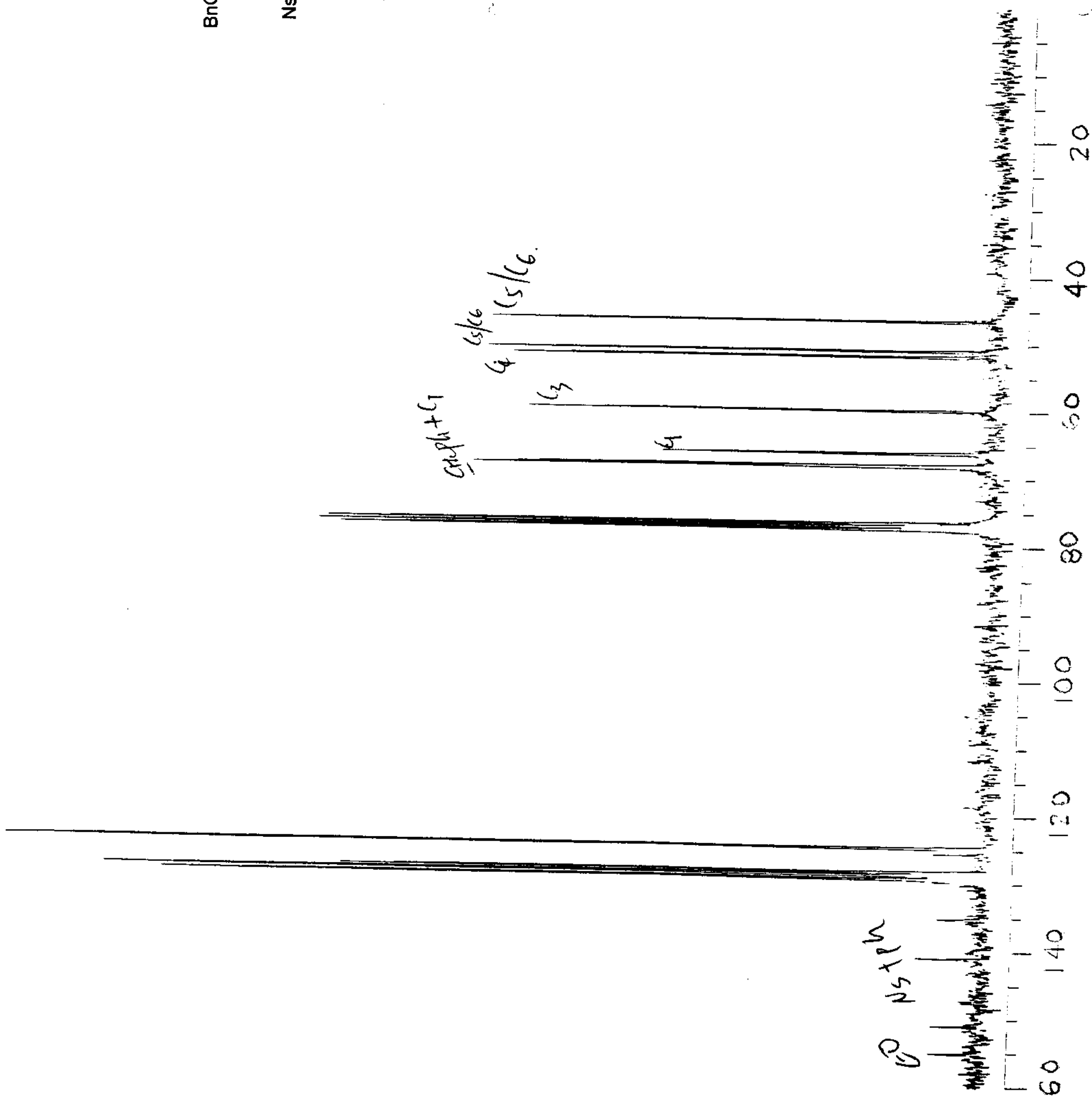

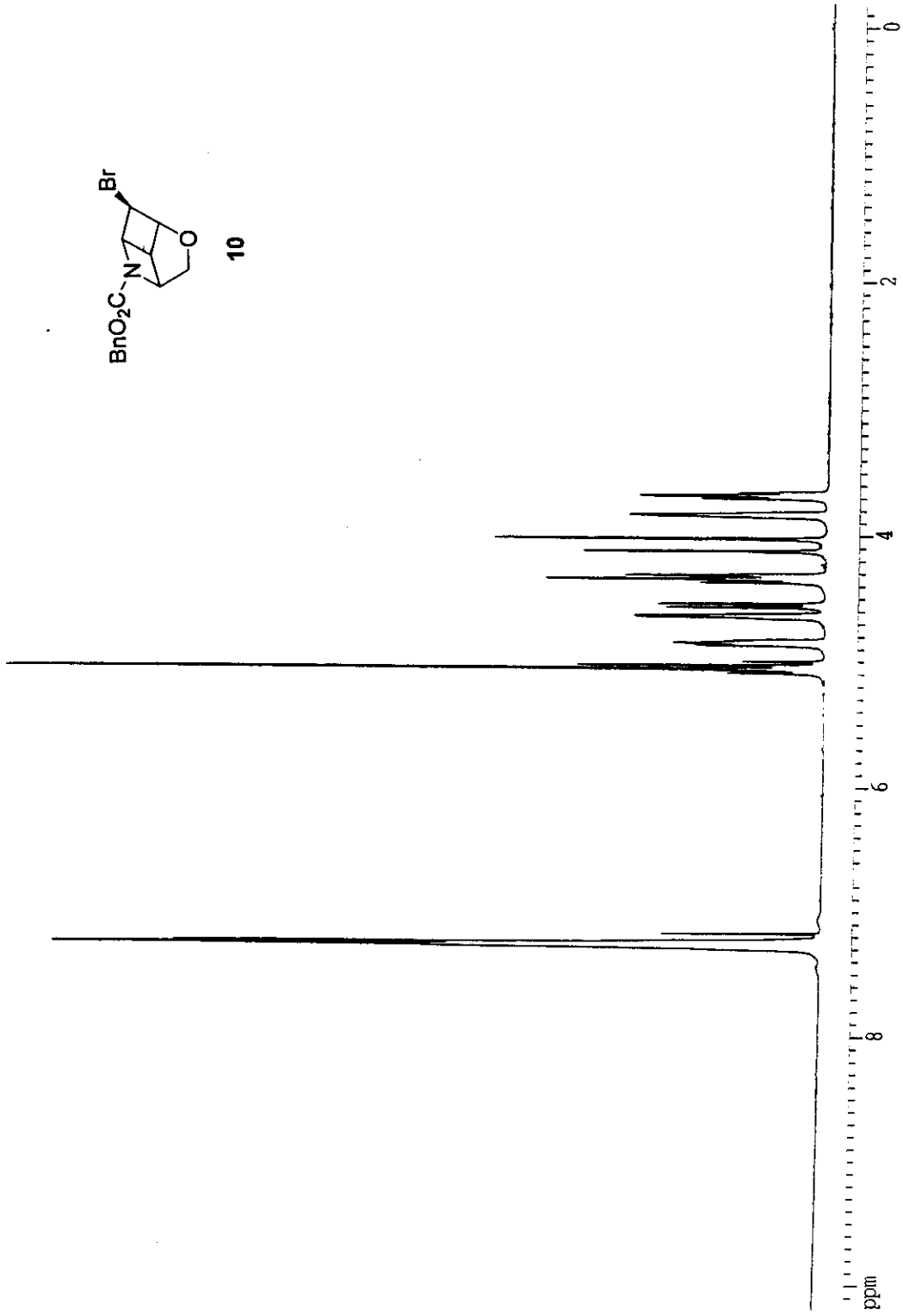
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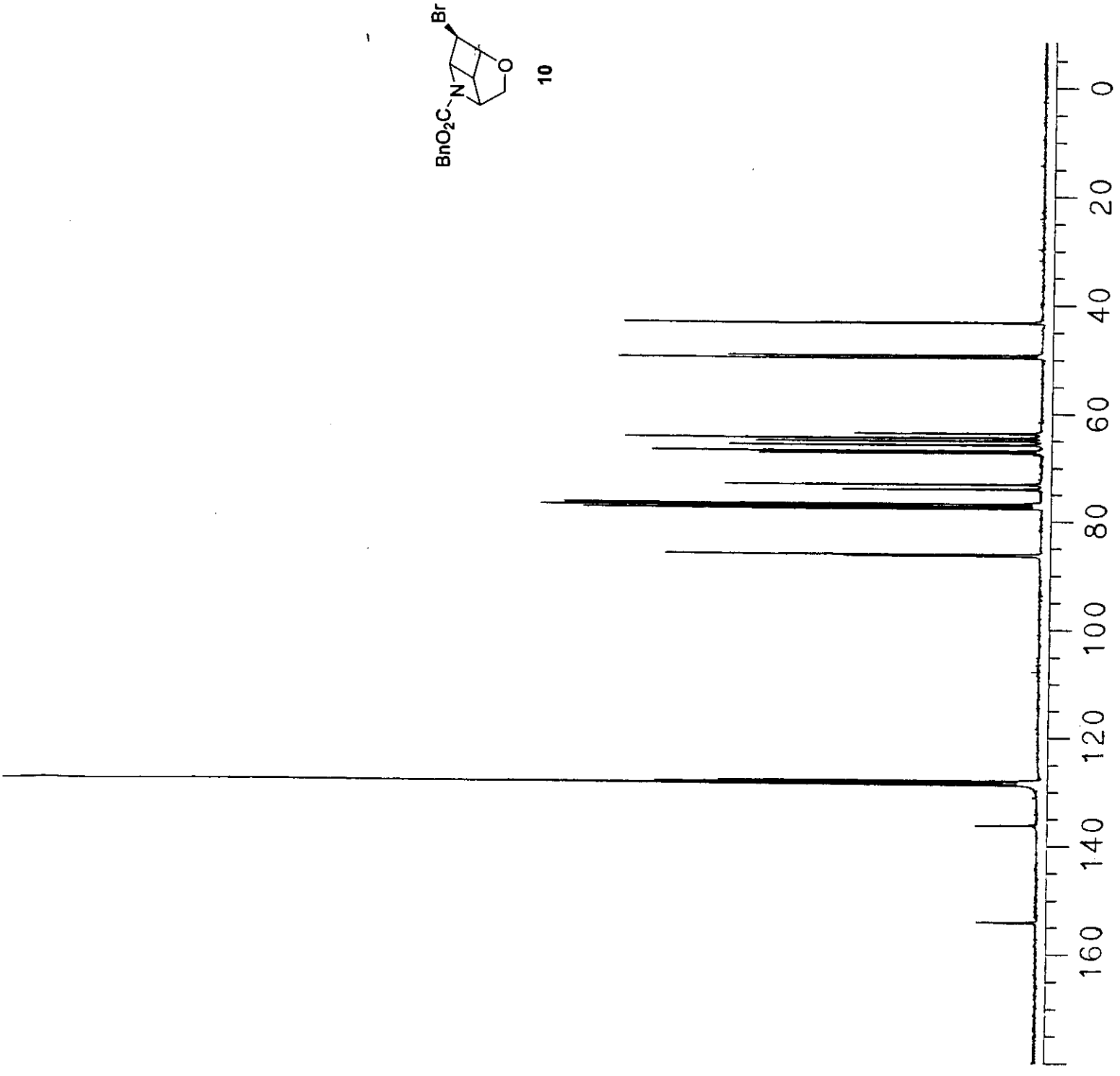
O
N
BnO2C
10
0
2
4
6
8
ppm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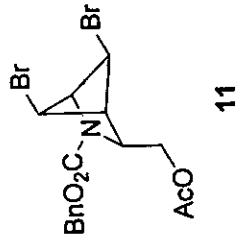
O
N
BnO2C
10
0
20
40
60
80
100
120
140
160



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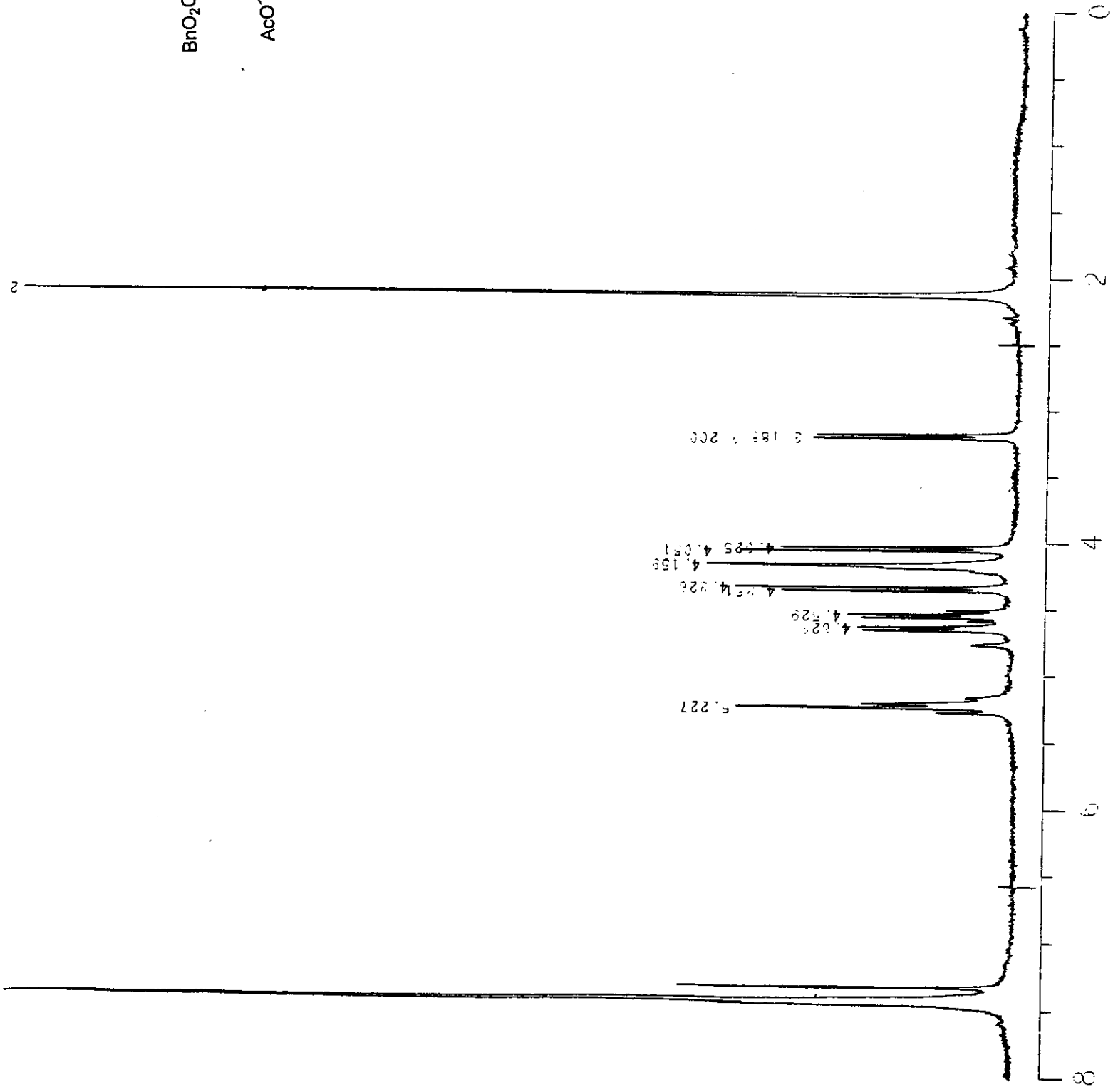

