Figure 1 x-ray structure of **6aa**

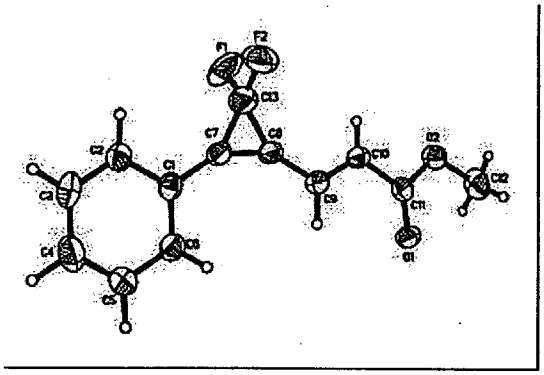


**Figure 1** X-ray structure of **6aa**. Selected bond lengths (Å), bond angles (°) and torsion angles (°): F (1)-C (13), 1.354 (4); F (2)-C (13), 1.367 (3); C (1)-C (7), 1.437 (3); C (7)-C (8), 1.328 (3); C (8)-C (9), 1.434 (3); C (7)-C (8)-C (13), 62.46 (17); C (7)-C (13)-C (8), 55.43 (17); C (6)-C (1)-C (7)-C (8), 178.8 (4); C (1)-C (7)-C (8)-C (13), 179.9 (5); C (13)-C (7)-C (8)-C (9), 179.9 (5).

Figure 2 x-ray structure of **8a-Z**

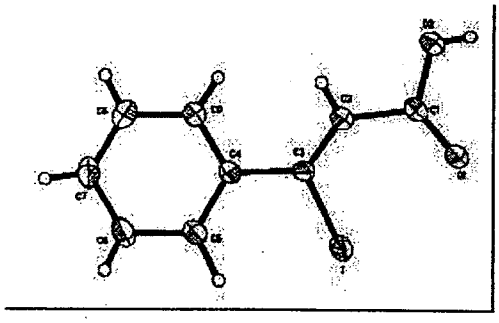


Figure 2 x-ray structure of **8a-Z**. Selected bond lengths (Å), bond angles (°) and torsion angles (°): I-C (3), 2.096 (4); C (1)-C (2), 1.466 (6); C (2)-C (3), 1.330 (6); C (3)-C (4), 1.480 (6); C (1)-C (2)-C (3), 128.3 (4); C (2)-C (3)-I, 122.7 (3); C (4)-C (3)-I, 114.8 (3); O (1)-C (1)-C (2)-C (3), -27.4 (8); O (2)-C (1)-C (2)-C (3), 154.7 (5); C (1)-C (2)-C (3)-I, -1.2 (7); C (2)-C (3)-C (4)-C (9), 37.5 (7); I-C (3)-C (4)-C (9), -139.4 (4).

**Figure 3** $^{1}H$-$^{13}C$ (HMBC) of **8f**

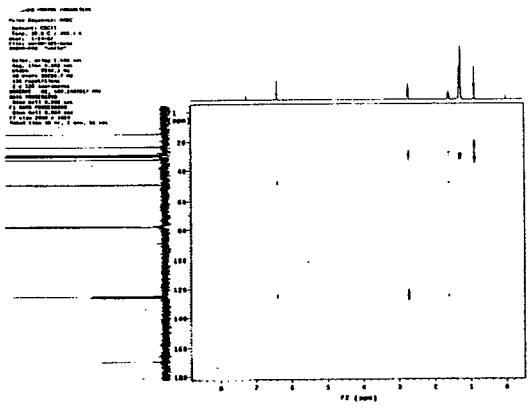
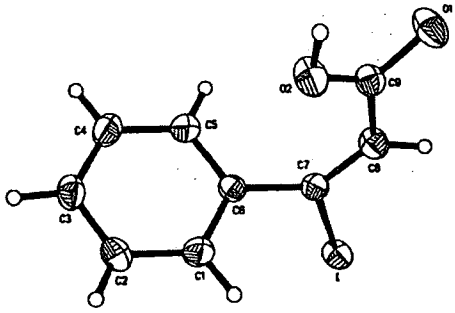
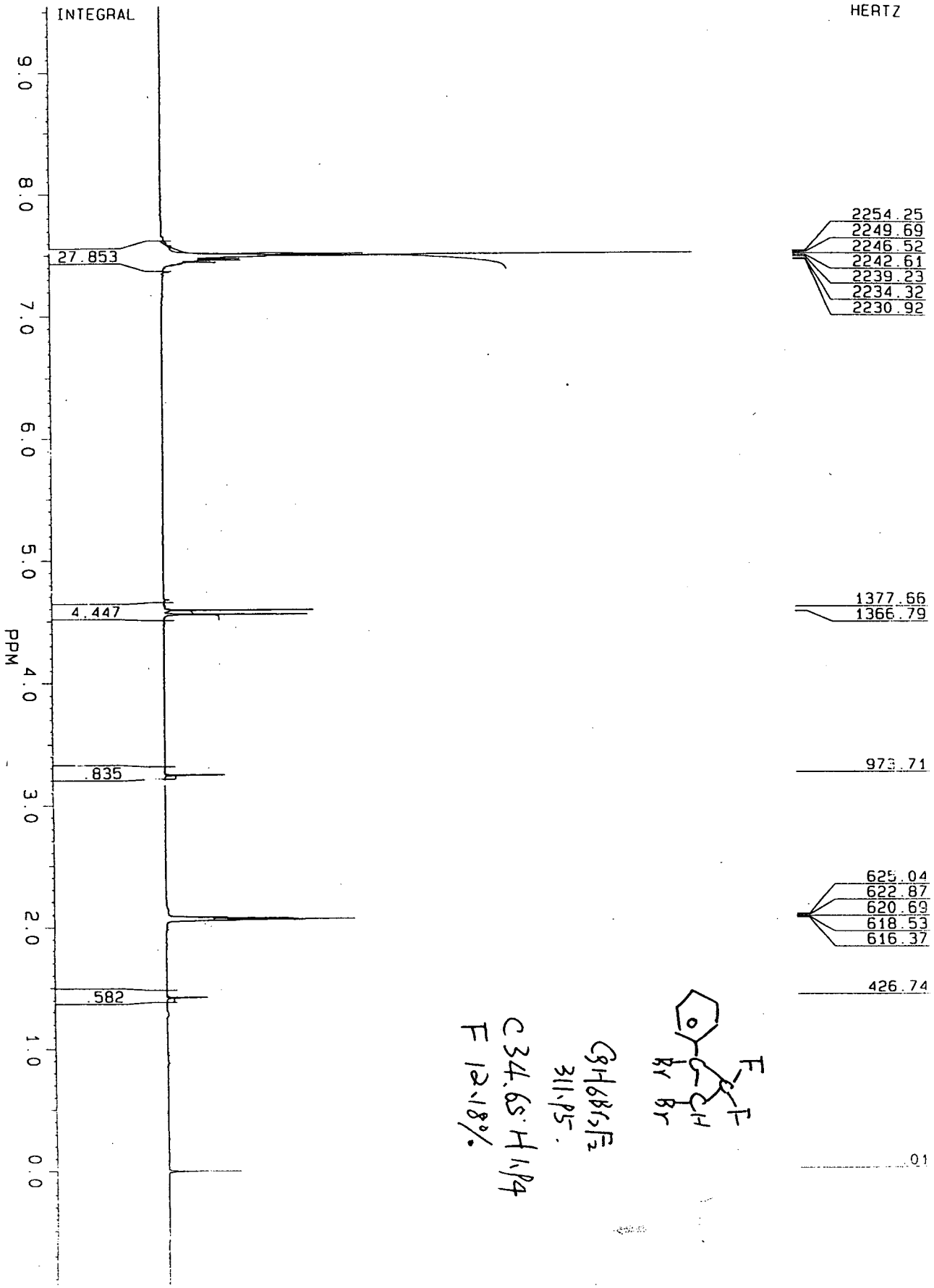


Figure 4. X-ray structure of 8a'.



Selected bond lengths (Å), bond angles (°) and torsion angles (°): I-C(7), 2.108(4); C(7)-C(8), 1.335(6); C(6)-C(7), 1.486(6); C(8)-C(9), 1.479(6); C(7)-C(8)-C(9), 124.5(4); C(8)-C(7)-I, 116.7(3); C(6)-C(7)-I, 114.4(3); C(6)-C(7)-C(8)-C(9), 0.9(8); C(5)-C(6)-C(7)-C(8), 74.4(6); I-C(7)-C(8)-C(9) , 178.6(4); C(1)-C(6)-C(7)-I, 75.2(5).

