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SUPPORTING INFORMATION

Title: Concise Synthesis of 2,6-Disubstituted Morpholines by Cyclization of Epoxy Alcohols
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Ref. No.: O200700011

Contents:

GeneralMethods

Procedure for synthesis of [1,4]-oxazepan-6-ol **13a**

References and notes

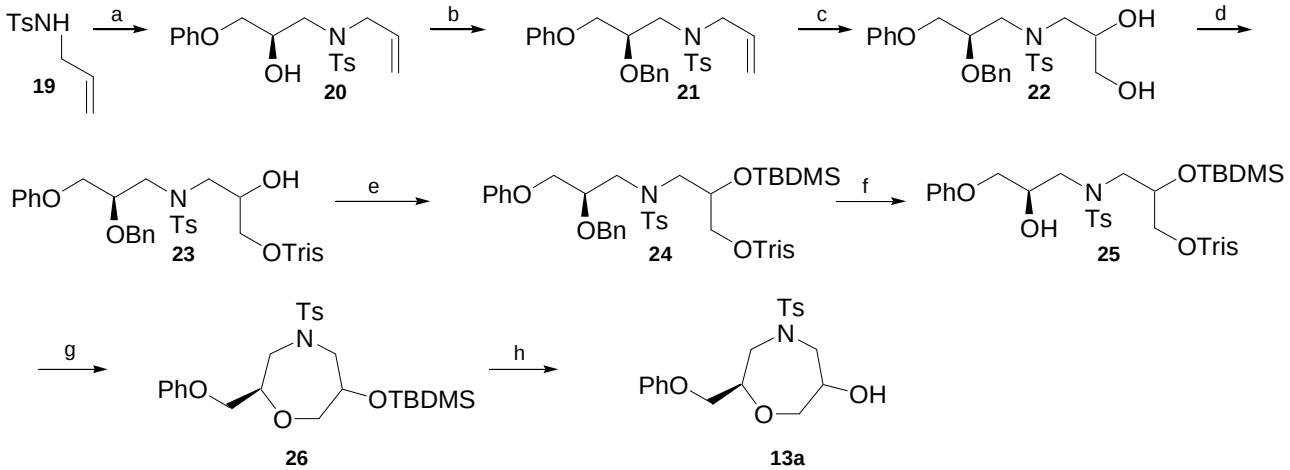
Copies of ^{1}H NMR and ^{13}C NMR spectra

General Methods. Melting points were determined on a BÜCHI 535 and are corrected. Infrared (IR) spectra were recorded on a Perkin Elmer 1725 X FT-IR spectrometer. NMR spectra were recorded on a Bruker AC 300 or AC 200 spectrometers, operating at 300.13 or 200.13 MHz for ^{1}H NMR and 75.3 or 50 MHz for ^{13}C NMR. Coupling constants *J* are in Hz. Chemical shifts were reported by using $CHCl_3$ as external standards (7.24 ppm for ^{1}H NMR and 77.0 for ^{13}C NMR). ^{1}H NMR resonances arising from the same proton in different diastereoisomers are reported as follows: [δ upfield resonance (multiplicity, coupling constant), δ downfield resonance (multiplicity, coupling constant), total integration for both resonances]. APT experiments were used in the assignment of carbon spectra. Optical rotations were measured with a Perkin Elmer 241 polarimeter; the $[\alpha]_D$ values are reported in 10^{-1} deg cm^{-2} g^{-1}, concentration (*c*) is reported in g per 100 mL. Mass spectra (ESI and APCI) were measured on a LCQ Advantage Thermo-Finnigan spectrometer. Column chromatography on silica gel (230-400 mesh) was performed by the flash technique or by using MPLC. Chiral HPLC separations were performed on a Agilent HP 1100 apparatus, equipped with a diode array detector, using mixtures of hexane/2-propanol as eluent, detection at 230 nm unless otherwise stated. The flux was set to 1 ml min^{-1} and the volume of injection was 20 μL. Petroleum ether (PE) refers to the fraction boiling in the range of 40-60 °C.

(*R*)-2-Phenoxymethyl-oxirane (**1a**) was prepared in 75% yield as previously described.[1] (*R*)-2-Benzyloxymethyl-oxirane (**1b**) was prepared through the *O*-alkylation of (*S*)-glycidol (**1c**).[2]

Synthesis of [1,4]-oxazepan-6-ol 13a (Scheme 1).

Scheme 1 Synthesis of [1,4]-oxazepan-6-ol **13a**.



Reagents and conditions: a) (*R*)-**1a**, K_2CO_3, TEBA, 3h, 88%; b) NaH, BnBr, THF, RT, 5h, 95%; c) AD-mix β, t-BuOH-H_2O 0 °C, 3d, 15%; d) Tris-Cl, Py, CH_2Cl_2, 2d, 56%; e) TBDMSCl, Im, CH_2Cl_2, 25 °C, 24 h, 83%; f) H_2, Pd/C, EtOH, 4 h, 97%; g) K_2CO_3, MeOH, 3 d, 25 °C, 32%; h) TBAF, 0 °C, 6 h, 97%.

(*R*)-*N*-Allyl-*N*-(2-hydroxy-3-phenoxy-propyl)-4-methylbenzenesulfonamide (20)

A screw cap vial was charged with epoxide (*R*)-**1a** (1.17 g, 7.39 mmol), **19**[8] (1.56 g, 7.39 mmol), K_2CO_3 (102 mg, 0.74 mmol), TEBA (169 mg, 0.74 mmol) and stirred at 90 °C for 3 h. After cooling the crude was diluted with Et_2O (15 mL) and washed with water (2 x 5 mL). After extraction of the aqueous phase with Et_2O, the combined organic extracts were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The resulting residue was purified by flash chromatography (AcOEt-PE 1:3) to give 2.35 g of **20**, yield 88%, as a colourless oil, $[\alpha]_D^{25}$ + 6.3 (c 0.88, EtOH), HPLC (Chiralpak AD, *i*PrOH-hexane 20-80) t_R (*R*) 13.1 min, t_R (*S*) 12.1, ee 98%. δ_H 2.45 (s, 3H), 2.97 (bs, 1H), 3.32 (m, 2H), 3.87 (dd, 2H, *J* = 15.3, 5.9), 3.99 (m, 2H), 4.20 (m, 1H), 5.13-5.20 (m, 2H), 5.55-5.75 (m, 1H), 6.88 (d, 2H, *J* = 7.7), 6.89 (t, 1H, *J* = 7.3), 7.28 (m, 4H), 7.72 (d, 2H, *J* = 8.5).

(*R*)-*N*-Allyl-*N*-(2-benzyloxy-3-phenoxy-propyl)-4-methylbenzenesulfonamide (21).

A stirred solution of (*R*)-**20** (2.26 g, 6.25 mmol) in anhydrous THF (6 mL) under nitrogen atmosphere was cooled to 0 °C and 60% NaH (0.36 g, 9.0 mmol) was added in two portions. After 30 min benzyl bromide (1.28 g, 7.5 mmol) was added dropwise and the temperature was allowed to warm to rt. After 5 h the excess NaH was destroyed at 0 °C by dropwise addition of NH_4Cl_{sat} and THF was evaporated in vacuo. The resulting aqueous phase was extracted with CH_2Cl_2 (2 x 10 mL) and the organic phase dried (Na_2SO_4), filtered and concentrated in vacuo. The residue was purified by flash chromatography (AcOEt-PE 1:6) to give 2.68 g of **21**, (yield 95%) as a colourless oil, $[\alpha]_D^{25}$ + 12.4 (c 1.0, $CHCl_3$). δ_H 2.41 (s, 3H), 3.18-3.50 (m, 2H), 3.85 (dd, 2H, *J* = 15.5, 6.6), 4.01-4.14 (m, 3H), 4.68 (AB q, 2H, *J* = 11.8), 4.73 (d, 1H, *J* = 11.8), 5.05 (m, 2H), 5.50 (m, 1H), 6.89 (d, 2H, *J* = 8.1), 6.96 (t, 1H, *J* = 7.3), 7.30 (m, 9H), 7.70 (d, 2H, *J* = 8.2). δ_C 21.5 (CH_3), 48.0 (CH_2), 52.3 (CH_2), 67.9 (CH_2), 72.6 (CH_2), 76.3 (CH), 114.5 (CH), 119.5 (CH_2), 120.9 (CH), 127.3 (CH), 127.7 (CH), 127.9 (CH), 128.4 (CH), 129.4 (CH), 129.7 (CH), 136.6 (C), 138.1 (C), 143.4 (C), 158.5 (C). ESI-MS *m/z* $[M + Na]^+$ 475.

***N*-[(*R*)-*2*-Benzyloxy-3-phenoxy-propyl]-*N*-(2,3-dihydroxypropyl)-4-methylbenzenesulfonamide (22).**

A round-bottomed flask, equipped with a magnetic stirrer, was charged with AD-mix-β (7.42 g), *t*-BuOH (26 mL) and water (26 mL). After formation of two clear phases the mixture was cooled to 0 °C and **21** (2.12 g, 4.69 mmol) was added. The heterogeneous slurry was stirred for 72 h at 0 °C. Solid sodium sulfite (2.80 g) was added and the mixture was allowed to warm to rt and stirred for 1 h. Methylene chloride (40 mL) was added and, after separation of the layers, the aqueous phase was further extracted with CH_2Cl_2 (3 x 10 mL). The combined organic extracts were dried (Na_2SO_4), filtered and concentrated *in vacuo*. The residue was purified by flash chromatography (AcOEt-PE 2:1) to give 1.55 g of (*R*)-**21** along with 0.39 g of (*R*)-**22** (yield 15%) as a colourless oil (1:1

inseparable diastereoisomeric mixture). HPLC (Chiralpak AD, *i*PrOH-hexane 20-80) 15.8, 17.0 min. δ_H 2.41 (s, 3H), 2.92 (m, 1H), 3.25 (m, 1H), 3.40-3.70 (m, 4H), 3.80-4.15 (m, 5H), 4.32 (bs, 1H), 4.60-4.80 (m, 2H), 6.88 (d, 2H, *J* = 7.7), 6.97 (t, 1H, *J* = 7.7), 7.26-7.33 (m, 9H), 7.67 (d, 2H, *J* = 7.8).

Sulfonate ester (23).

In a round-bottomed flask, **22** (530 mg, 1.09 mmol) was dissolved in CH_2Cl_2 (10 mL) and pyridine (4.6 mL) was added. After cooling to 0 °C, 2,4,6-*tris*-isopropylbenzenesulfonyl chloride (1.03 g, 3.40 mmol) was added and the temperature was allowed to warm to rt. After 48 h the reaction mixture was made acidic with 10% aq HCl. The organic solution was dried (Na_2SO_4), filtered, concentrated *in vacuo* and purified by flash column chromatography [MTBE/PE 1:1] affording 467 mg of **23**, yield 56%, as colourless oil (inseparable diastereoisomeric mixture). δ_H 1.23 (d, 12H, *J* = 4.1), 1.25 (d, 6H, *J* = 4.2), 2.41 (s, 3H), 2.87-3.65 (m, 5H), 3.90-4.41 (m, 8H), 4.57-4.77 (m, 2H), 6.85 (d, 2H, *J* = 7.9), 6.95 (t, 1H, *J* = 7.3), 7.15 (s, 2H), 7.24-7.30 (m, 9H), 7.66 (d, 2H, *J* = 8.1).

2-(*tert*-Butyldimethylsilanyloxy)sulfonate ester (24).

To a stirred solution of **23** (453 mg, 0.60 mmol) in CH_2Cl_2 (2 mL), cooled to 0 °C, were added imidazole (61 mg, 0.90 mmol) and *t*-$BuMe_2SiCl$ (136 mg, 0.90 mmol) and the temperature was allowed to warm to rt. After 24 h the crude was diluted with CH_2Cl_2 (10 mL), washed with water (5 mL), dried (Na_2SO_4), filtered, concentrated *in vacuo* and purified by flash column chromatography [AcOEt/PE 1:6] affording 429 mg of **24** (83% yield) as a colourless oil (inseparable diastereoisomeric mixture). HPLC (ChiralPak AD, *i*PrOH-hexane 5-95) t_R 7.7, 8.2 min. δ_H 0.00 (s, 3H), 0.01 (s, 3H), [0.79 (s), 0.81 (s), 9H], 1.24 (d, 18H, *J* = 6.9), 2.39 (s, 3H), 2.89 (m, 1H), 2.98-3.50 (m, 3H), 3.60-3.68 (m, 1H), 3.90-4.30 (m, 8H), [4.42 (ABq, *J* = 11.8), 4.51 (ABq, *J* = 11.4), 2H], 6.84 (m, 2H), 6.95 (m, 1H), 7.17-7.30 (m, 11H), 7.65 (m, 2H).

Sulfonate ester (25).

The benzyl ether **24** (0.42 g, 0.48 mmol) was dissolved in EtOH (5 mL) and 10% Pd/C (51 mg) was added. The resulting heterogeneous mixture was subjected to hydrogenation under atmospheric pressure after three vacuum/H_2 cycles to remove air from the reaction vessel. After 4 h at rt. the crude was filtered through celite, dried (Na_2SO_4) and the solvent evaporated at reduced pressure affording 363 mg of **25** (inseparable diastereoisomeric mixture), yield 97%. δ_H [0.07 (s), 0.08 (s), 0.09 (s), 0.11 (s), 6H], [0.84 (s), 0.85 (s), 9H], 1.25 (d, 18H, *J* = 7.0), 2.42 (s, 3H), 2.87-3.60 (m, 5H), 3.88-4.46 (m, 8H), 6.86-6.96 (m, 2H), 6.95 (t, 1H, *J* = 8.3), 7.24-7.31 (m, 4H), 7.66 (d, 2H, *J* = 8.4), 7.67 (d, 2H, *J* = 8.4).

6-(*tert*-Butyldimethylsilanyloxy)-(*R*)-2-phenoxymethyl-4-(toluene-4-sulfonyl)-[1,4]oxazepane (26). To a stirred solution of **25** (348 mg, 0.49 mmol) in MeOH (3.5 mL) was added K_2CO_3 (311 mg, 2.25 mmol). After stirring at rt for 3 days, MeOH was evaporated, AcOEt (10 mL) and water (5

mL) were added and the resulting layers were separated. The organic phase was dried (Na_2SO_4), filtered and the solvent evaporated. The crude was purified by MPLC (MTBE/PE 1:4) to give 77 mg of **26**, yield 32%. Pure diastereoisomers could be obtained along with a diastereoisomeric mixture through chromatography.

26 (major). $[\alpha]_D^{25}$ + 30.8 (c 0.35, $CHCl_3$), HPLC (Chiralpak AD, *i*PrOH-hexane 20-80) t_R 5.2 min, δ_H 0.09 (s, 6H), 0.90 (s, 9H), 2.45 (s, 3H), 2.84 (m, 2H), 3.78-4.12 (m, 7H), 4.20 (m, 1H), 6.90 (d, 2H, *J* = 8.2), 6.95 (t, 1H, *J* = 8.2), 7.28-7.32 (m, 4H), 7.71 (d, 2H, *J* = 8.2). δ_C – 4.7 (CH_3), – 4.8 (CH_3), 21.5 (CH_3), 25.8 (CH_3), 53.4 (CH_2), 54.1 (CH_2), 68.5 (CH_2), 72.2 (CH), 76.8 (CH_2), 81.1 (CH), 114.6 (CH), 121.2 (CH), 126.9 (CH), 129.5 (CH), 129.9 (CH), 136.2 (C), 143.5 (C), 158.4 (C).

26 (minor). HPLC (Chiralpak AD, *i*PrOH-hexane 20-80) t_R 6.5 min, δ_H 0.09 (s, 3H), 0.12 (s, 3H), 0.91 (s, 9H), 2.45 (s, 3H), 3.25-3.60 (m, 4H), 3.90-4.15 (m, 6H), 6.90 (d, 2H, *J* = 8.2), 6.95 (t, 1H, *J* = 7.4), 7.29 (m, 4H), 7.74 (d, 2H, *J* = 8.2). δ_C (selected peaks) 51.9 (CH_2), 54.5 (CH_2), 68.5 (CH_2), 70.3 (CH), 74.0 (CH_2), 78.2 (CH).

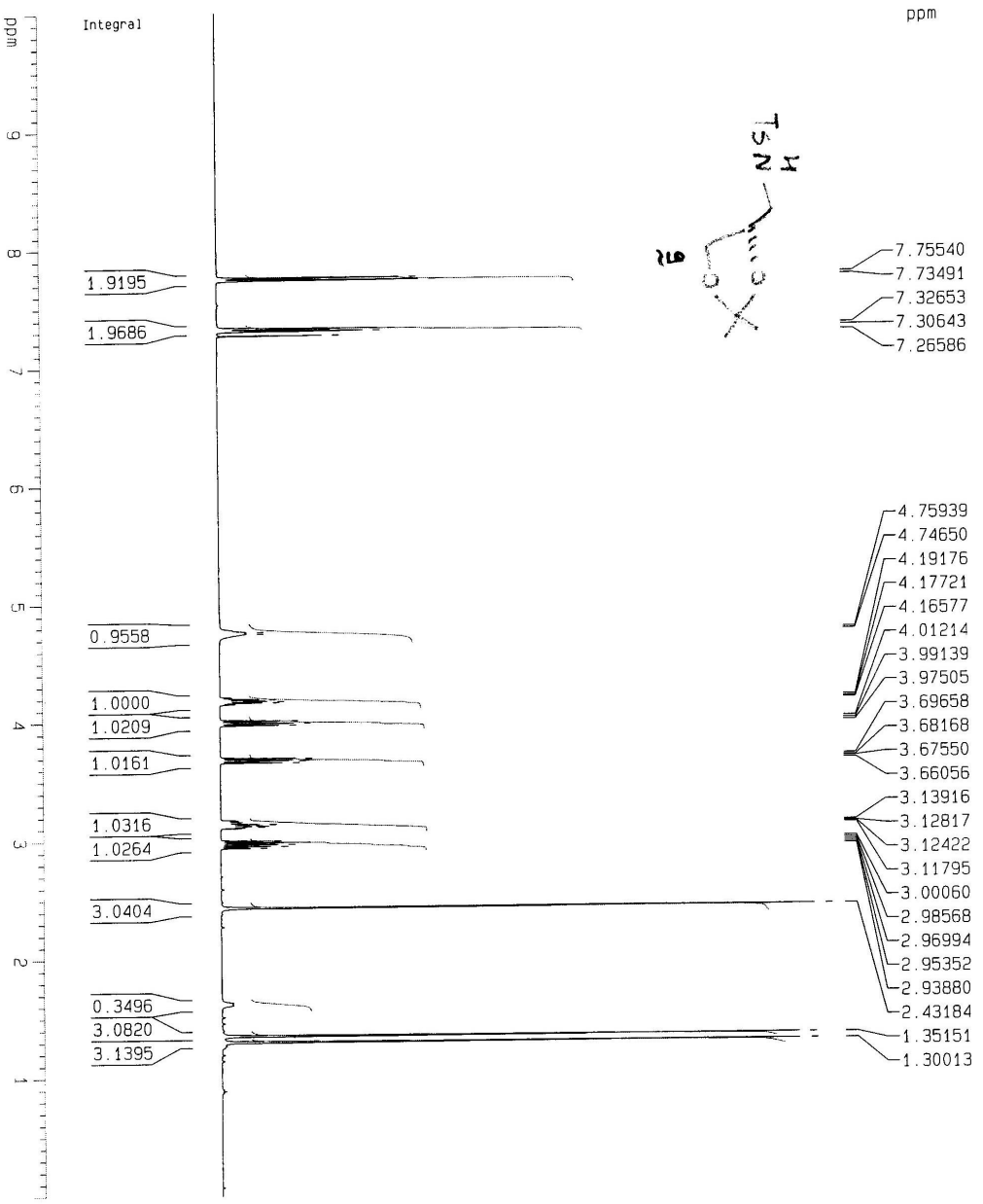
***N*-(tosyl)-(*R*)-2-phenoxymethyl-[1,4]-oxazepan-6-ol (13a).** To a stirred solution of **26** (3/1 diastereoisomeric mixture) (36 mg, 0.074 mmol) in THF (1 mL) was added TBAF·$3H_2O$ (23 mg, 0.074 mmol). After stirring at 0 °C for 6 h, THF was evaporated and the resulting crude dissolved in CH_2Cl_2 (5 mL) and washed with water (2 mL). The organic phase was dried (Na_2SO_4), filtered and the solvent evaporated. The crude was purified by MPLC (MTBE-PE 1:1) affording **13a** in 97% yield (2 mg of a single diastereoisomer along with 25 mg of a diastereoisomeric mixture). The minor compound was found to be identical to that obtained as a byproduct during the cyclisation of (*R,S*)-**12a** (Table 2).

13a (major): $[\alpha]_D^{25}$ – 2.85 (c 0.1, $CHCl_3$), HPLC (Chiralpak AD, *i*PrOH-hexane 20-80) t_R (*2R,6R*) 18.1 min. δ_H 3.18-3.38 (m, 2H), 3.52-3.71 (m, 2H), 3.85-4.15 (m, 6H), 6.92 (m, 3H), 7.29 (m, 4H), 7.68 (d, 2H, *J* = 8.3). δ_C 21.5 (CH_3), 52.9 (CH_2), 54.4 (CH_2), 68.3 (CH_2), 69.9 (CH), 73.8 (CH_2), 79.3 (CH), 114.6 (CH), 121.2 (CH), 127.0 (CH), 129.5 (CH), 129.9 (CH), 143.7 (C), 158,3 (C). APCI-MS *m/z* 378 $[M + H]^+$;

13a (minor): HPLC (Chiralpak AD, *i*PrOH-hexane 20-80) t_R (*2R,6S*) 16.2 min. δ_H 2.43 (s, 3H), 2.93 (dd, 1H, *J* = 10.7, 14.3), 3.19 (dd, 1H, *J* = 3.7, 14.7), 3.59 (dd, 1H, *J* = 7.7, 12.9), 3.76 (m, 1H), 3.92-4.15 (m, 5H), 4.29 (dd, 1H, *J* = 5.9, 12.9), 6.88 (d, 2H, *J* = 8.1), 6.96 (t, 1H, *J* = 7.4), 7.21-7.34 (m, 4H), 7.69 (d, 1H, *J* = 8.1). δ_C (selected peaks) 53.6 (CH_2), 55.0 (CH_2), 68.3 (CH_2), 69.9 (CH), 73.5 (CH_2), 80.8 (CH).

References and notes

1. Waagen, V.; Hollings? ter, I.; Partali, V.; Thorstad, O.; Anthonsen, T. *Tetrahedron: Asymmetry* **1993**, *4*, 2265.
2. Tse, B. *J. Am. Chem. Soc.* **1996**, *118*, 7094. (*R*)-**1b** is also commercially available.
3. Diastereoisomeric mixture [(*R*,*S*) + (*R*,*R*)]-**6a** was obtained through dihydroxylation of **20** with AD-mix β.
4. Diastereoisomeric mixture [(*R*,*S*) + (*R*,*R*)]-**6b** was obtained through ring opening of (±)-**1b** with **9**, followed by treatment with 80% CH_3COOH.
5. Diastereoisomeric mixtures [(*R*,*S*) + (*R*,*R*)]-**12a,b** were obtained through sulfonylation of [(*R*,*S*) + (*R*,*R*)]-**6a,b** with Tris-Cl.
6. Diastereoisomeric mixture [(*R*,*S*) + (*R*,*R*)]-**5a** was obtained through cyclization of [(*R*,*S*) + (*R*,*R*)]-**12a**.
7. Diastereoisomeric mixture [S,*R*) + (*S*,*S*)]-**18** was obtained by treating (*R*,*S*)-**11c** with NaH and *N*-tosylimidazole.
8. Miyata, O.; Ozawa, Y.; Ninomiya, I.; Naito, T. *Tetrahedron* **2000**, *56*, 6199.