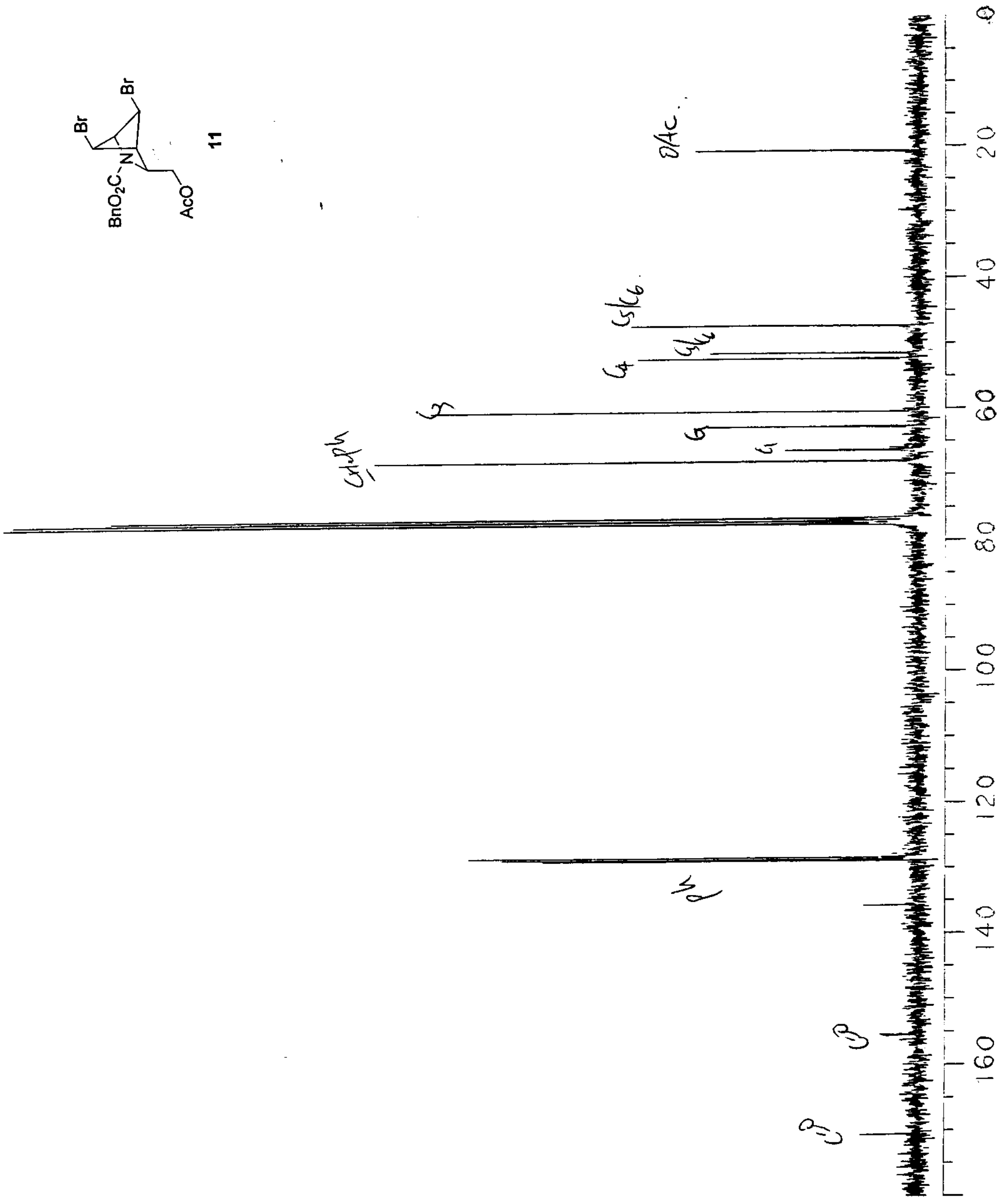

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Br
Br
AcO
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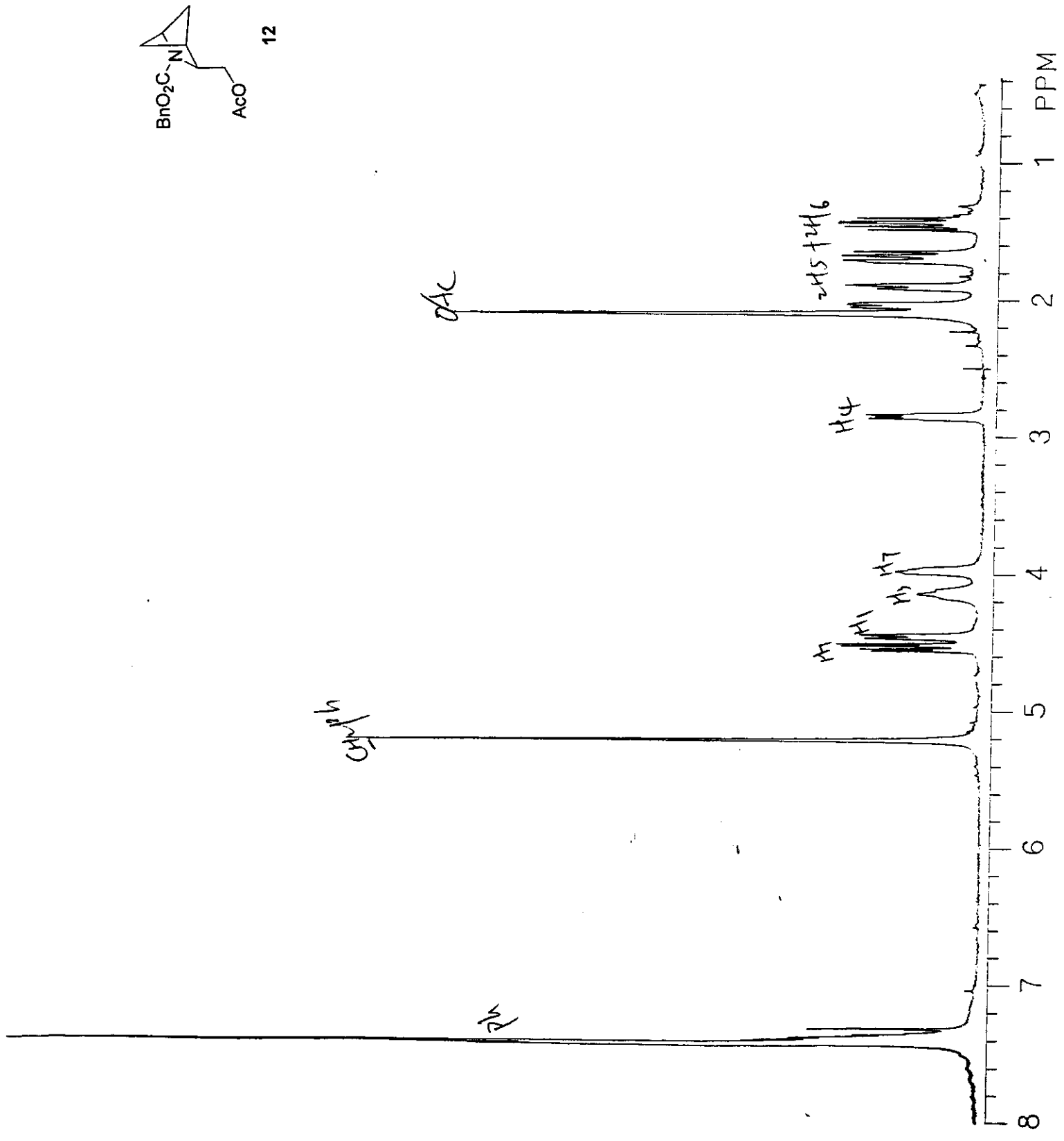
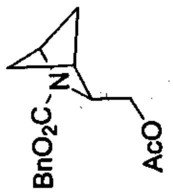
0
20
40
60
80
100
120
140
160


BnO2C
N
AcO
12
PPM
1
2
3
4
5
6
7
8



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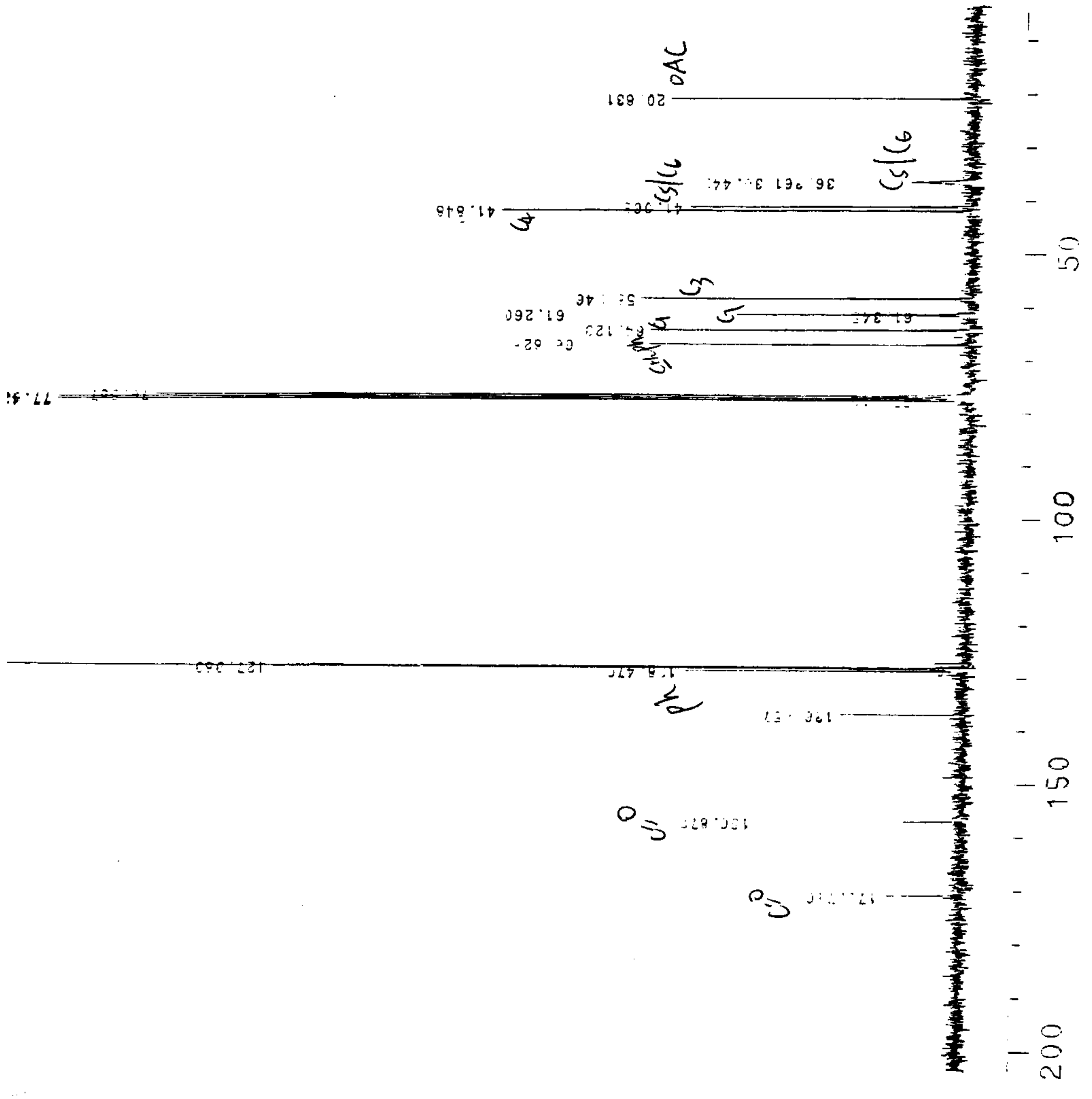
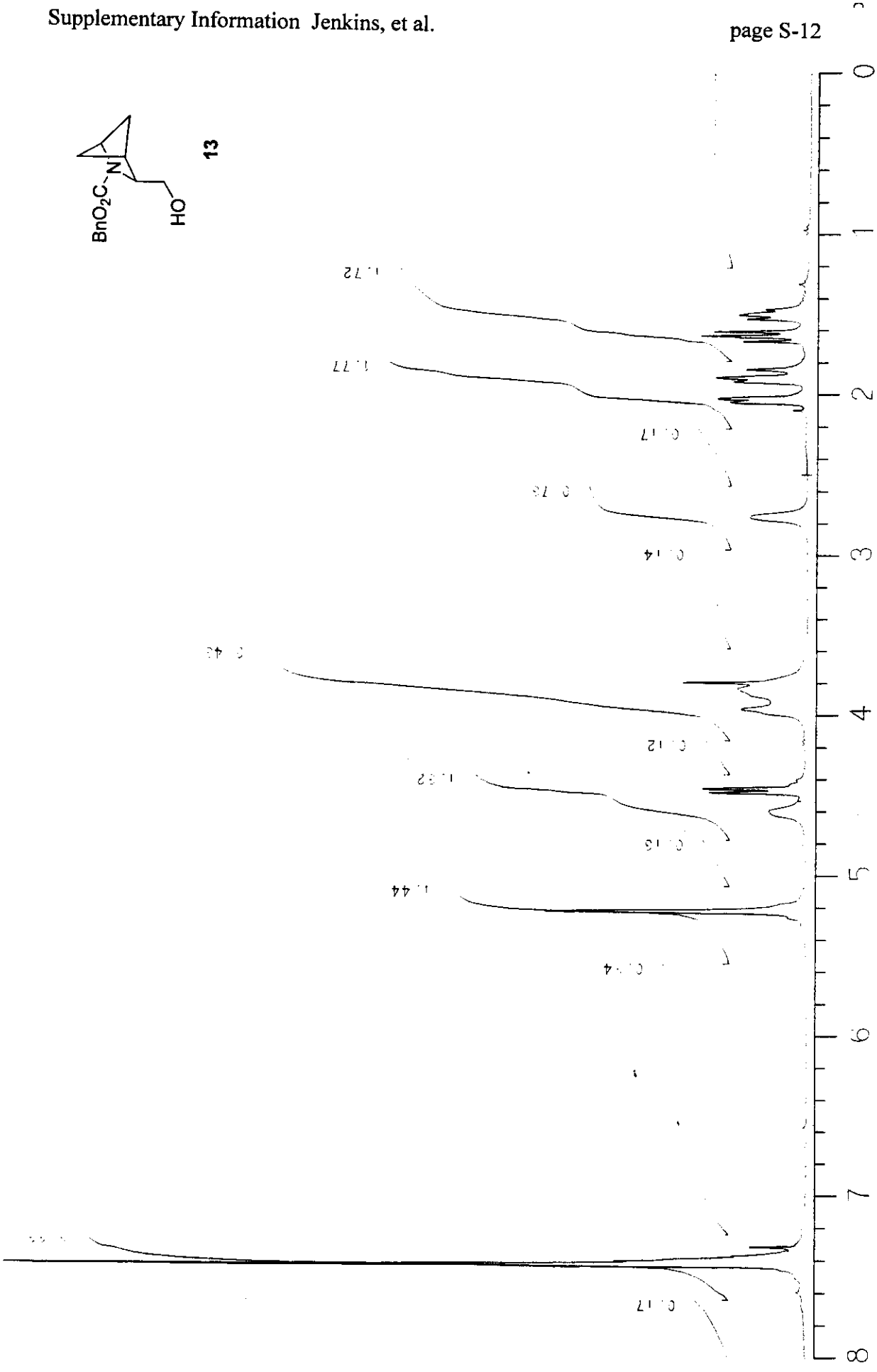
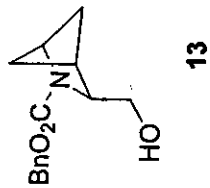
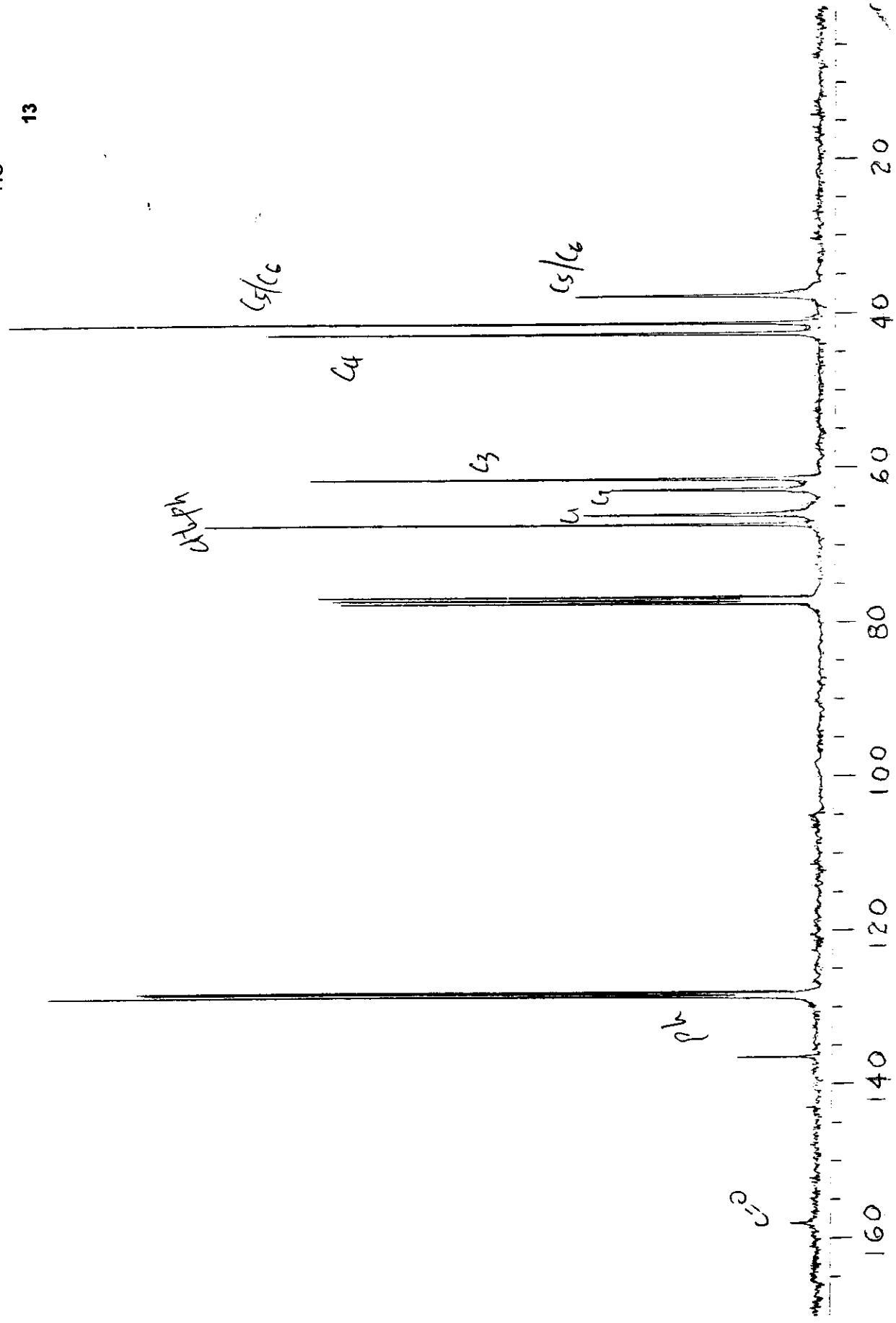
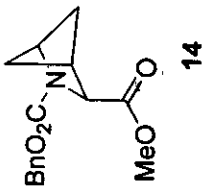



BnO2C
N
HO
13


BnO2C
N
HO

13


C5/C6
C5/C6
C4
C3
C2
C1
Ph
Ph
C=O
20
40
60
80
100
120
140
160



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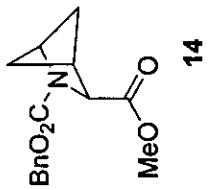