2

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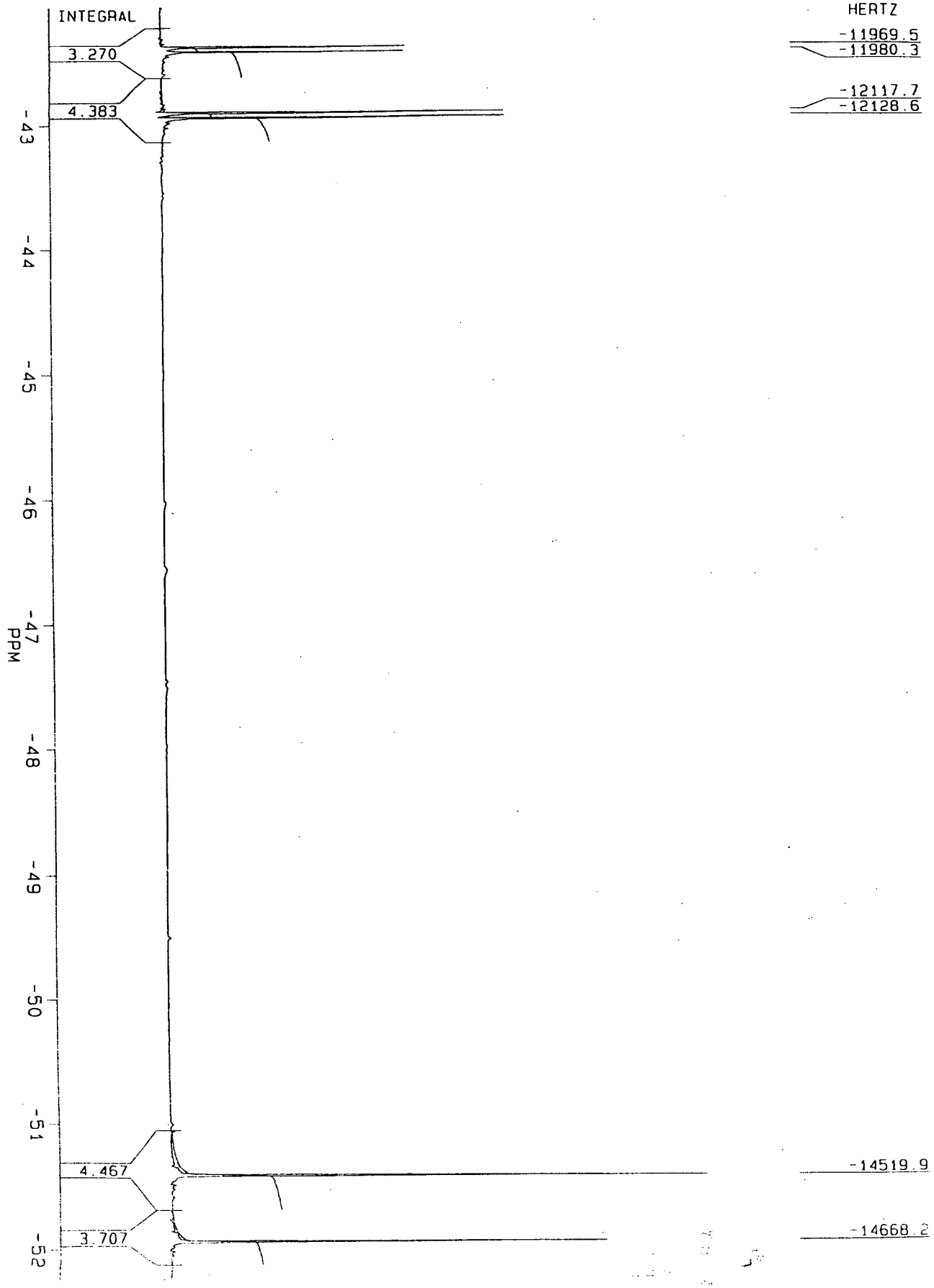
F 12.18%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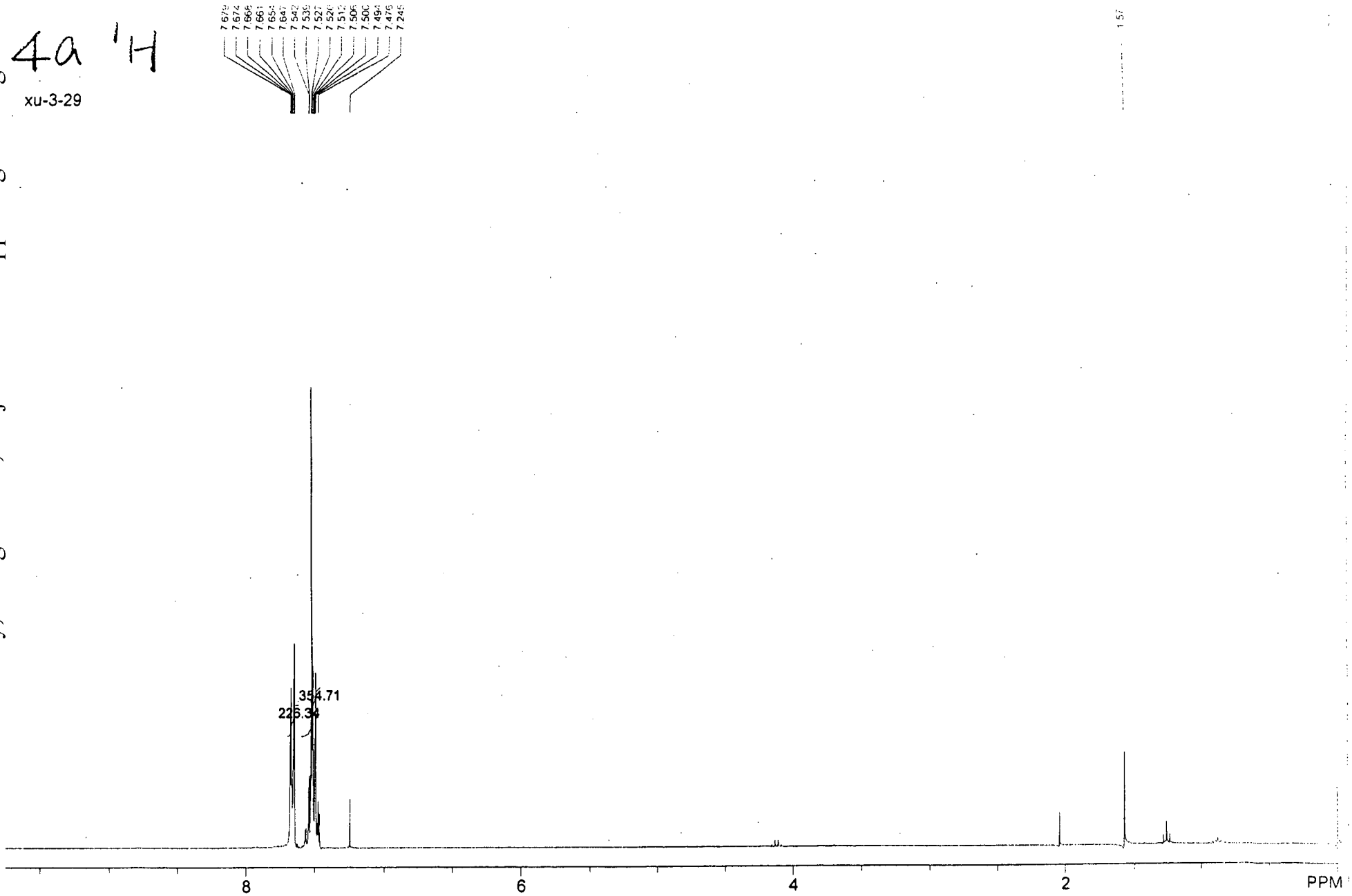
4a $^1$H