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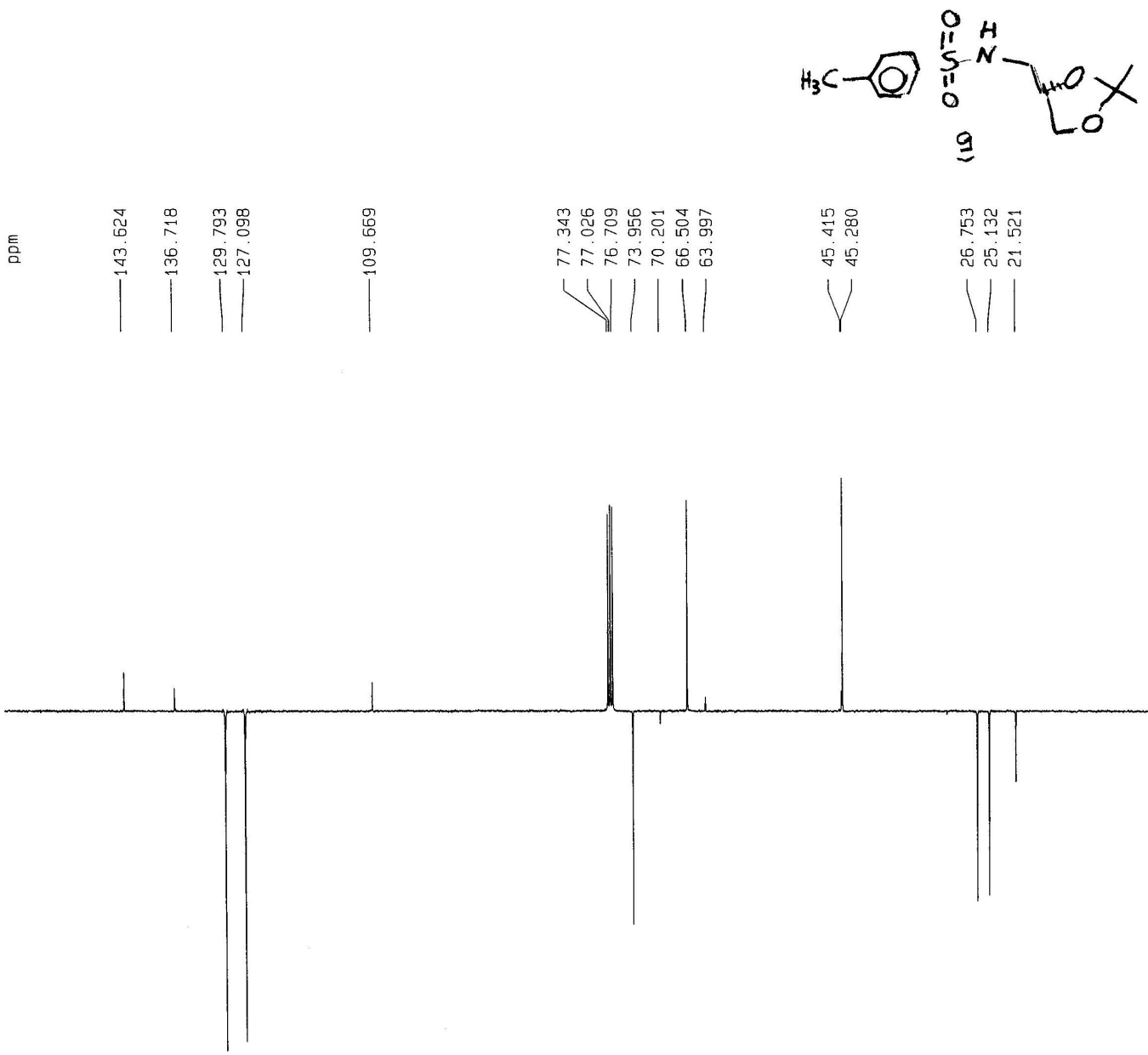

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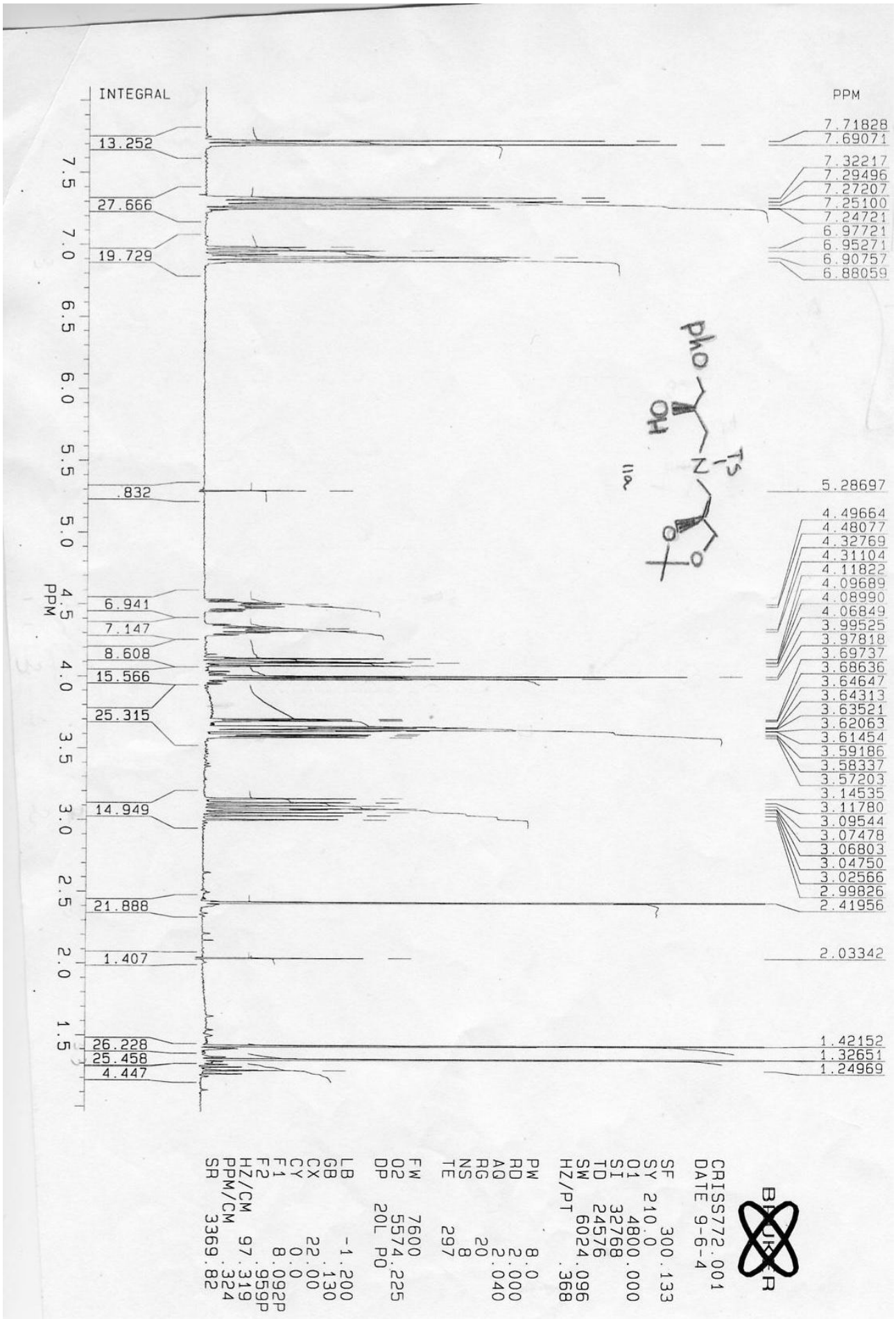
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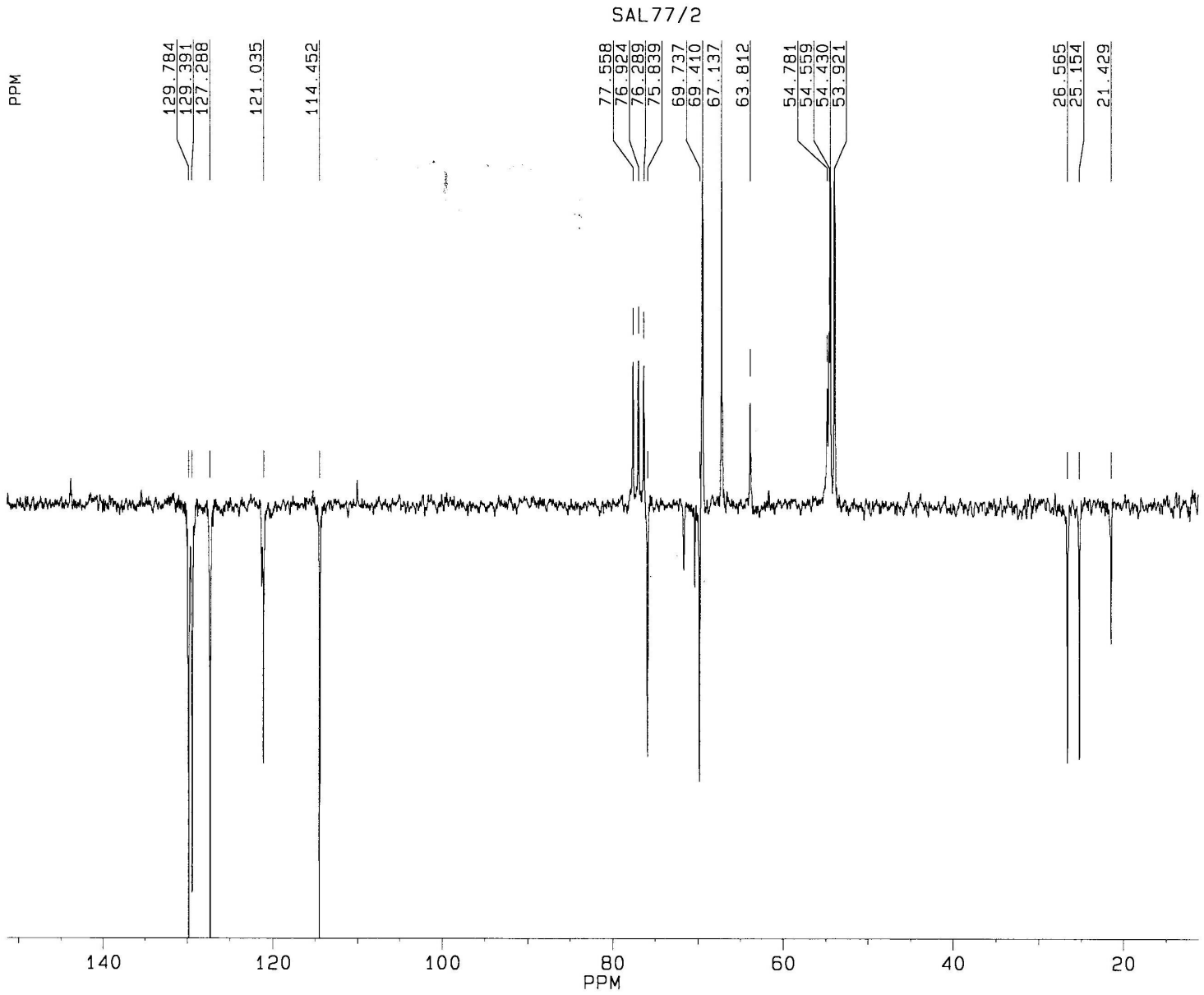

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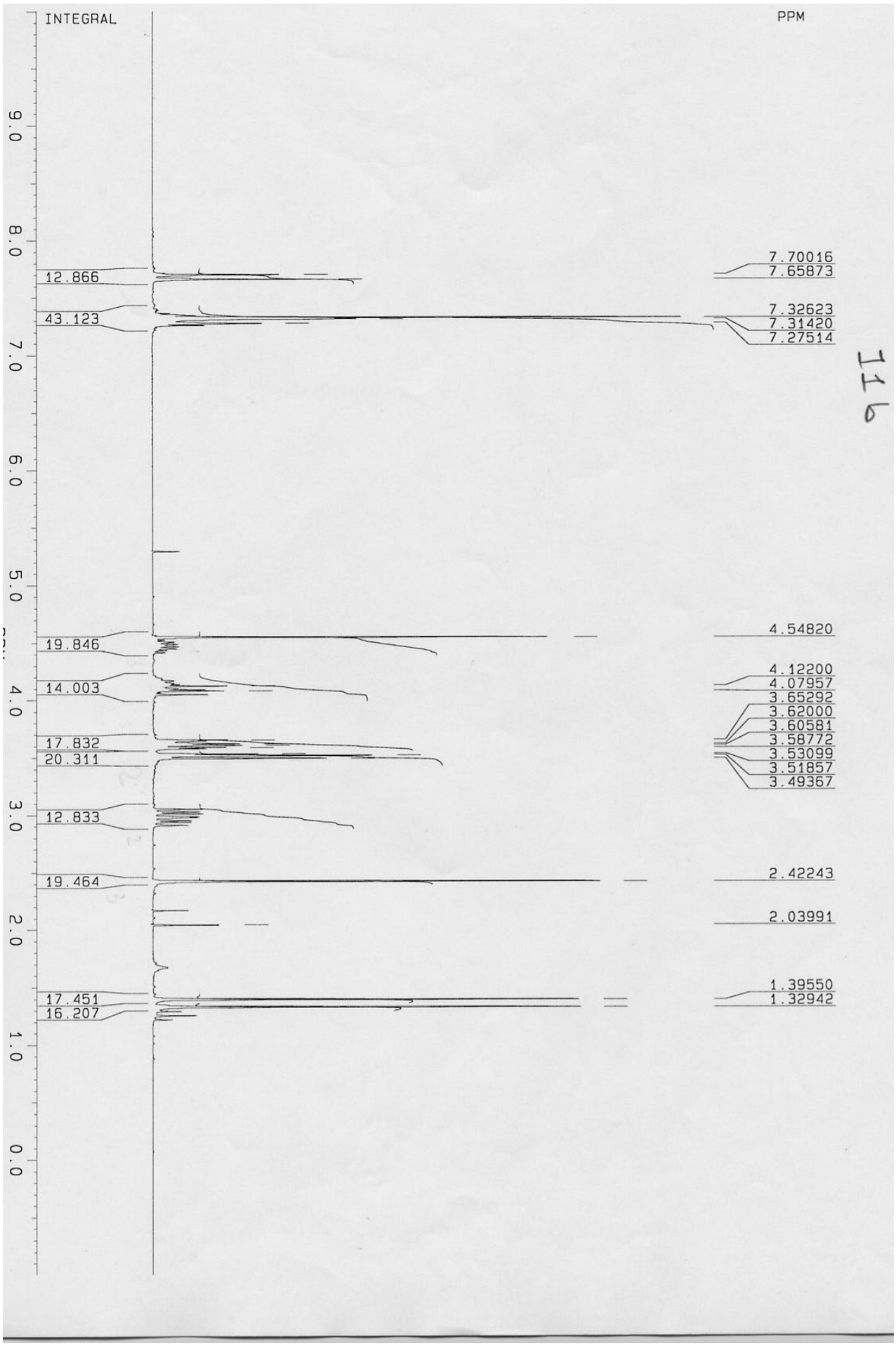
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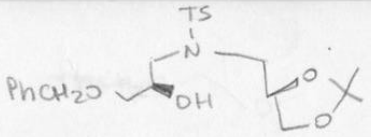

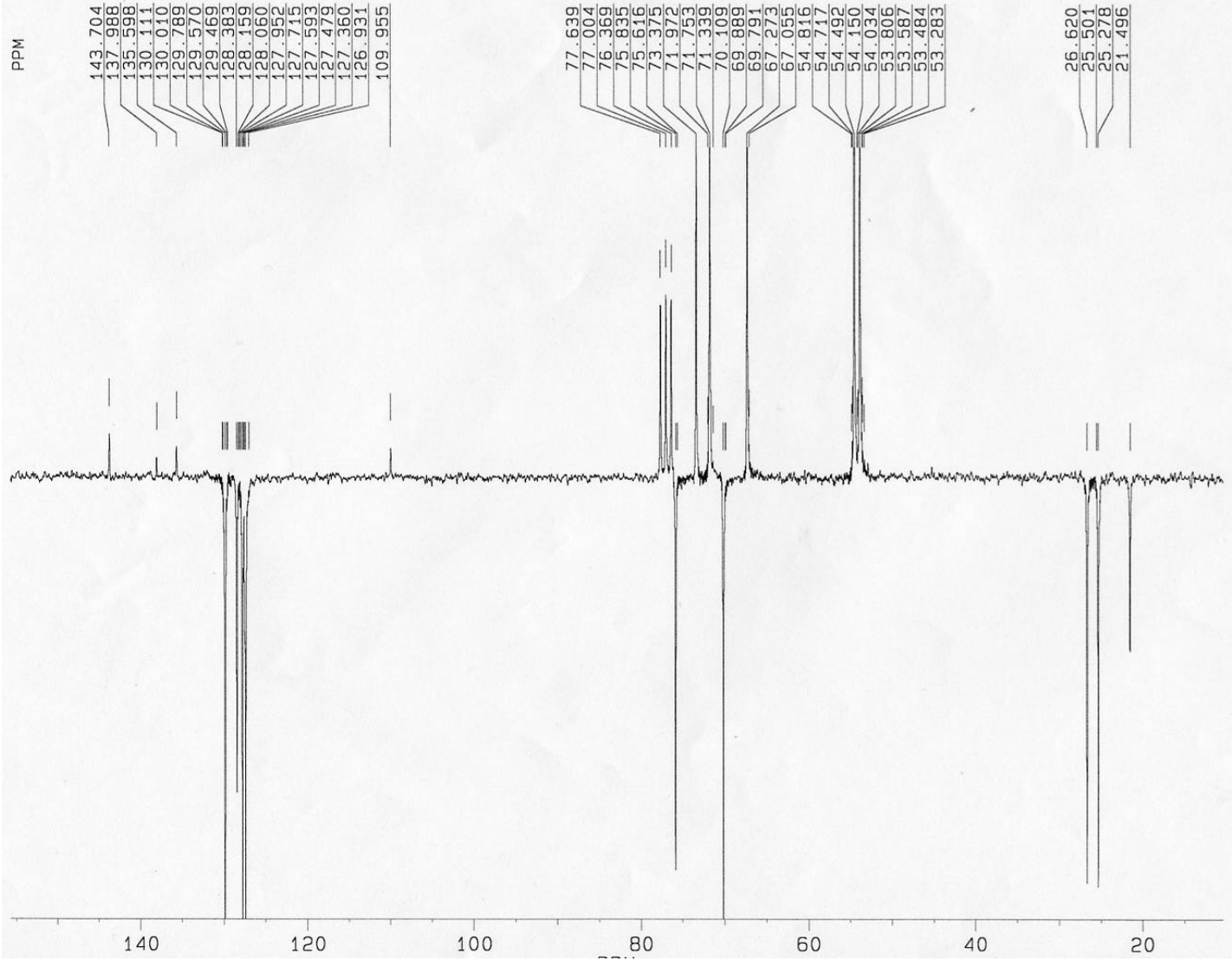

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O1 8600.000
SI 131072
TD 5128
SW 12820.513
HZ/PT .196

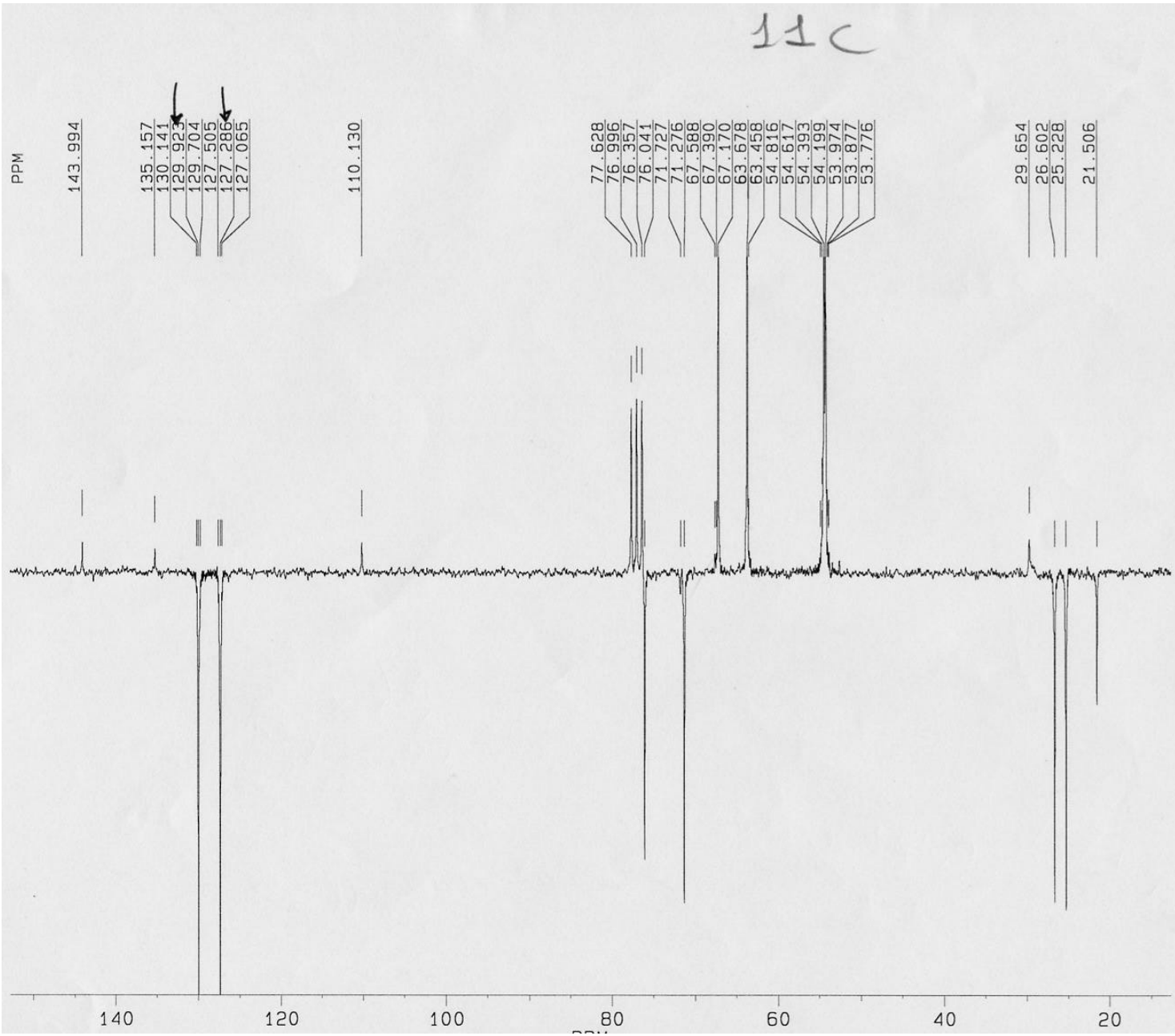
PW 0.0
RD 0.0
AQ .200
RG 3200
NS 318199
TE 297

FW 16100
O2 3400.000
DP 16H PO

LB 3.500
GB 0.0
CX 22.00
CY 0.0
F1 155.630P
F2 10.339P
HZ/CM 332.341
PPM/CM 6.604
SR 3317.58

ppm (f1)
7.0
6.0
5.0
4.0
3.0
2.0
1.00
1.01
0.49
1.16
0.49
2.10
0.87
1.11
1.80
1.73
0
50
100
7.691
7.663
7.332
7.305
4.447
4.091
4.069
4.030
4.018
3.831
3.678
3.665
3.649
3.570
3.621
3.598
3.593
3.532
3.522
3.502
3.488
3.452
3.439
2.991
2.963
2.941
2.914
2.424
1.411
1.338
11c
Ts
N
OH
HO

11c

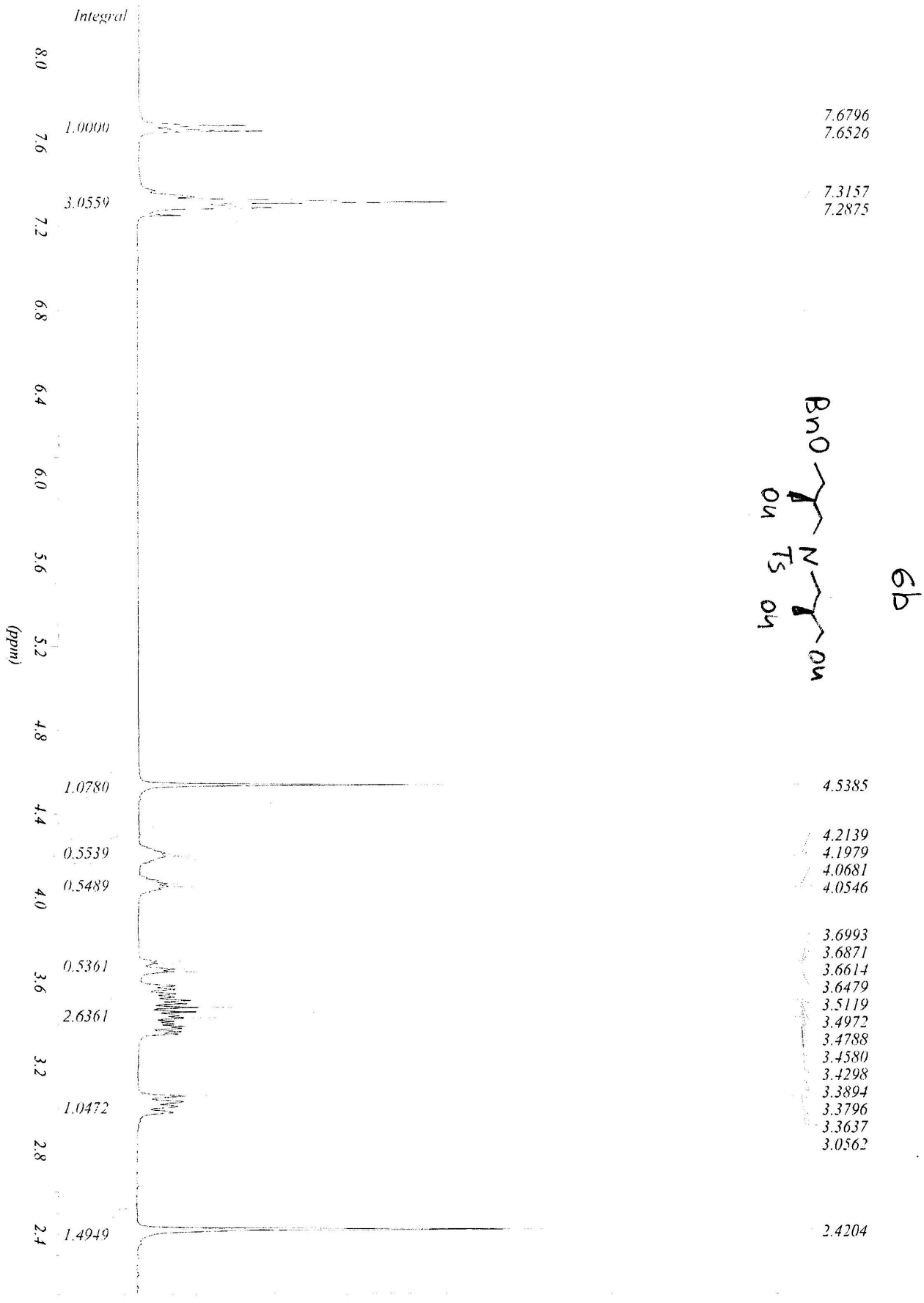


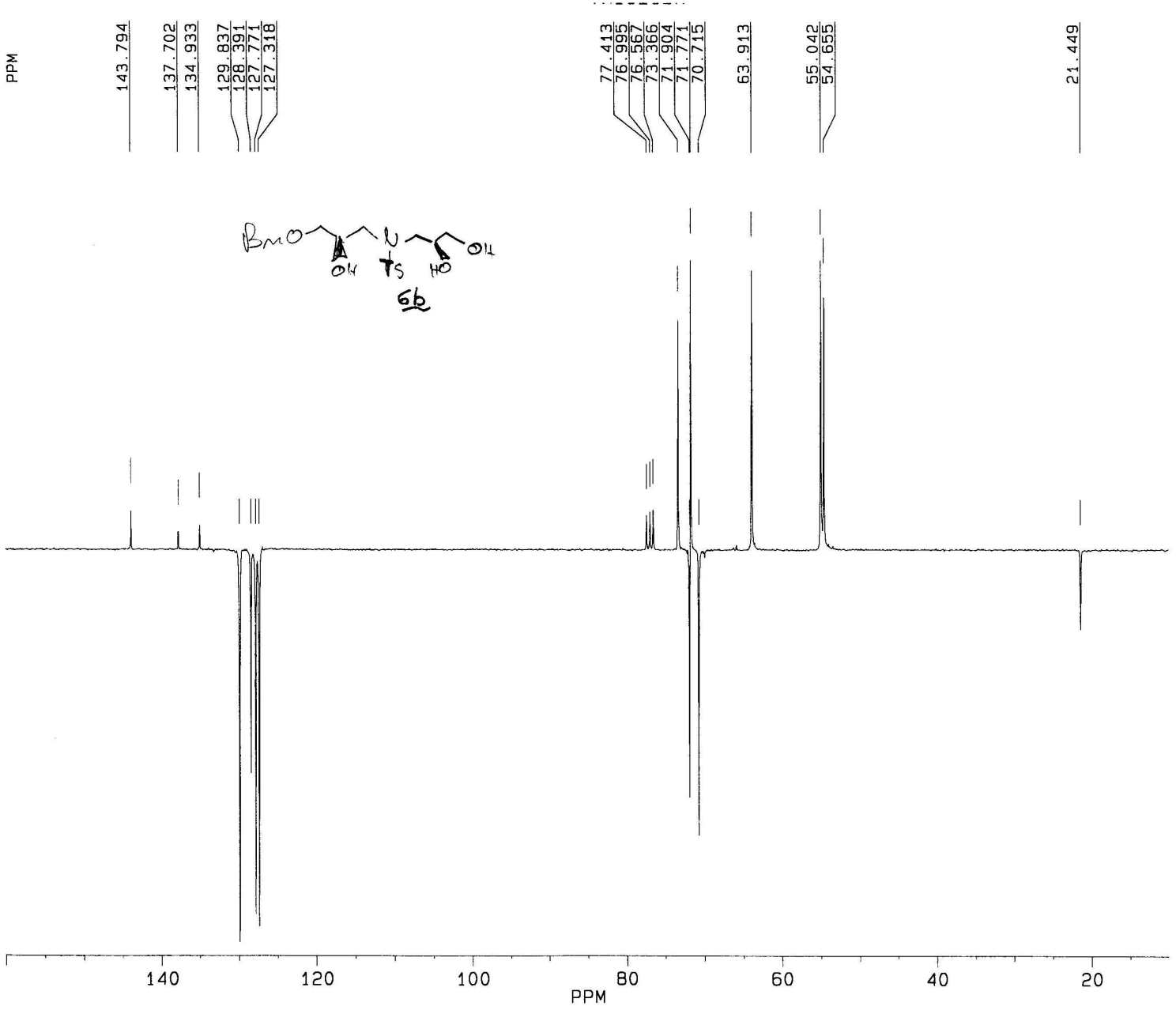
DOMENIC8.001
AU PROG:
JMODXH.AU
DATE 20-9-4