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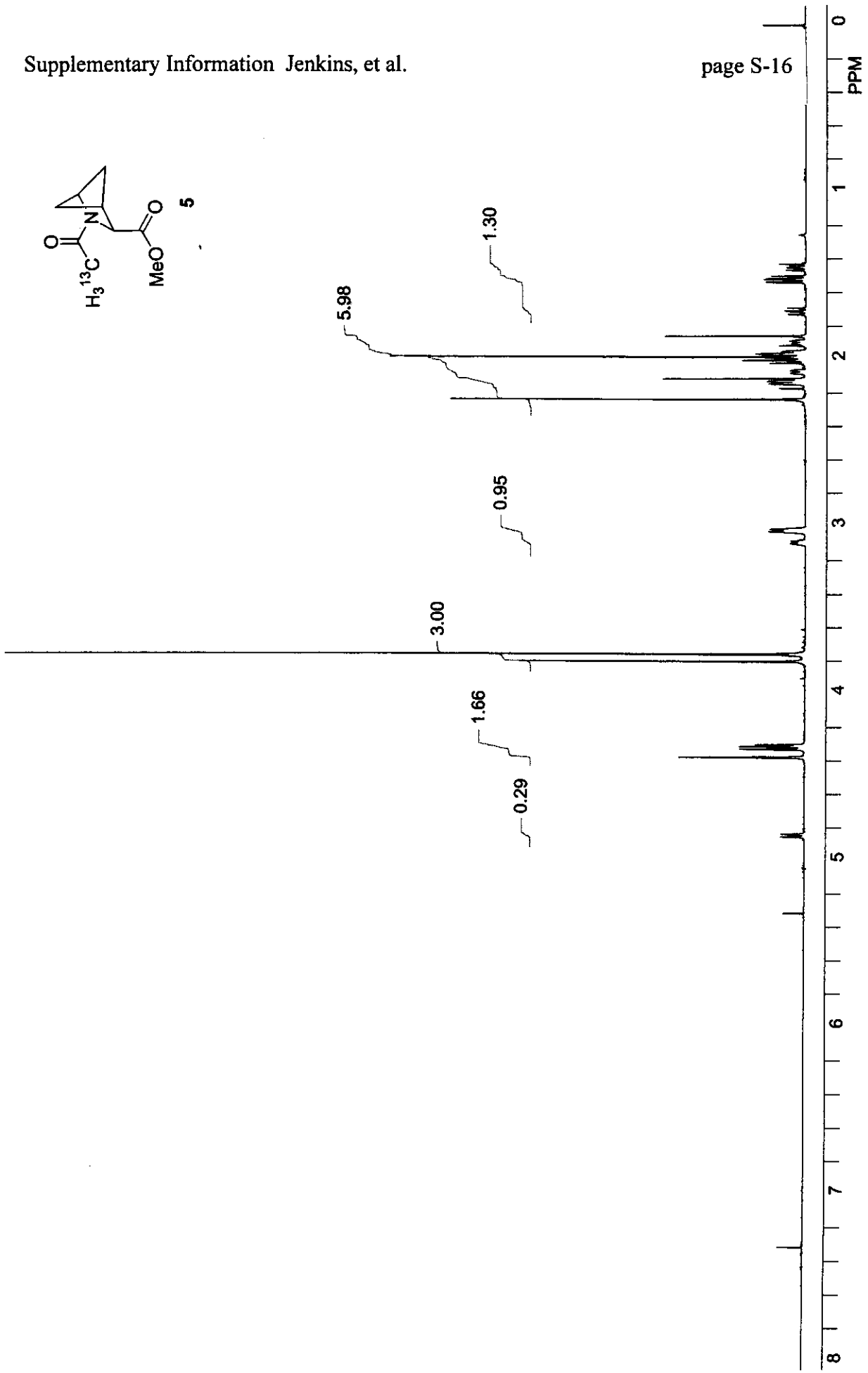
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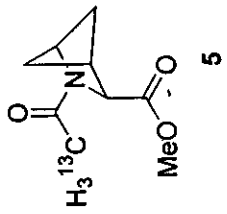
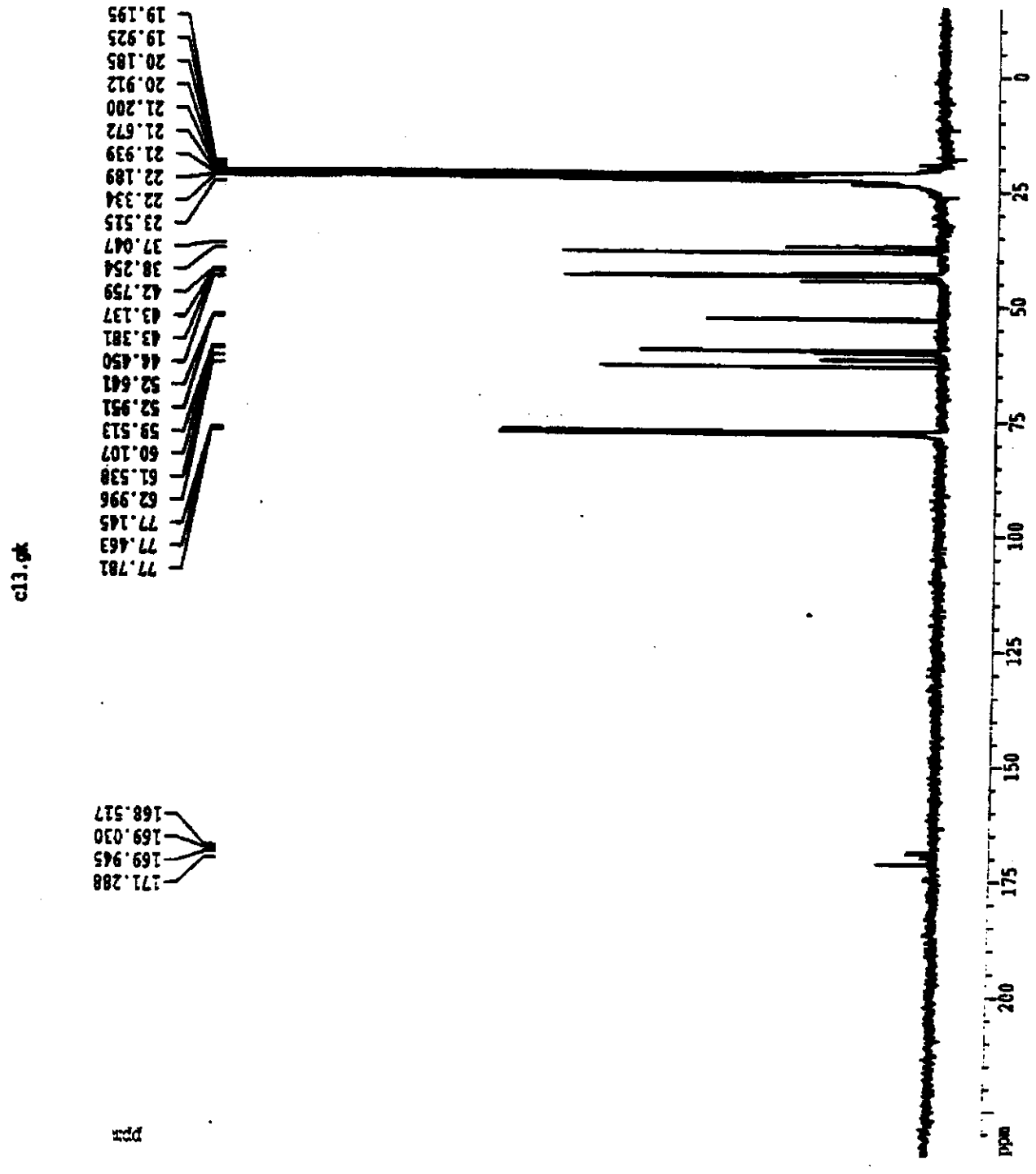
$H_3{}^{13}C$
O
N
O
MeO
O
5
5.98
1.30
0.95
3.00
1.66
0.29
PPM
0
1
2
3
4
5
6
7
8


O
N
O
O
$H_3{}^{13}C$
MeO

5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20.185
20.912
21.200
21.672
21.939
22.189
22.334
23.515
37.047
38.254
42.759
43.137
43.381
44.450
52.641
52.951
59.513
60.107
61.538
62.996
77.145
77.463
77.781
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169.030
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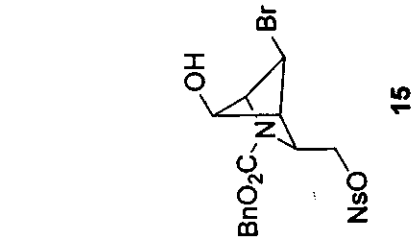
0
25
50
75
100
125
150
175
200
ppm



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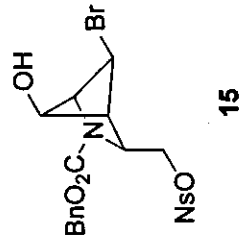