xu-3-29

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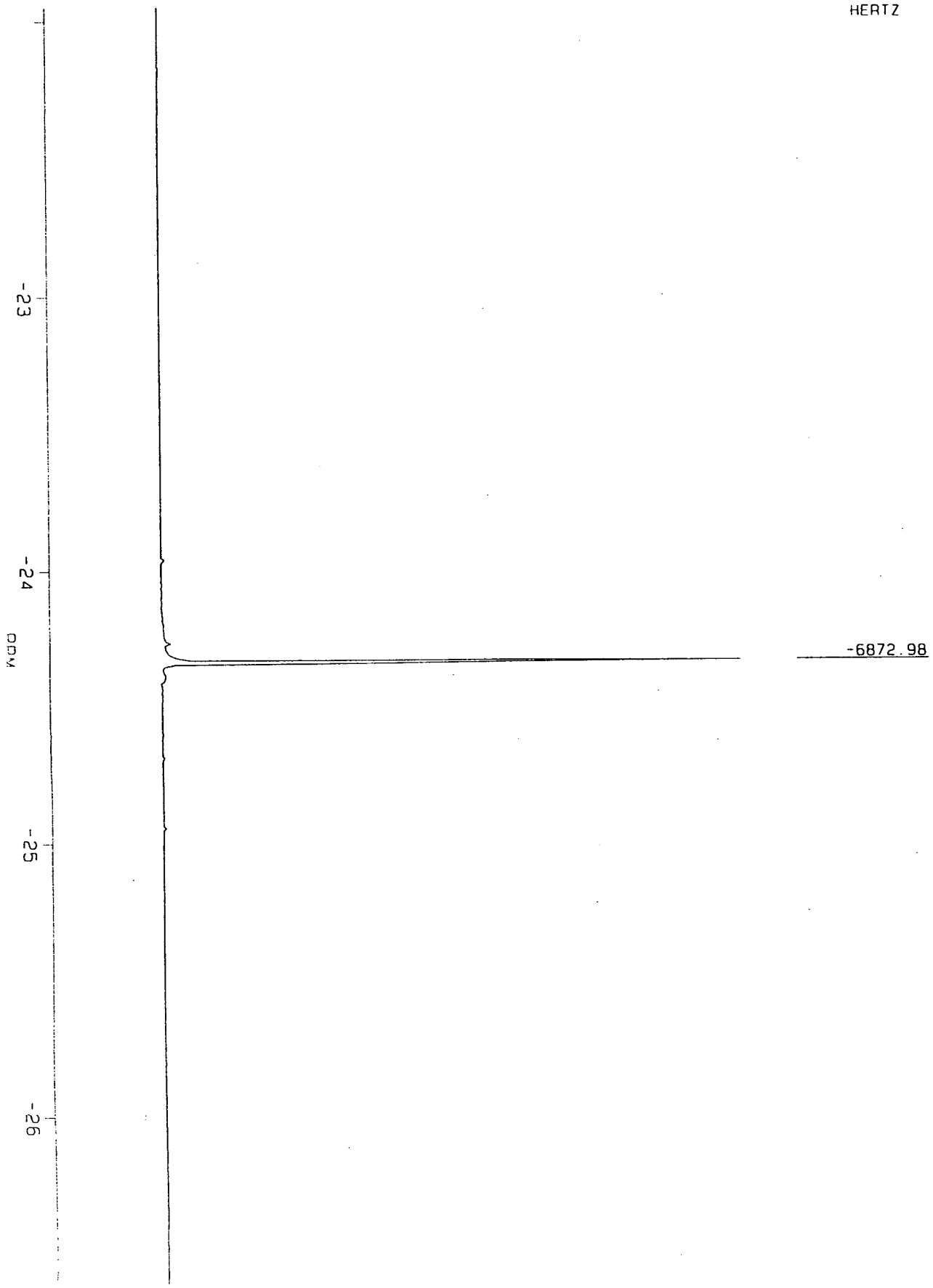
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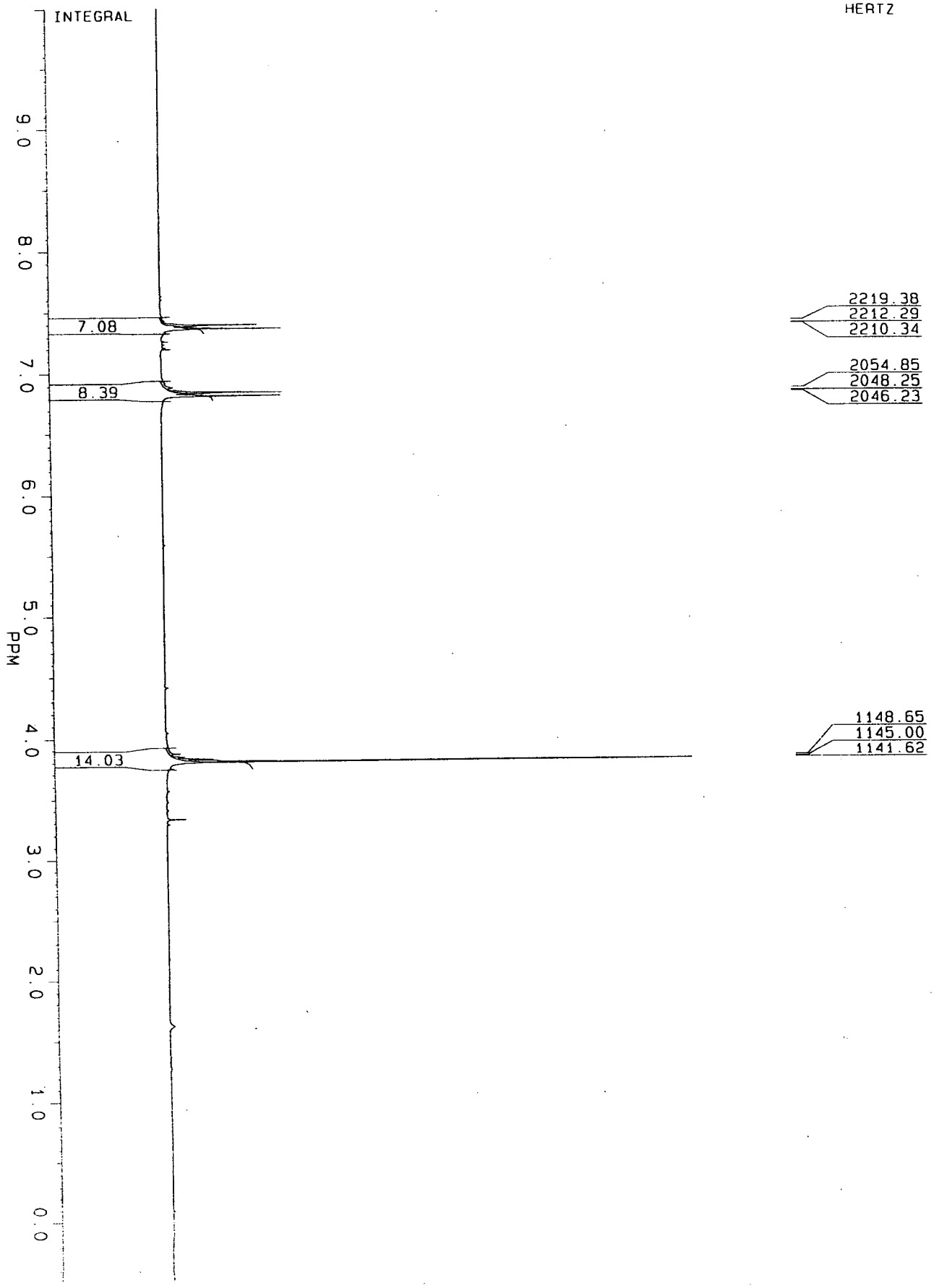
$^1$H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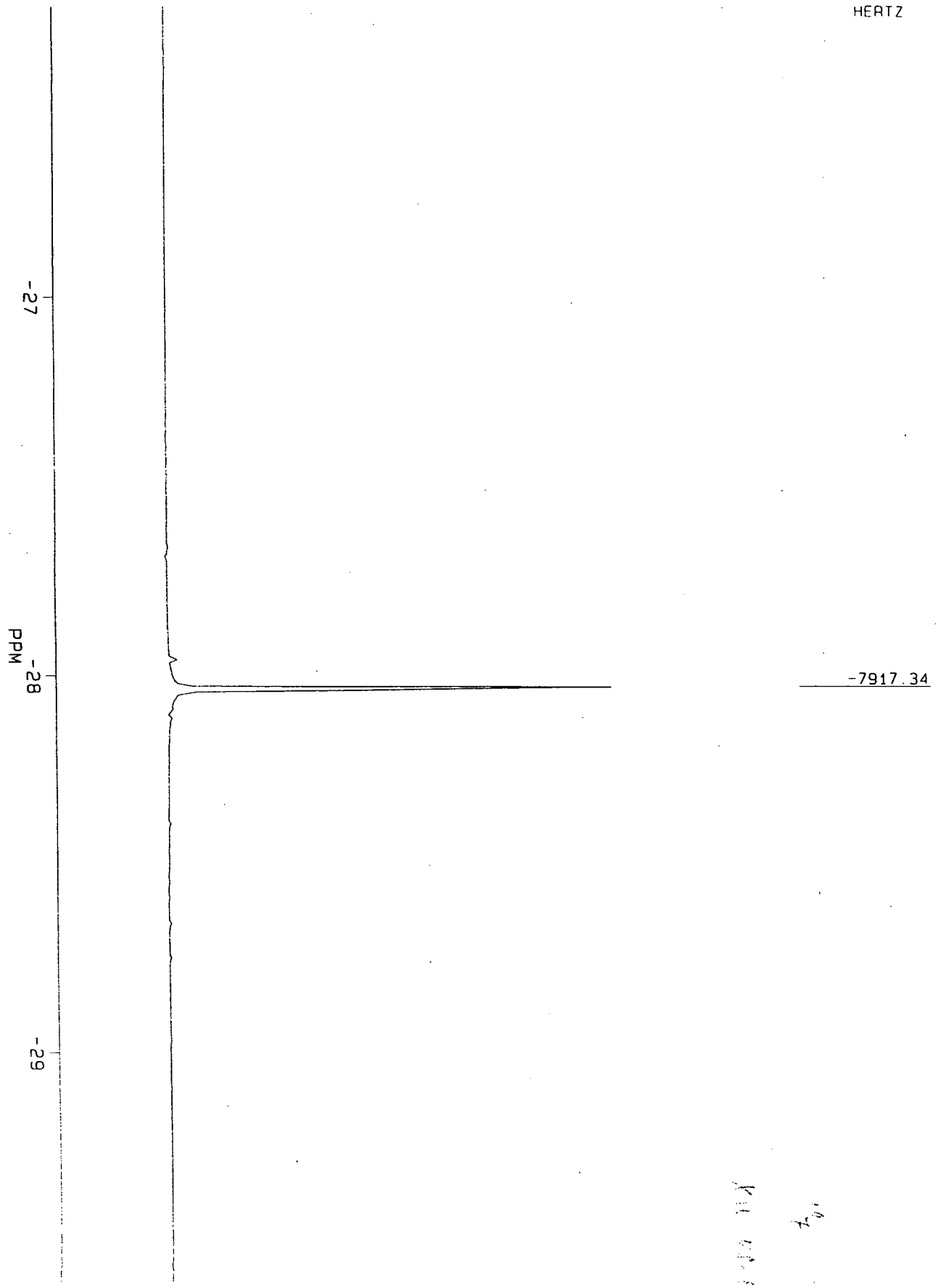