SF	50.323
SY	50.0600000
O1	8600.000
SI	131072
TD	5128
SW	12820.513
HZ/PT	.196
PW	0.0
RD	0.0
AQ	.200
RG	3200
NS	317744
TE	297
FW	16100
O2	3400.000
DP	16H PO
LB	3.500
GB	0.0
CX	22.00
CY	0.0
F1	152.780P
F2	12.606P
HZ/CM	320.639
PPM/CM	6.372
SR	3317.77

ppm (f1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.00
2.14
1.38
0.58
0.62
1.17
0.57
0.77
0.30
0.56
1.04
1.60
0.31
7.713
7.686
7.336
7.309
7.302
7.277
7.253
6.964
6.902
6.876
4.397
4.380
4.123
4.109
3.991
3.976
3.972
3.558
3.388
3.217
3.188
3.167
3.146
3.138
3.119
3.097
3.069
2.427
2.075
6a
Ts
0
50
100

158.2793
144.0329
134.7634
129.9
129.5065
127.3602
121.2635
114.5135
77.4044
77.0000
76.5645
71.8676
70.4367
69.5035
65.9575
63.9356
55.0394
54.6972
21.5074
(ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
3e
OH
N
Ts
OH
OH

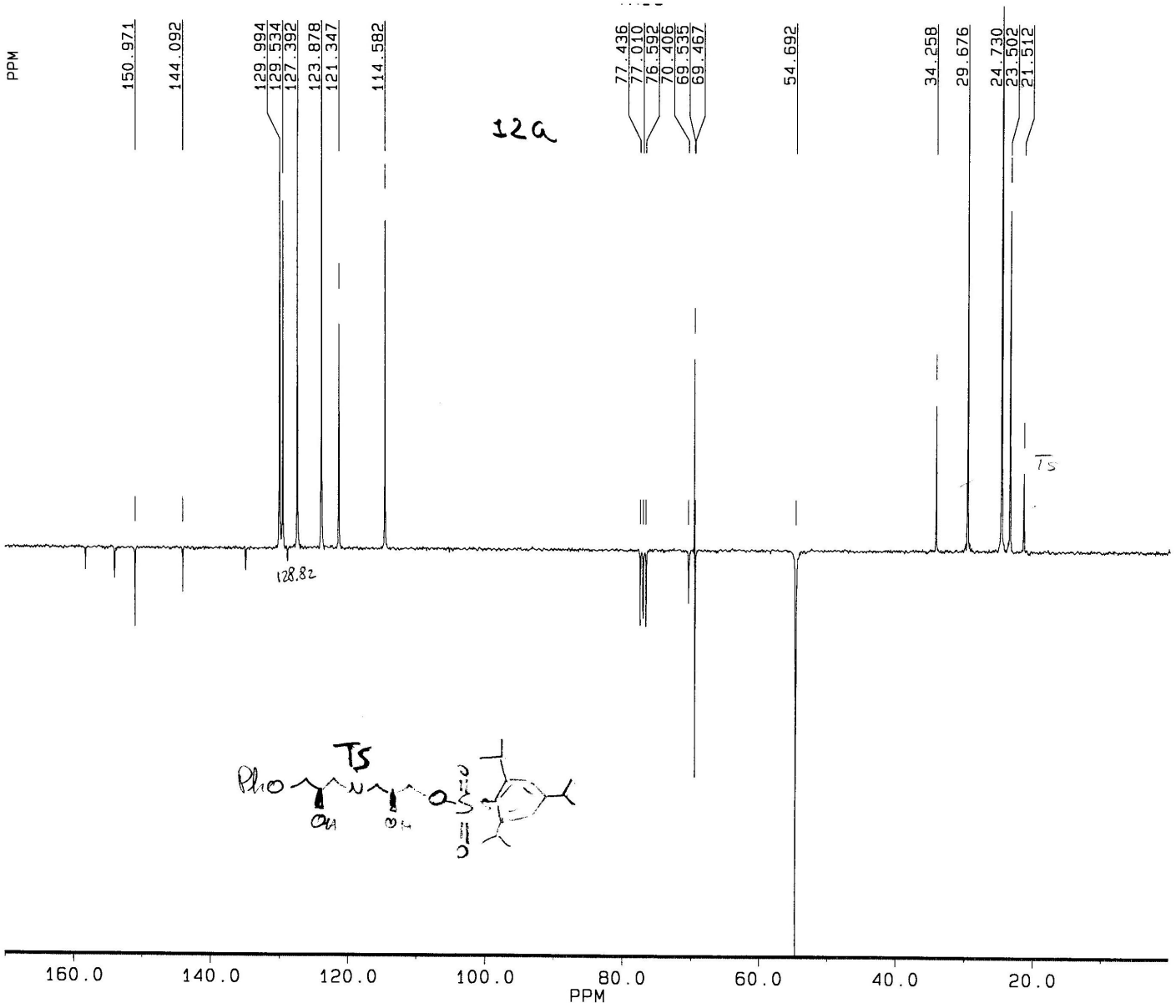

Integral
8.0
7.6
7.2
6.8
6.4
6.0
5.6
5.2
4.8
4.4
4.0
3.6
3.2
2.8
2.4
(ppm)
1.0000
3.0559
1.0780
0.5539
0.5489
0.5361
2.6361
1.0472
1.4949
7.6796
7.6526
7.3157
7.2875
4.5385
4.2139
4.1979
4.0681
4.0546
3.6993
3.6871
3.6614
3.6479
3.5119
3.4972
3.4788
3.4580
3.4298
3.3894
3.3796
3.3637
3.0562
2.4204
BnO
OH
N
Ts
OH
OH
6b



DOMEDT15.001
AU PROG:
JMODXH.AU
DATE 8-9-5

SF	75.469
SY	75.0
O1	6534.949
SI	16384
TD	10714
SW	19230.769
HZ/PT	2.348
PW	0.0
RD	0.0
AQ	.279
RG	3200
NS	71298
TE	297
FW	24100
O2	6000.000
DP	18H PO
LB	3.000
GB	0.0
CX	23.00
CY	0.0
F1	160.021
F2	10.029
HZ/CM	492.160
PPM/CM	6.521
SR	-1400.63
D1	.500000
S1	23H
P9	100.00
D2	.005000
S2	18H
P1	5.00
VD	.007000
P2	10.00
RD	0.0
PW	0.0
DE	35.00
NS	71298
DS	0
NE	1

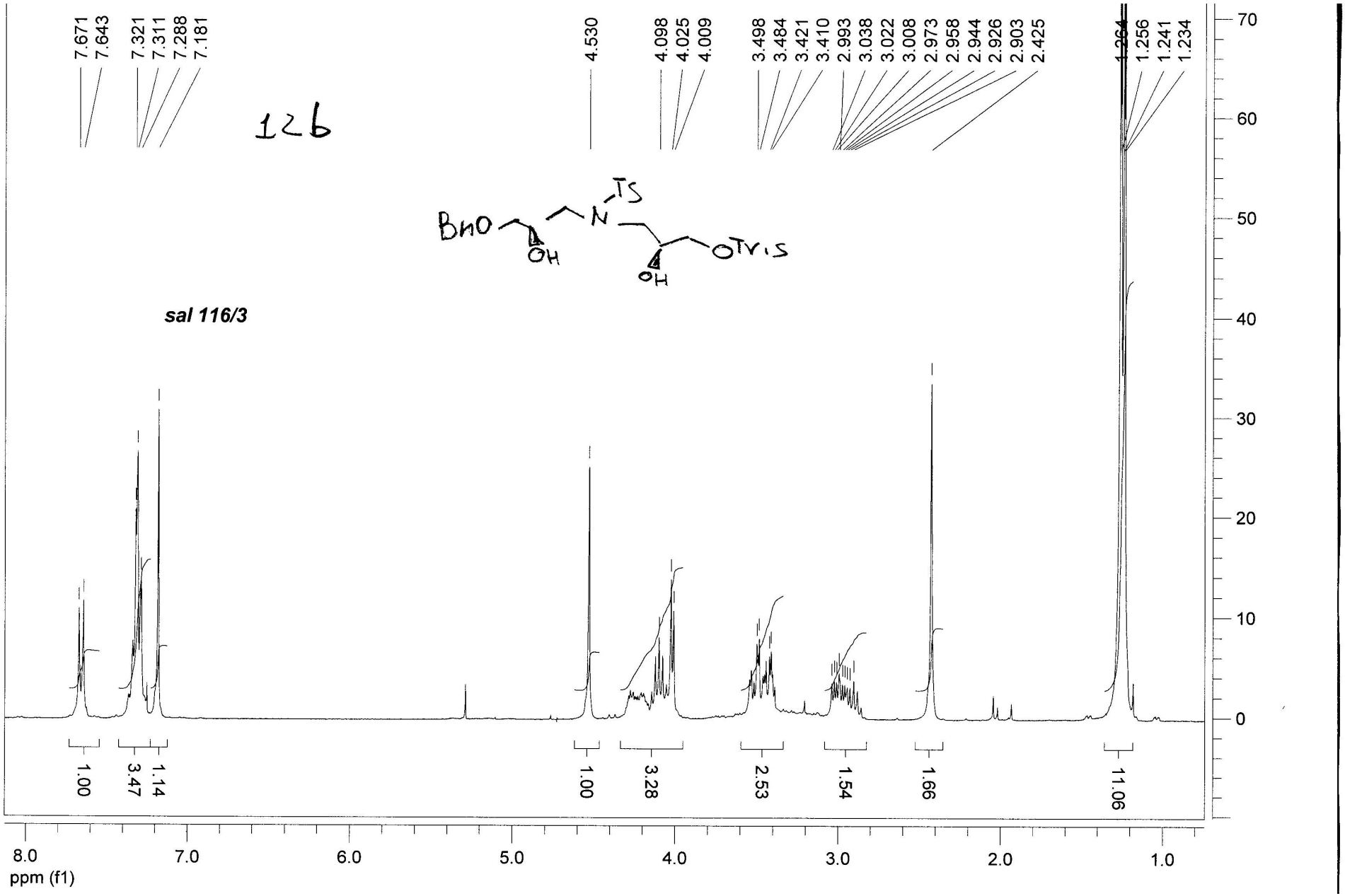
ppm (f1)
7.0
6.0
5.0
4.0
3.0
2.0
1.00
2.46
1.11
1.02
3.39
1.11
1.10
0.45
1.61
11.33
7.699
7.672
7.332
7.253
7.184
6.962
6.896
6.871
4.368
4.351
4.318
4.300
4.059
4.096
3.974
3.528
3.501
3.138
3.109
2.906
2.428
1.266
1.260
1.243
PhO
OH
N
Ts
OH
OTrio
12a
0
50
100



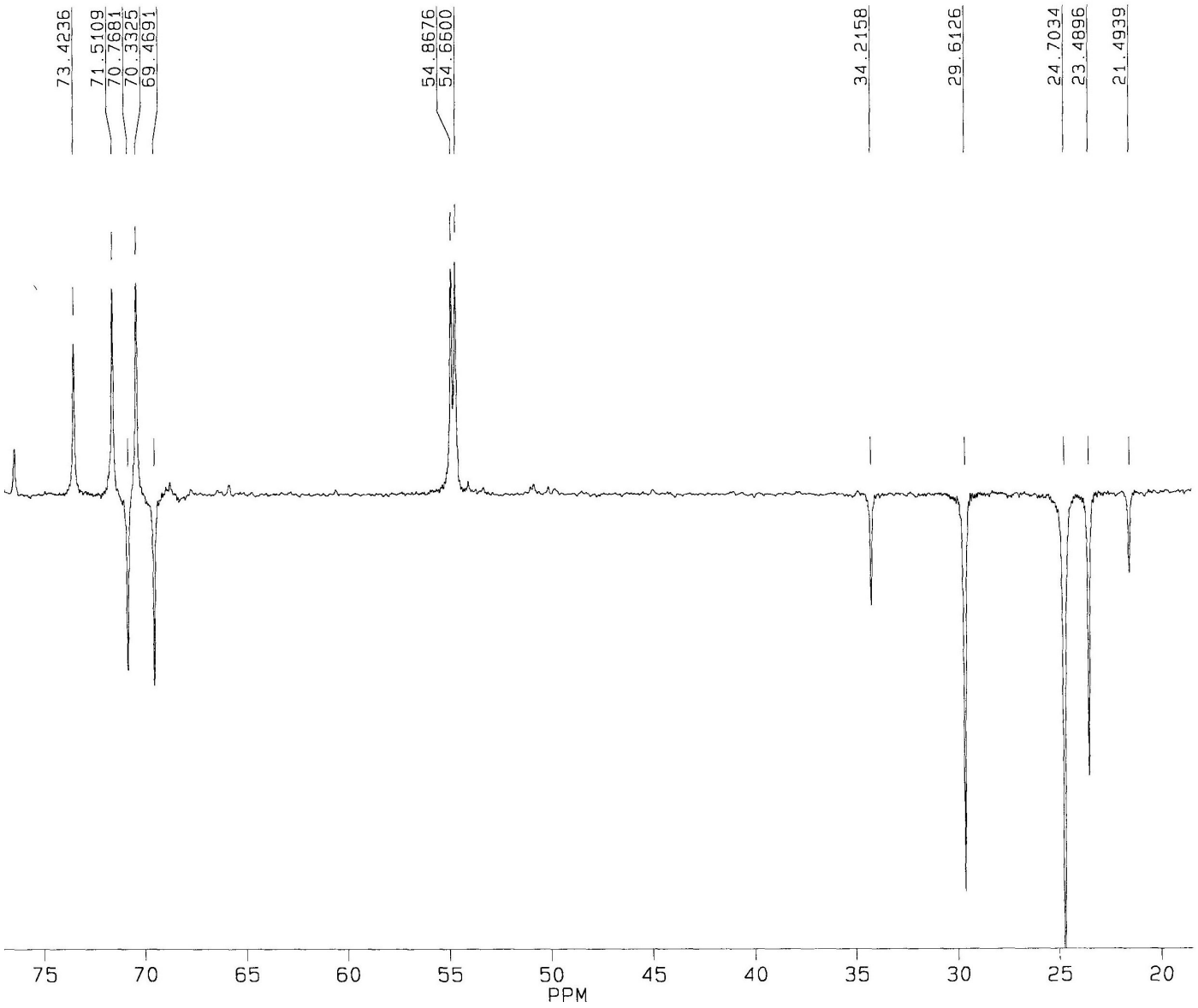
BRUKER

ALBATRIS.001
AU PROG:
JMODXH.AU
DATE 2-9-5

SF	75.469
SY	75.0
O1	6534.949
SI	16384
TD	10714
SW	19230.769
HZ/PT	2.348
PW	0.0
RD	0.0
AQ	.279
RG	3200
NS	68437
TE	297
FW	24100
O2	6000.000
DP	18H CPD
LB	3.000
GB	0.0
CX	23.00
CY	0.0
F1	170.006
F2	.013
HZ/CM	557.788
PPM/CM	7.391
SR	-1405.32
D1	.500000
S1	23H
P9	100.00
D2	.005000
S2	18H
P1	5.00
VD	.007000
P2	10.00
RD	0.0
PW	0.0
DE	35.00
NS	68437
DS	0
NE	1


7.671
7.643
7.321
7.311
7.288
7.181
4.530
4.098
4.025
4.009
3.498
3.484
3.421
3.410
2.993
3.038
3.022
3.008
2.973
2.958
2.944
2.926
2.903
2.425
1.264
1.256
1.241
1.234
126
BnO
OH
N
Ts
OTIPS
OH
sal 116/3
1.00
3.47
1.14
1.00
3.28
2.53
1.54
1.66
11.06
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)
70
60
50
40
30
20
10
0

1eb

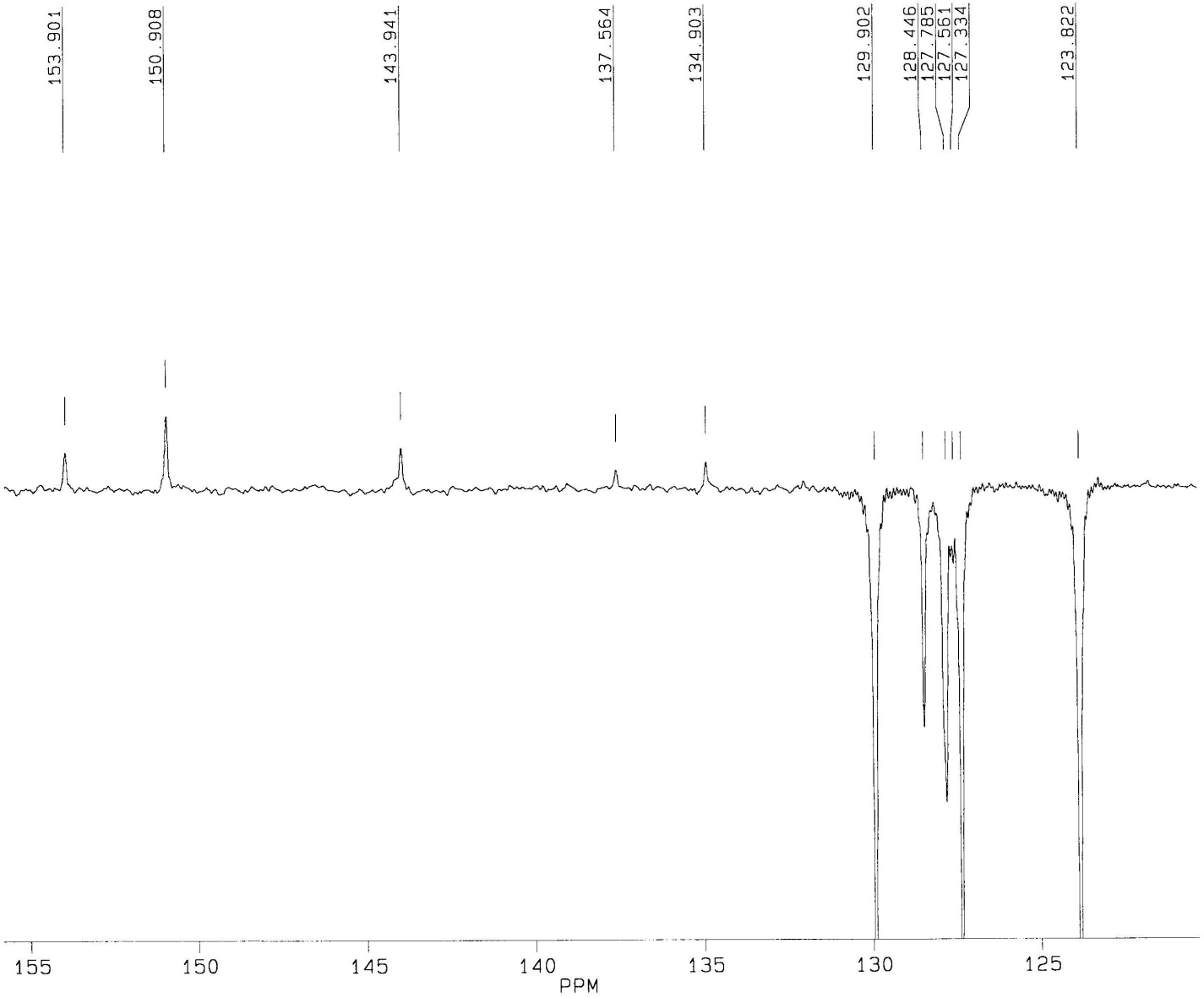


BRUKER

ALBATRIS.001
AU PROG:
JMODXH.AU
DATE 14-10-4

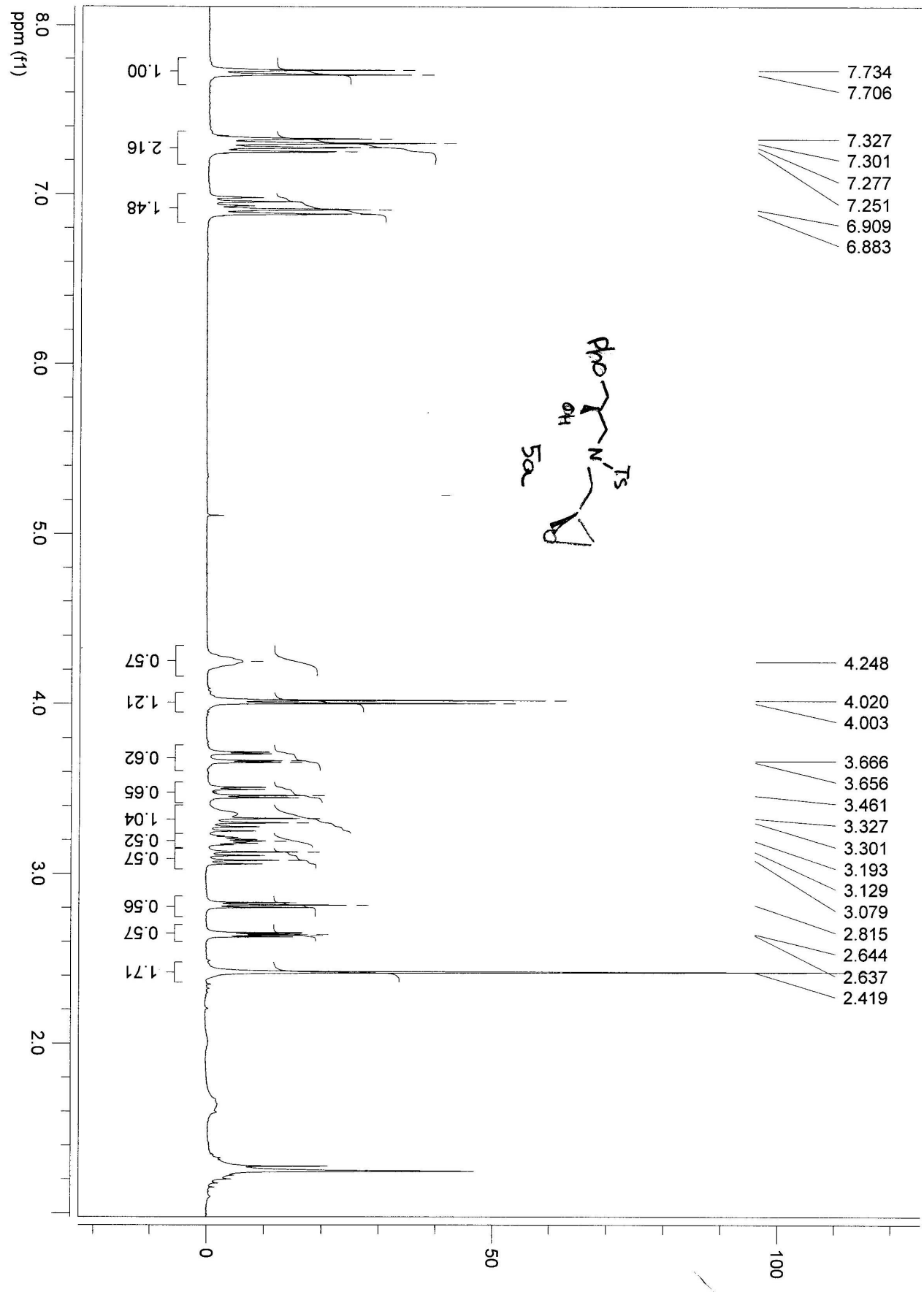
SF	50.323
SY	50.0600000
O1	8600.000
SI	131072
TD	5128
SW	12820.513
HZ/PT	.196
PW	0.0
RD	0.0
AQ	.200
RG	3200
NS	76581
TE	297
FW	16100
O2	3400.000
DP	16H PO
LB	3.500
GB	0.0
CX	22.00
CY	0.0
F1	80.044P
F2	18.413P
HZ/CM	140.975
PPM/CM	2.801
SR	3319.14