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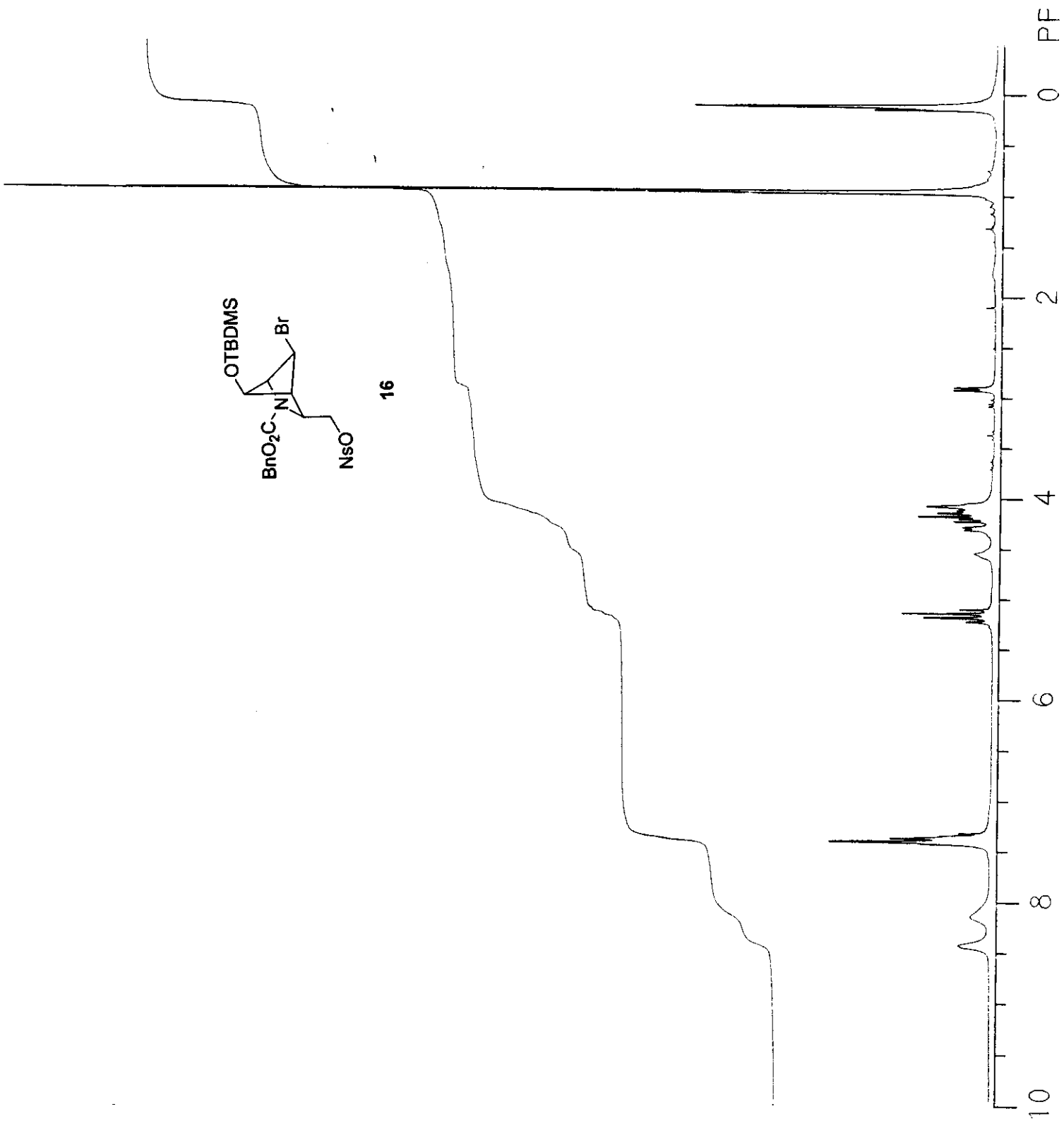
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N
BnO2C
NsO
16
PF
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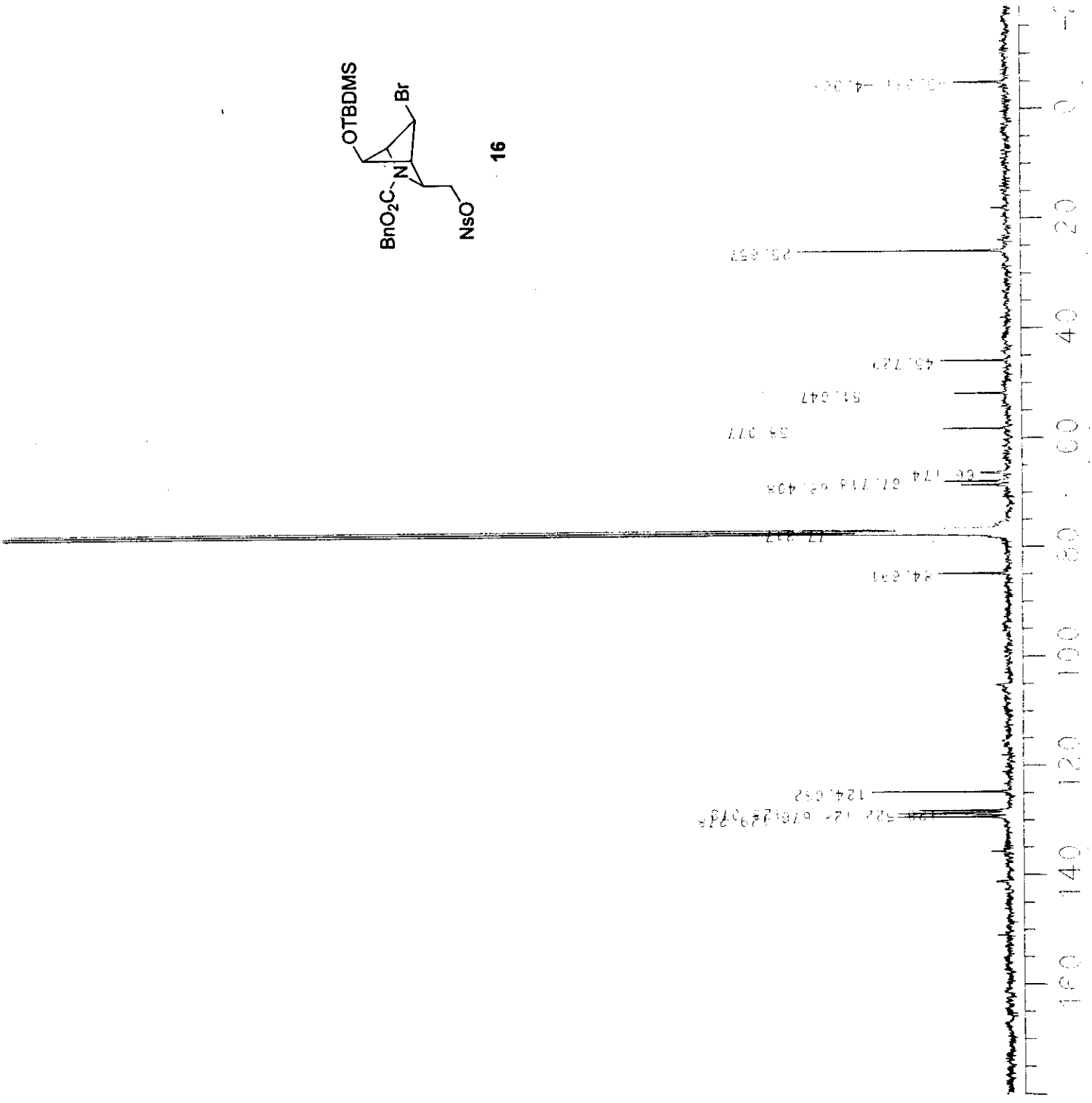
2
4
6
8
10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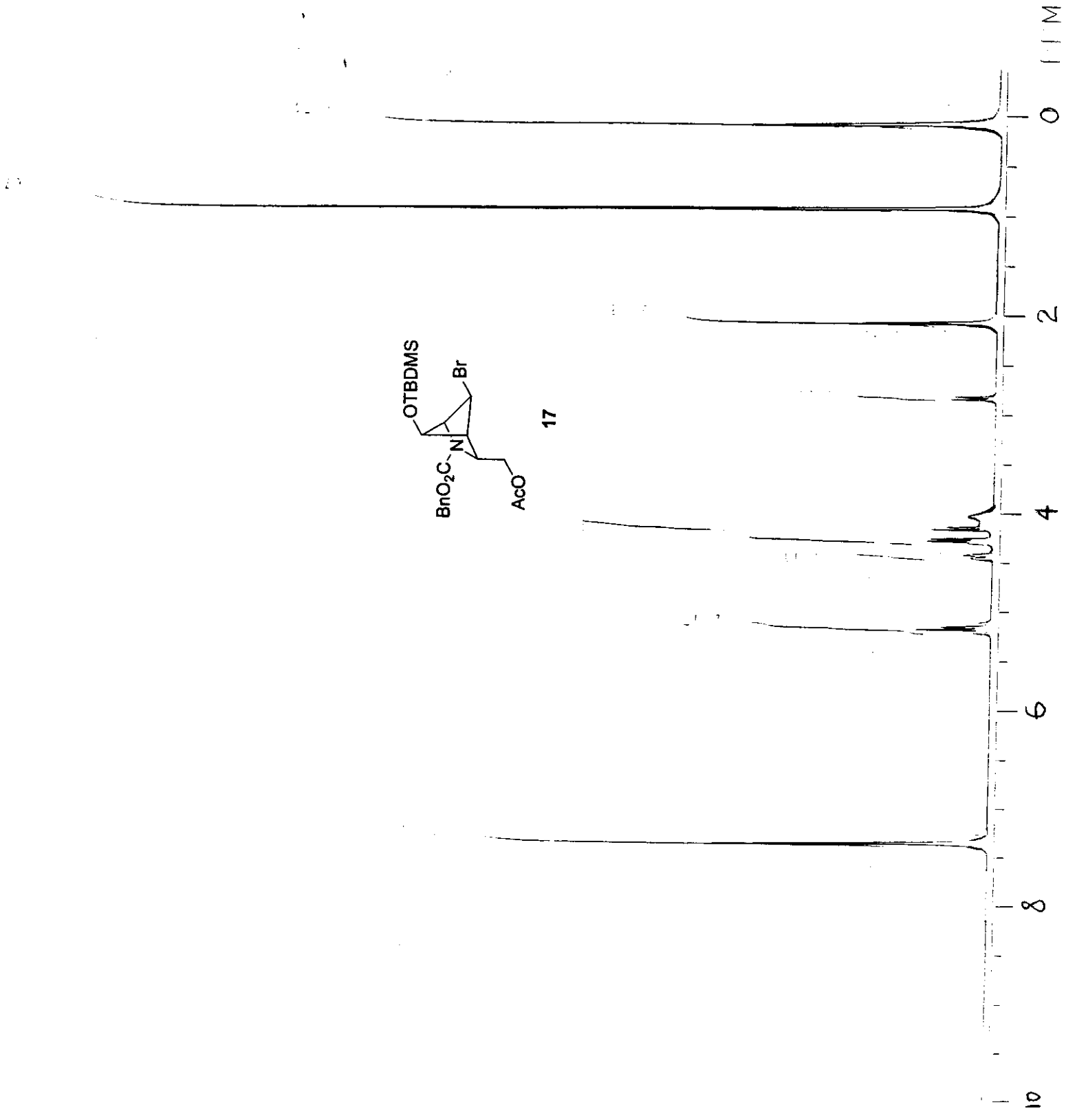
N
BnO2C
NsO
16
PPM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BnO2C
AcO
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2
4
6
8
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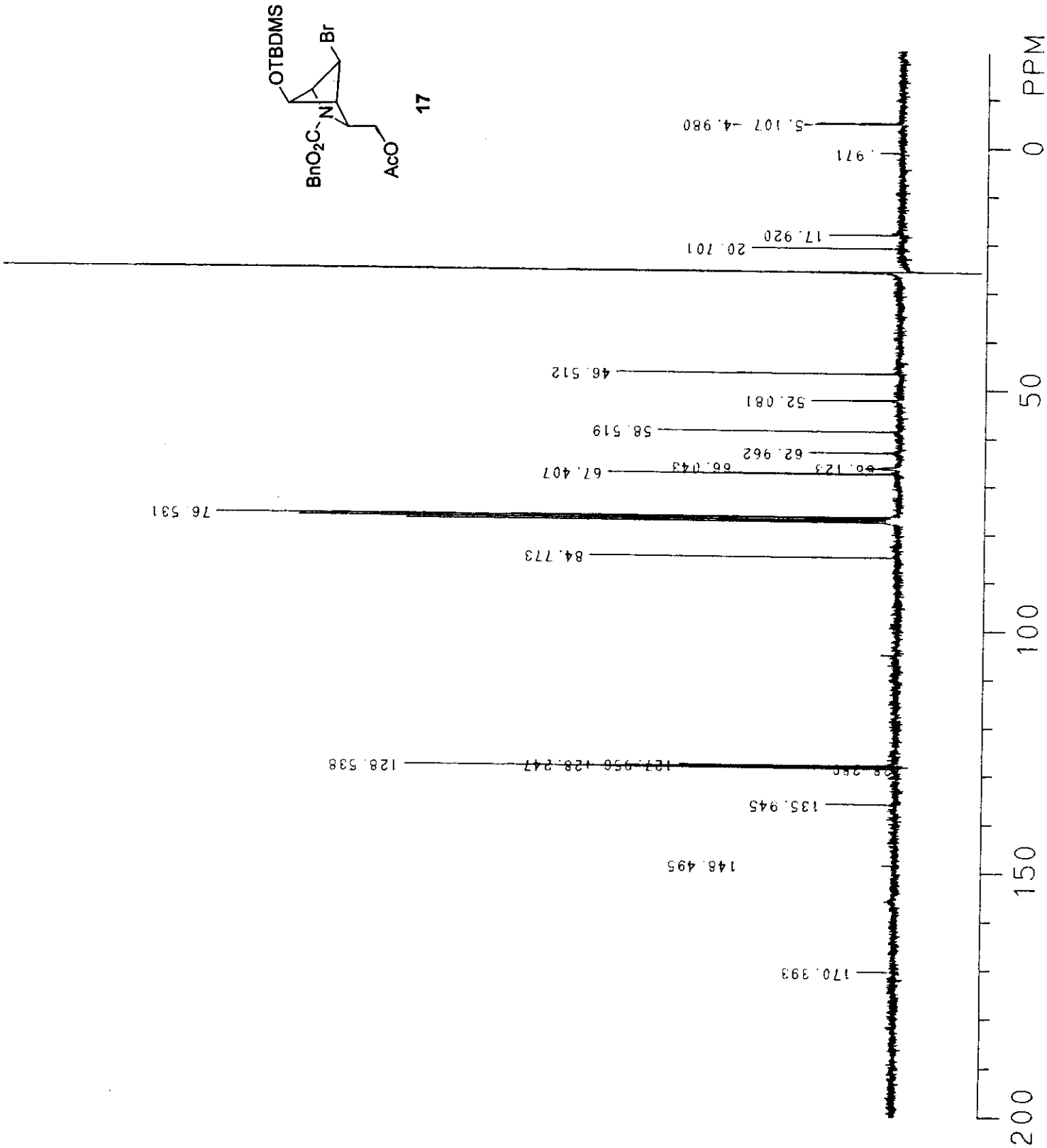
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Br
N
BnO2C
AcO
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-4.980
.971
17.920
20.101
46.512
52.081
58.519
62.962
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76.531
84.773
128.538
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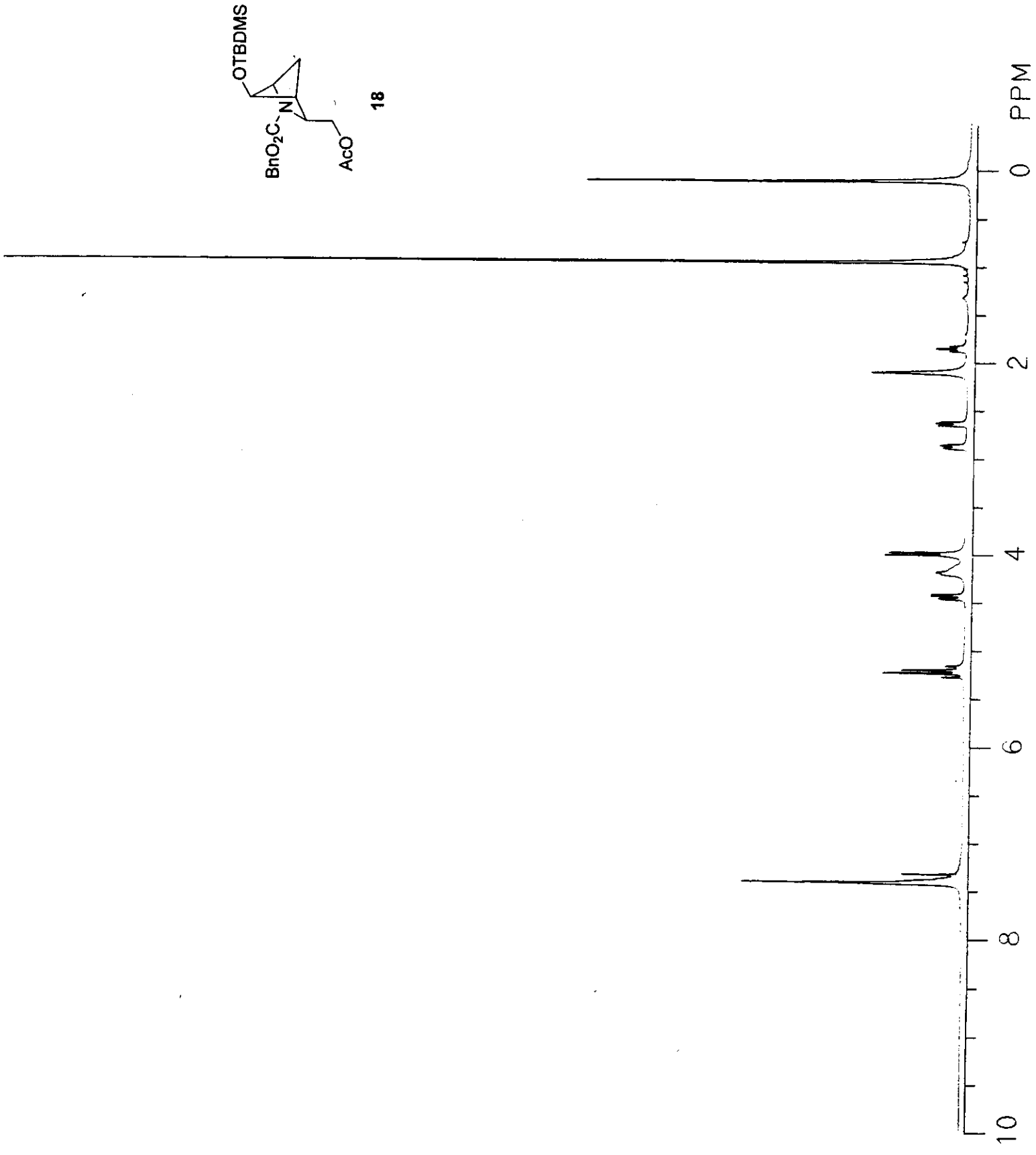
170.393
0 PPM
50
100
150
200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BnO2C
AcO
18
PPM
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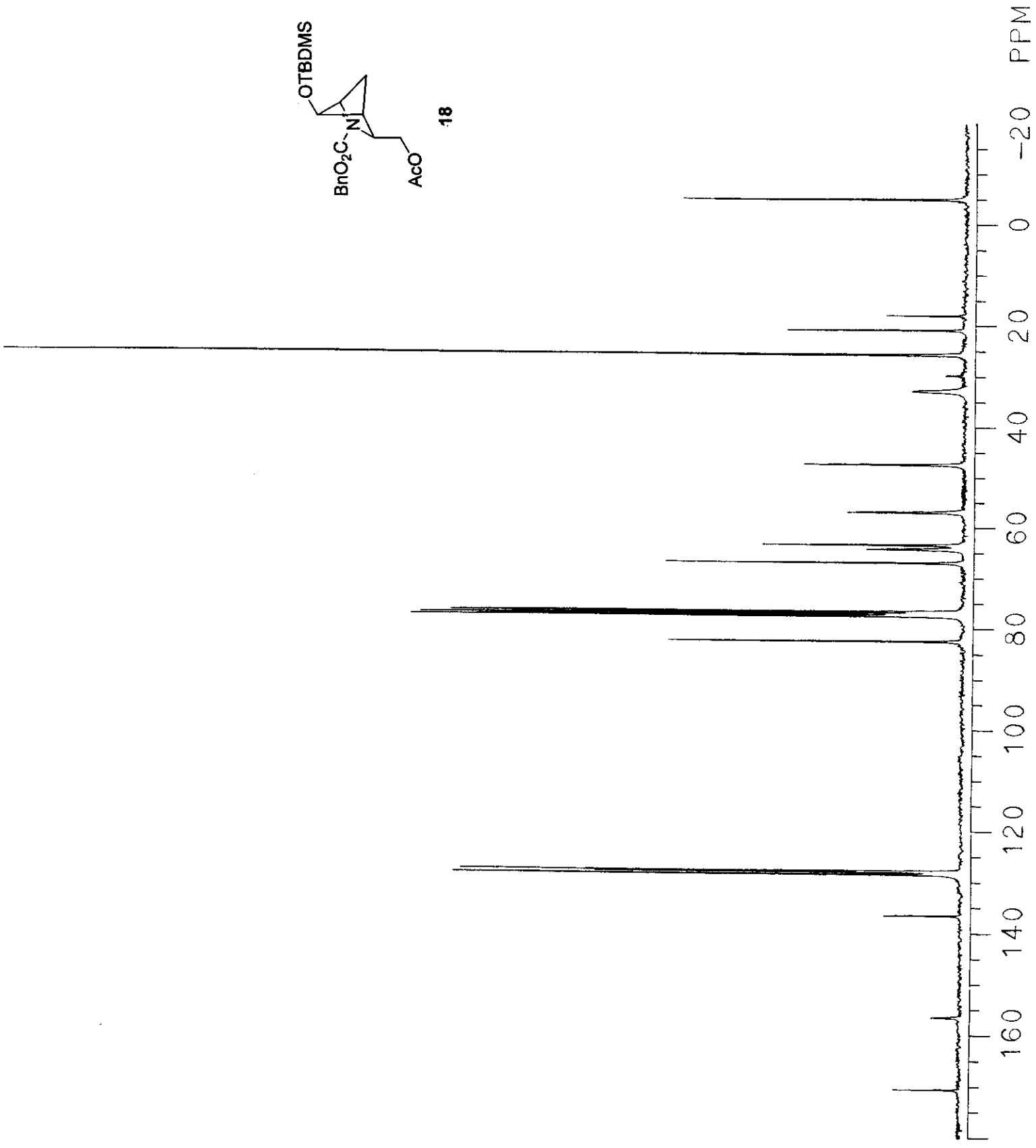
2
4
6
8
10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BnO2C
AcO
18
PPM
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120
100
80
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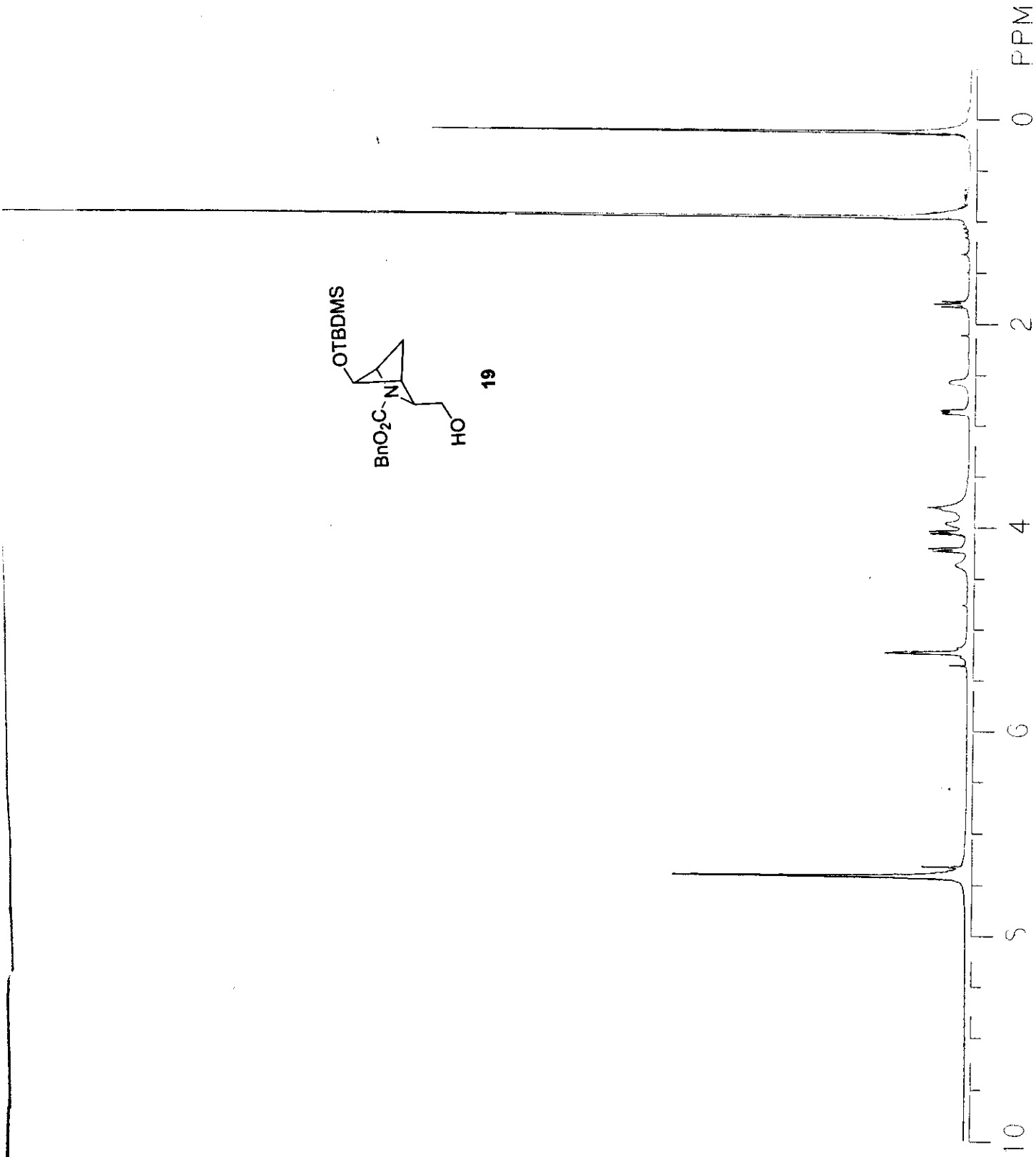