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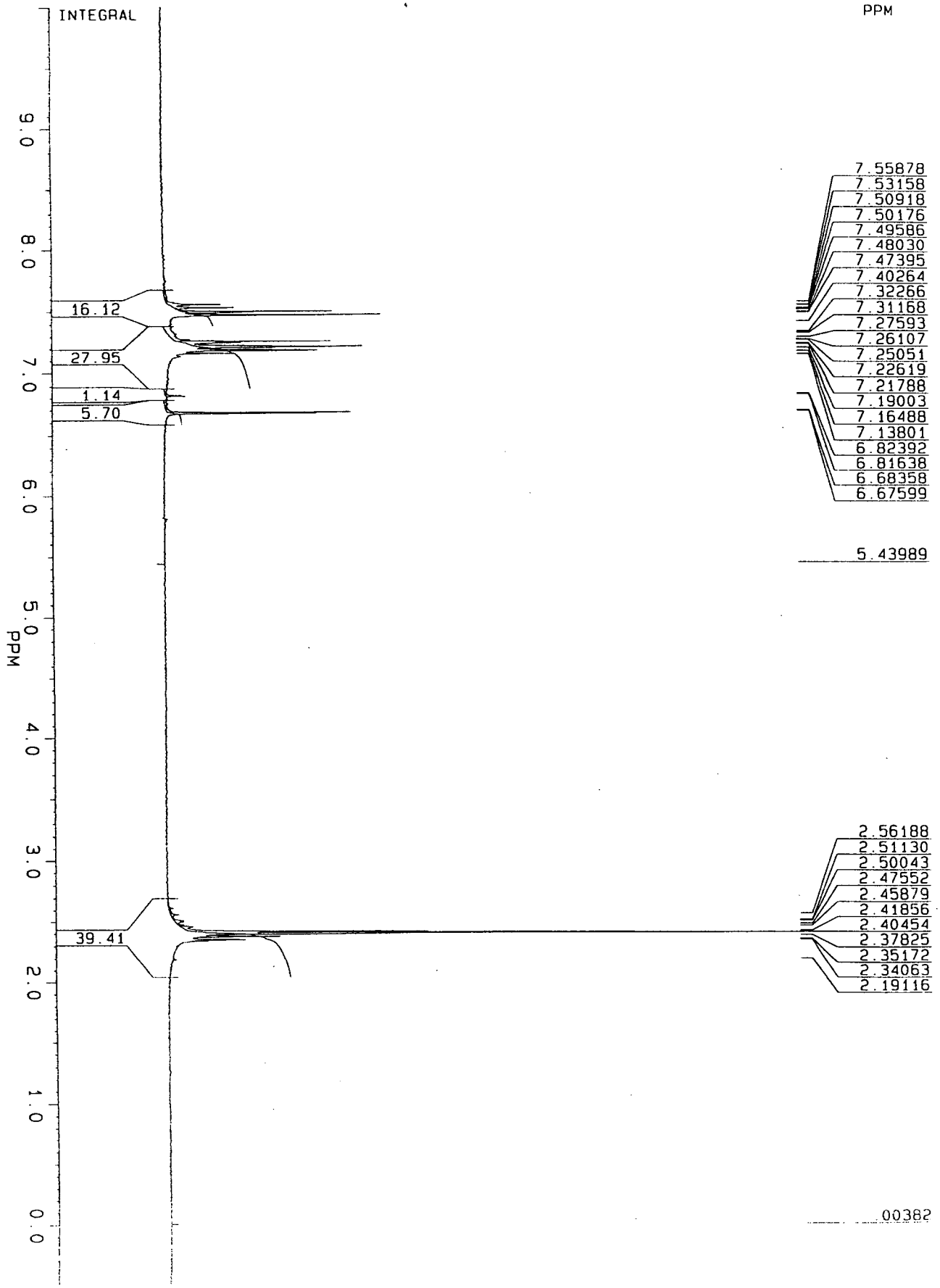
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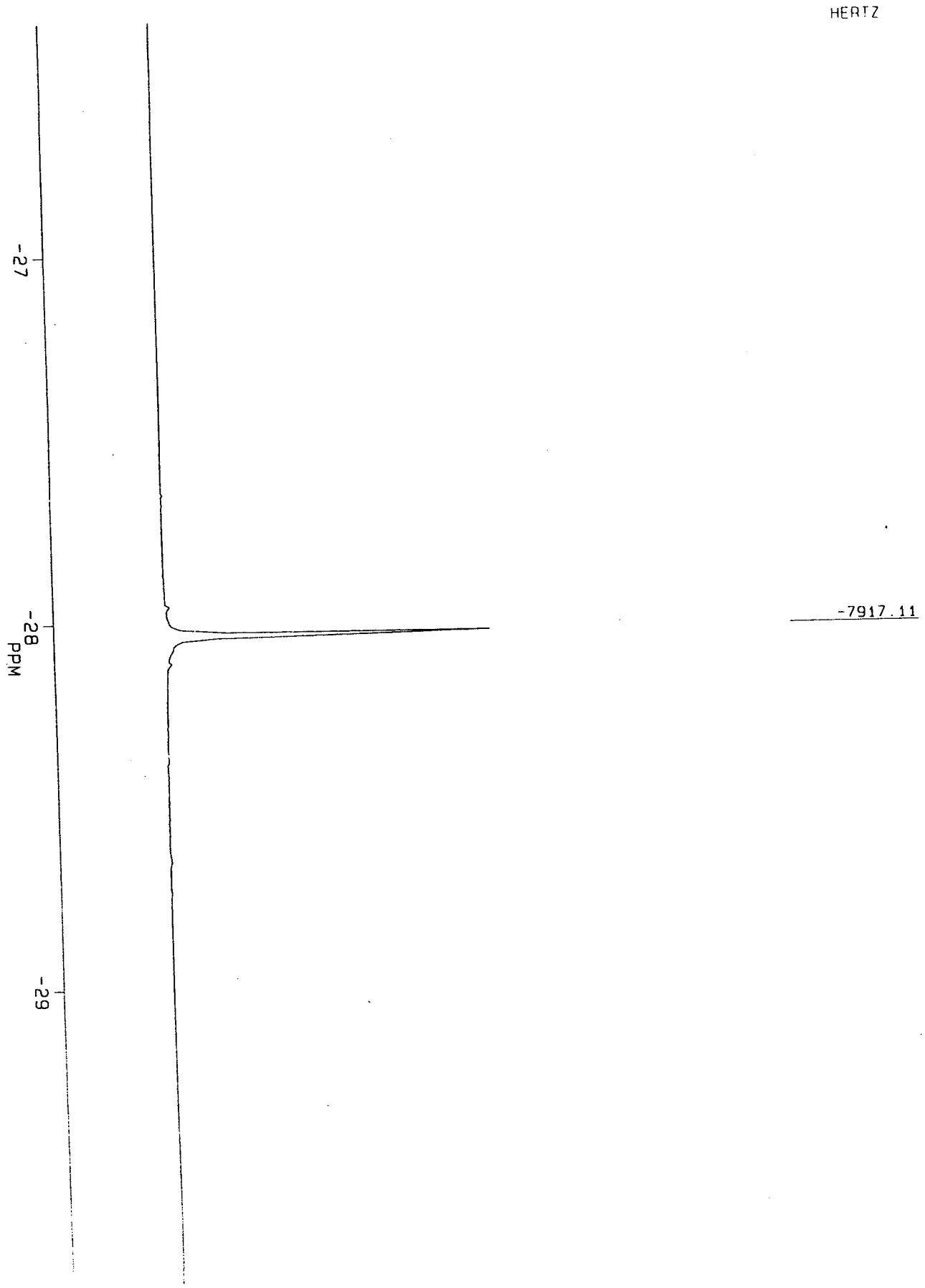
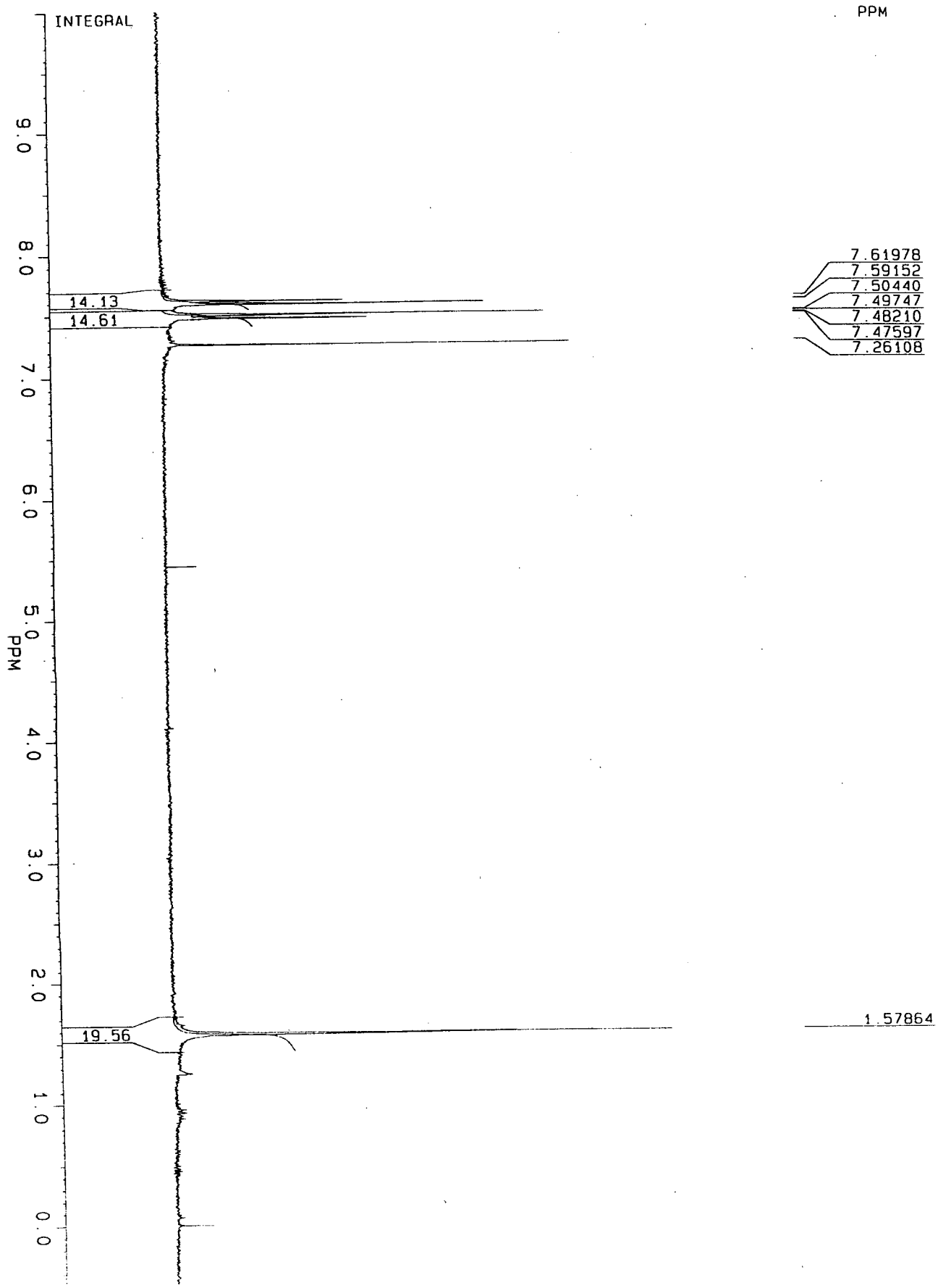
$^{19}$F