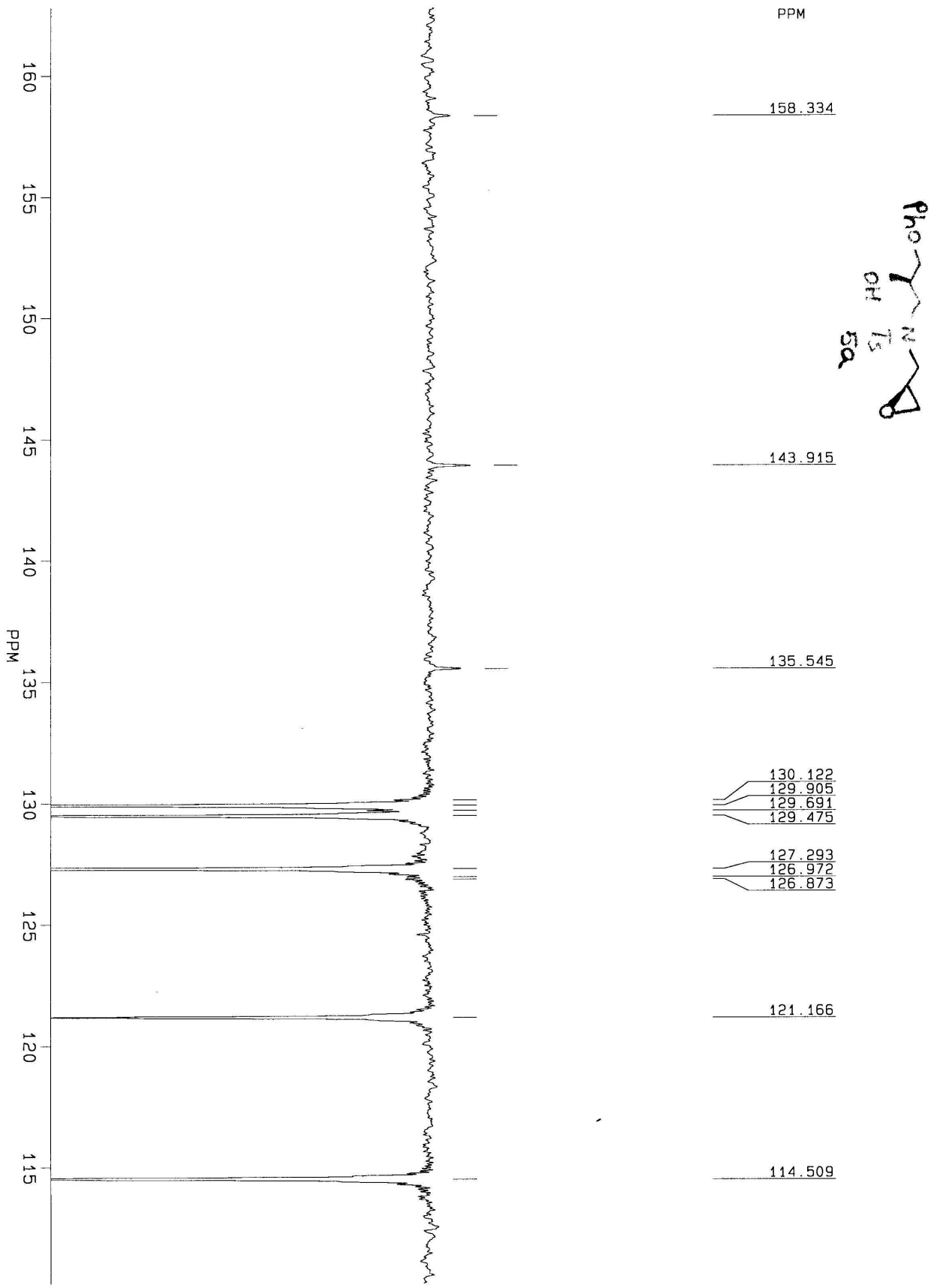
12b

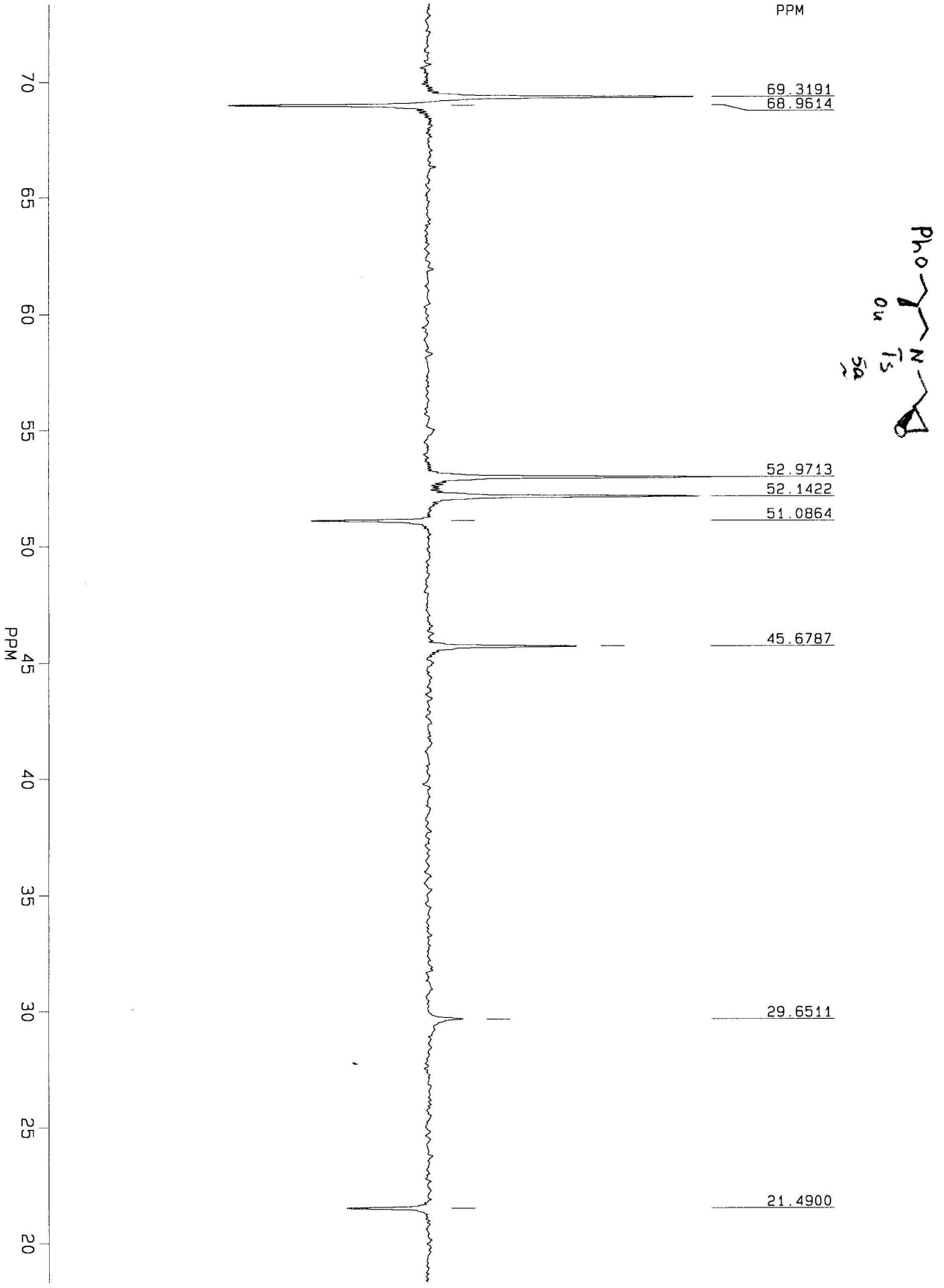


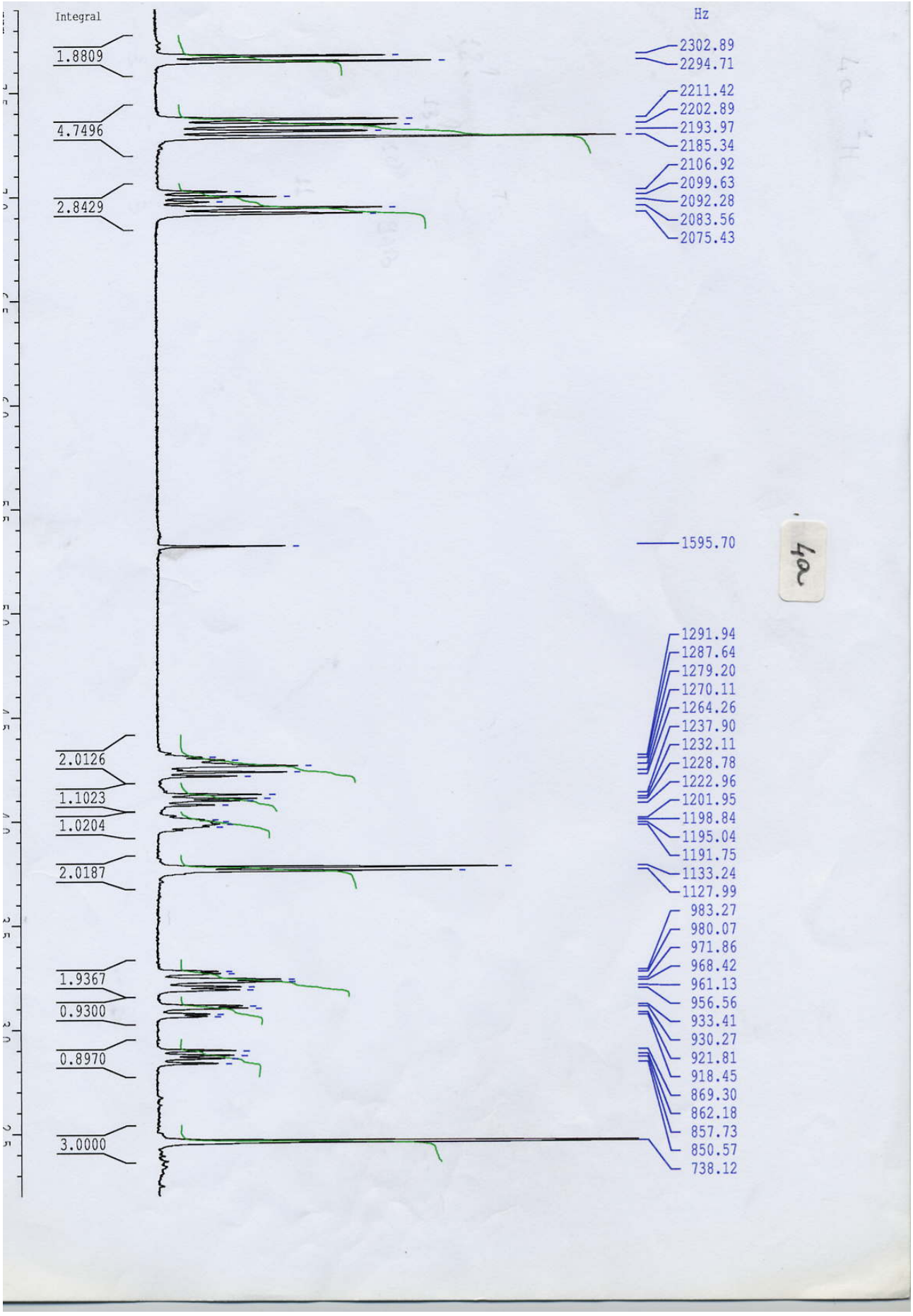
ALBATRIS.001
AU PROG:
JMODXH.AU
DATE 14-10-4

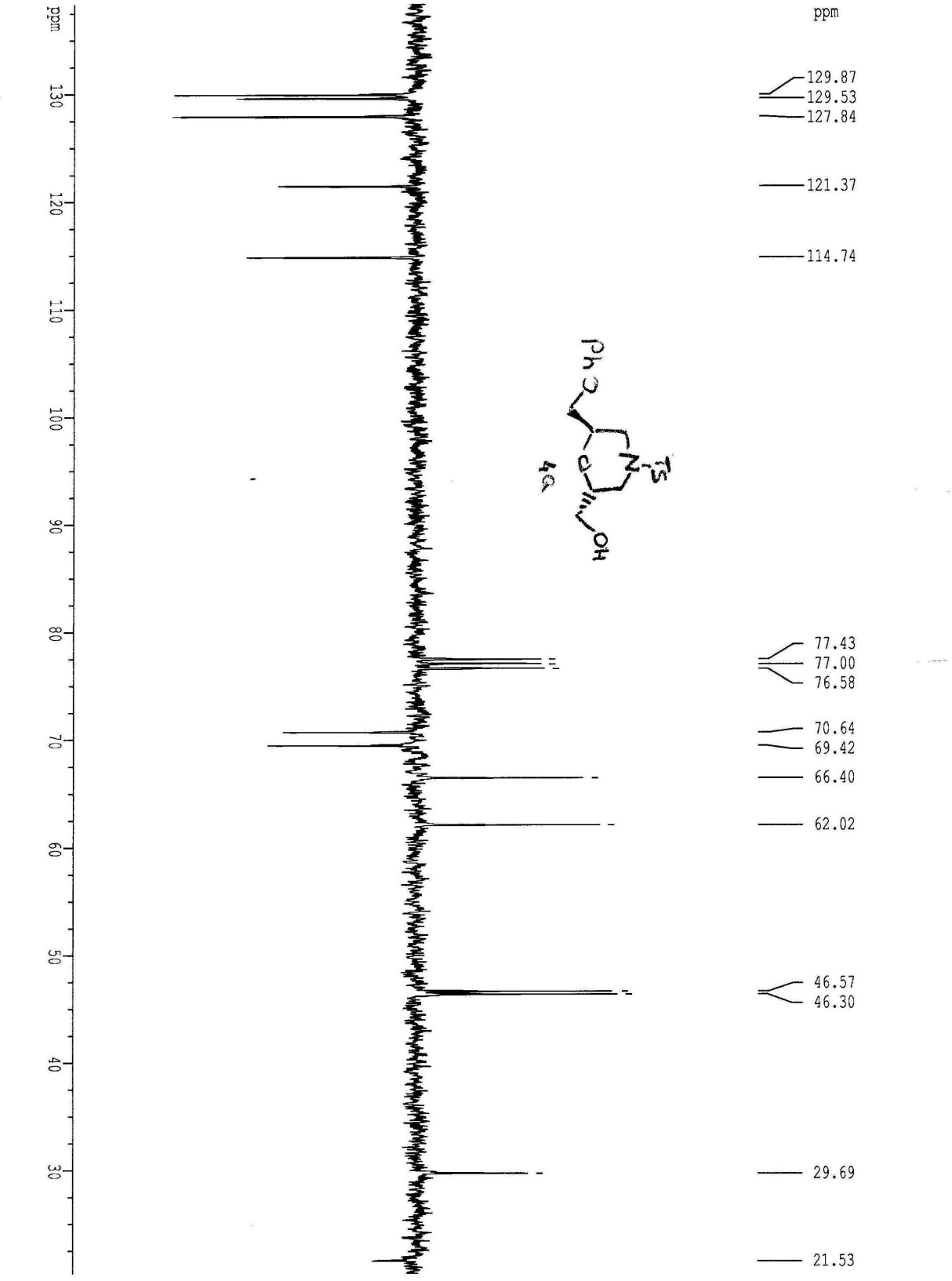
SF	50.323
SY	50.0600000
O1	8600.000
SI	131072
TD	5128
SW	12820.513
HZ/PT	.196
PW	0.0
RD	0.0
AQ	.200
RG	3200
NS	76581
TE	297
FW	16100
O2	3400.000
DP	16H PO
LB	3.500
GB	0.0
CX	22.00
CY	0.0
F1	157.189P
F2	120.317P
HZ/CM	84.341
PPM/CM	1.676
SR	3319.14


ppm (f1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
0
50
100
1.00
2.16
1.48
0.57
1.21
0.62
0.65
1.04
0.52
0.57
0.56
0.57
1.71
7.734
7.706
7.327
7.301
7.277
7.251
6.909
6.883
4.248
4.020
4.003
3.666
3.656
3.461
3.327
3.301
3.193
3.129
3.079
2.815
2.644
2.637
2.419
5a
Ph
OH
Ts
N

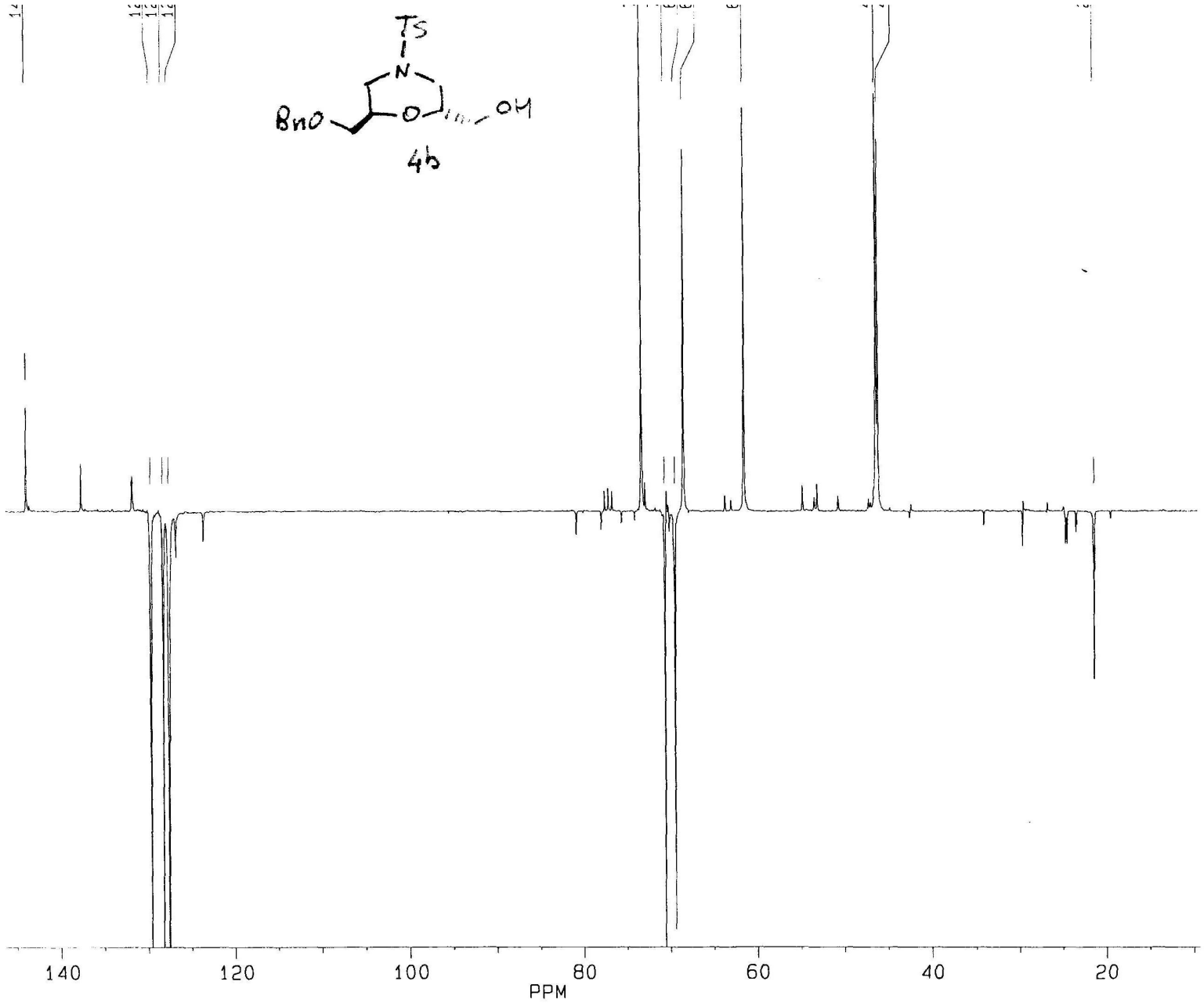

PPM
158.334
143.915
135.545
130.122
129.905
129.691
129.475
127.293
126.972
126.873
121.166
114.509
160
155
150
145
140
135
130
125
120
115
PPM

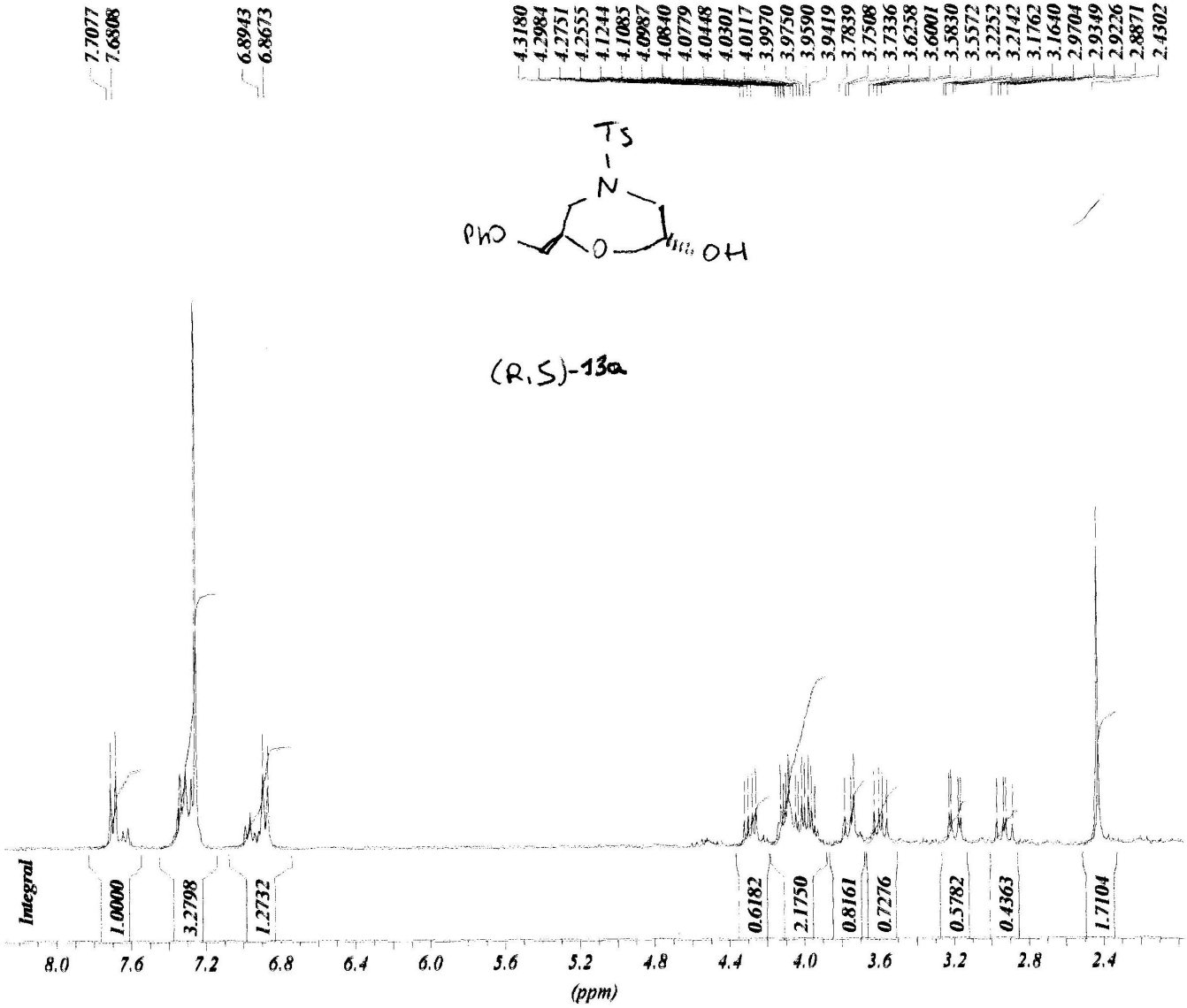

PPM
69.3191
68.9614
52.9713
52.1422
51.0864
45.6787
29.6511
21.4900
PPM
70
65
60
55
50
45
40
35
30
25
20
Pho
Ou
N
Is
Sa