20
0
−20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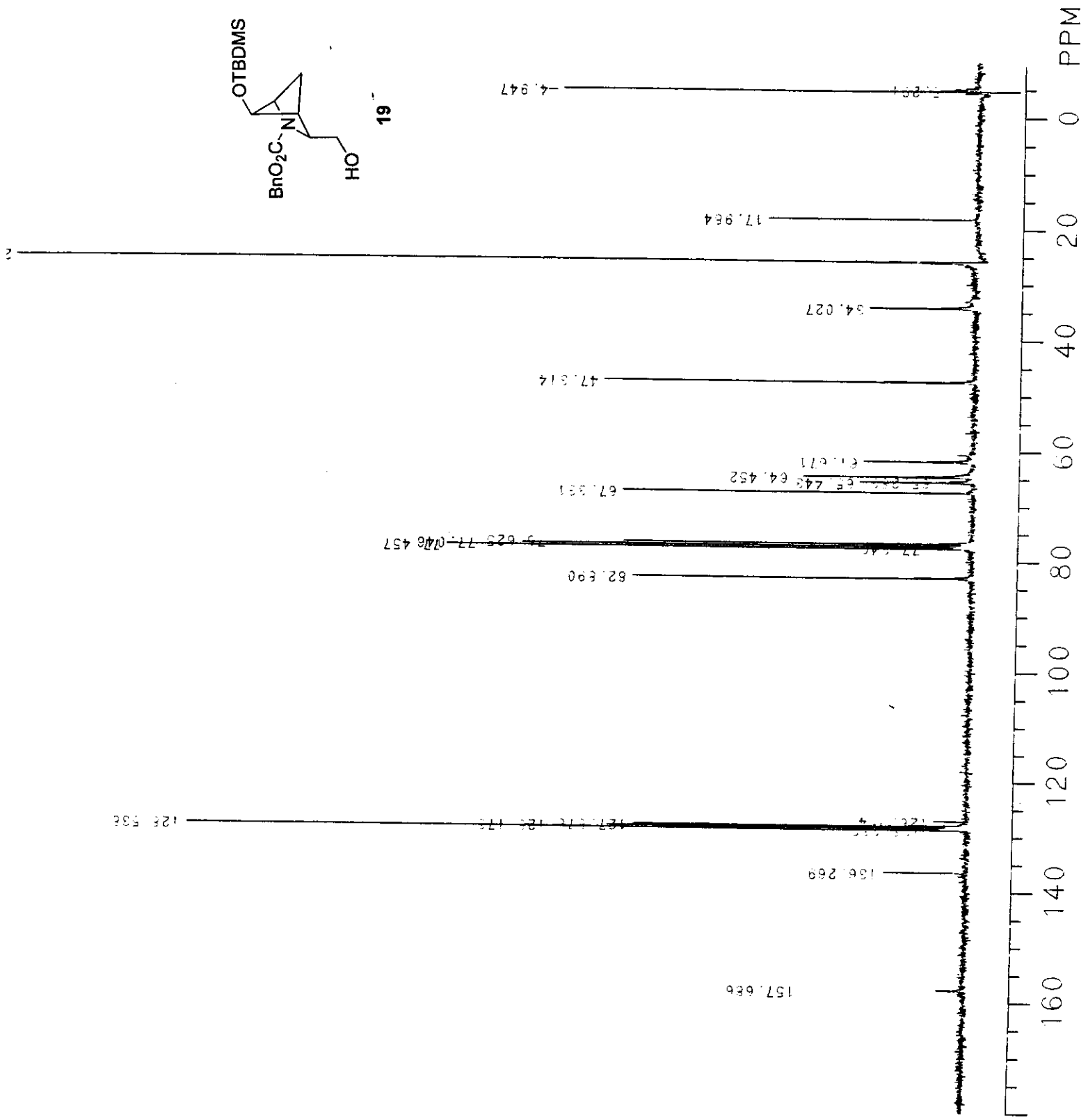
BnO2C
HO
19
10
5
6
4
2
0
PPM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BnO2C
HO
19
PPM
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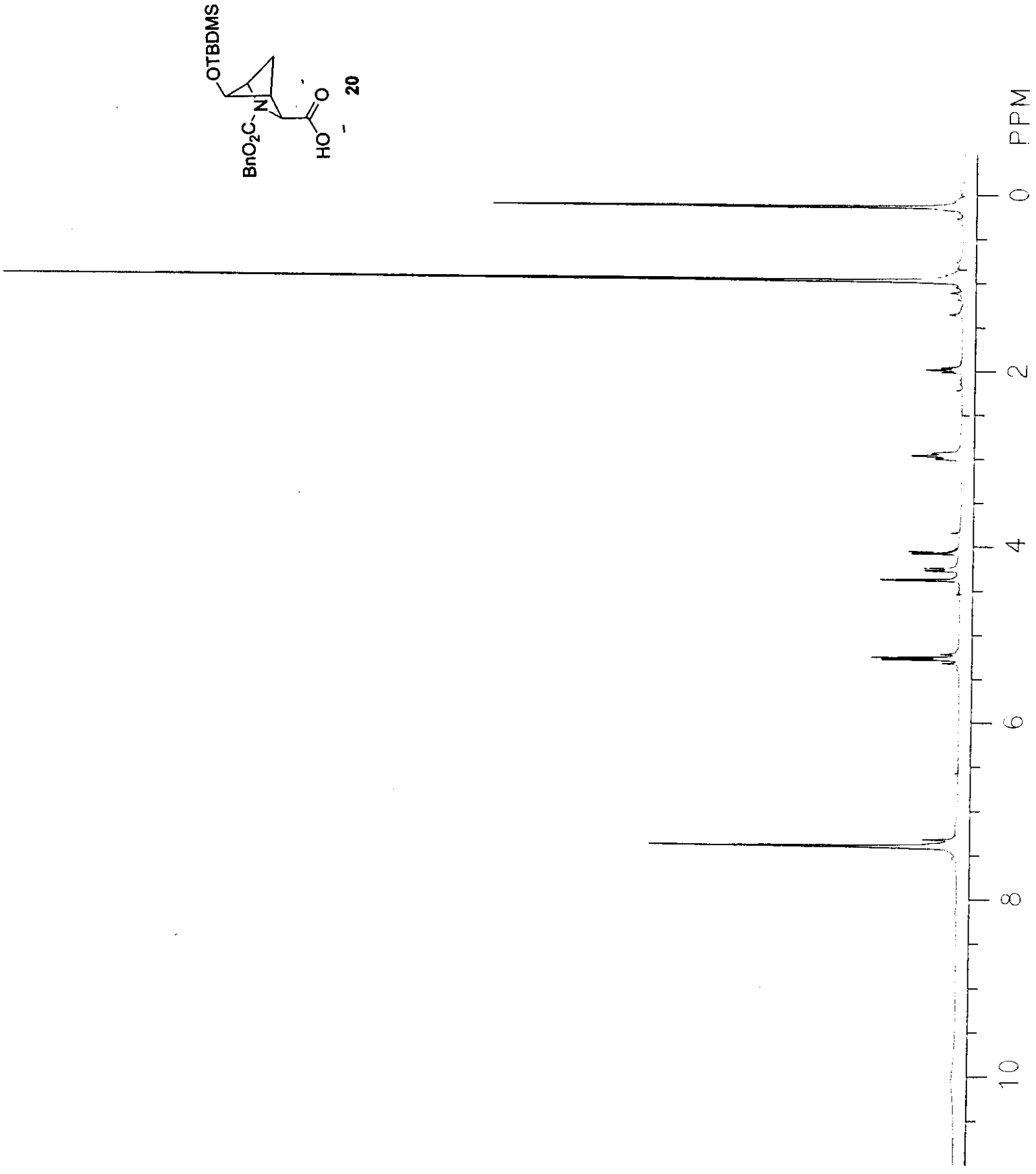
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BnO2C
O
HO
20
PPM
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2
4
6
8
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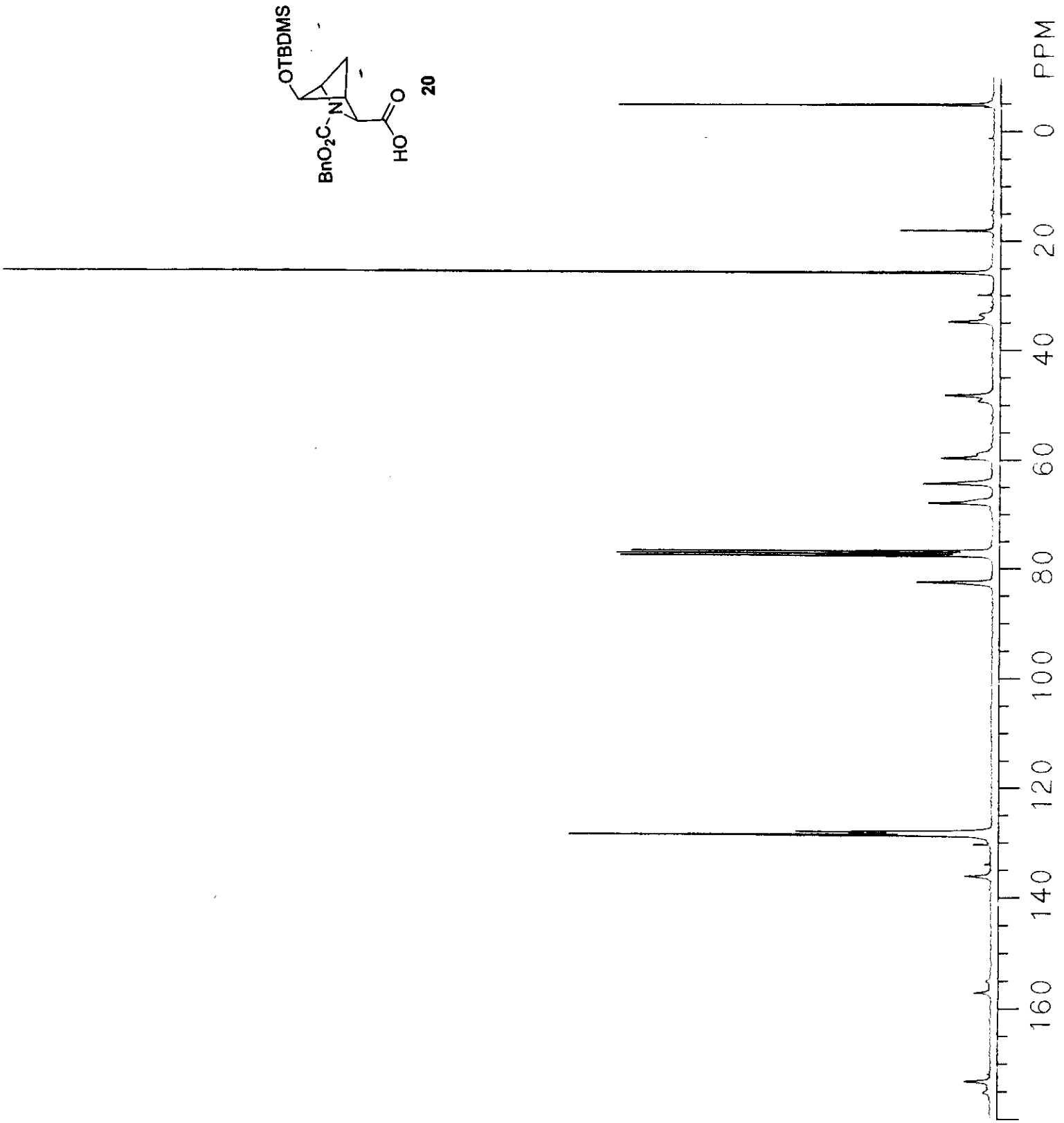
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BnO2C
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PPM
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20
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60
80
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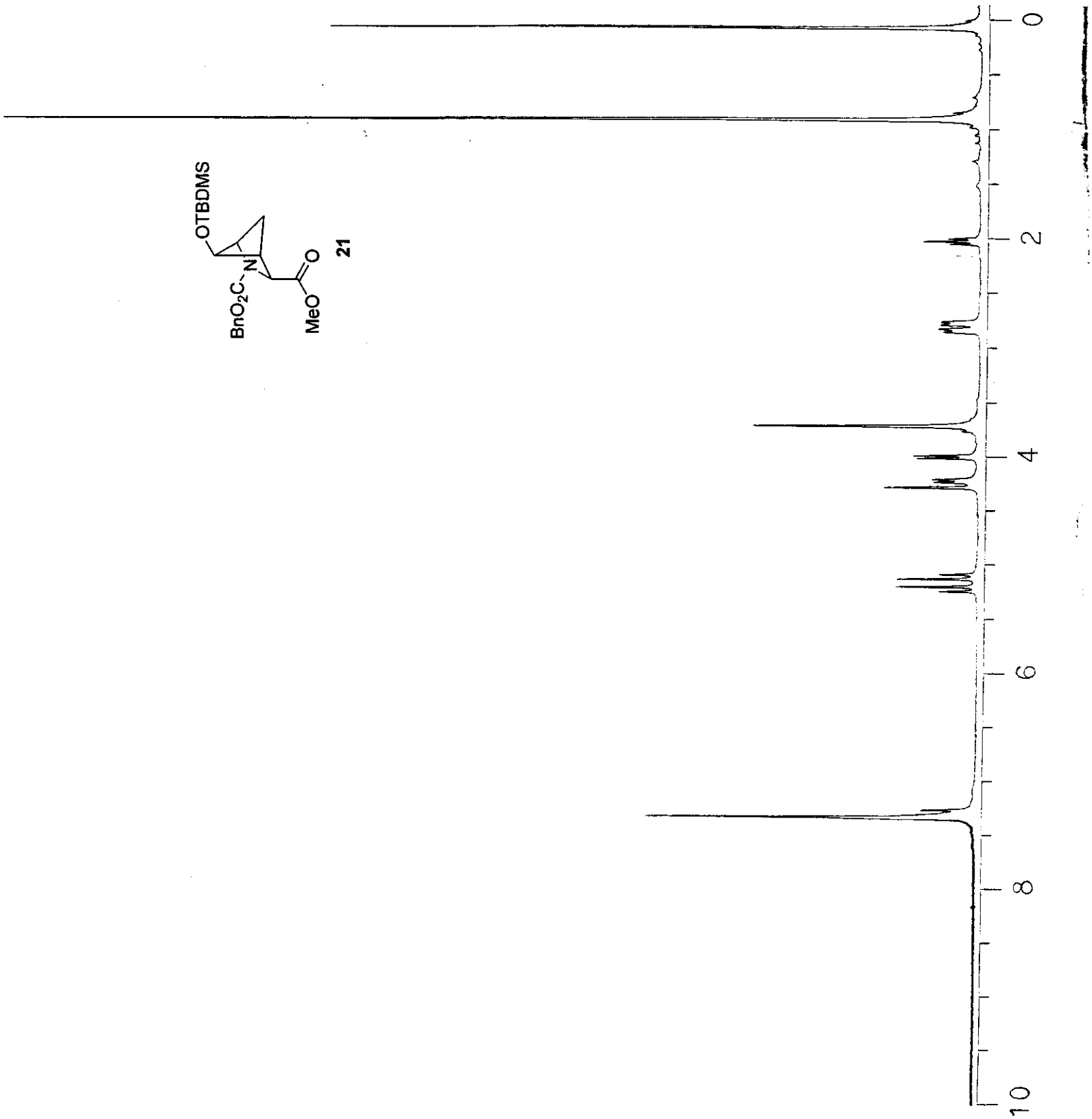
120
140
160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BnO2C
MeO
O
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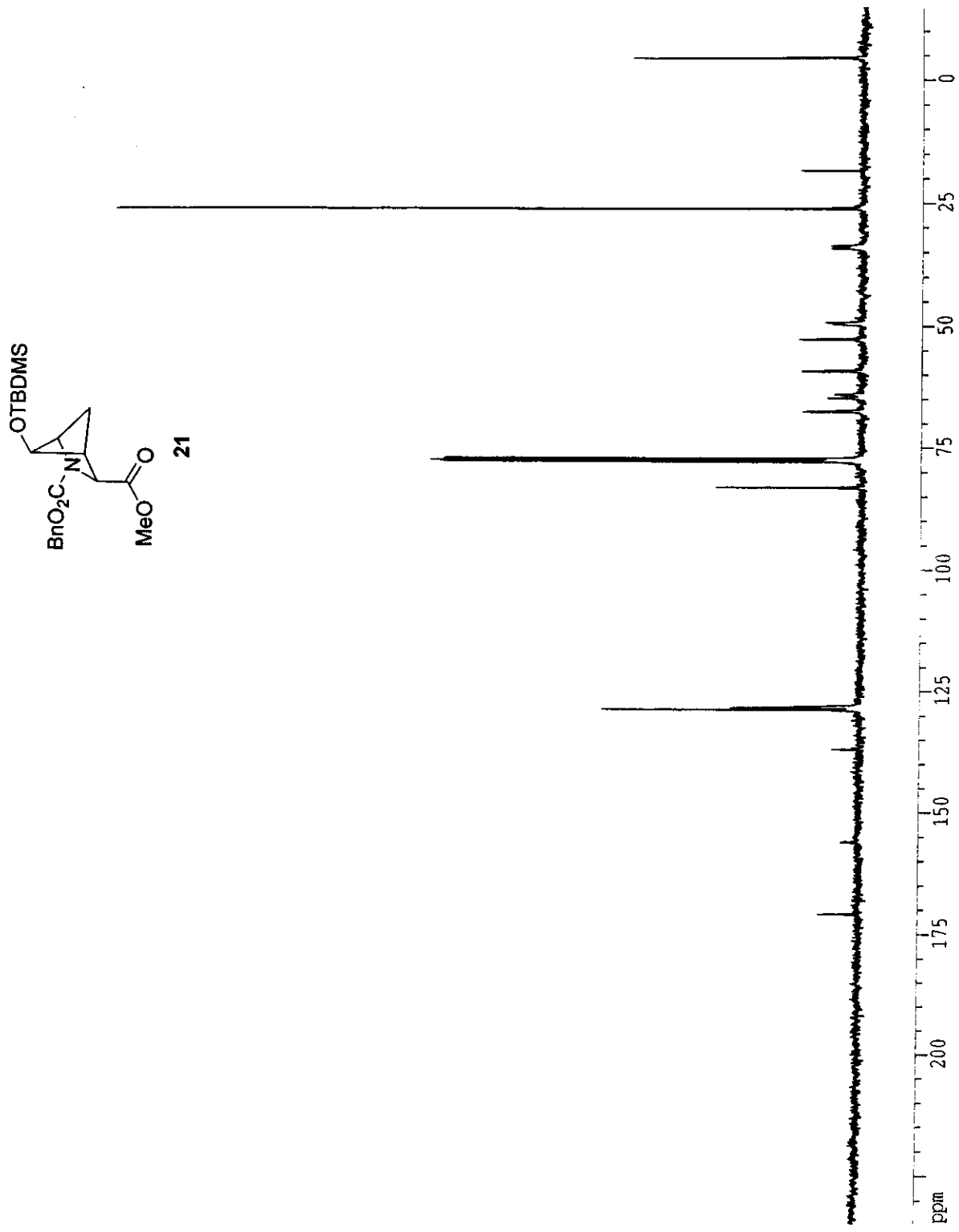
4
6
8
10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BnO2C
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MeO
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50
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125
150
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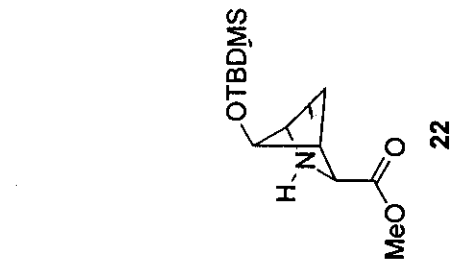
200
ppm