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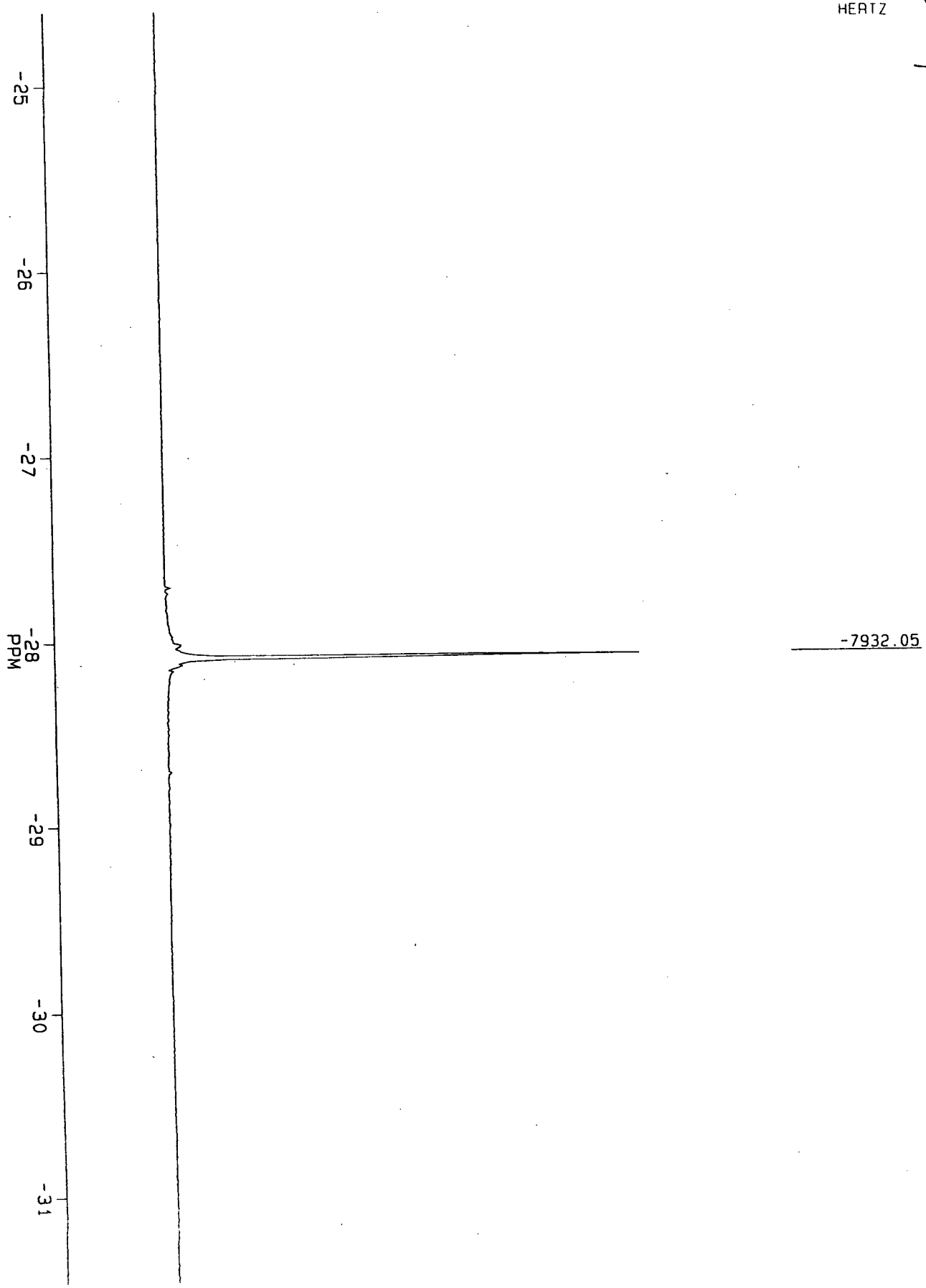
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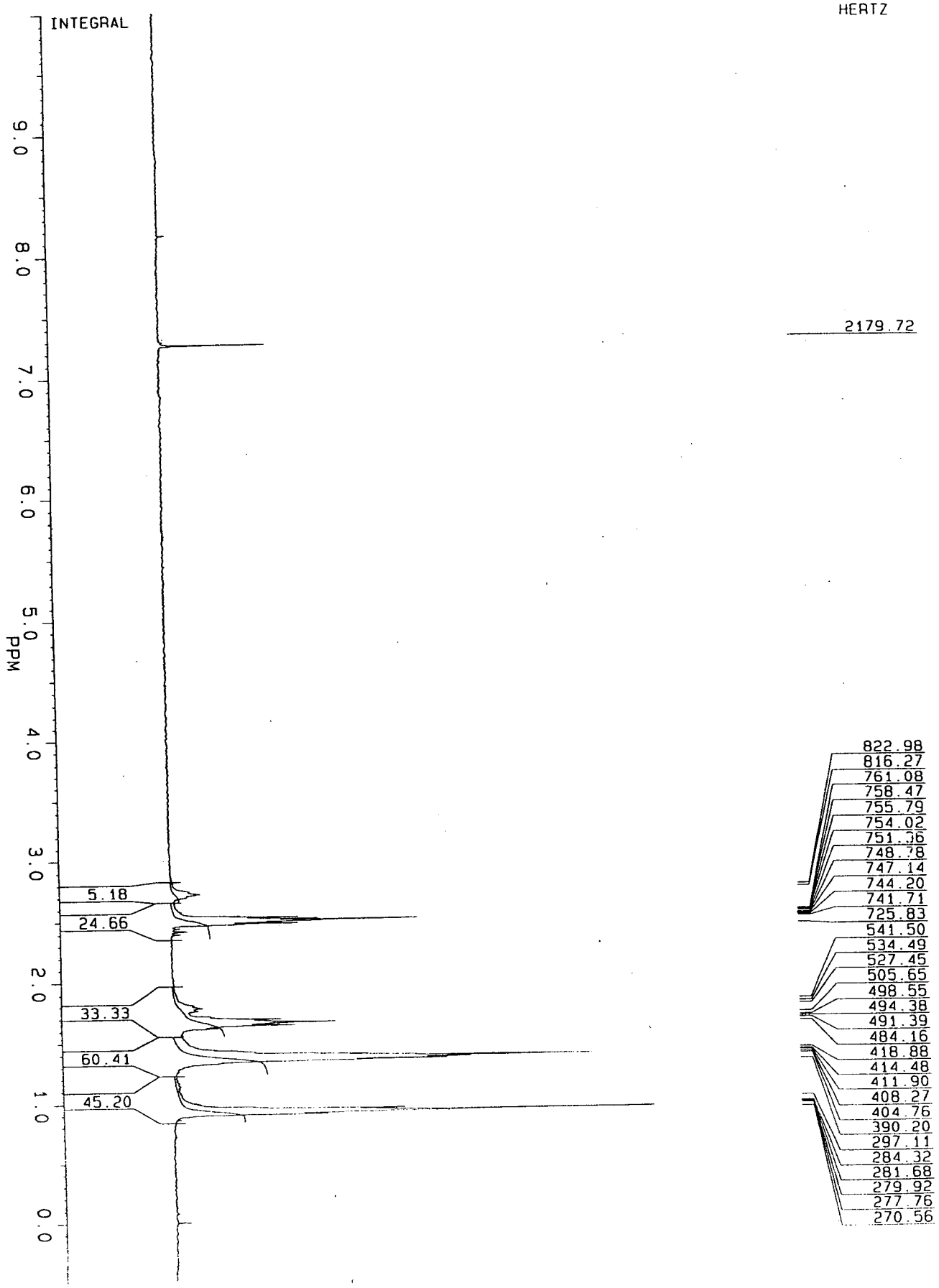
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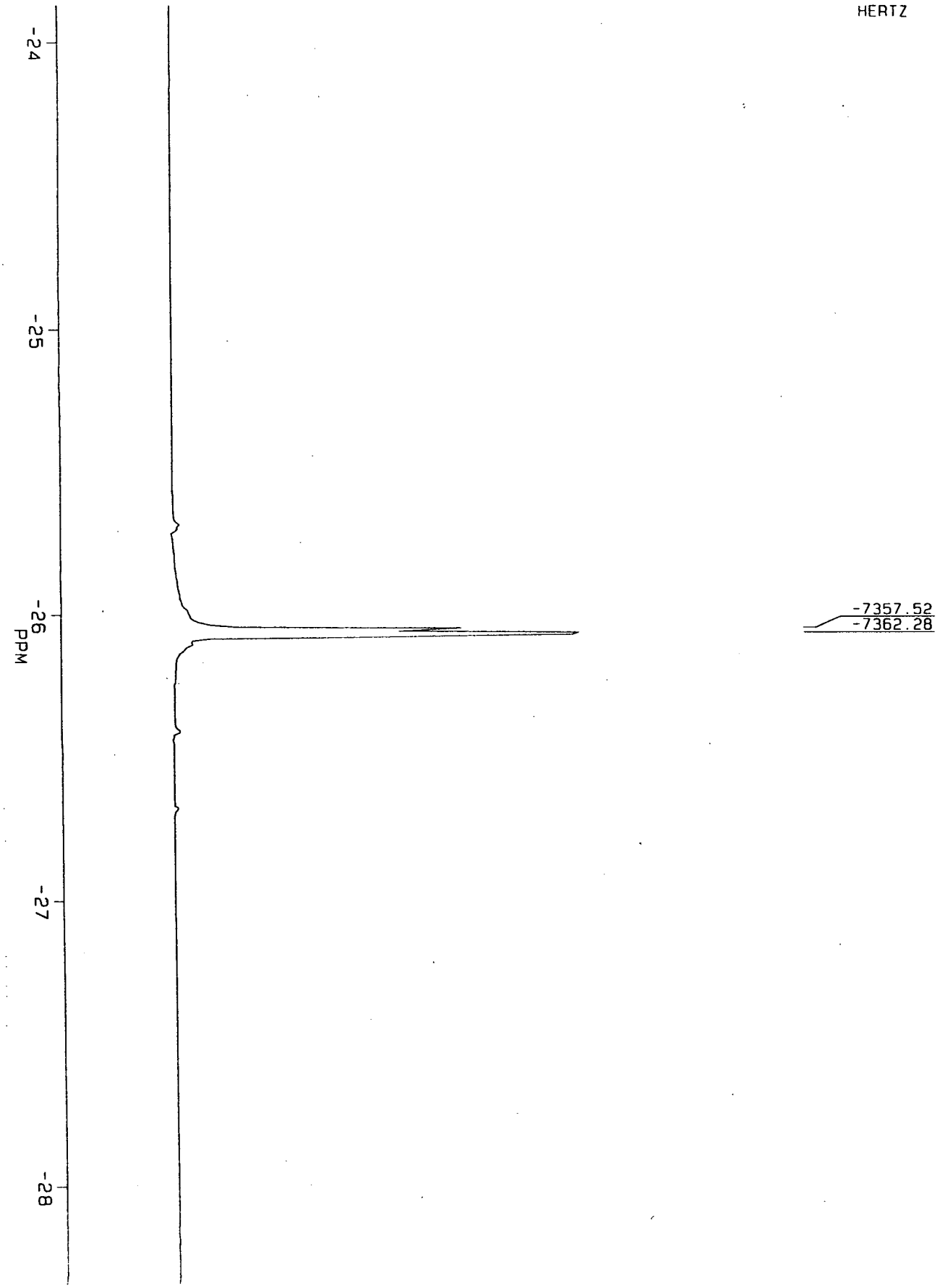
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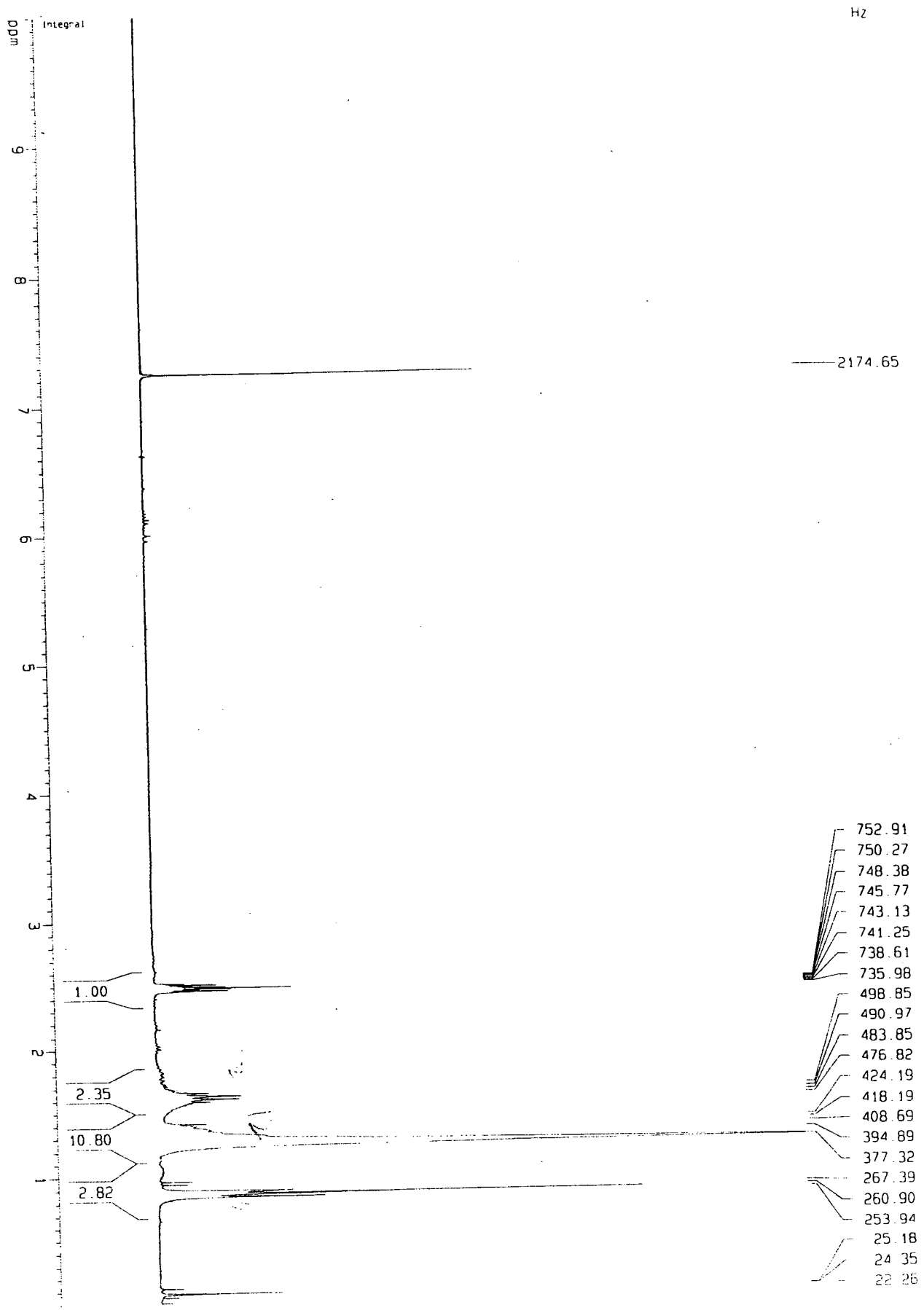
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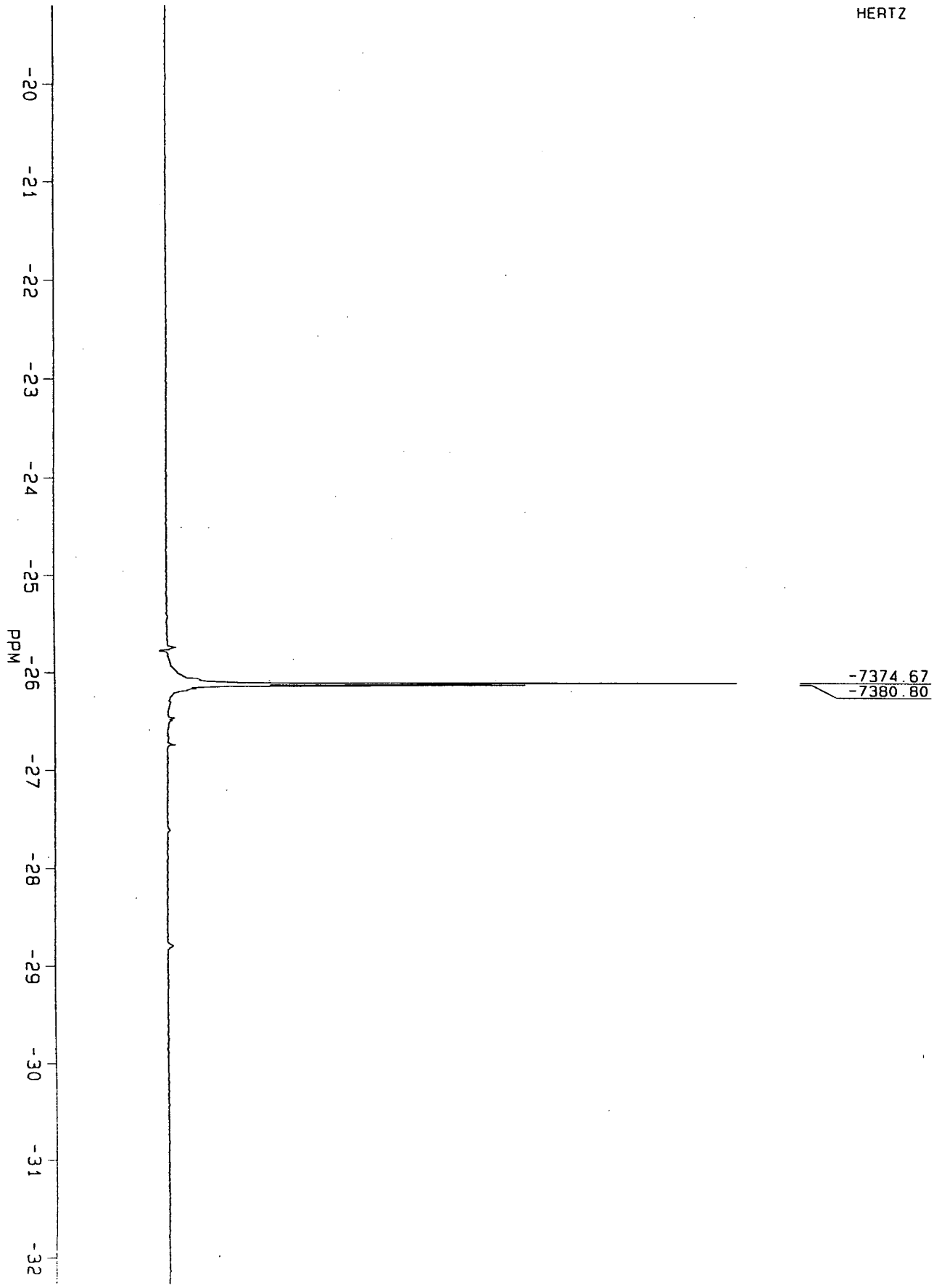
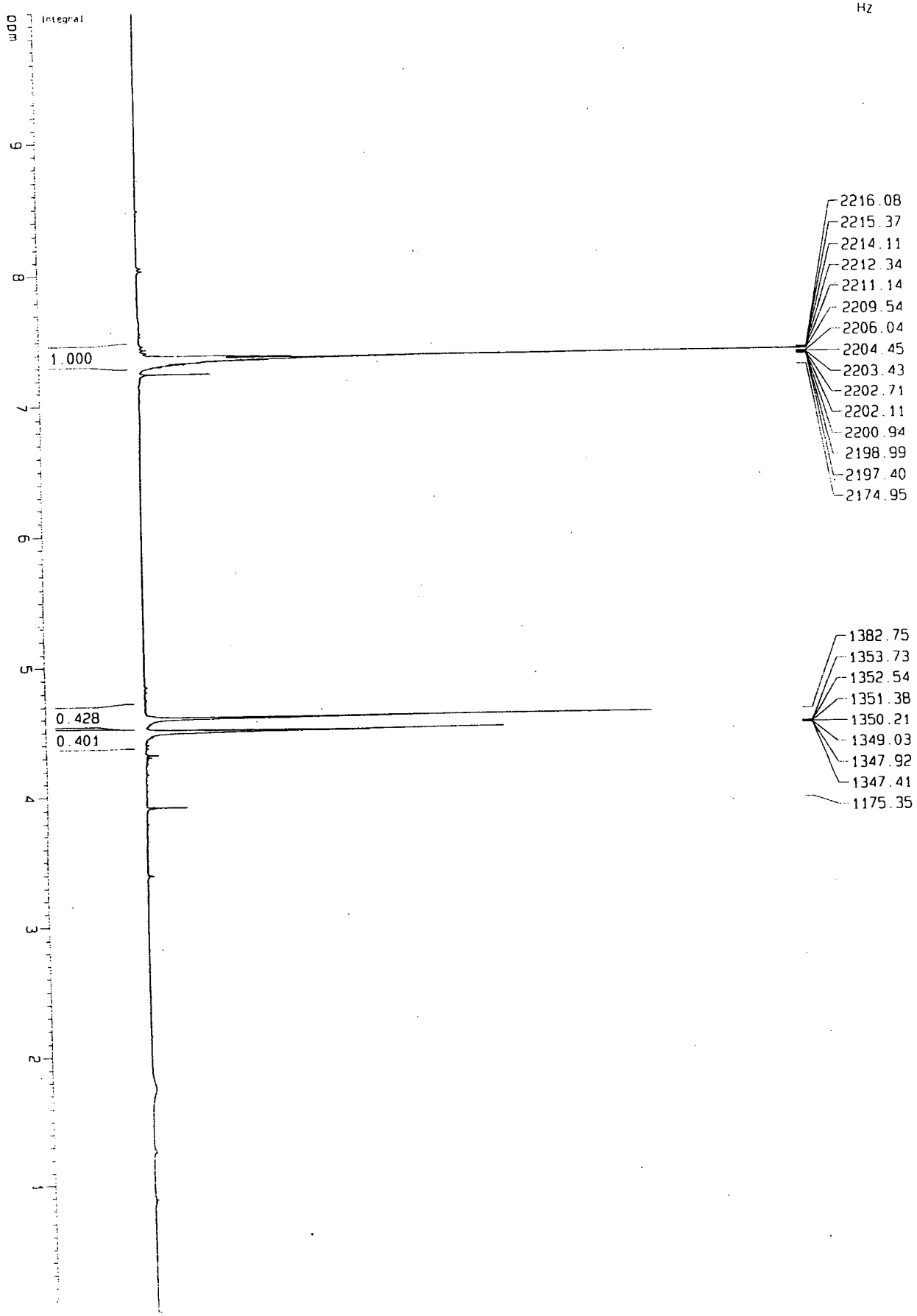
4b