Integral
1.8809
4.7496
2.8429
2.0126
1.1023
1.0204
2.0187
1.9367
0.9300
0.8970
3.0000
Hz
2302.89
2294.71
2211.42
2202.89
2193.97
2185.34
2106.92
2099.63
2092.28
2083.56
2075.43
1595.70
1291.94
1287.64
1279.20
1270.11
1264.26
1237.90
1232.11
1228.78
1222.96
1201.95
1198.84
1195.04
1191.75
1133.24
1127.99
983.27
980.07
971.86
968.42
961.13
956.56
933.41
930.27
921.81
918.45
869.30
862.18
857.73
850.57
738.12
4a


ppm
130
120
110
100
90
80
70
60
50
40
30
ppm
129.87
129.53
127.84
121.37
114.74
77.43
77.00
76.58
70.64
69.42
66.40
62.02
46.57
46.30
29.69
21.53
Ts
N
Ph
OH
4a

ppm (f1)
7.0
6.0
5.0
4.0
3.0
0
50
100
0.56
1.95
0.61
0.30
0.32
1.31
0.84
0.60
1.00
7.621
7.593
7.328
7.311
4.554
4.542
4.594
4.519
4.502
4.069
4.055
4.040
3.883
3.872
3.866
3.859
3.848
3.689
3.675
3.655
3.634
3.613
3.201
3.150
3.144
3.108
3.093
2.913
2.901
BnO
Ts
4b


Ts
N
O
BnO
OH
4b
140
120
100
80
60
40
20
PPM



*** Current Data Parameters ***

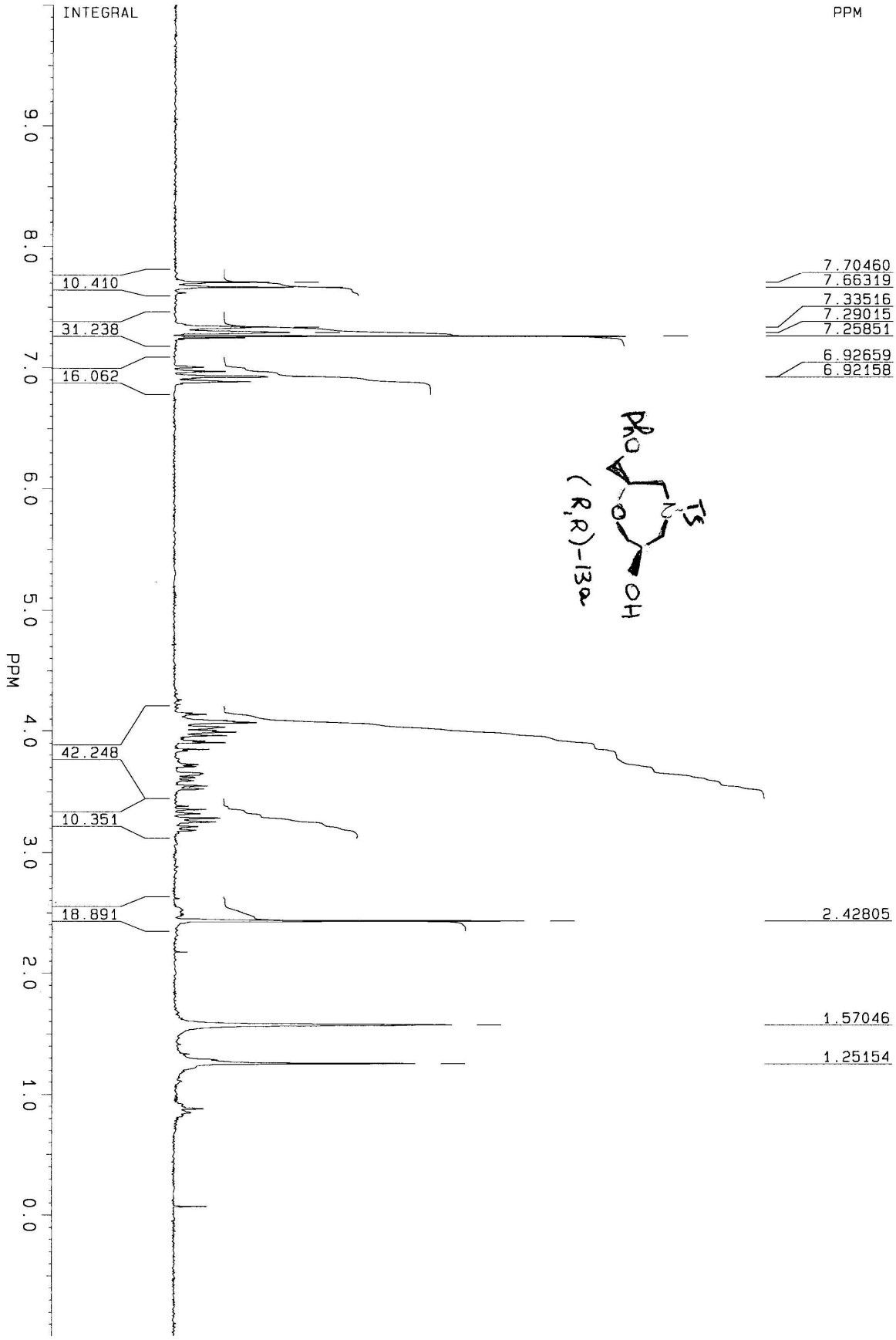
NAME	:	TEOSC7
EXPNO	:	1
PROCNO	:	2

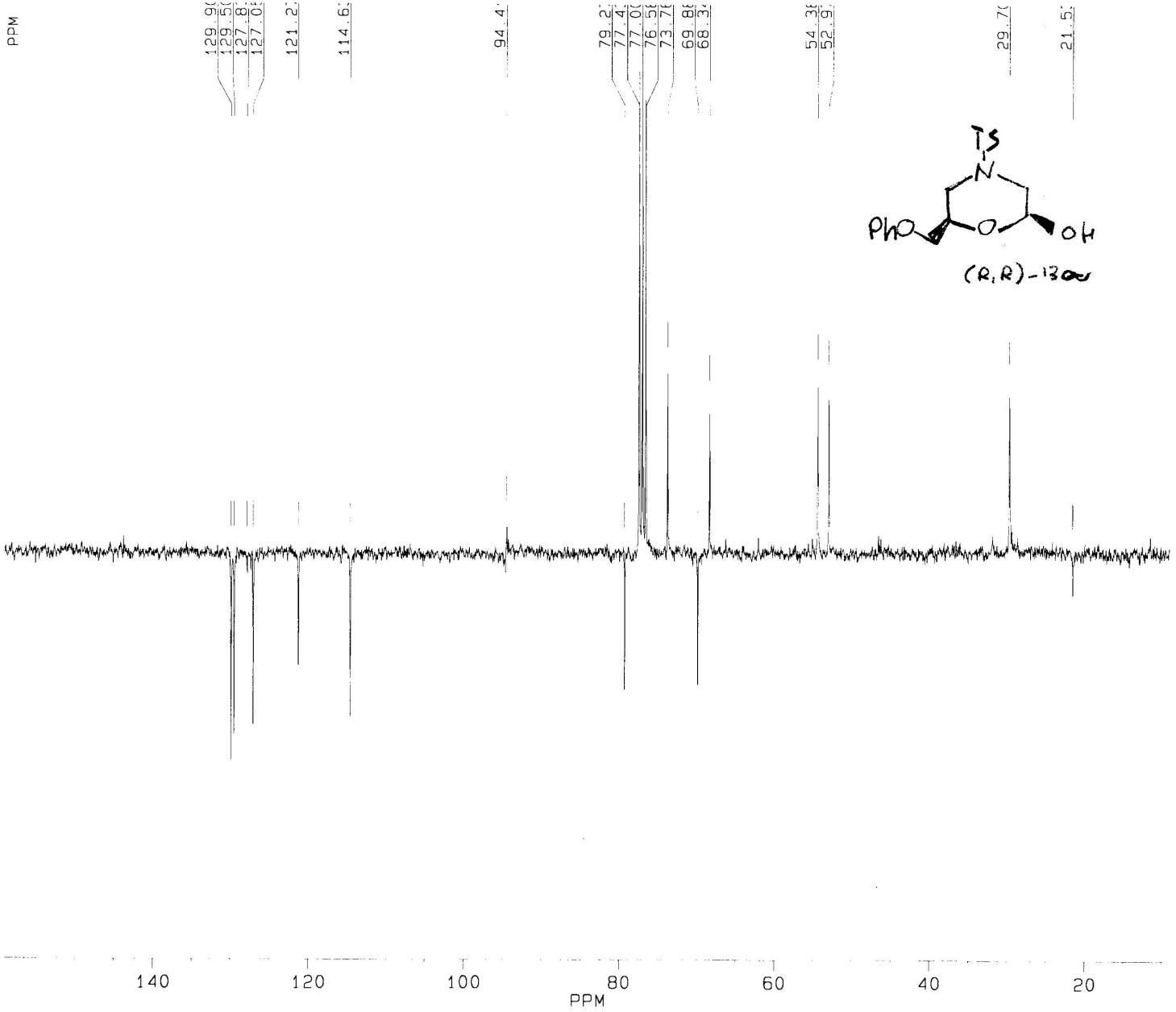
*** Acquisition Parameters ***

AQ_mod	:	qseq
AUNM	:	PRESAT.AUR
BF1	:	300.1300000 MHz
BF2	:	0.0000000 MHz
DEC_NMR	:	PO
DEC_MC	:	PO
DECSTAT	:	CPD
DP3000	:	148 dB
DS	:	0
FMFLAG	:	0
FW	:	7600.00 Hz
INSTRUM	:	AM
LOCNUC	:	Lock ?
NS	:	64
NUCLEUS	:	Nuc ?
O1	:	4800.00 Hz
O2	:	5574.22 Hz
PULPROG	:	
RO	:	20 Hz
SFO1	:	300.1348000 MHz
SOLVENT	:	Solvent ?
SW	:	20.0714 ppm
SW_h	:	6024.096 Hz
TD	:	24576
TE	:	297 K
VD	:	0.0000000 sec
YMAX_a		91788.8125000
YMIN_a		-91788.8125000

*** 1D NMR Plot Parameters ***

NUCLEUS	:	?

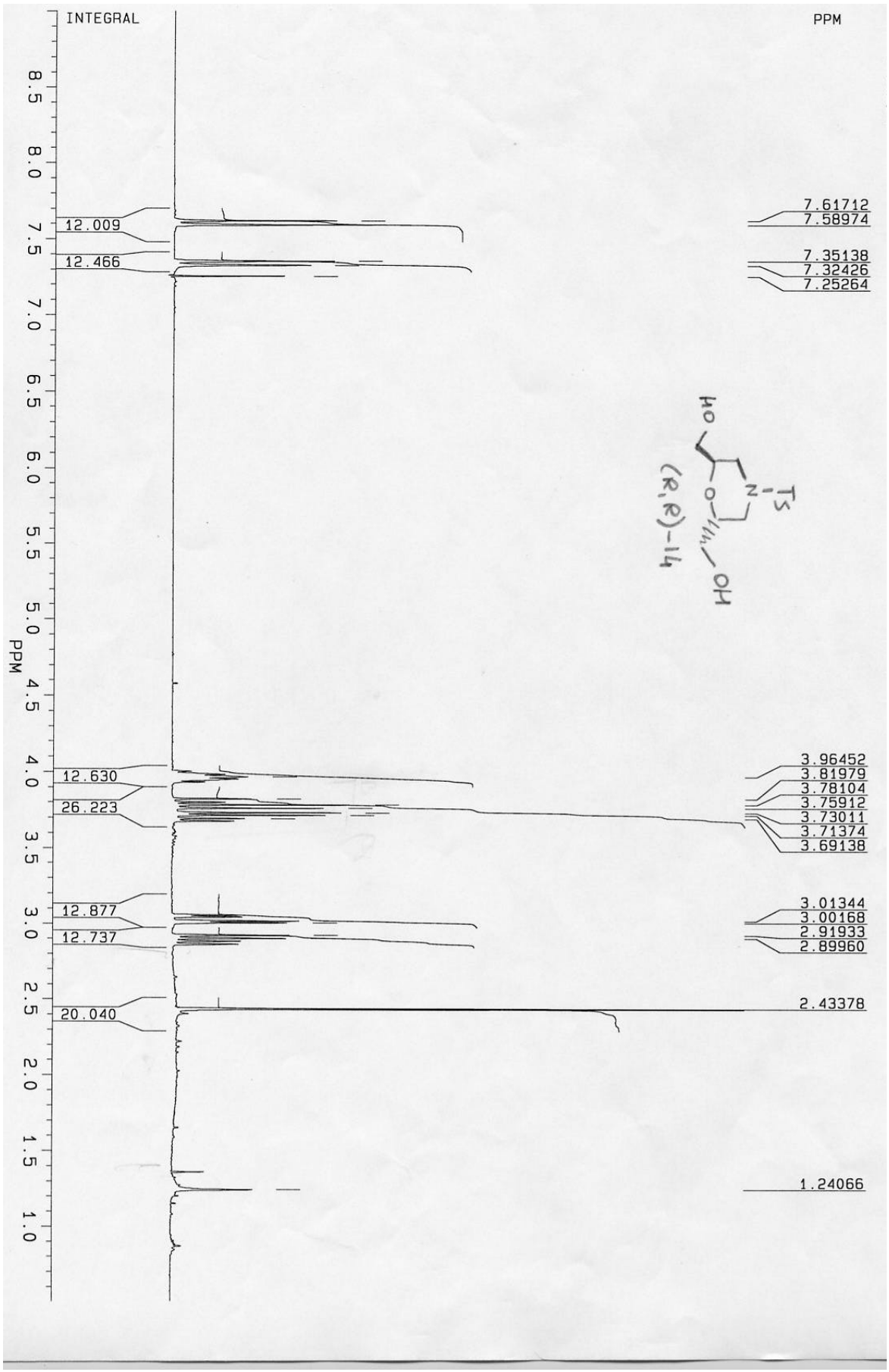

INTEGRAL
PPM
10.410
31.238
16.062
42.248
10.351
18.891
7.70460
7.66319
7.33516
7.29015
7.25851
6.92659
6.92158
2.42805
1.57046
1.25154
PPM
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
Ph
Ts
OH
(R,R)-13a

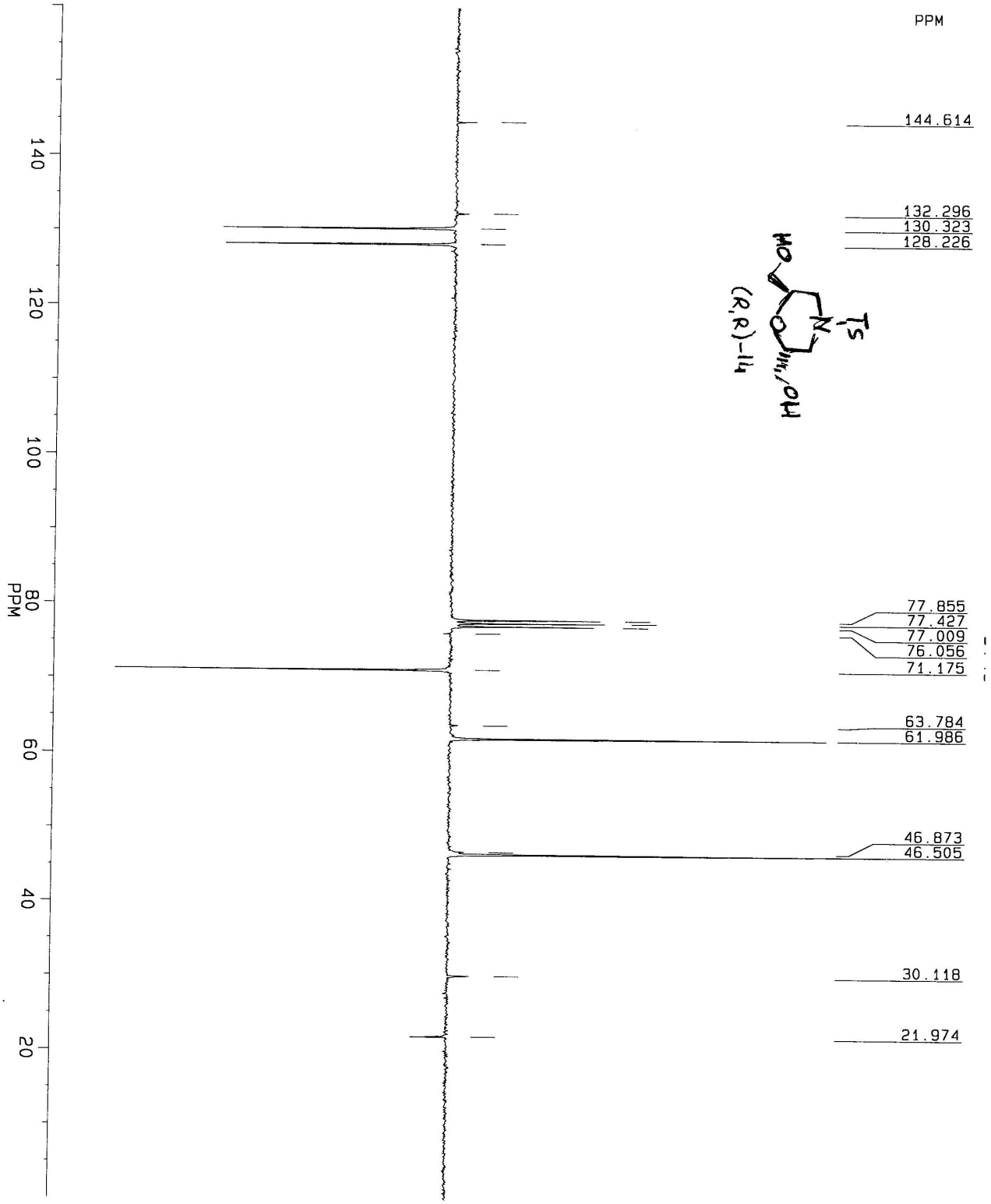


BRUKER

ALBAS863.002
AU PROG:
JMODXH.AU
DATE 26-7-4

SF	75.469
SY	75.0
O1	6534.949
SI	16384
TD	10714
SW	19230.769
HZ/PT	2.348
PW	0.0
RD	0.0
AQ	.279
RG	3200
NS	286422
TE	297
FW	24100
O2	6000.000
DP	18H CPD
LB	3.000
GB	0.0
CX	23.00
CY	0.0
F1	159.026
F2	8.910
HZ/CM	492.568
PPM/CM	6.527
SR	-1405.32
D1	.500000
S1	23H
P9	100.00
D2	.005000
S2	18H
P1	5.00
VD	.007000
P2	10.00
RD	0.0
PW	0.0
DE	35.00
NS	286422
DS	0
NE	1


INTEGRAL
PPM
12.009
12.466
12.630
26.223
12.877
12.737
20.040
7.61712
7.58974
7.35138
7.32426
7.25264
3.96452
3.81979
3.78104
3.75912
3.73011
3.71374
3.69138
3.01344
3.00168
2.91933
2.89960
2.43378
1.24066
Ts
N
O
OH
HO
(R,R)-14



ALBADT49.'
AU PROG:
JMODXH.A'
DATE 12-9

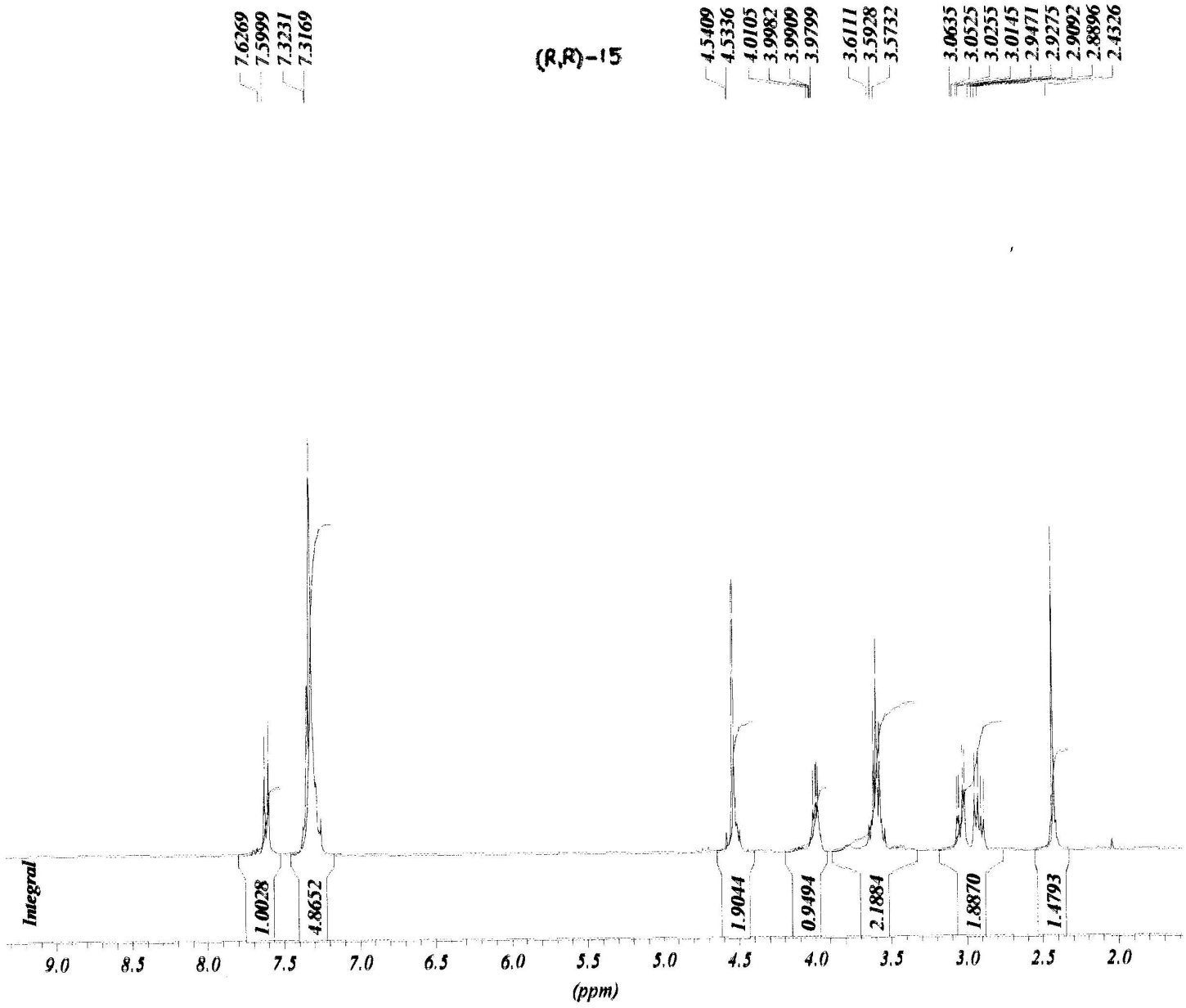
SF 75
SY 75.0
O1 6534
SI 16384
TD 10714
SW 19230
HZ/PT 2

PW 0
RD 0
AQ
RG 3200
NS 288252
TE 297

FW 24100
O2 6000
DP 18H C'