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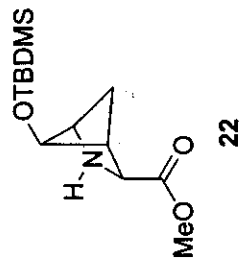

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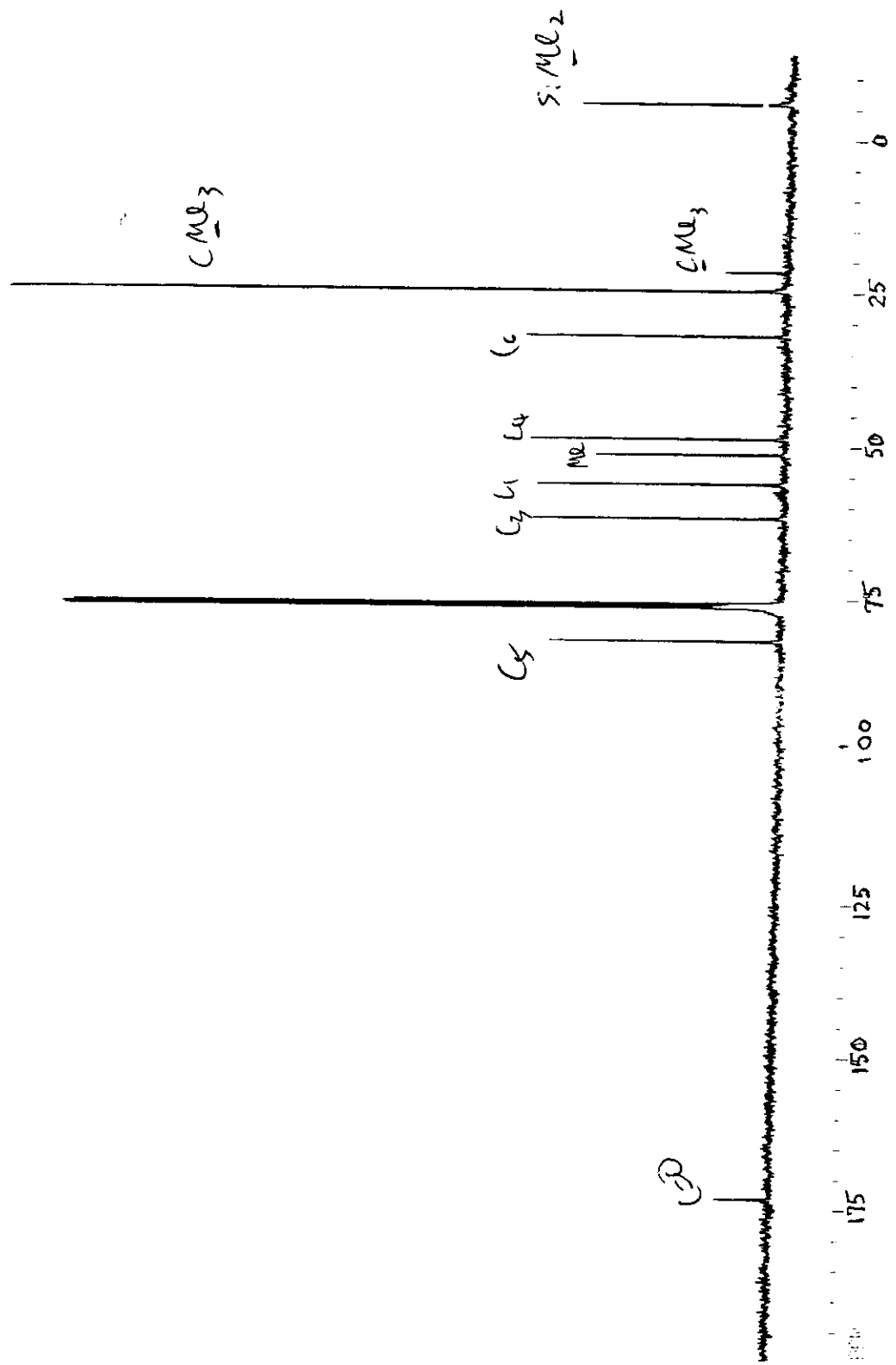
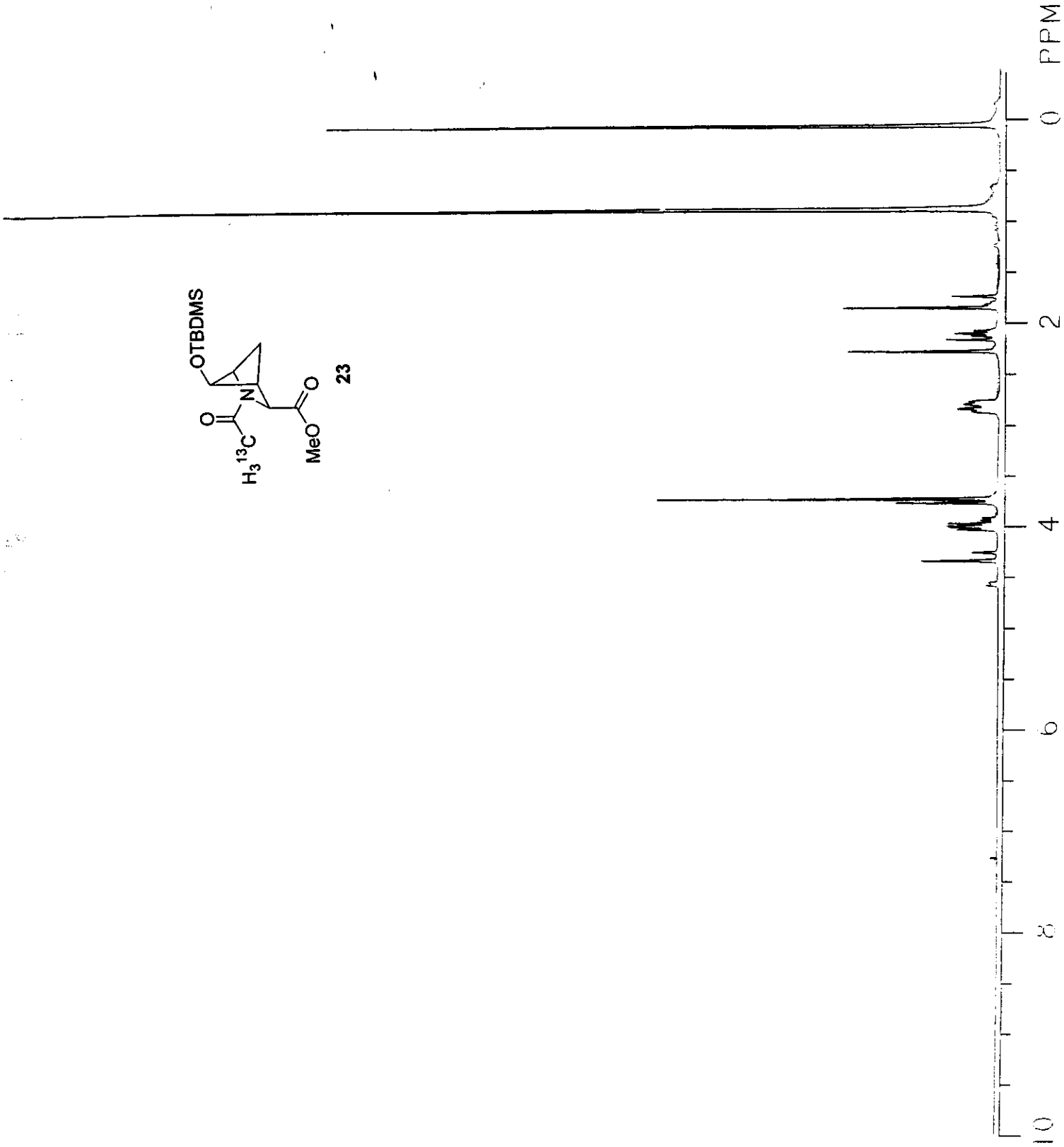
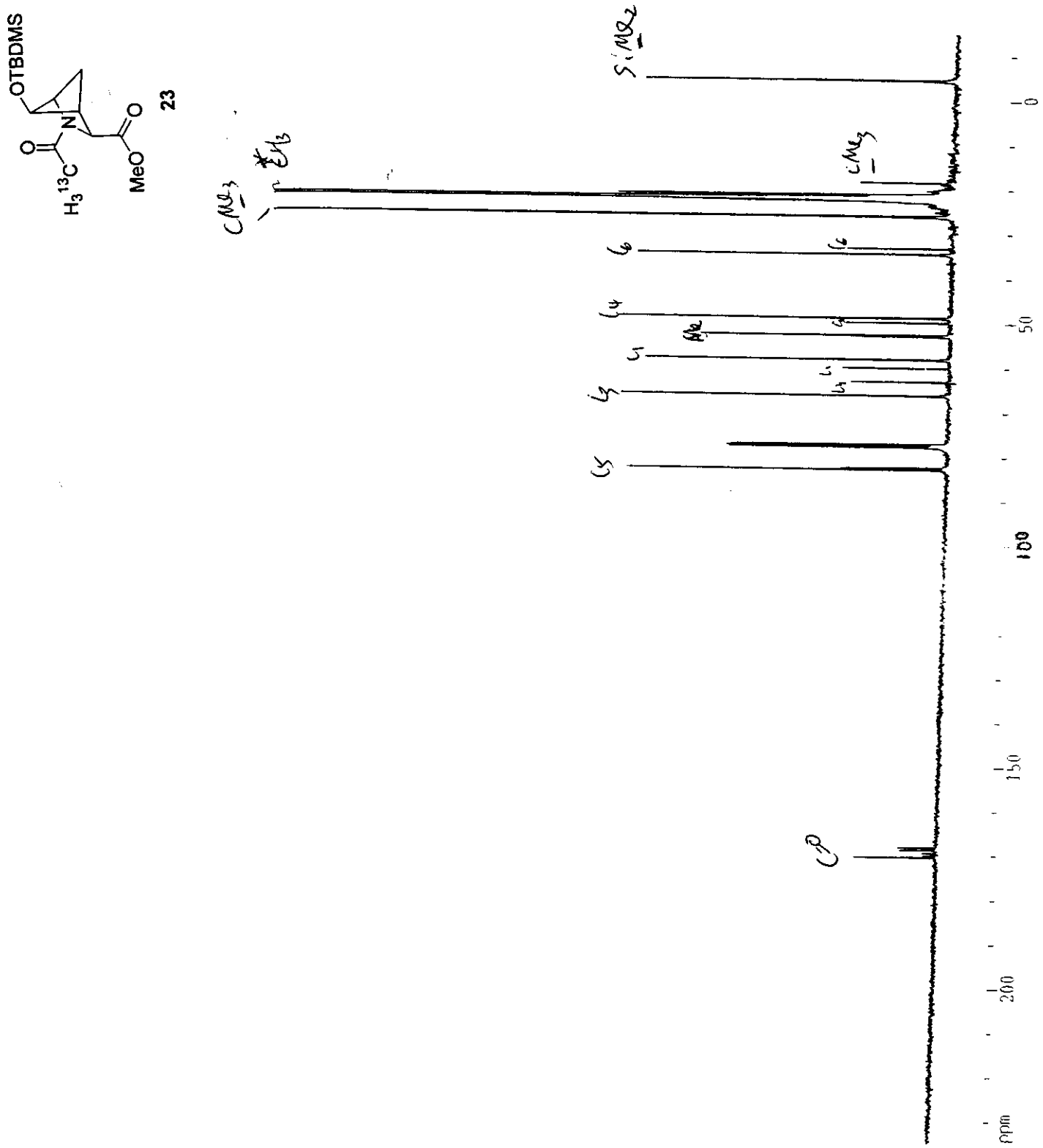



OTBDMS
N
O
$H_3{}^{13}C$
O
MeO
23
0
2
4
6
8
10
PPM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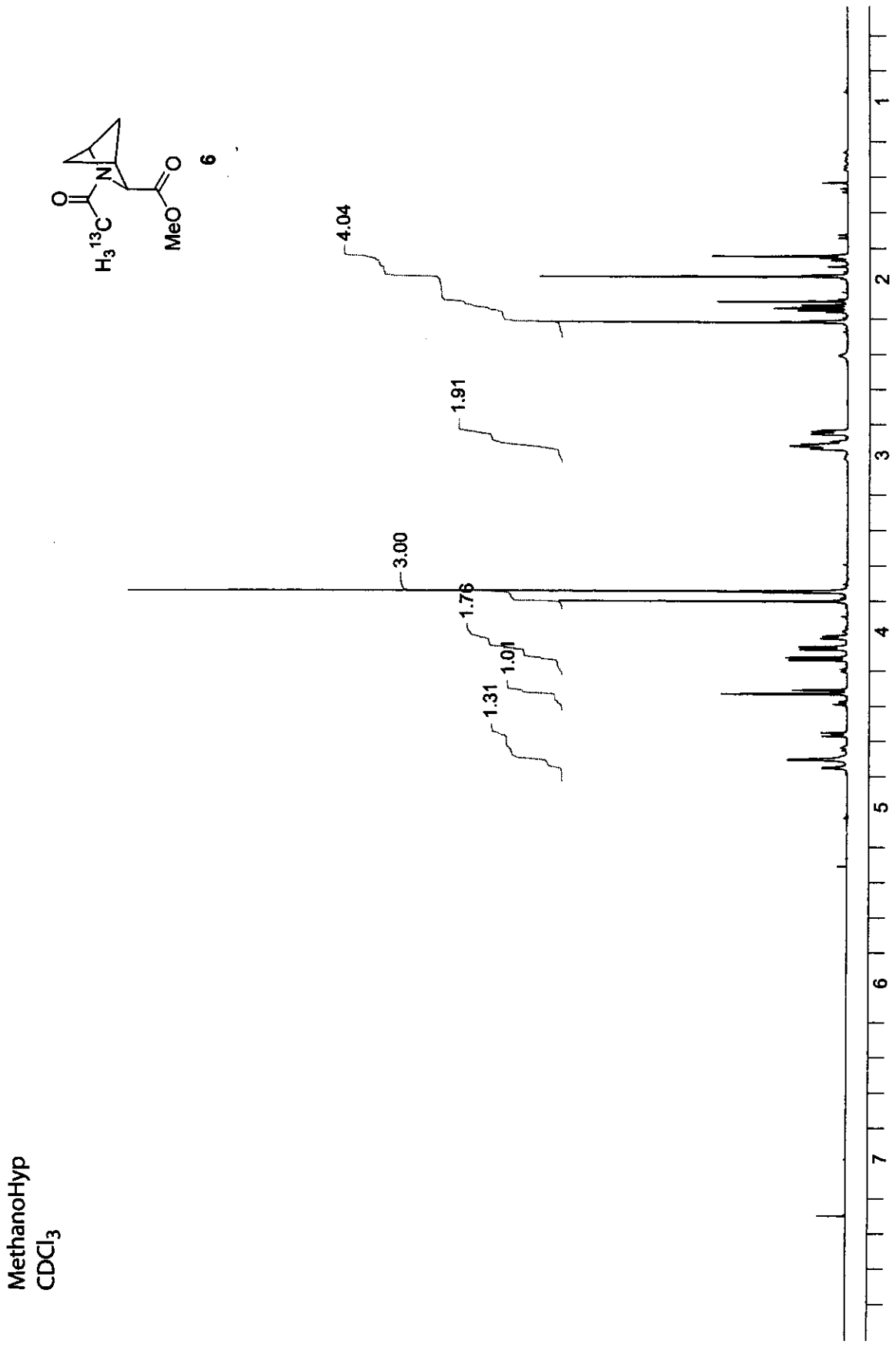
O
O
MeO
$H_3{}^{13}C$
23
ppm
200
150
100
50
0


MethanoHyp
$CDCl_3$
$H_3{}^{13}C$
O
N
O
MeO
O
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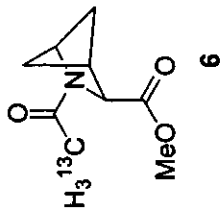
1.91
3.00
1.76
1.01
1.31
1
2
3
4
5
6
7



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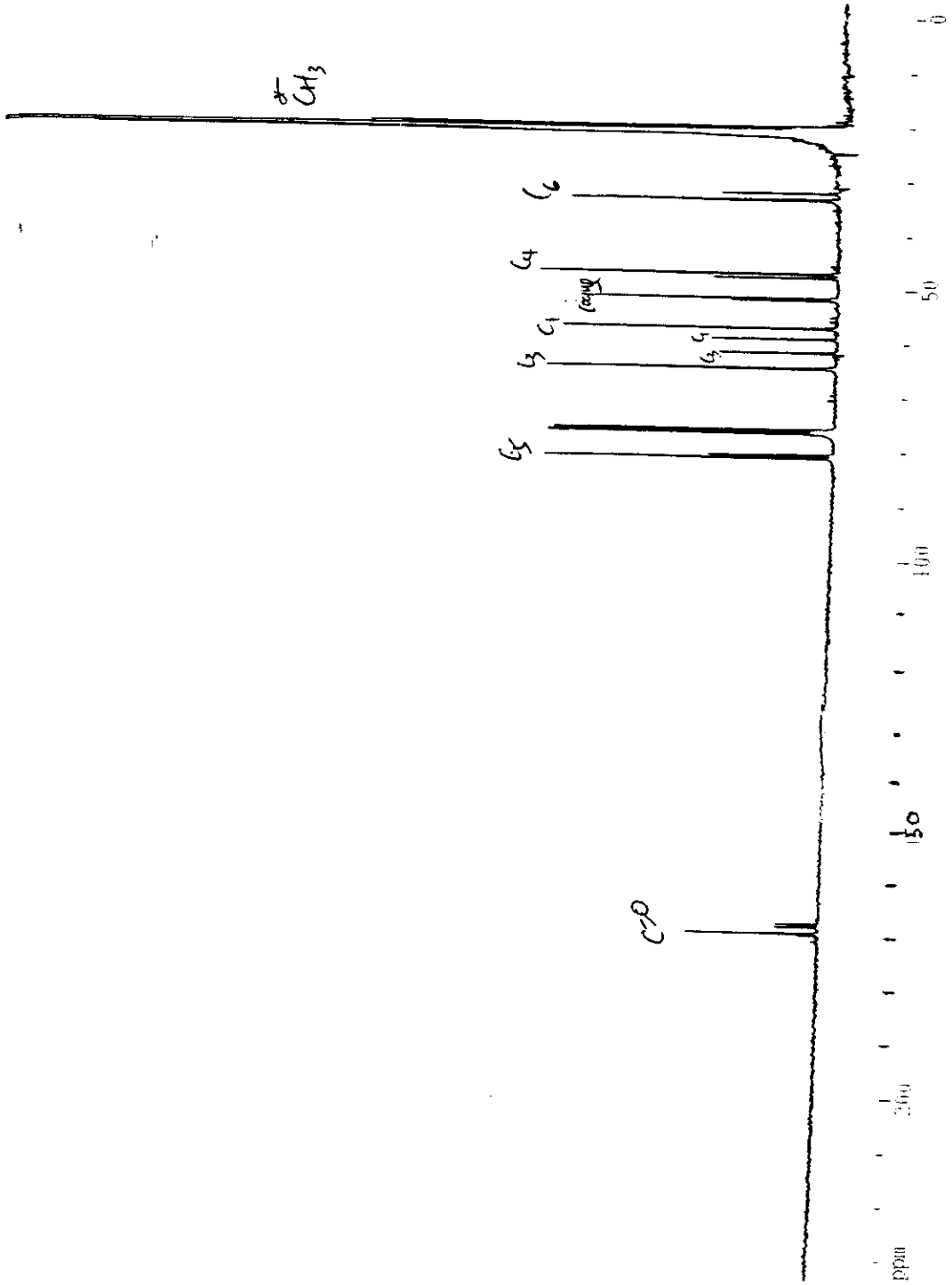