$^{19}$F

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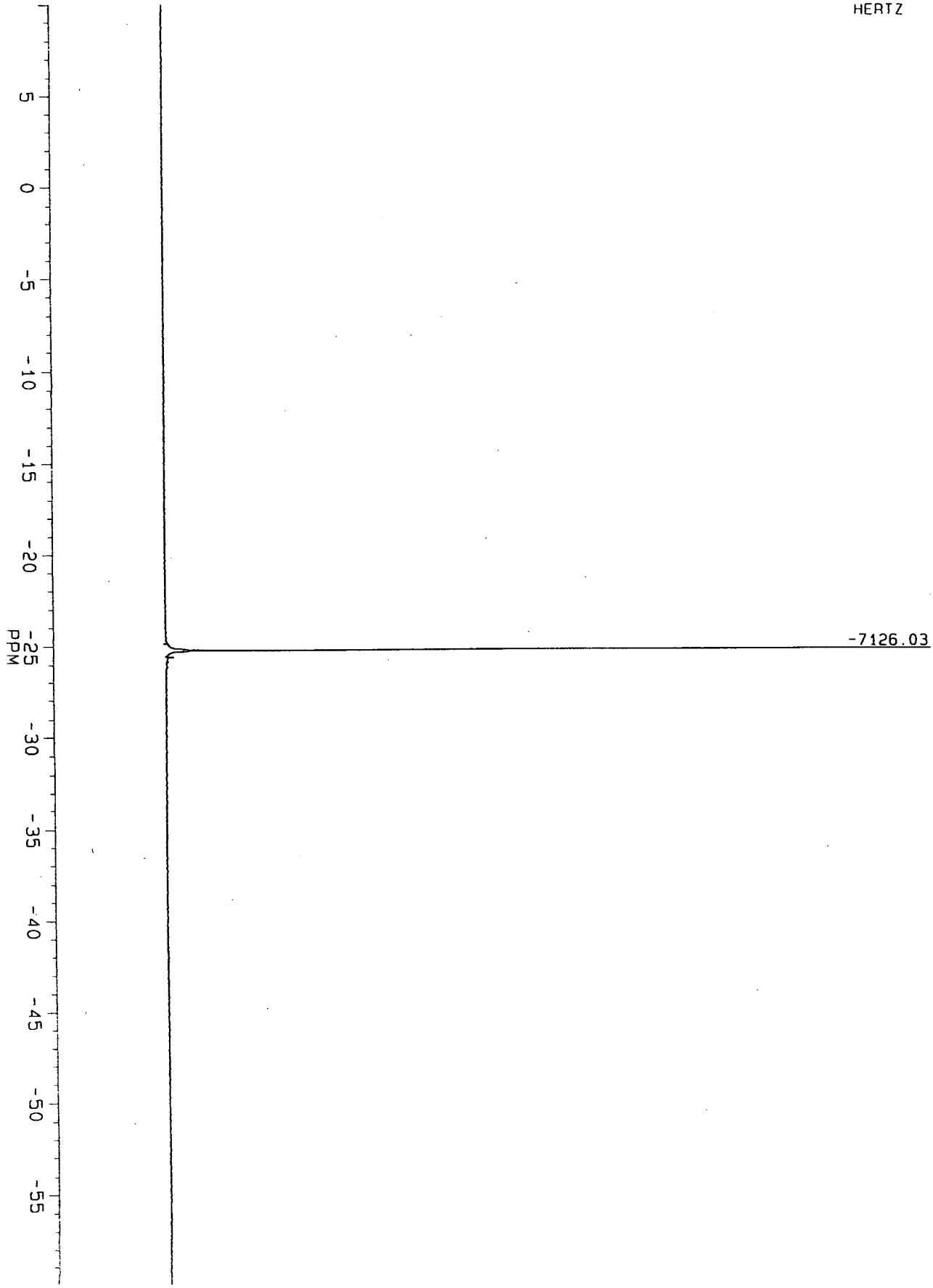
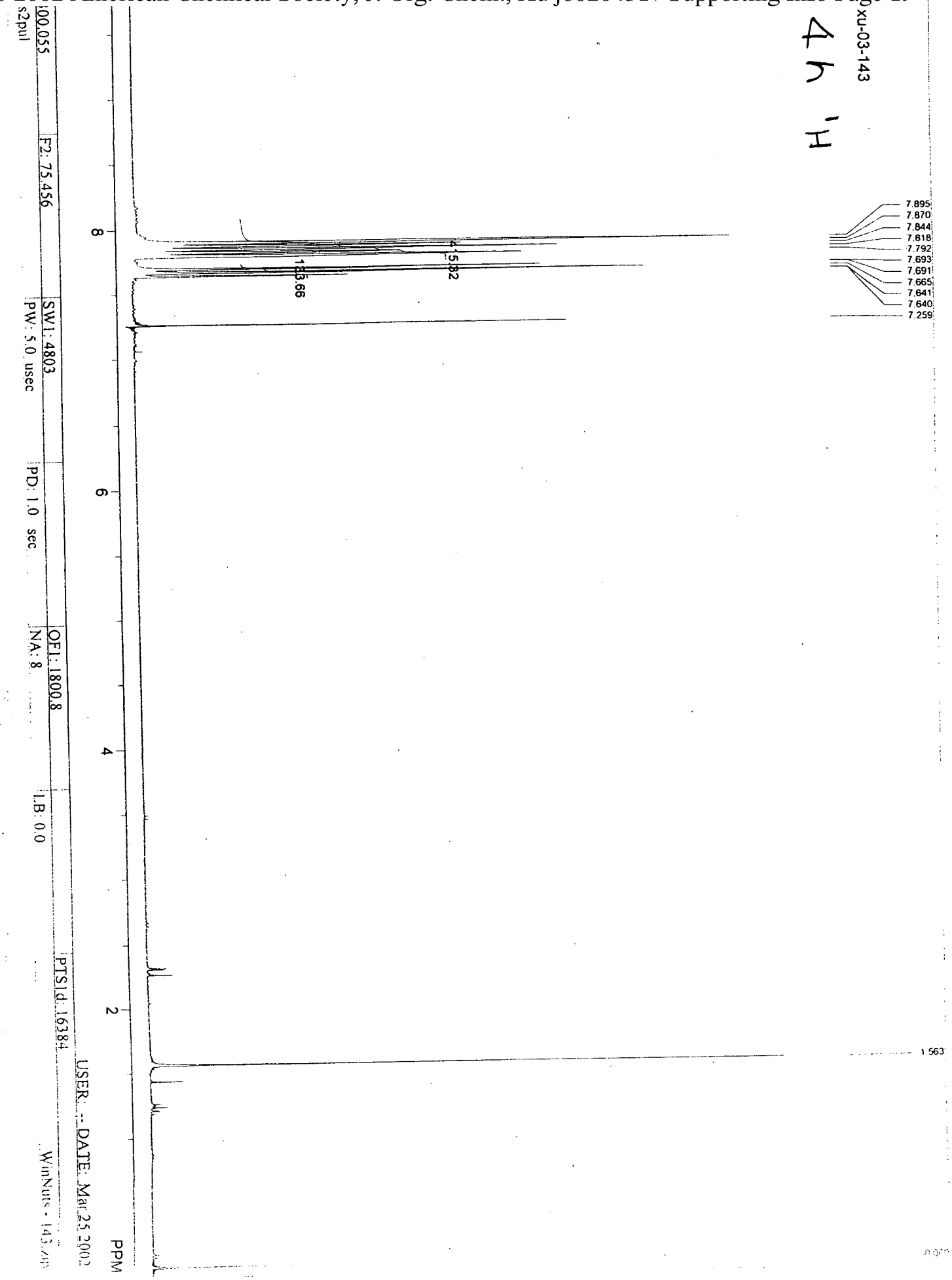
$^{19}F$