LB 3
GB 0
CX 24
CY 0
F1 160
F2
HZ/CM 503
PPM/CM 6
SR -1437

D1 .50'
S1 23H
P9 10'
.00'
D2
S2 18H
P1
VD .00
P2 1'
RD 0.0
PW
DE 3'
NS 2882'
DS
NE



*** Current Data Parameters ***

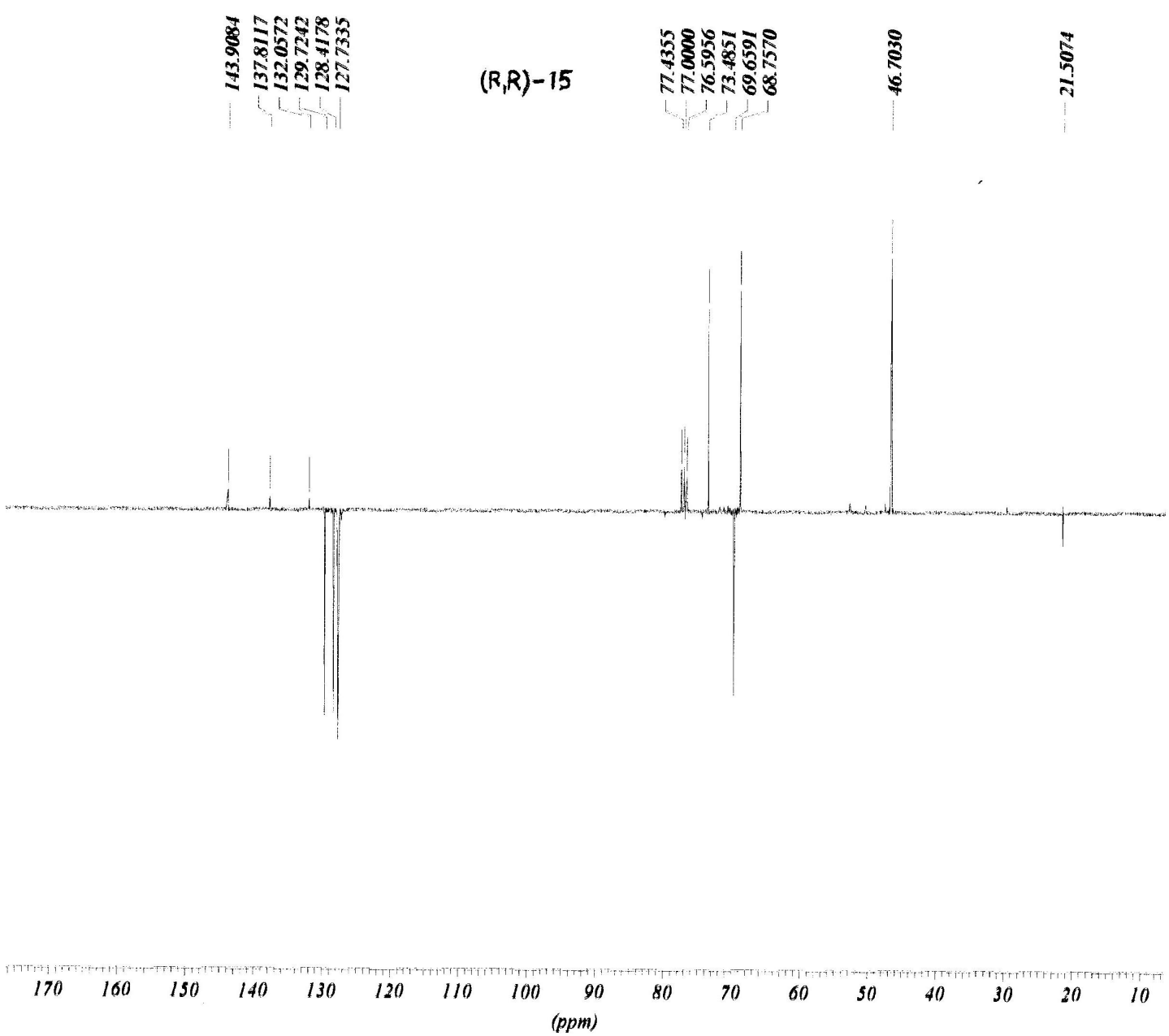
NAME	:	ALBABIBN
EXPNO	:	1
PROCNO	:	2

*** Acquisition Parameters ***

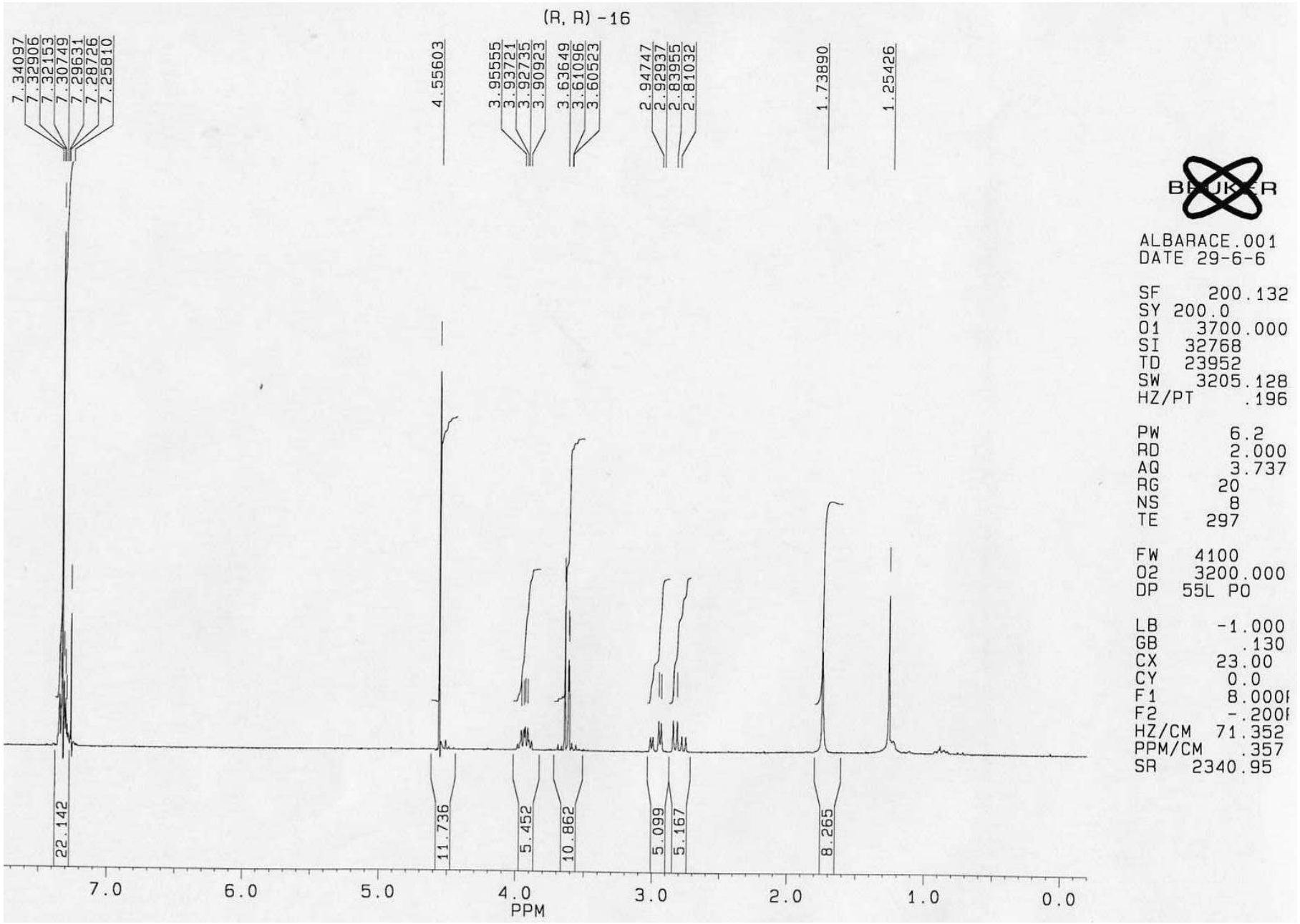
AQ_mod	:	qseq
AUNM	:	PRESAT.AUR
BF1	:	300.1300000 MHz
BF2	:	0.0000000 MHz
DEC_NMR	:	PO
DEC_MC	:	PO
DECSTAT	:	CPD
DP3000	:	148 dB
DS	:	0
FMFLAG	:	0
FW	:	7600.00 Hz
INSTRUM	:	AM
LOCNUC	:	Lock ?
NS	:	8
NUCLEUS	:	Nuc ?
O1	:	4800.00 Hz
O2	:	5574.22 Hz
PULPROG	:	
RO	:	20 Hz
SFO1	:	300.1348000 MHz
SOLVENT	:	Solvent ?
SW	:	20.0714 ppm
SW_h	:	6024.096 Hz
TD	:	24576
TE	:	297 K
VD	:	0.0000000 sec
YMAX_a	:	2130.0932617
YMIN_a	:	-2130.0932617

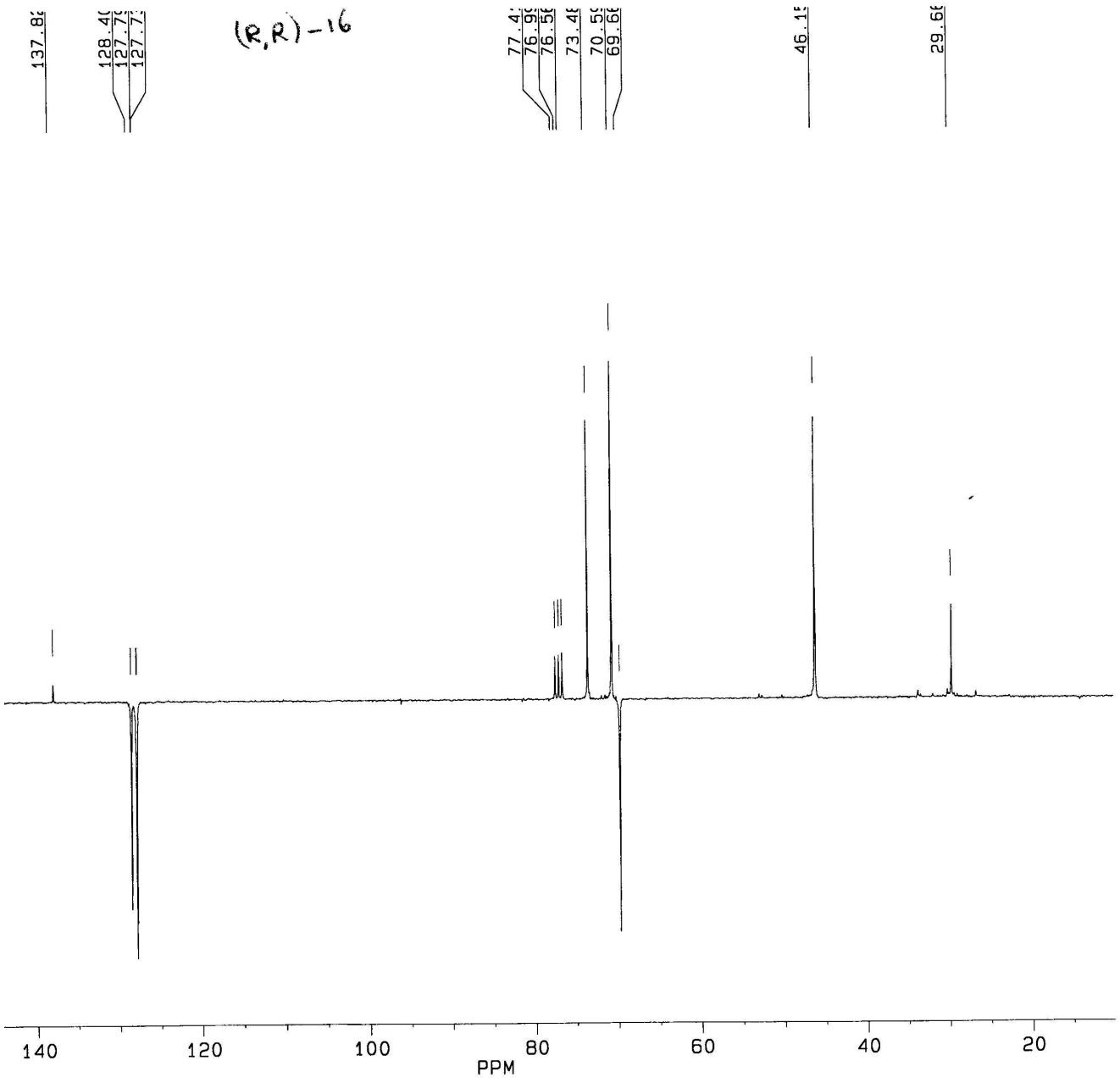
*** 1D NMR Plot Parameters ***

NUCLEUS	:	?



*** Current Data Parameters ***
NAME : ALBABENZ
EXPNO : 1
PROCNO : 2
*** Acquisition Parameters ***
AQ_mod : qseq
AUNM : JMODXH.AU
BF1 : 75.4700000 MHz
BF2 : 0.0000000 MHz
DEC_NMR : CPD
DEC_MC : PO
DECSTAT : PO
DP3000 : 18 dB
DS : 0
FMFLAG : 0
FW : 24100.00 Hz
INSTRUM : AM
LOCNUC : Lock ?
NS : 69238
NUCLEUS : Nuc ?
O1 : 6534.95 Hz
O2 : 6000.00 Hz
PULPROG :
RO : 20 Hz
SFO1 : 75.4765349 MHz
SOLVENT : Solvent ?
SW : 254.8183 ppm
SW_h : 19230.769 Hz
TD : 10714
TE : 297 K
VD : 0.0000000 sec
YMAX_a :3217565.7500000
YMIN_a :-3217565.7500000
*** 1D NMR Plot Parameters ***
NUCLEUS : ?


(R, R) -16
7.34097
7.32906
7.32153
7.30749
7.29631
7.28726
7.25810
4.55603
3.95555
3.93721
3.92735
3.90923
3.63649
3.61096
3.60523
2.94747
2.92937
2.83955
2.81032
1.73890
1.25426
22.142
11.736
5.452
10.862
5.099
5.167
8.265
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
PPM
ALBARACE.001
DATE 29-6-6
SF 200.132
SY 200.0
O1 3700.000
SI 32768
TD 23952
SW 3205.128
HZ/PT .196
PW 6.2
RD 2.000
AQ 3.737
RG 20
NS 8
TE 297
FW 4100
O2 3200.000
DP 55L PO
LB -1.000
GB .130
CX 23.00
CY 0.0
F1 8.000
F2 -.200
HZ/CM 71.352
PPM/CM .357
SR 2340.95

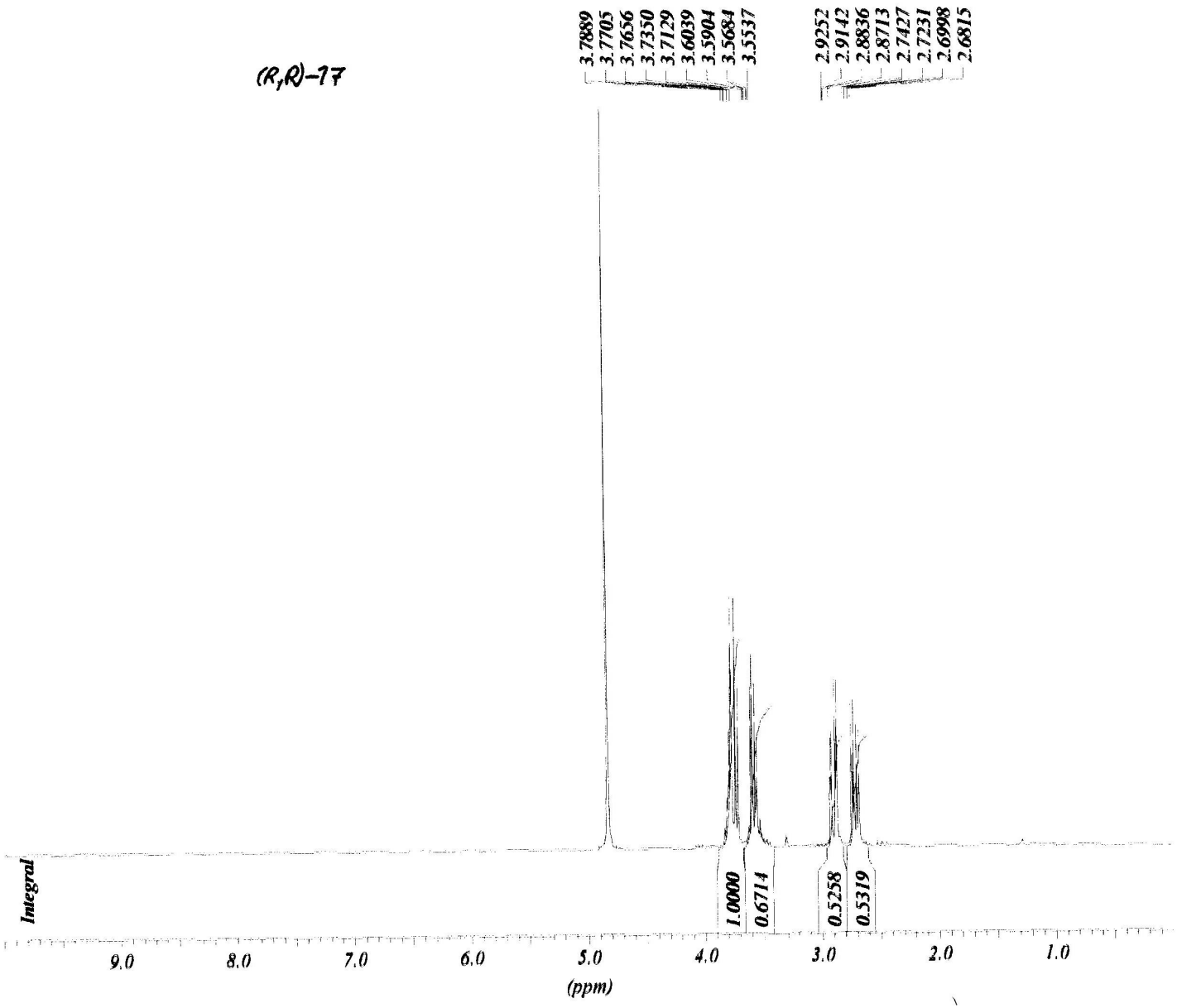


BRUKER

DOMECARB.002
AU PROG:
JMODXH.AU
DATE 21-6-6

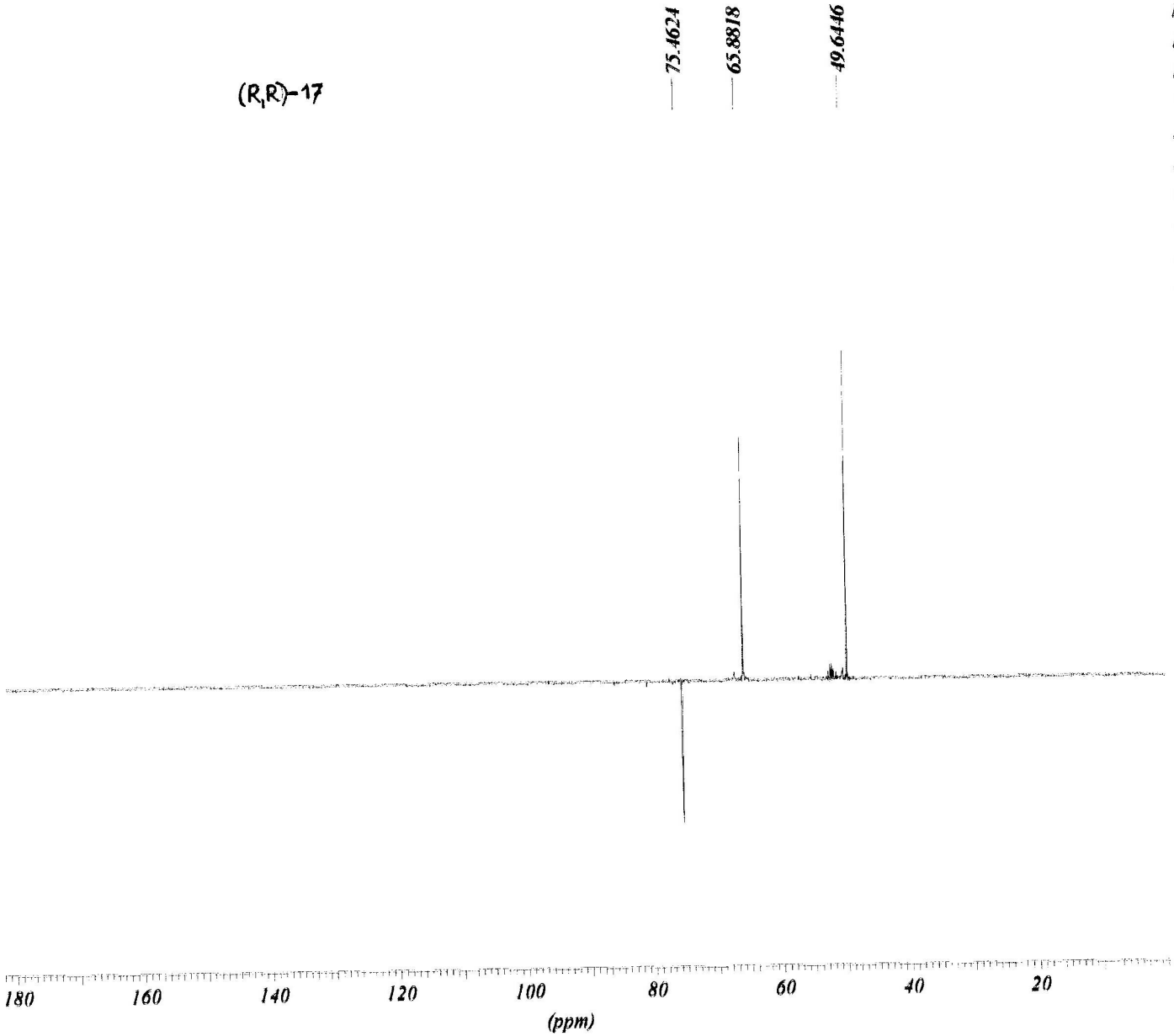
SF	75.469
SY	75.0
O1	6534.949
SI	16384
TD	10714
SW	19230.769
HZ/PT	2.348
PW	0.0
RD	0.0
AQ	.279
RG	3200
NS	69340
TE	297
FW	24100
O2	6000.000
DP	23H PO
LB	3.000
GB	0.0
CX	23.00
CY	0.0
F1	160.021
F2	10.029
HZ/CM	492.160
PPM/CM	6.521
SR	-1402.97
D1	.500000
S1	26H
P9	100.00
D2	.005000
S2	23H
P1	5.00
VD	.007000
P2	10.00
RD	0.0
PW	0.0
DE	35.00
NS	69340
DS	0
NE	1

(R,R)-77

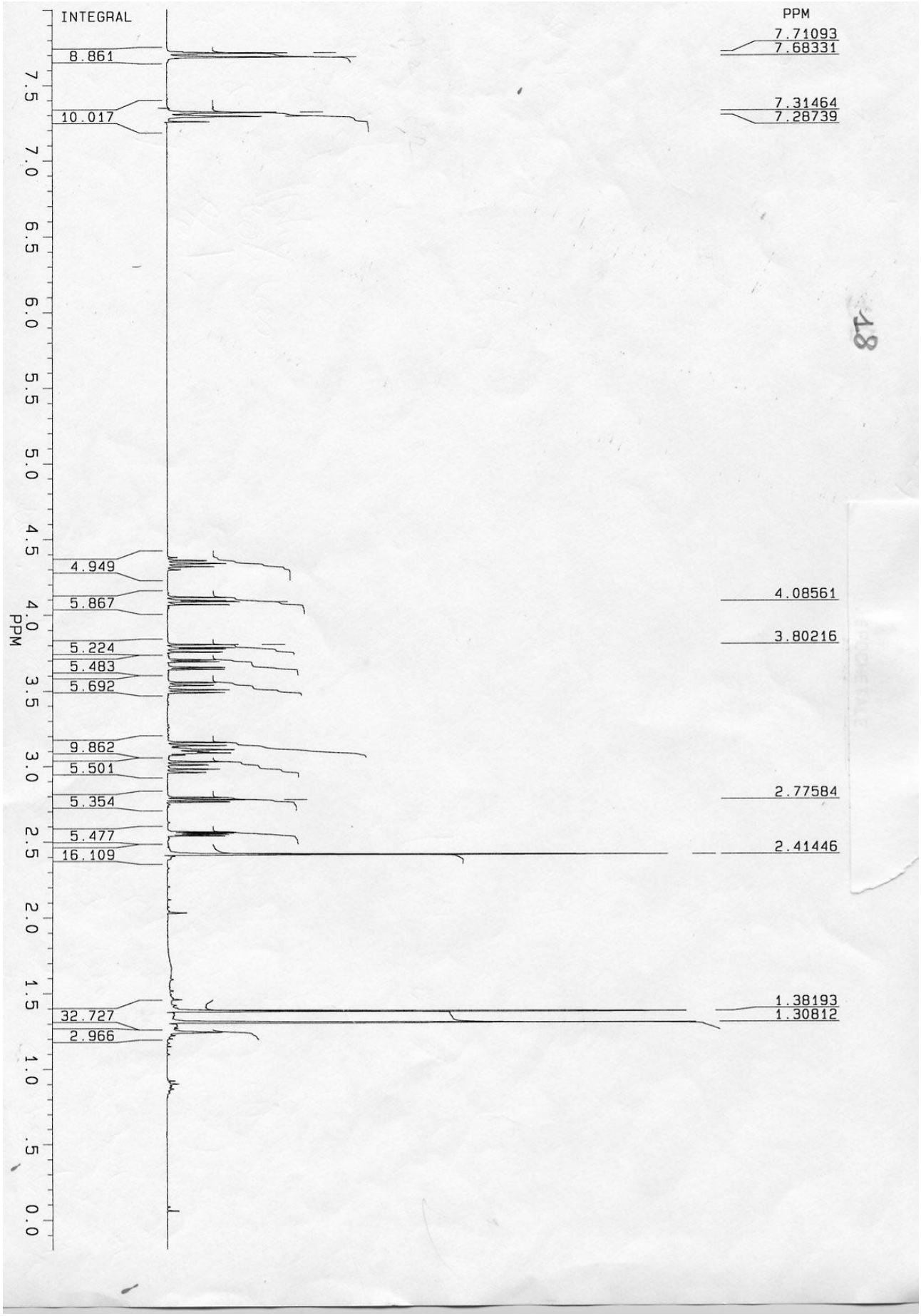


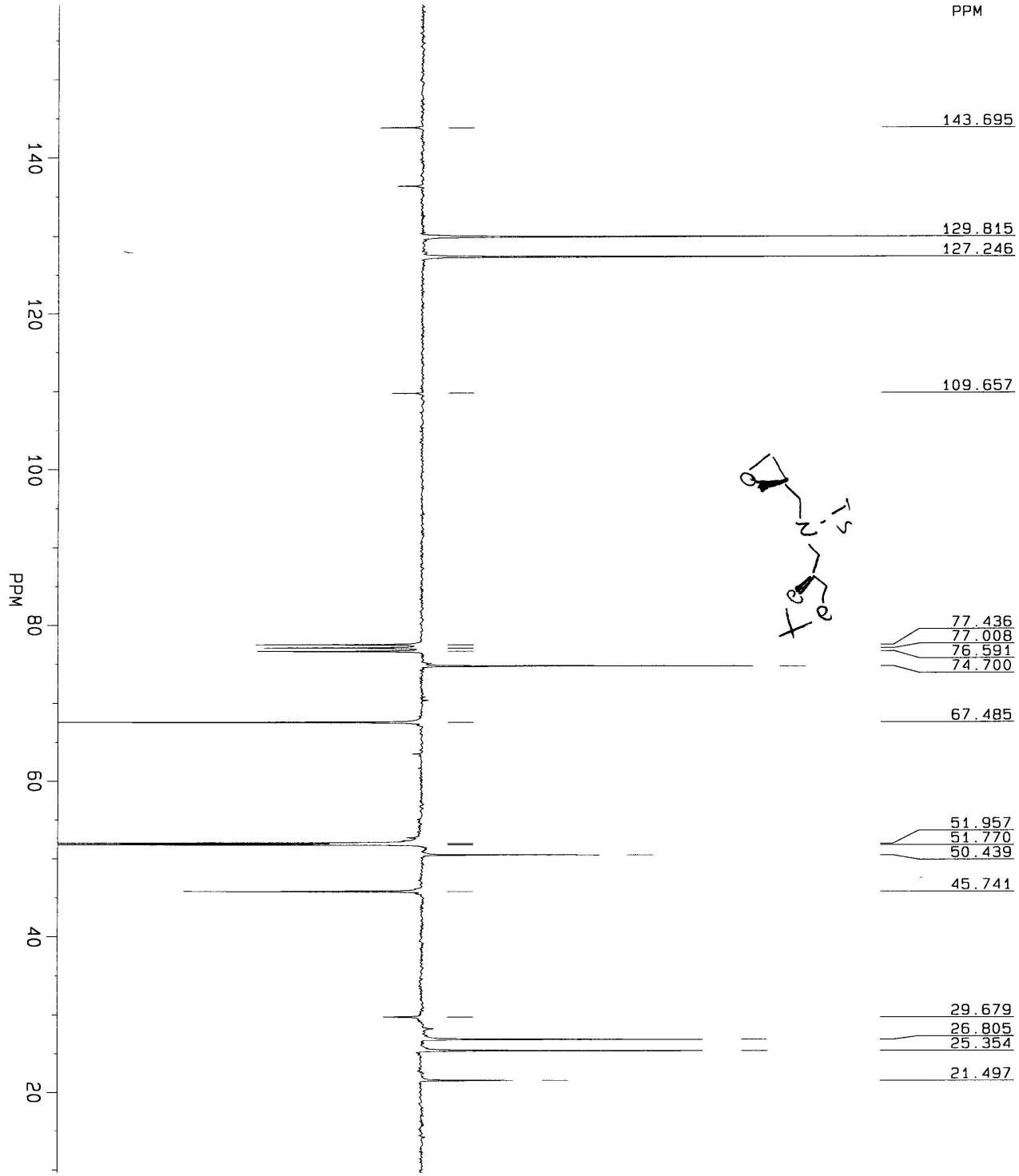
*** Current Data Parameters ***
NAME : DOMEDT94
EXPNO : 1
PROCNO : 2
*** Acquisition Parameters ***
AQ_mod : qseq
AUNM : PRESAT.AUR
BF1 : 300.1300000 MHz
BF2 : 0.0000000 MHz
DEC_NMR : PO
DEC_MC : PO
DECSTAT : CPD
DP3000 : 148 dB
DS : 0
FMFLAG : 0
FW : 7600.00 Hz
INSTRUM : AM
LOCNUC : Lock ?
NS : 8
NUCLEUS : Nuc ?
O1 : 6000.00 Hz
O2 : 5574.22 Hz
PULPROG :
RO : 20 Hz
SFO1 : 300.1360000 MHz
SOLVENT : Solvent ?
SW : 20.0713 ppm
SW_h : 6024.096 Hz
TD : 24576
TE : 297 K
VD : 0.0000000 sec
YMAX_a : 5528.5722656
YMIN_a : -5528.5722656
*** 1D NMR Plot Parameters ***
NUCLEUS : ?
SOLVENT : ?