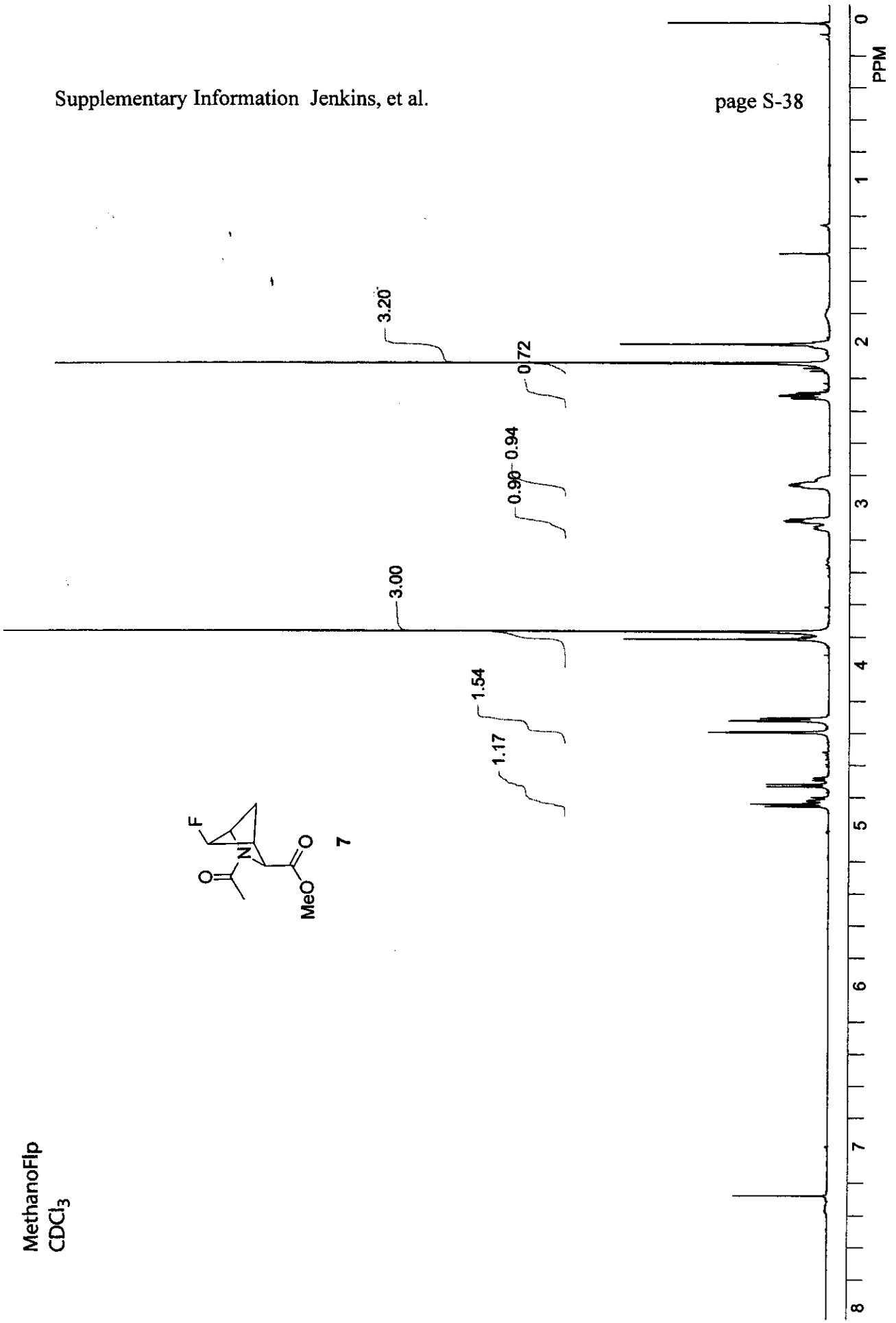
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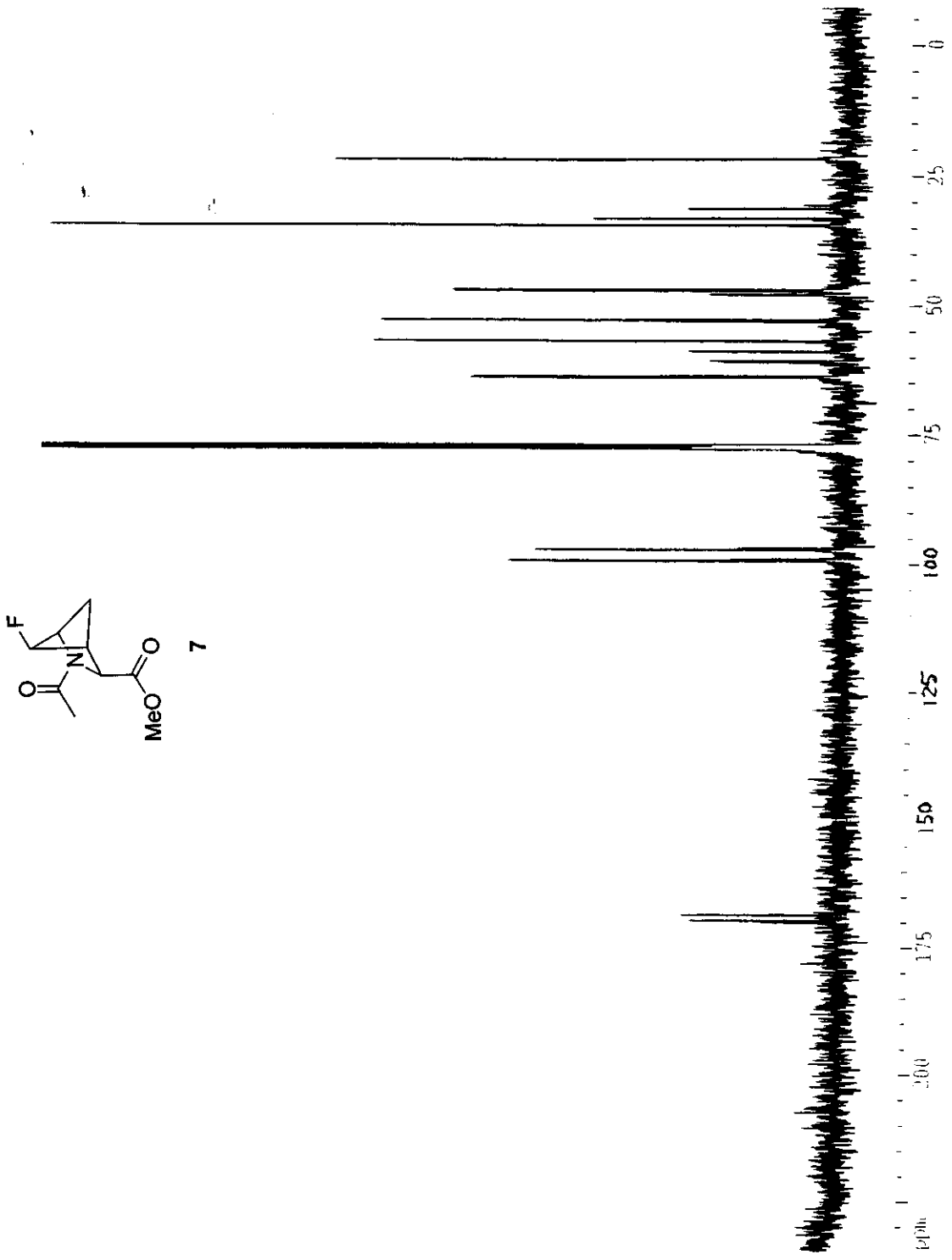
0.72
0.94
0.90
3.00
1.54
1.17
F
N
O
O
MeO
7
PPM
0
1
2
3
4
5
6
7
8


F
N
O
O
MeO
7
0
25
50
75
100
125
150
175
200
ppm

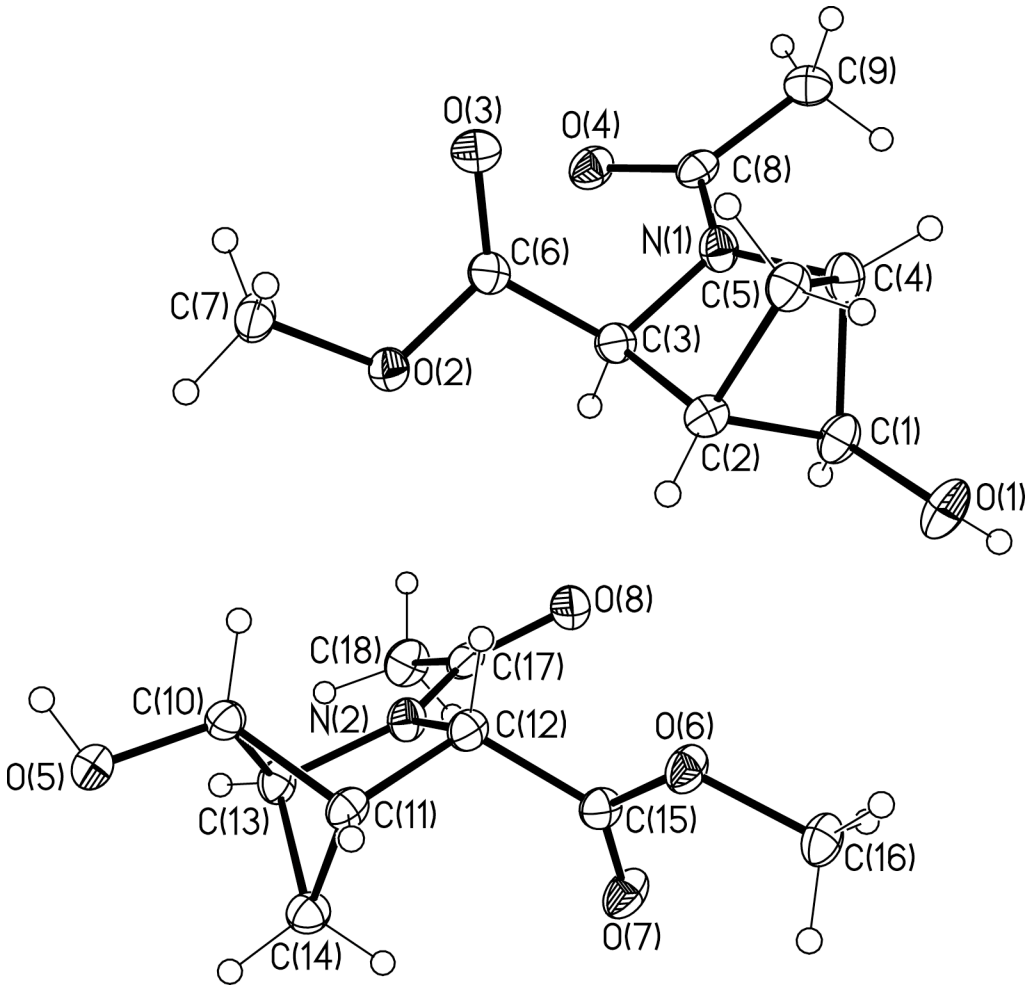


Figure S-1. The crystal structure of Ac–methano-hyp–OMe (6). Top: Molecule A; Bottom: Molecule B. The Supporting Information uses the nomenclature in this figure.

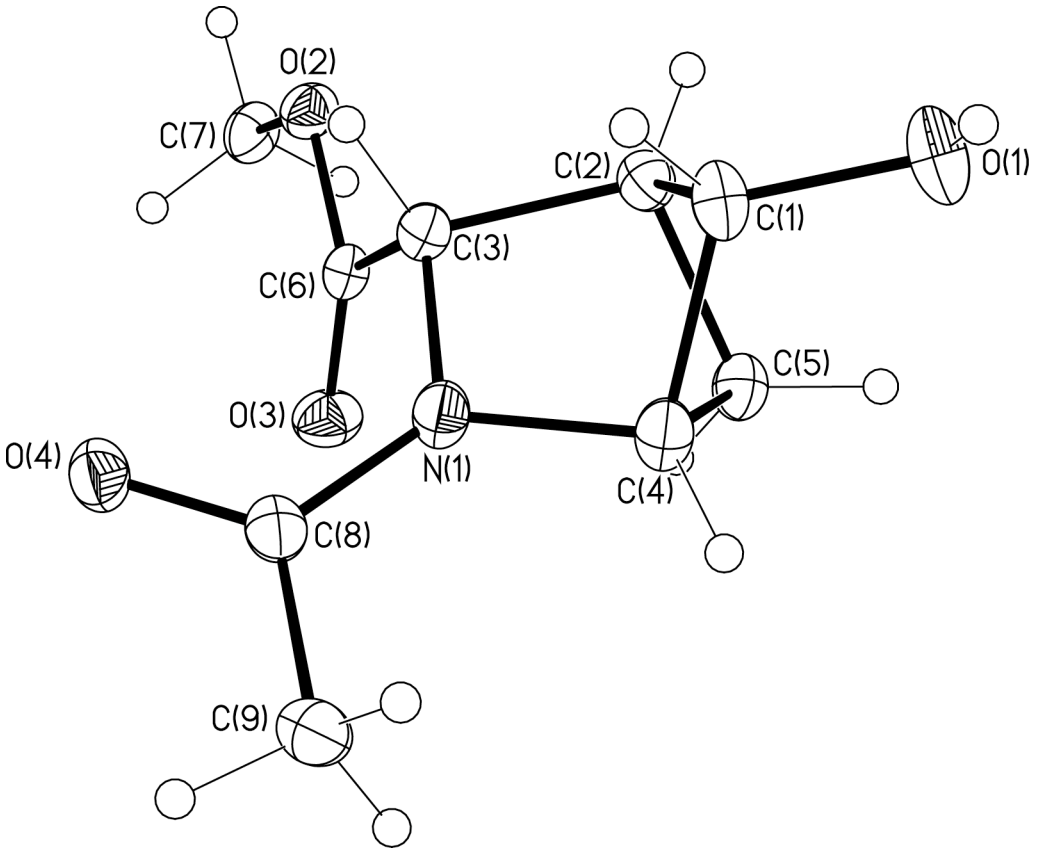


Figure S-2. Molecule A of Ac–methano-hyp–OMe (6).

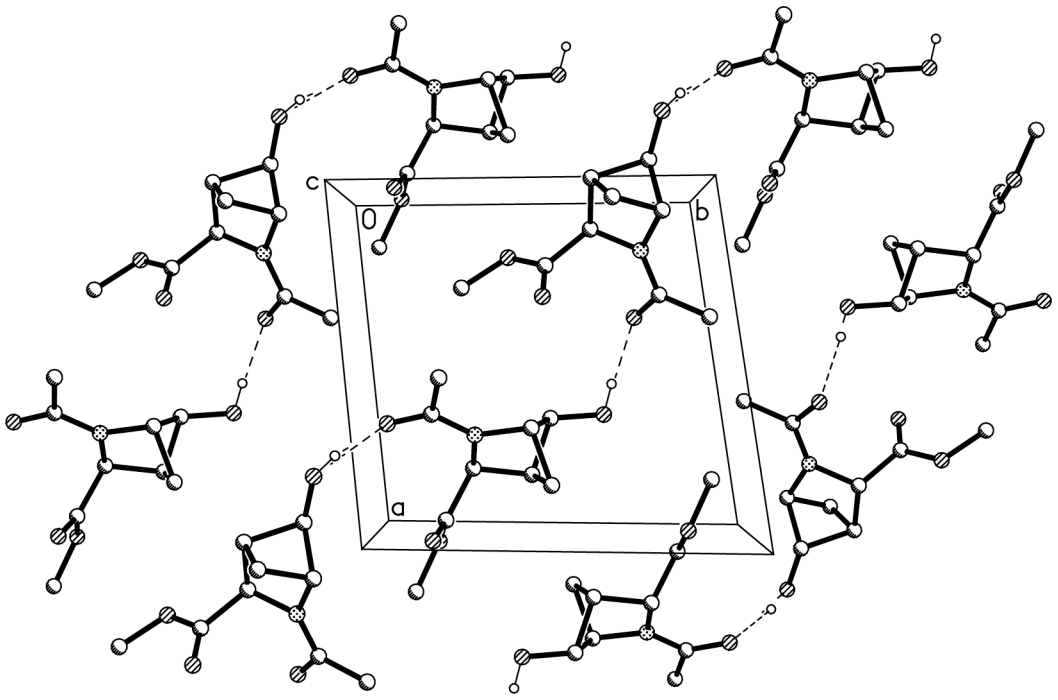


Figure S-3. Packing diagram of Ac–methano-hyp–OMe (6) viewed in the *c* direction.