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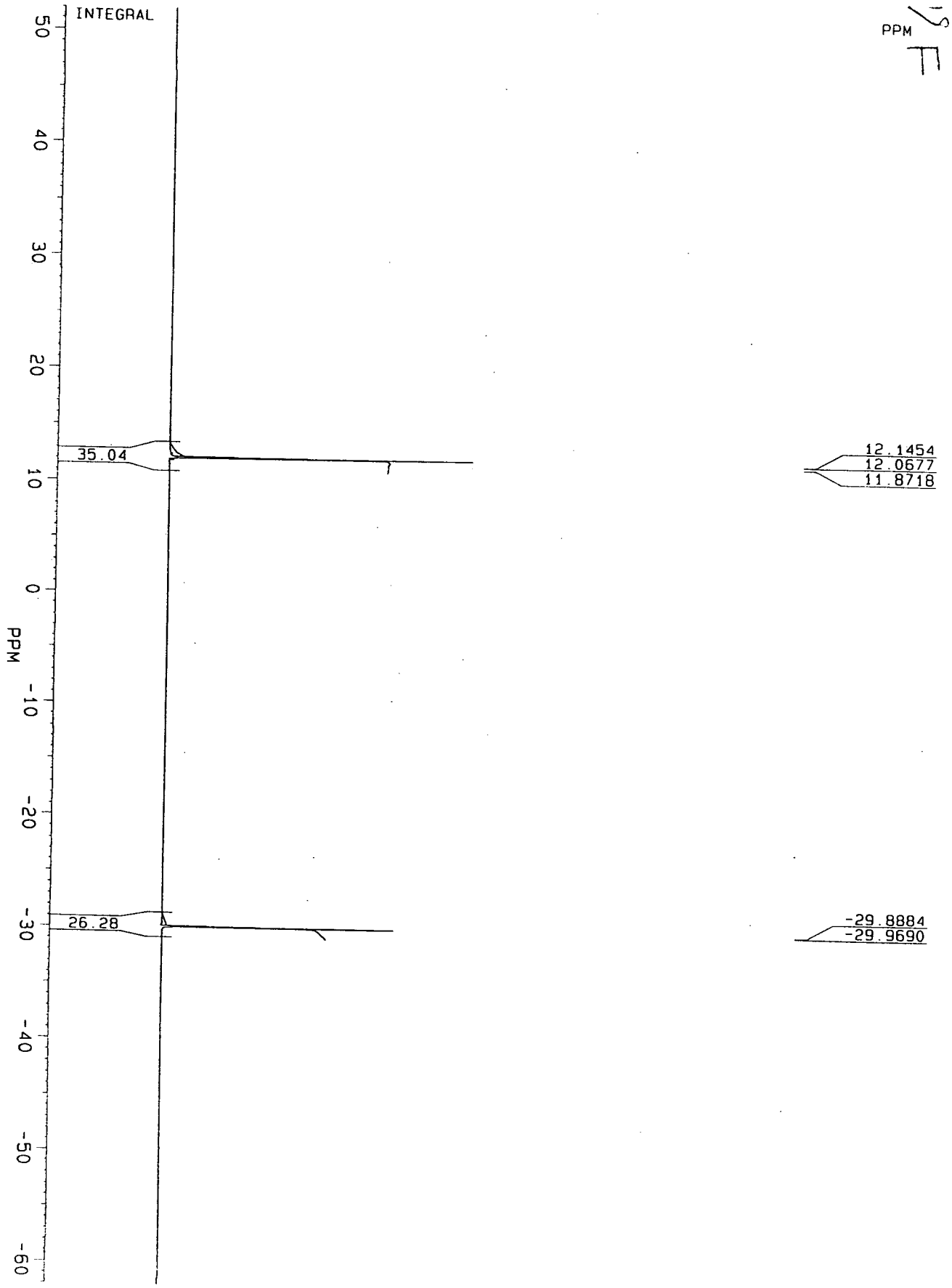
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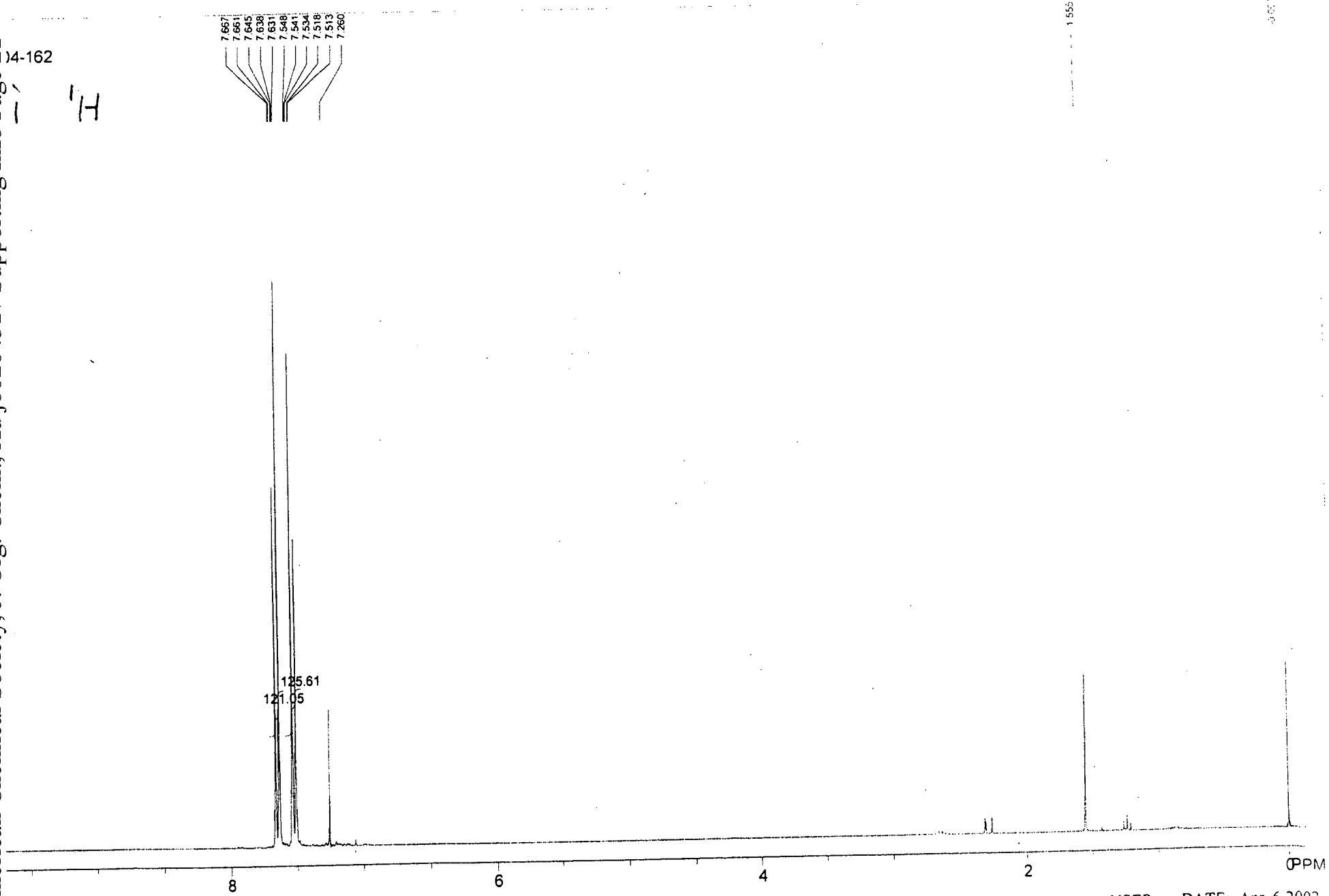