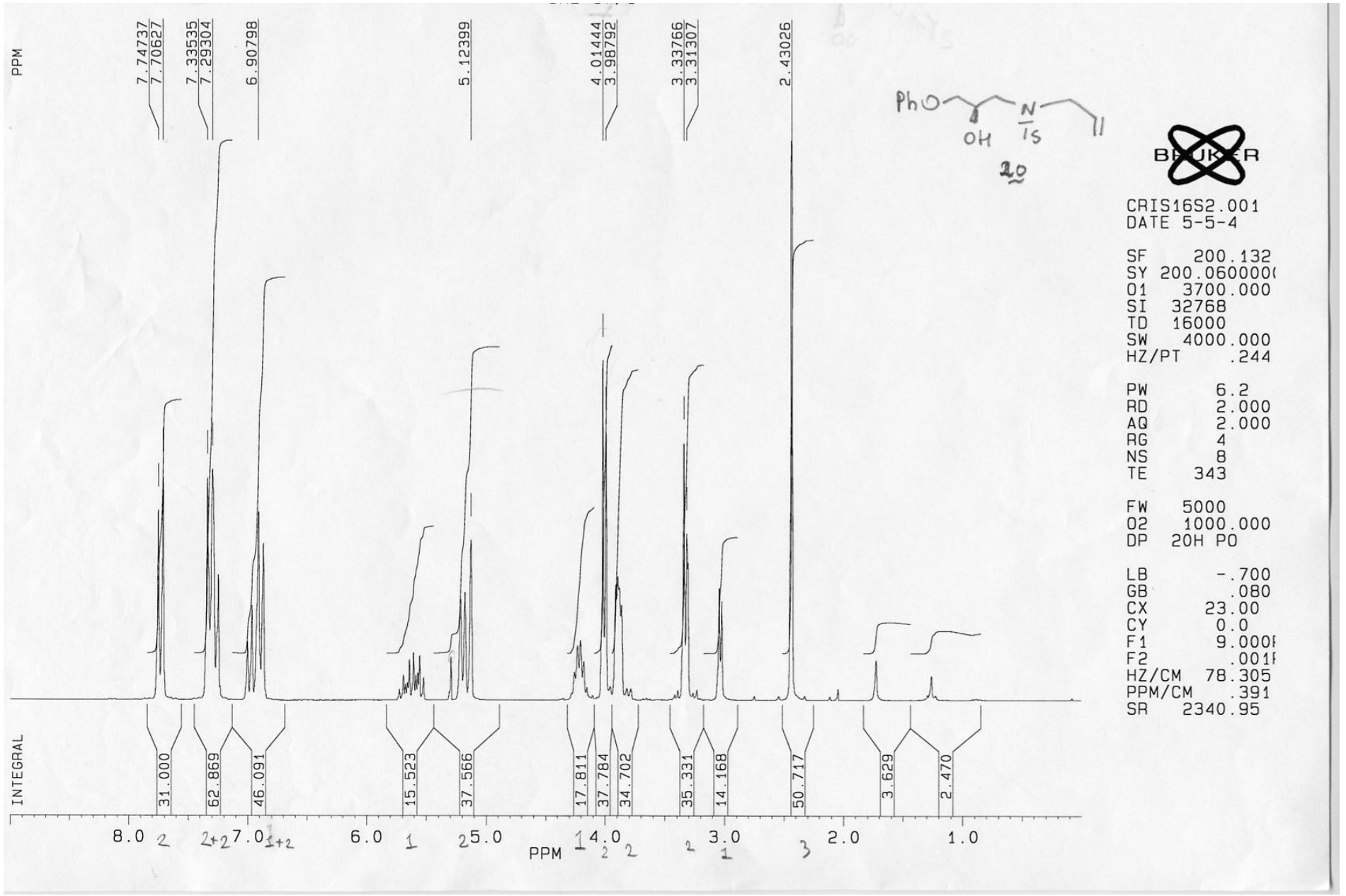
(R,R)-17

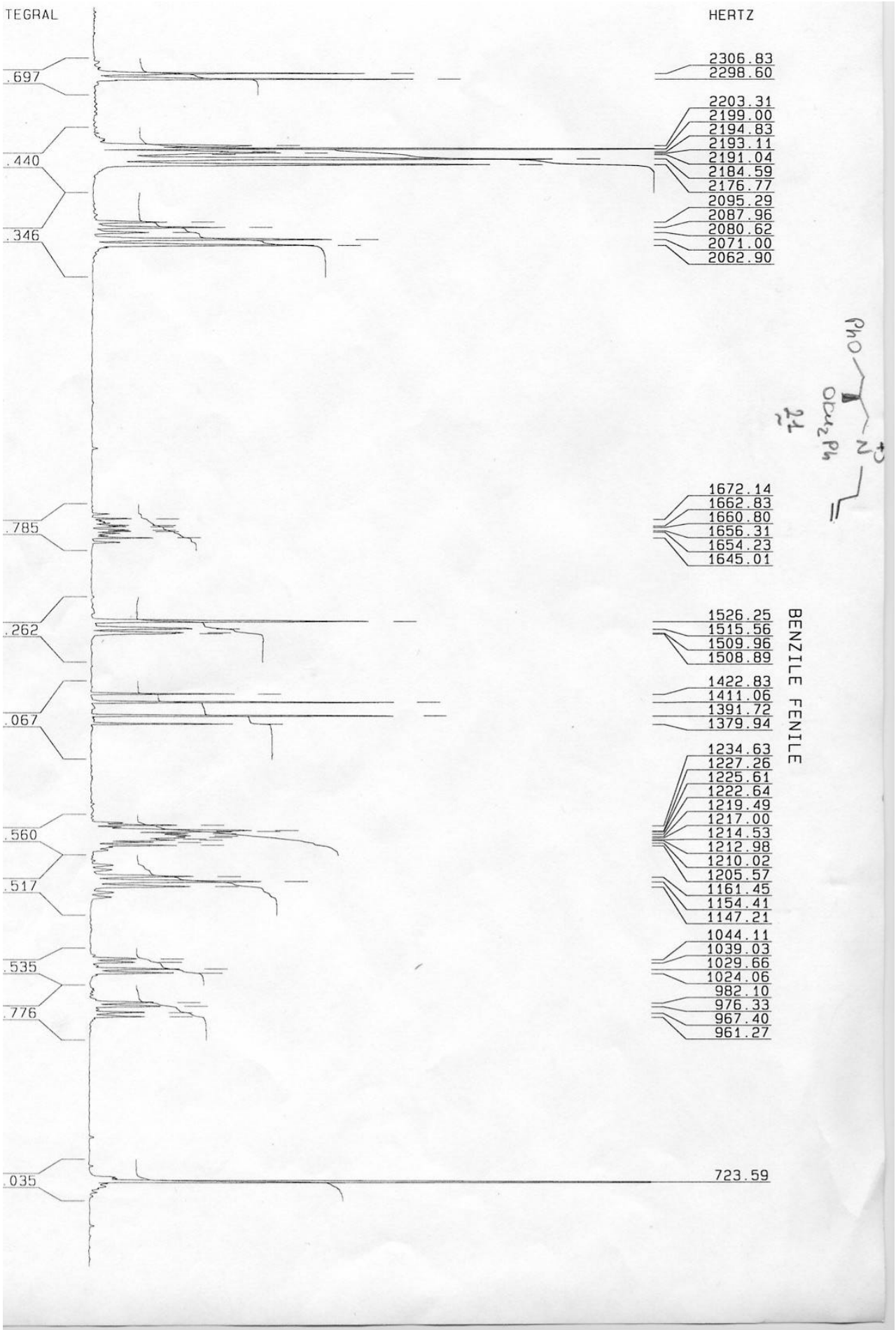


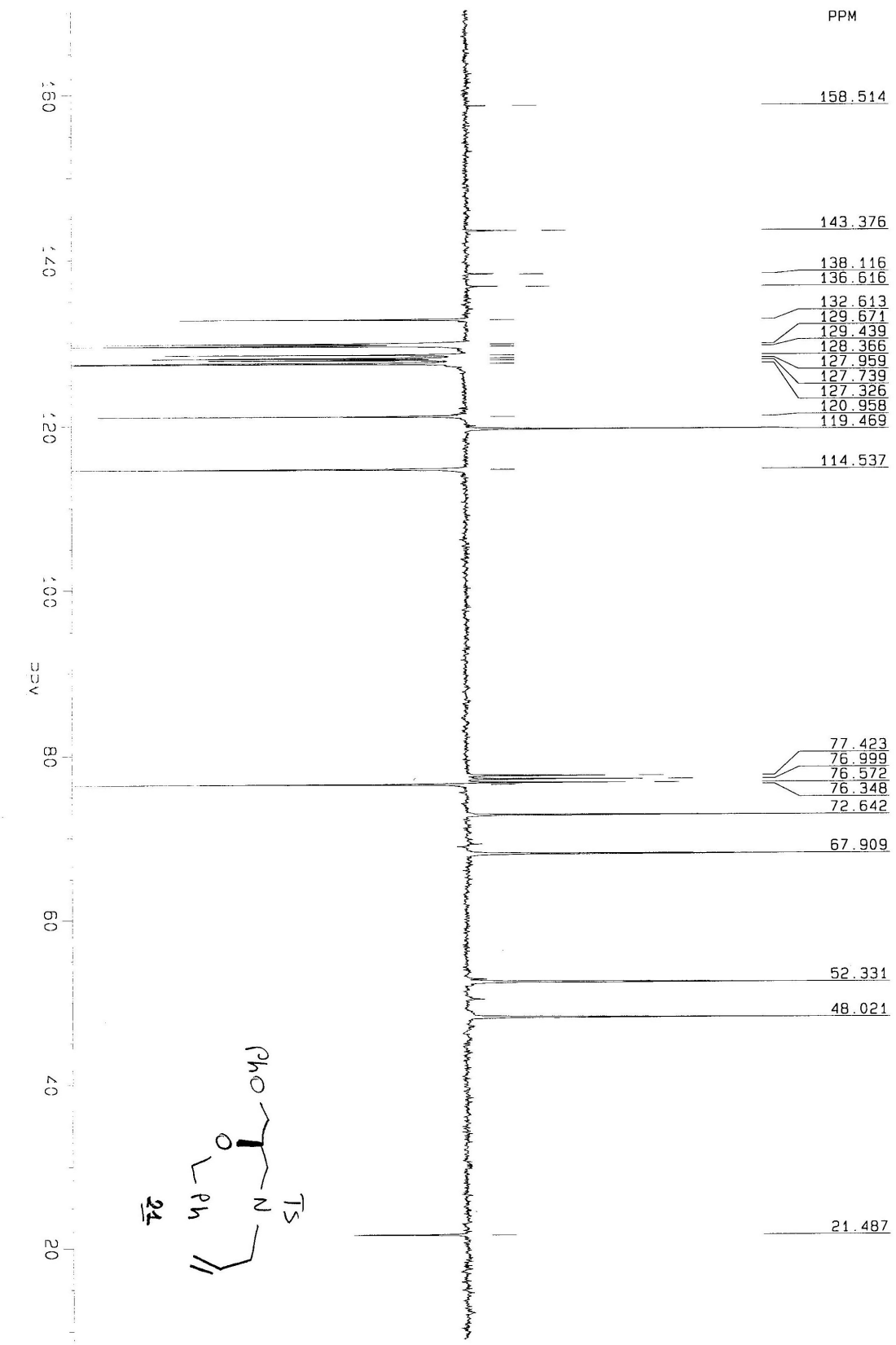
*** Current Data Parameters ***
NAME : DOMEDT94
EXPNO : 2
PROCNO : 2
*** Acquisition Parameters ***
AQ_mod : qseq
AUNM : JMODXH.AU
BF1 : 75.4700000 MHz
BF2 : 0.0000000 MHz
DEC_NMR : CPD
DEC_MC : PO
DECSTAT : PO
DP3000 : 18 dB
DS : 0
FMFLAG : 0
FW : 24100.00 Hz
INSTRUM : AM
LOCNUC : Lock ?
NS : 5905
NUCLEUS : Nuc ?
O1 : 6534.95 Hz
O2 : 6000.00 Hz
PULPROG :
RO : 20 Hz
SFO1 : 75.4765349 MHz
SOLVENT : Solvent ?
SW : 254.8183 ppm
SW_h : 19230.769 Hz
TD : 10714
TE : 297 K
VD : 0.0000000 sec
YMAX_a : 2251658.0000000
YMIN_a : -2251658.0000000
*** 1D NMR Plot Parameters ***
NUCLEUS : ?

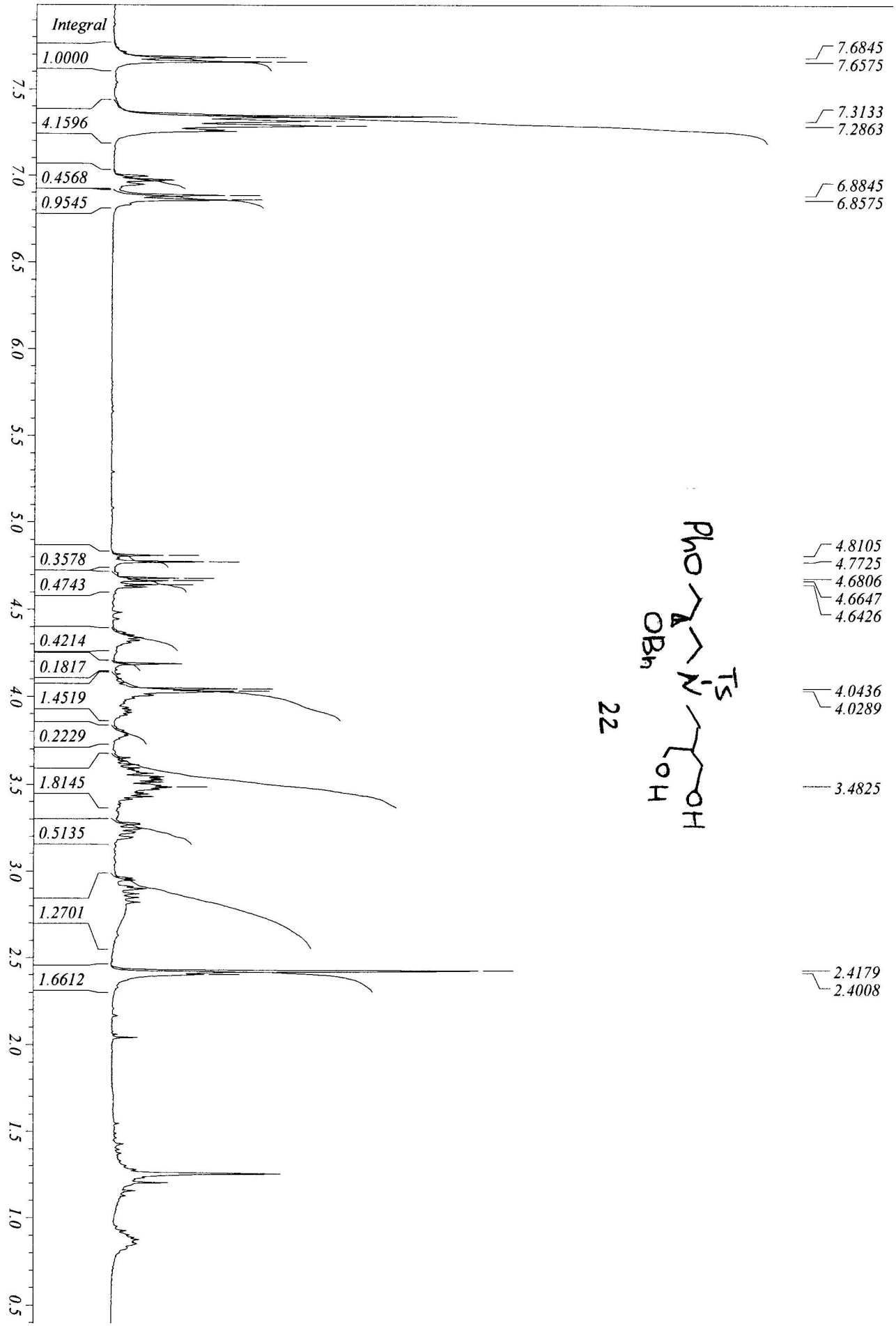

INTEGRAL
PPM
8.861
10.017
4.949
5.867
5.224
5.483
5.692
9.862
5.501
5.354
5.477
16.109
32.727
2.966
7.71093
7.68331
7.31464
7.28739
4.08561
3.80216
2.77584
2.41446
1.38193
1.30812
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0.0
PPM

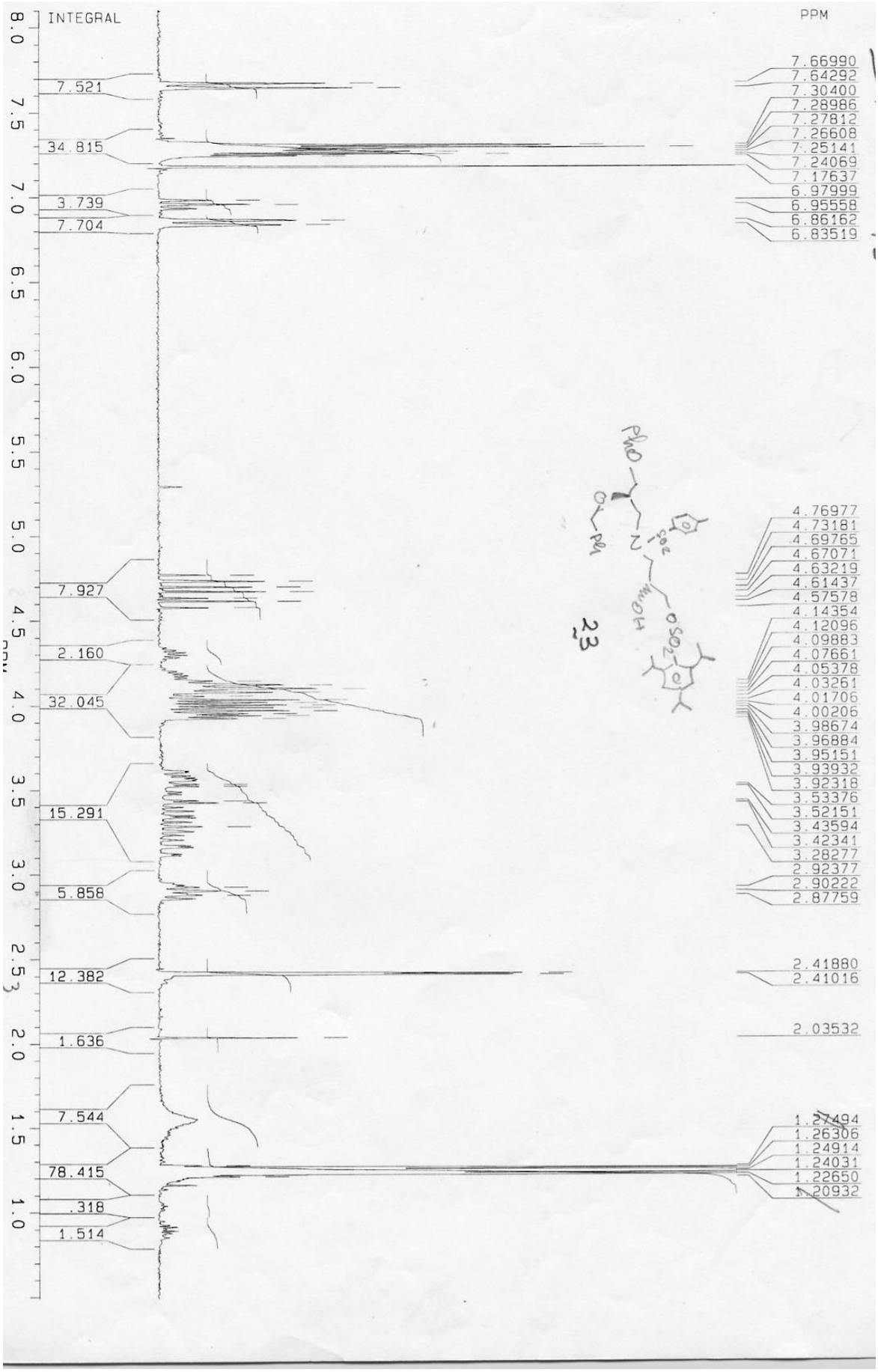

PPM
143.695
129.815
127.246
109.657
77.436
77.008
76.591
74.700
67.485
51.957
51.770
50.439
45.741
29.679
26.805
25.354
21.497
PPM
140
120
100
80
60
40
20
Ts
N

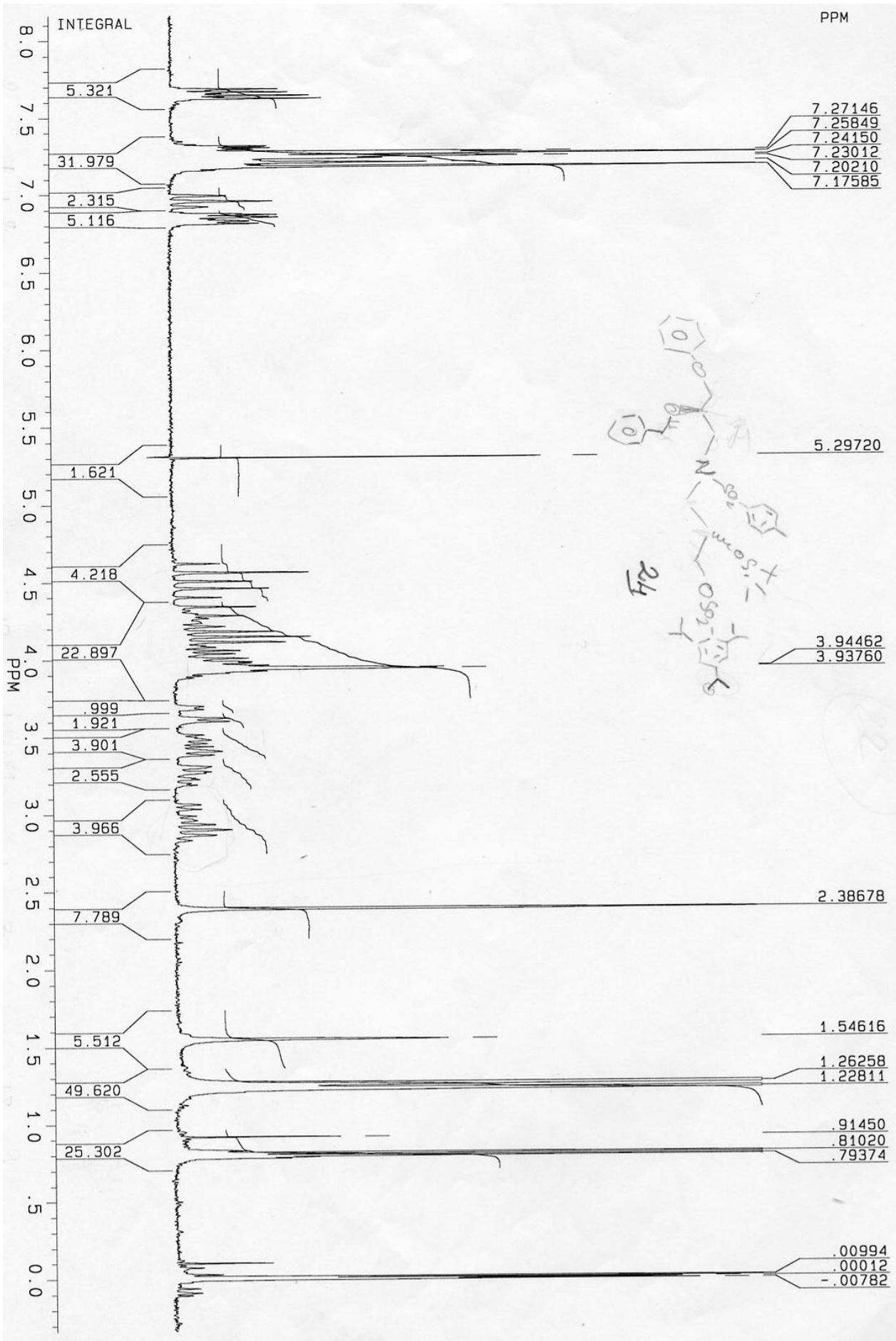

PPM
7.74737
7.70627
7.33535
7.29304
6.90798
5.12399
4.01444
3.98792
3.33766
3.31307
2.43026
INTEGRAL
31.000
62.869
46.091
15.523
37.566
17.811
37.784
34.702
35.331
14.168
50.717
3.629
2.470
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
PPM
PhO
OH
N
Ts
20
BRUKER
CRIS16S2.001
DATE 5-5-4
SF 200.132
SY 200.060000
O1 3700.000
SI 32768
TD 16000
SW 4000.000
HZ/PT .244
PW 6.2
RD 2.000
AQ 2.000
RG 4
NS 8
TE 343
FW 5000
O2 1000.000
DP 20H PO
LB -.700
GB .080
CX 23.00
CY 0.0
F1 9.000
F2 .001
HZ/CM 78.305
PPM/CM .391
SR 2340.95