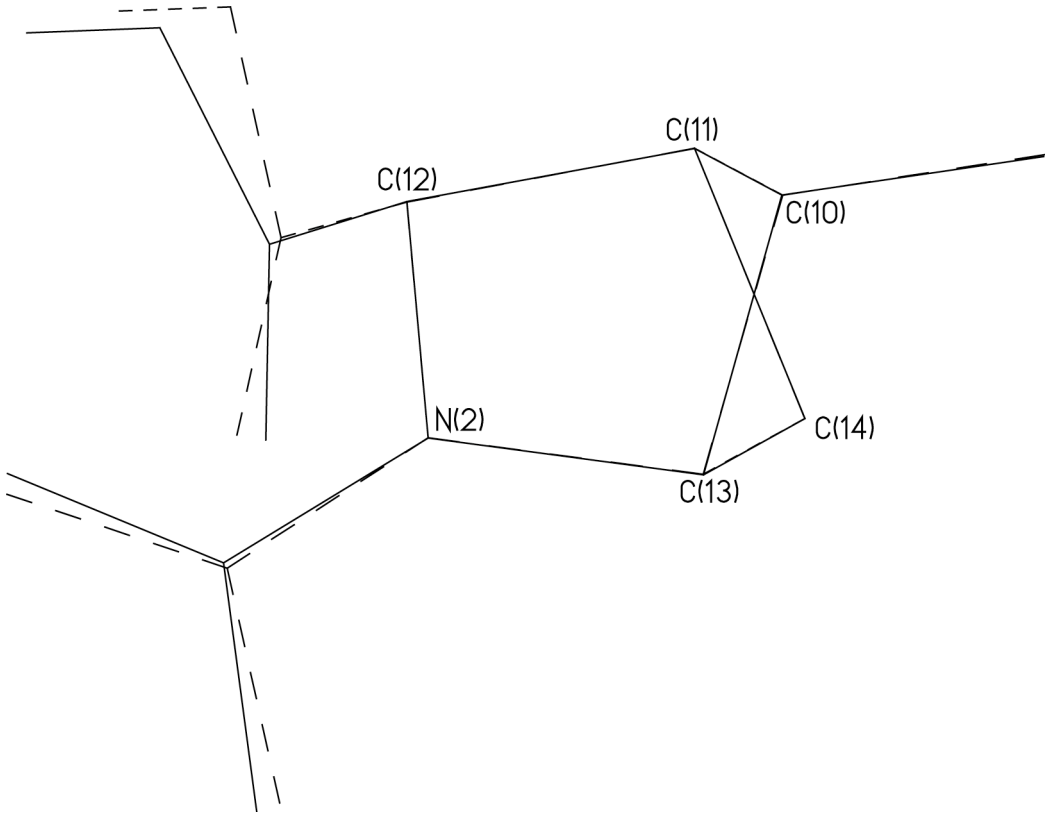


Figure S-4. Superposition of the two crystallographically independent molecules of Ac–methano-hyp–OMe (6).

Table S-1. Crystal data and structure refinement for Ac–methano-hyp–OMe (6).

Identification code	rai03	
Empirical formula	$C_9H_{13}NO_4$	
Formula weight	199.20	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 9.6797(10) Å	α = 80.629(2)°
	b = 9.963(1) Å	β = 72.380(2)°
	c = 10.7145(10) Å	γ = 80.362(1)°
Volume	963.98(17) Å^3	
Z	4	
Density (calculated)	1.373 Mg/m^3	
Absorption coefficient	0.108 mm^{-1}	
F(000)	424	
Crystal size	0.50 × 0.40 × 0.40 mm^3	
Theta range for data collection	2.01–26.35°	
Index ranges	$-11 \le h \le 12$, $-12 \le k \le 12$, $0 \le l \le 13$	
Reflections collected	12437	
Independent reflections	3638 [R(int) = 0.0284]	
Completeness to theta = 26.35°	92.2%	
Absorption correction	Empirical with SADABS	
Max. and min. transmission	0.9579 and 0.9478	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3638 / 0 / 259	
Goodness-of-fit on F^2	1.000	
Final R indices [$I > 2\sigma$(I)]	$R1$ = 0.0735, $wR2$ = 0.2132	
R indices (all data)	$R1$ = 0.0822, $wR2$ = 0.2199	
Largest diff. peak and hole	0.341 and –0.391 e.Å^{-3}	

Table S-2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for crystalline Ac–methano-hyp–OMe (6). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	*y*	*z*	*U*(eq)
O(1)	6543(2)	6489(2)	5853(2)	43(1)
O(2)	10187(2)	1683(2)	4942(2)	31(1)
O(3)	10004(2)	1630(2)	7091(2)	39(1)
O(4)	6762(2)	827(2)	8093(2)	36(1)
O(5)	11863(2)	1075(2)	388(2)	35(1)
O(6)	7908(2)	5524(2)	2673(2)	34(1)
O(7)	6757(2)	4747(2)	1450(2)	39(1)
O(8)	6213(2)	2369(2)	3947(2)	37(1)
N(1)	7079(2)	3049(2)	7515(2)	30(1)
N(2)	8063(2)	2036(2)	2142(2)	30(1)
C(1)	6644(3)	5066(3)	6186(3)	32(1)
C(2)	8246(3)	4390(3)	5720(3)	28(1)
C(3)	8059(3)	2864(3)	6186(3)	28(1)
C(4)	6876(3)	4536(3)	7575(3)	32(1)
C(5)	8470(3)	4877(3)	6956(3)	31(1)
C(6)	9507(3)	1985(3)	6176(3)	27(1)
C(7)	11629(3)	893(3)	4769(3)	34(1)
C(8)	6485(3)	2022(3)	8382(3)	29(1)
C(9)	5481(3)	2377(3)	9695(3)	35(1)
C(10)	10578(3)	1539(3)	1325(3)	28(1)
C(11)	10053(3)	3099(3)	1027(3)	28(1)
C(12)	8680(3)	3269(3)	2215(3)	28(1)
C(13)	9123(3)	1401(3)	1026(3)	30(1)
C(14)	9437(3)	2666(3)	–18(3)	31(1)
C(15)	7646(3)	4571(3)	2063(3)	29(1)
C(16)	7045(3)	6855(3)	2586(3)	36(1)
C(17)	6837(3)	1674(3)	3015(3)	29(1)
C(18)	6210(3)	459(3)	2841(3)	40(1)

Table S-3. Bond lengths [Å] and angles [°] for crystalline Ac–methano-hyp–OMe (6). Symmetry transformations used to generate equivalent atoms: molecule A: $-x + 1, -y + 1, -z + 1$; molecule B: $-x + 2, -y, -z + 1$.

O(1)–C(1)	1.399(3)	N(2)–C(12)	1.475(3)
O(2)–C(6)	1.346(3)	C(1)–C(2)	1.549(4)
O(2)–C(7)	1.458(3)	C(1)–C(4)	1.565(4)
O(3)–C(6)	1.198(3)	C(2)–C(3)	1.544(4)
O(4)–C(8)	1.244(3)	C(2)–C(5)	1.568(4)
O(5)–C(10)	1.404(3)	C(3)–C(6)	1.521(4)
O(6)–C(15)	1.333(3)	C(4)–C(5)	1.555(4)
O(6)–C(16)	1.450(3)	C(8)–C(9)	1.506(4)
O(7)–C(15)	1.207(3)	C(10)–C(11)	1.565(4)
O(8)–C(17)	1.250(3)	C(10)–C(13)	1.568(4)
N(1)–C(8)	1.344(4)	C(11)–C(12)	1.545(4)
N(1)–C(4)	1.471(3)	C(11)–C(14)	1.563(4)
N(1)–C(3)	1.474(3)	C(12)–C(15)	1.518(4)
N(2)–C(17)	1.333(4)	C(13)–C(14)	1.548(4)
N(2)–C(13)	1.472(3)	C(17)–C(18)	1.502(4)

C(6)–O(2)–C(7)	114.9(2)	O(2)–C(6)–C(3)	108.7(2)
C(15)–O(6)–C(16)	116.6(2)	O(4)–C(8)–N(1)	120.4(3)
C(8)–N(1)–C(4)	131.4(2)	O(4)–C(8)–C(9)	122.0(2)
C(8)–N(1)–C(3)	123.8(2)	N(1)–C(8)–C(9)	117.6(2)
C(4)–N(1)–C(3)	104.8(2)	O(5)–C(10)–C(11)	113.1(2)
C(17)–N(2)–C(13)	133.5(2)	O(5)–C(10)–C(13)	115.1(2)
C(17)–N(2)–C(12)	121.8(2)	C(11)–C(10)–C(13)	81.53(19)
C(13)–N(2)–C(12)	104.7(2)	C(12)–C(11)–C(14)	102.6(2)
O(1)–C(1)–C(2)	111.0(2)	C(12)–C(11)–C(10)	99.9(2)
O(1)–C(1)–C(4)	115.2(2)	C(14)–C(11)–C(10)	86.28(19)
C(2)–C(1)–C(4)	81.87(19)	N(2)–C(12)–C(15)	112.0(2)
C(3)–C(2)–C(1)	100.9(2)	N(2)–C(12)–C(11)	97.24(19)
C(3)–C(2)–C(5)	102.3(2)	C(15)–C(12)–C(11)	114.4(2)
C(1)–C(2)–C(5)	86.5(2)	N(2)–C(13)–C(14)	101.4(2)
N(1)–C(3)–C(6)	114.2(2)	N(2)–C(13)–C(10)	99.4(2)
N(1)–C(3)–C(2)	97.0(2)	C(14)–C(13)–C(10)	86.7(2)
C(6)–C(3)–C(2)	112.2(2)	C(13)–C(14)–C(11)	82.22(19)
N(1)–C(4)–C(5)	101.1(2)	O(7)–C(15)–O(6)	124.6(2)
N(1)–C(4)–C(1)	99.7(2)	O(7)–C(15)–C(12)	126.0(2)
C(5)–C(4)–C(1)	86.4(2)	O(6)–C(15)–C(12)	109.3(2)
C(4)–C(5)–C(2)	81.60(19)	O(8)–C(17)–N(2)	119.4(3)
O(3)–C(6)–O(2)	124.2(2)	O(8)–C(17)–C(18)	121.2(3)
O(3)–C(6)–C(3)	127.0(2)	N(2)–C(17)–C(18)	119.4(2)

Table S-4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for Ac–methano-hyp–OMe (6). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	33(1)	25(1)	63(2)	6(1)	–11(1)	–2(1)
O(2)	34(1)	29(1)	31(1)	–8(1)	–12(1)	2(1)
O(3)	41(1)	44(1)	35(1)	–6(1)	–18(1)	1(1)
O(4)	41(1)	26(1)	41(1)	0(1)	–16(1)	–5(1)
O(5)	35(1)	31(1)	36(1)	–3(1)	–10(1)	4(1)
O(6)	42(1)	22(1)	44(1)	–8(1)	–21(1)	–1(1)
O(7)	44(1)	28(1)	55(1)	–8(1)	–31(1)	2(1)
O(8)	36(1)	37(1)	36(1)	–8(1)	–10(1)	2(1)
N(1)	31(1)	25(1)	33(1)	–6(1)	–5(1)	–5(1)
N(2)	36(1)	21(1)	35(1)	–7(1)	–11(1)	–5(1)
C(1)	29(1)	23(1)	44(2)	0(1)	–10(1)	–5(1)
C(2)	28(1)	27(1)	31(1)	–1(1)	–11(1)	–6(1)
C(3)	33(1)	24(1)	28(1)	–4(1)	–11(1)	–5(1)
C(4)	31(1)	26(1)	37(2)	–6(1)	–5(1)	–5(1)
C(5)	31(1)	27(1)	37(2)	–5(1)	–11(1)	–6(1)
C(6)	33(1)	21(1)	29(1)	–4(1)	–10(1)	–7(1)
C(7)	33(1)	29(1)	42(2)	–10(1)	–14(1)	4(1)
C(8)	29(1)	27(1)	34(1)	0(1)	–16(1)	–4(1)
C(9)	36(1)	40(2)	30(1)	1(1)	–10(1)	–9(1)
C(10)	34(1)	24(1)	28(1)	–3(1)	–11(1)	–1(1)
C(11)	31(1)	22(1)	33(1)	–2(1)	–14(1)	–4(1)
C(12)	35(1)	22(1)	32(1)	–6(1)	–15(1)	–3(1)
C(13)	34(1)	23(1)	34(2)	–8(1)	–10(1)	–3(1)
C(14)	35(1)	30(1)	32(1)	–4(1)	–14(1)	–4(1)
C(15)	34(1)	23(1)	31(1)	–3(1)	–12(1)	–7(1)
C(16)	41(2)	23(1)	48(2)	–8(1)	–16(1)	–2(1)
C(17)	31(1)	24(1)	32(1)	0(1)	–14(1)	2(1)
C(18)	43(2)	28(2)	50(2)	–2(1)	–12(1)	–11(1)

Table S-5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for Ac–methano-hyp–OMe (6).

	x	*y*	*z*	*U*(eq)
H(1)	5677	6804	5869	64
H(5)	12402	519	770	53
H(1A)	5916	4616	5961	39
H(2)	8875	4672	4816	34
H(3)	7551	2505	5647	33
H(4)	6231	4940	8381	38
H(5A)	9208	4281	7334	37
H(5B)	8586	5860	6864	37
H(7A)	12293	1443	4932	51
H(7B)	12007	652	3866	51
H(7C)	11557	54	5393	51
H(9A)	5036	1565	10191	53
H(9B)	4712	3110	9553	53
H(9C)	6040	2686	10194	53
H(10)	10580	1239	2262	34
H(11)	10766	3785	760	33
H(12)	8957	3188	3053	34
H(13)	8970	524	777	35
H(14A)	8557	3258	–165	37
H(14B)	10175	2470	–858	37
H(16A)	7198	7231	1657	54
H(16B)	7345	7476	3049	54
H(16C)	6008	6758	2992	54
H(18A)	5971	–139	3679	60
H(18B)	6928	–52	2168	60
H(18C)	5321	775	2563	60

Table S-6. Torsion angles [°] for Ac–methano-hyp–OMe (6). Symmetry transformations used to generate equivalent atoms: molecule A: *–x* + 1,*–y* + 1,*–z* + 1; molecule B: *–x* + 2, *–y*,*–z* + 1.

O(1)–C(1)–C(2)–C(3)	–179.6(2)	C(17)–N(2)–C(12)–C(11)	178.1(2)
C(4)–C(1)–C(2)–C(3)	66.4(2)	C(13)–N(2)–C(12)–C(11)	1.1(2)
O(1)–C(1)–C(2)–C(5)	78.6(3)	C(14)–C(11)–C(12)–N(2)	42.4(2)
C(4)–C(1)–C(2)–C(5)	–35.43(18)	C(10)–C(11)–C(12)–N(2)	–46.0(2)
C(8)–N(1)–C(3)–C(6)	–65.0(3)	C(14)–C(11)–C(12)–C(15)	–75.7(3)
C(4)–N(1)–C(3)–C(6)	118.7(2)	C(10)–C(11)–C(12)–C(15)	–164.1(2)
C(8)–N(1)–C(3)–C(2)	176.8(2)	C(17)–N(2)–C(13)–C(14)	138.8(3)
C(4)–N(1)–C(3)–C(2)	0.5(2)	C(12)–N(2)–C(13)–C(14)	–44.6(2)
C(1)–C(2)–C(3)–N(1)	–45.3(2)	C(17)–N(2)–C(13)–C(10)	–132.7(3)
C(5)–C(2)–C(3)–N(1)	43.5(2)	C(12)–N(2)–C(13)–C(10)	43.8(2)
C(1)–C(2)–C(3)–C(6)	–165.1(2)	O(5)–C(10)–C(13)–N(2)	–177.2(2)
C(5)–C(2)–C(3)–C(6)	–76.3(3)	C(11)–C(10)–C(13)–N(2)	–65.5(2)
C(8)–N(1)–C(4)–C(5)	139.5(3)	O(5)–C(10)–C(13)–C(14)	–76.2(2)
C(3)–N(1)–C(4)–C(5)	–44.6(2)	C(11)–C(10)–C(13)–C(14)	35.44(18)
C(8)–N(1)–C(4)–C(1)	–132.3(3)	N(2)–C(13)–C(14)–C(11)	63.6(2)
C(3)–N(1)–C(4)–C(1)	43.7(2)	C(10)–C(13)–C(14)–C(11)	–35.40(18)
O(1)–C(1)–C(4)–N(1)	–174.4(2)	C(12)–C(11)–C(14)–C(13)	–63.8(2)
C(2)–C(1)–C(4)–N(1)	–64.9(2)	C(10)–C(11)–C(14)–C(13)	35.52(18)
O(1)–C(1)–C(4)–C(5)	–73.7(2)	C(16)–O(6)–C(15)–O(7)	0.4(4)
C(2)–C(1)–C(4)–C(5)	35.77(18)	C(16)–O(6)–C(15)–C(12)	178.0(2)
N(1)–C(4)–C(5)–C(2)	63.9(2)	N(2)–C(12)–C(15)–O(7)	–29.0(4)
C(1)–C(4)–C(5)–C(2)	–35.30(18)	C(11)–C(12)–C(15)–O(7)	80.4(3)
C(3)–C(2)–C(5)–C(4)	–64.7(2)	N(2)–C(12)–C(15)–O(6)	153.5(2)
C(1)–C(2)–C(5)–C(4)	35.72(19)	C(11)–C(12)–C(15)–O(6)	–97.1(3)
C(7)–O(2)–C(6)–O(3)	–1.2(4)	C(13)–N(2)–C(17)–O(8)	173.7(3)
C(7)–O(2)–C(6)–C(3)	177.3(2)	C(12)–N(2)–C(17)–O(8)	–2.4(4)
N(1)–C(3)–C(6)–O(3)	–12.6(4)	C(13)–N(2)–C(17)–C(18)	–7.8(4)
C(2)–C(3)–C(6)–O(3)	96.6(3)	C(12)–N(2)–C(17)–C(18)	176.2(2)
N(1)–C(3)–C(6)–O(2)	169.0(2)		
C(2)–C(3)–C(6)–O(2)	–81.9(3)		
C(4)–N(1)–C(8)–O(4)	176.2(2)		
C(3)–N(1)–C(8)–O(4)	0.9(4)		
C(4)–N(1)–C(8)–C(9)	–3.5(4)		
C(3)–N(1)–C(8)–C(9)	–178.8(2)		
O(5)–C(10)–C(11)–C(12)	–179.2(2)		
C(13)–C(10)–C(11)–C(12)	67.1(2)		
O(5)–C(10)–C(11)–C(14)	78.7(2)		
C(13)–C(10)–C(11)–C(14)	–35.05(18)		
C(17)–N(2)–C(12)–C(15)	–61.9(3)		
C(13)–N(2)–C(12)–C(15)	121.1(2)		

Table S-7. Hydrogen bonds for Ac–methano-hyp–OMe (6) [Å and °]. Symmetry transformations used to generate equivalent atoms: molecule A: $-x + 1, -y + 1, -z + 1$; molecule B: $-x + 2, -y, -z + 1$.

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
O(1)–H(1)···O(8) (molecule A)	0.84	1.84	2.678(3)	173(1)
O(5)–H(5)···O(4) (molecule B)	0.84	1.91	2.734(3)	168(1)