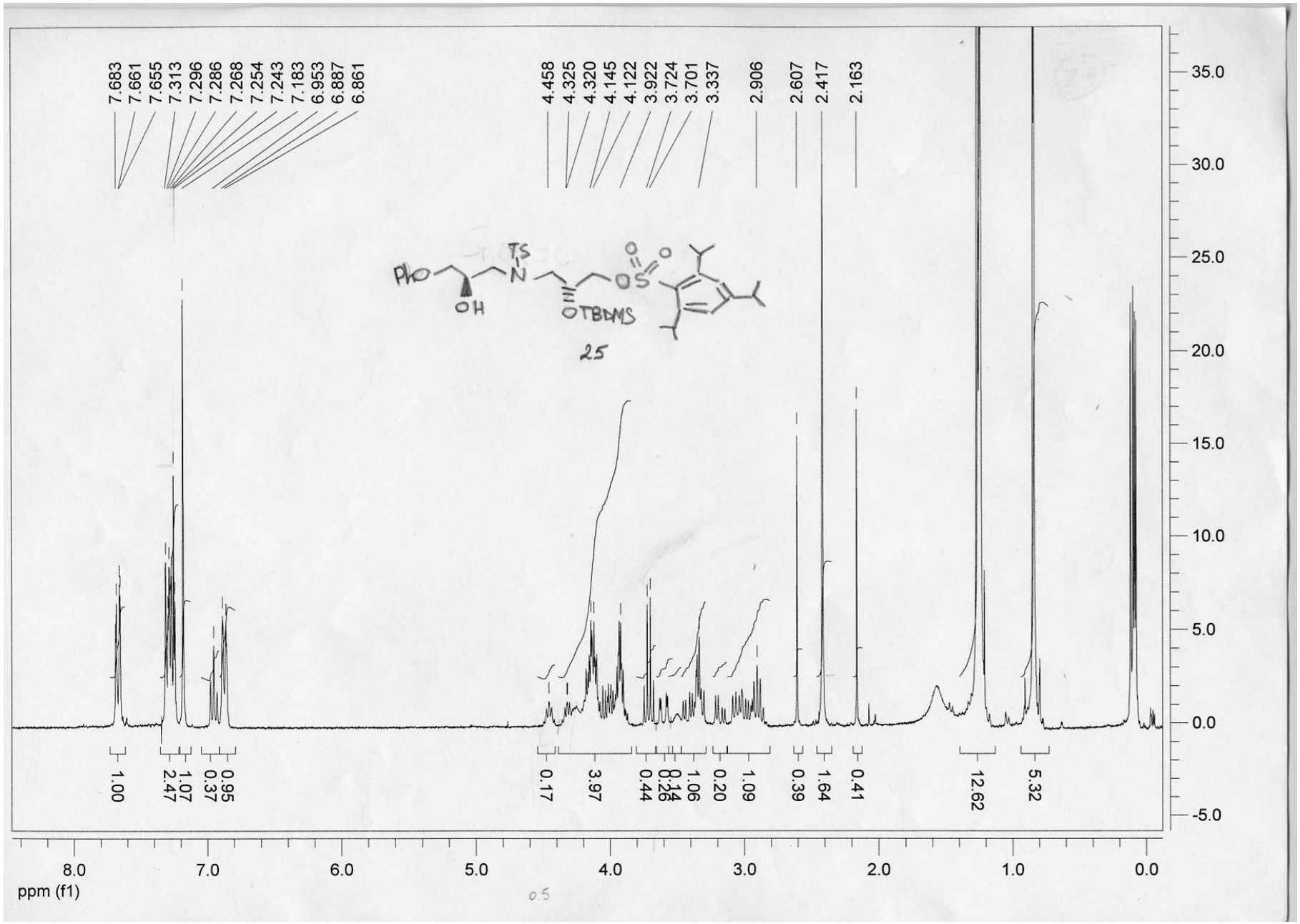

TEGRAL
HERTZ
.697
.440
.346
.785
.262
.067
.560
.517
.535
.776
.035
2306.83
2298.60
2203.31
2199.00
2194.83
2193.11
2191.04
2184.59
2176.77
2095.29
2087.96
2080.62
2071.00
2062.90
1672.14
1662.83
1660.80
1656.31
1654.23
1645.01
1526.25
1515.56
1509.96
1508.89
1422.83
1411.06
1391.72
1379.94
1234.63
1227.26
1225.61
1222.64
1219.49
1217.00
1214.53
1212.98
1210.02
1205.57
1161.45
1154.41
1147.21
1044.11
1039.03
1029.66
1024.06
982.10
976.33
967.40
961.27
723.59
BENZILE FENILE

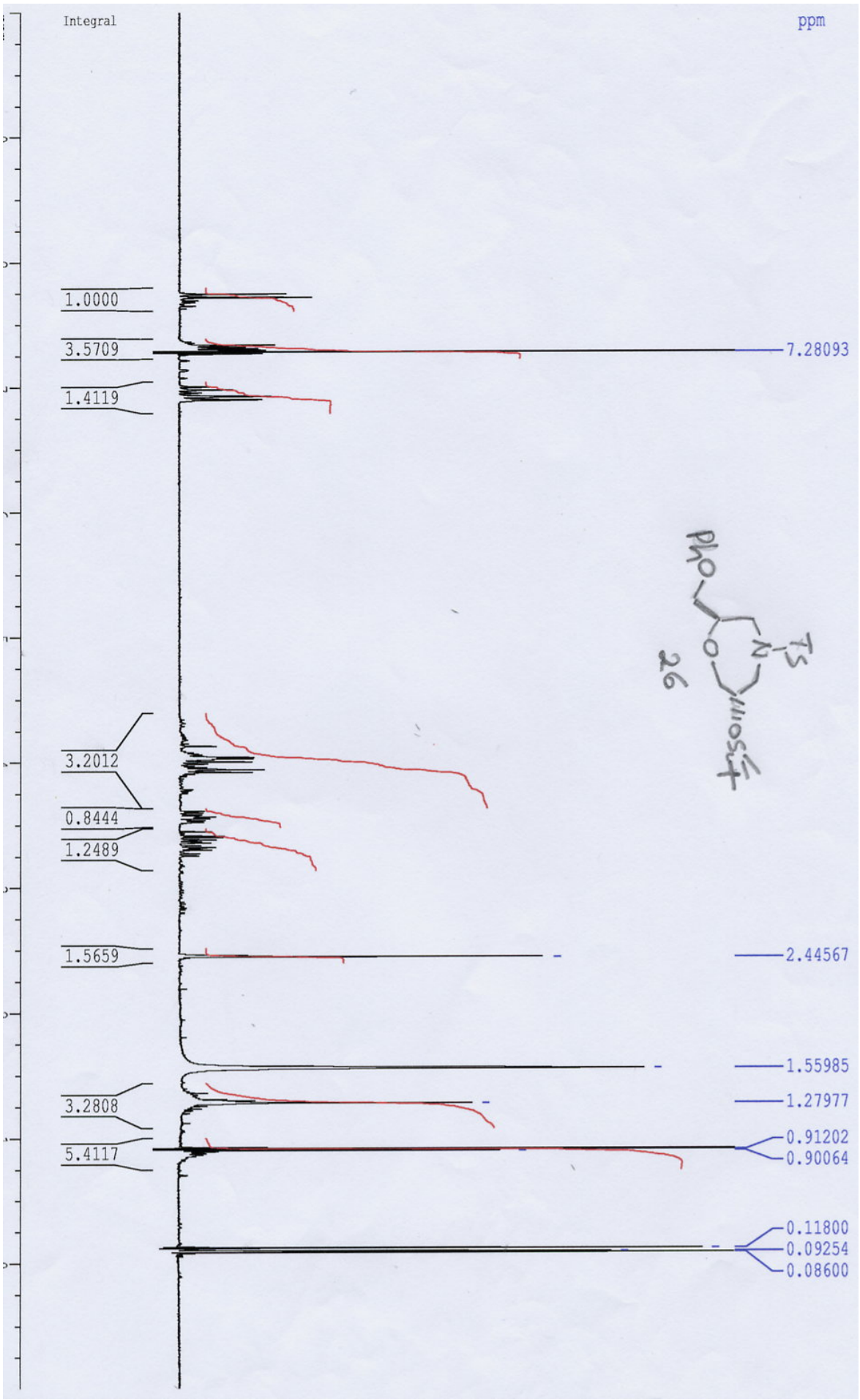

PPM
158.514
143.376
138.116
136.616
132.613
129.671
129.439
128.366
127.959
127.739
127.326
120.958
119.469
114.537
77.423
76.999
76.572
76.348
72.642
67.909
52.331
48.021
21.487
160
140
120
100
80
60
40
20
ppm
Ph
O
N
Ts
OH

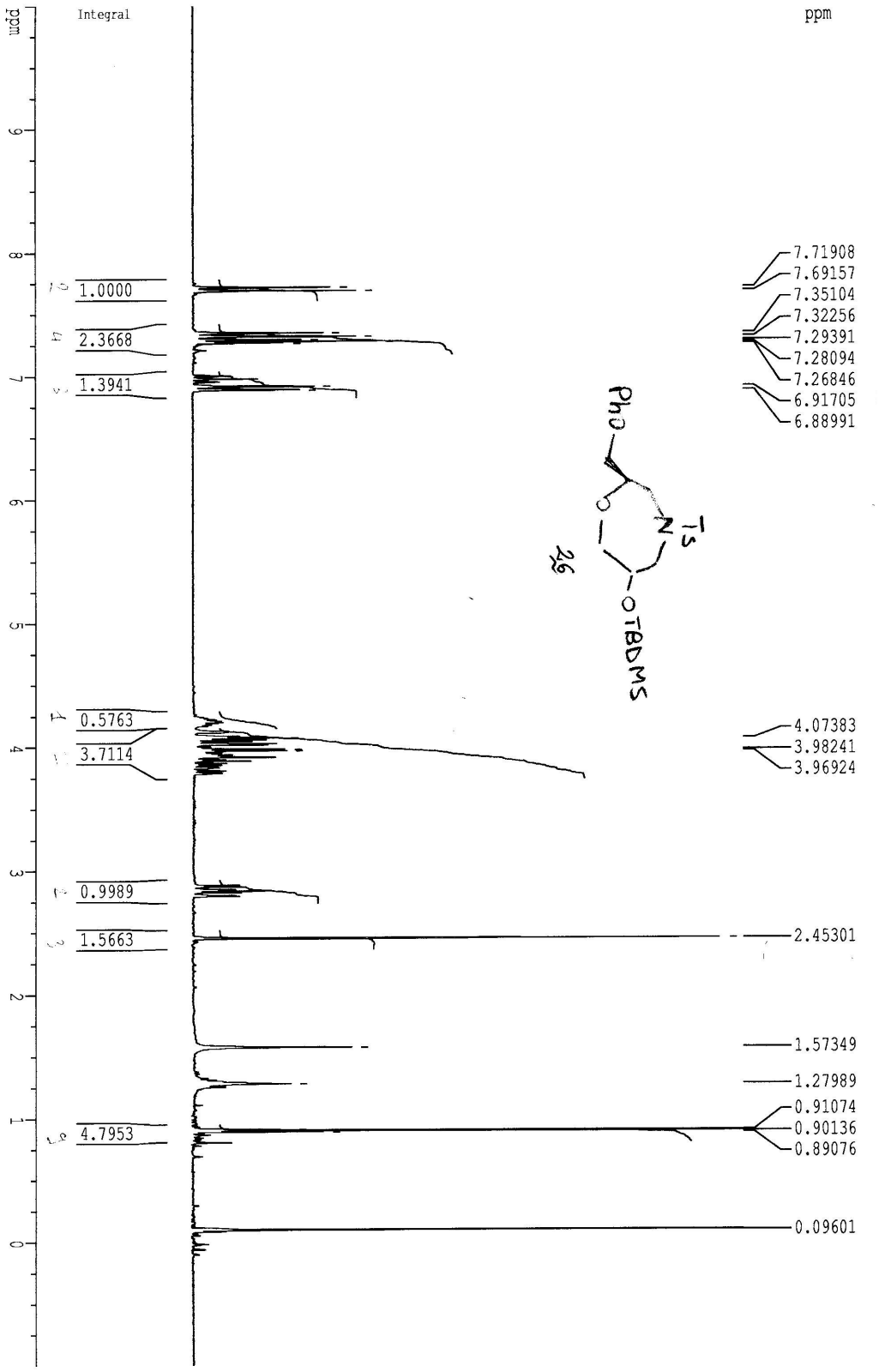

Integral
1.0000
4.1596
0.4568
0.9545
0.3578
0.4743
0.4214
0.1817
1.4519
0.2229
1.8145
0.5135
1.2701
1.6612
7.6845
7.6575
7.3133
7.2863
6.8845
6.8575
4.8105
4.7725
4.6806
4.6647
4.6426
4.0436
4.0289
3.4825
2.4179
2.4008
PhO
OBn
N
Ts
OH
22

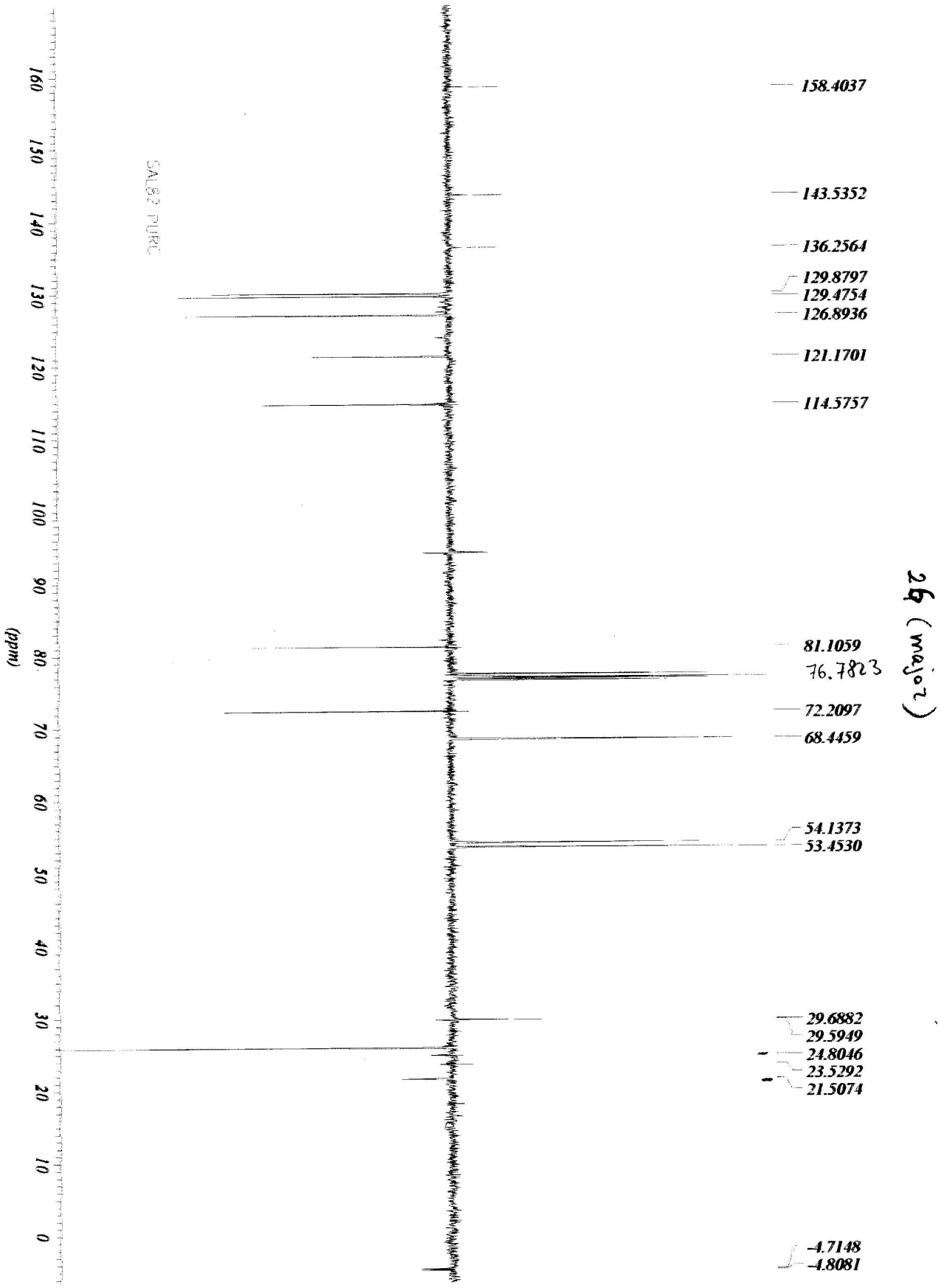

INTEGRAL
PPM
7.521
34.815
3.739
7.704
7.927
2.160
32.045
15.291
5.858
12.382
1.636
7.544
78.415
.318
1.514
7.66990
7.64292
7.30400
7.28986
7.27812
7.26608
7.25141
7.24069
7.17637
6.97999
6.95558
6.86162
6.83519
4.76977
4.73181
4.69765
4.67071
4.63219
4.61437
4.57578
4.14354
4.12096
4.09883
4.07661
4.05378
4.03261
4.01706
4.00206
3.98674
3.96884
3.95151
3.93932
3.92318
3.53376
3.52151
3.43594
3.42341
3.28277
2.92377
2.90222
2.87759
2.41880
2.41016
2.03532
1.27494
1.26306
1.24914
1.24031
1.22650
1.20932
23


INTEGRAL
PPM
5.321
31.979
2.315
5.116
1.621
4.218
22.897
.999
1.921
3.901
2.555
3.966
7.789
5.512
49.620
25.302
7.27146
7.25849
7.24150
7.23012
7.20210
7.17585
5.29720
3.94462
3.93760
2.38678
1.54616
1.26258
1.22811
.91450
.81020
.79374
.00994
.00012
-.00782
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
.5
0.0
PPM

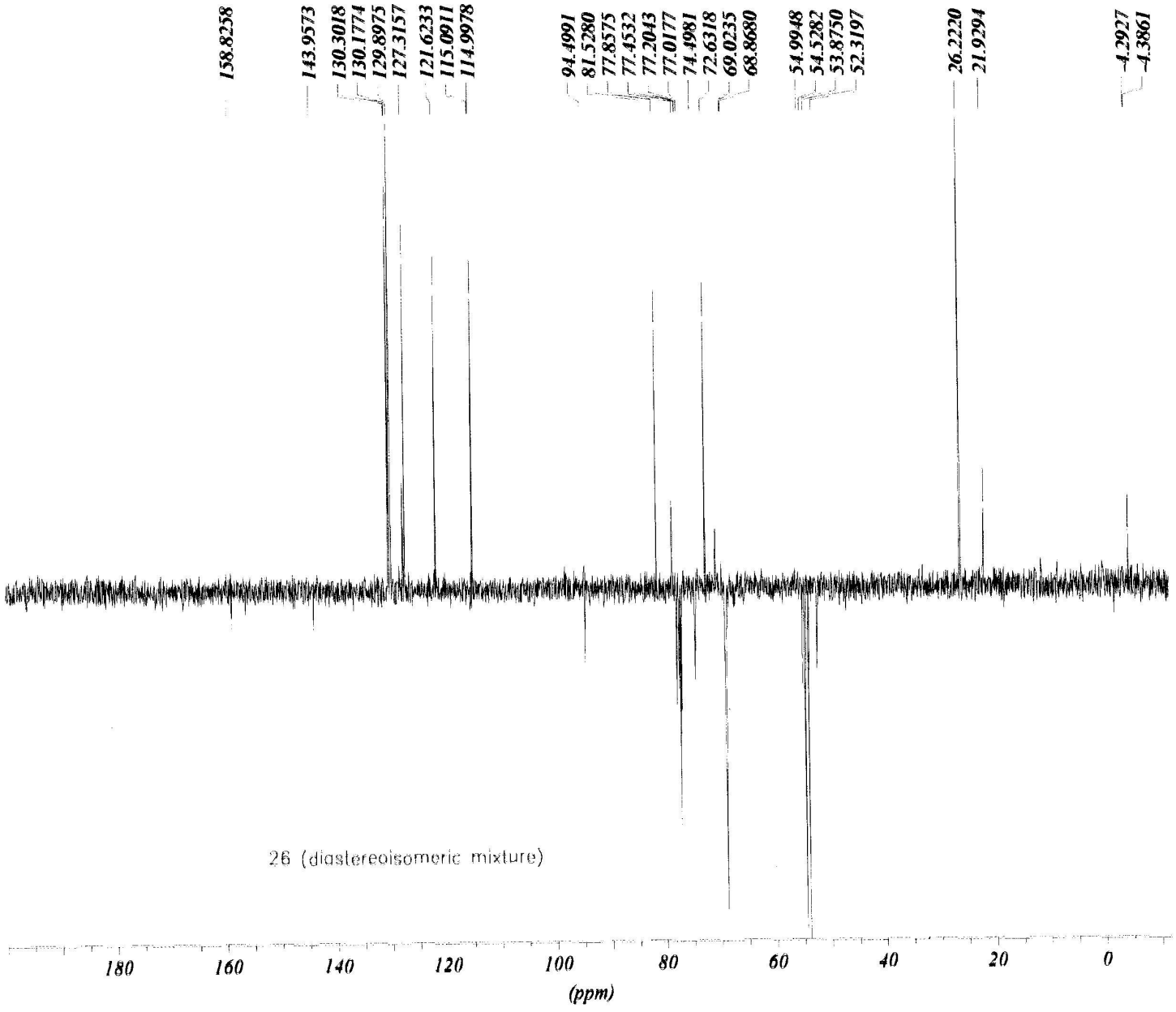

7.683
7.661
7.655
7.313
7.296
7.286
7.268
7.254
7.243
7.183
6.953
6.887
6.861
4.458
4.325
4.320
4.145
4.122
3.922
3.724
3.701
3.337
2.906
2.607
2.417
2.163
PhO
OH
TS
N
O
S
O
O
OTBDMS
25
1.00
2.47
1.07
0.37
0.95
0.17
3.97
0.44
0.26
0.14
1.06
0.20
1.09
0.39
1.64
0.41
12.62
5.32
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
-5.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


Integral
ppm
1.0000
3.5709
1.4119
3.2012
0.8444
1.2489
1.5659
3.2808
5.4117
7.28093
2.44567
1.55985
1.27977
0.91202
0.90064
0.11800
0.09254
0.08600
PhO
N
Ts
O
26


ppm
Integral
1.0000
2.3668
1.3941
0.5763
3.7114
0.9989
1.5663
4.7953
7.71908
7.69157
7.35104
7.32256
7.29391
7.28094
7.26846
6.91705
6.88991
4.07383
3.98241
3.96924
2.45301
1.57349
1.27989
0.91074
0.90136
0.89076
0.09601
Ph
O
N
Ts
OTBDMS


158.4037
143.5352
136.2564
129.8797
129.4754
126.8936
121.1701
114.5757
81.1059
76.7823
72.2097
68.4459
54.1373
53.4530
29.6882
29.5949
24.8046
23.5292
21.5074
-4.7148
-4.8081
(ppm)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

2g (major)



*** Current Data Parameters ***

NAME	:	DOMESA82
EXPNO	:	1
PROCNO	:	2

*** Acquisition Parameters ***

AQ_mod	:	qseq
AUNM	:	JMODXH.AU
BF1	:	75.4700000 MHz
BF2	:	0.0000000 MHz
DEC_NMR	:	CPD
DEC_MC	:	PO
DECSTAT	:	PO
DP3000	:	18 dB
DS	:	0
FMFLAG	:	0
FW	:	24100.00 Hz
INSTRUM	:	AM
LOCNUC	:	Lock ?
NS	:	6291
NUCLEUS	:	Nuc ?
O1	:	6534.95 Hz
O2	:	6000.00 Hz
PULPROG	:	
RO	:	20 Hz
SFO1	:	75.4765349 MHz
SOLVENT	:	Solvent ?
SW	:	254.8183 ppm
SW_h	:	19230.769 Hz
TD	:	10714
TE	:	297 K
VD	:	0.0000000 sec
YMAX_a		566639.3125000
YMIN_a		:-566639.3125000

*** 1D NMR Plot Parameters ***

NUCLEUS	:	?