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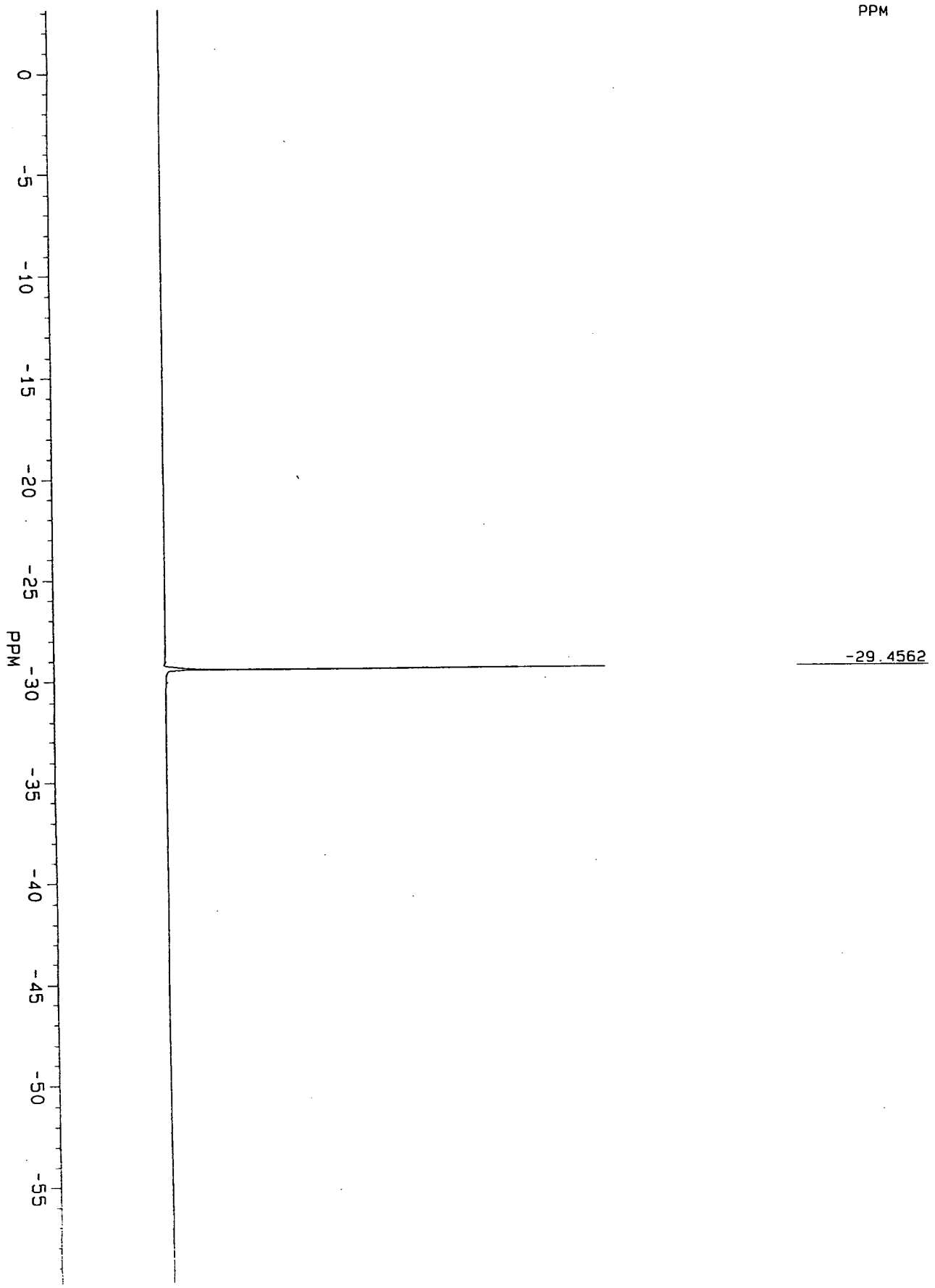
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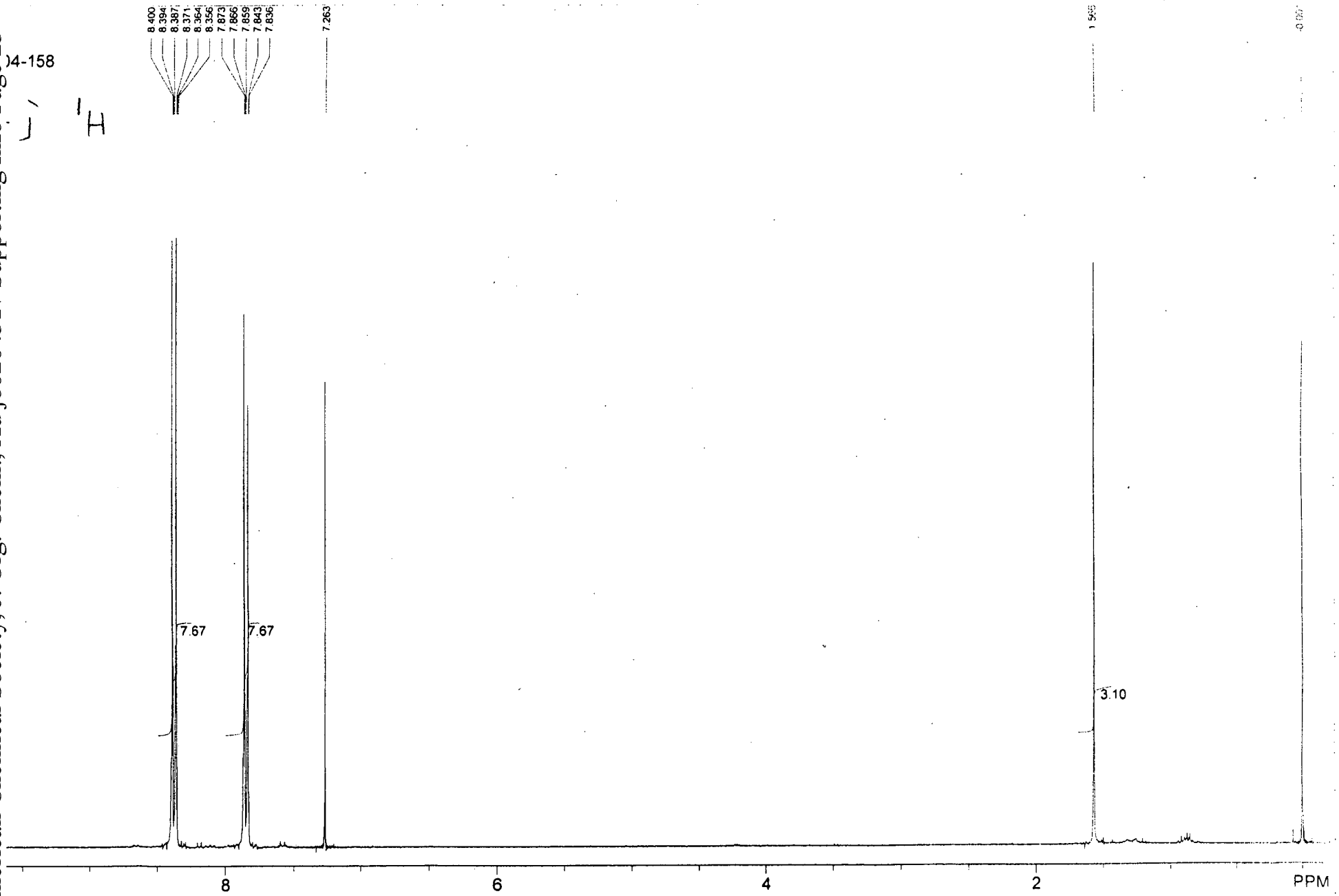
)4-158

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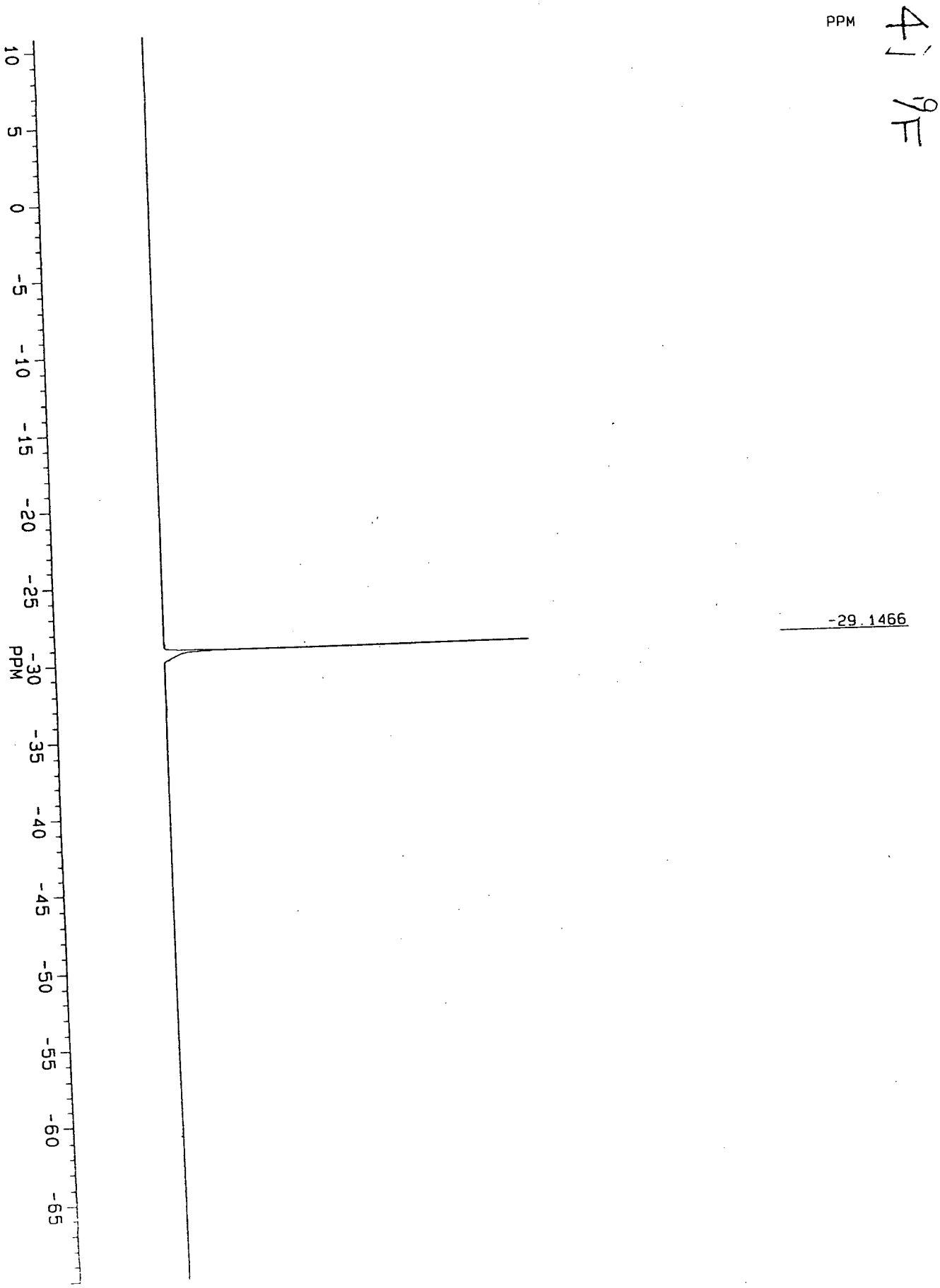
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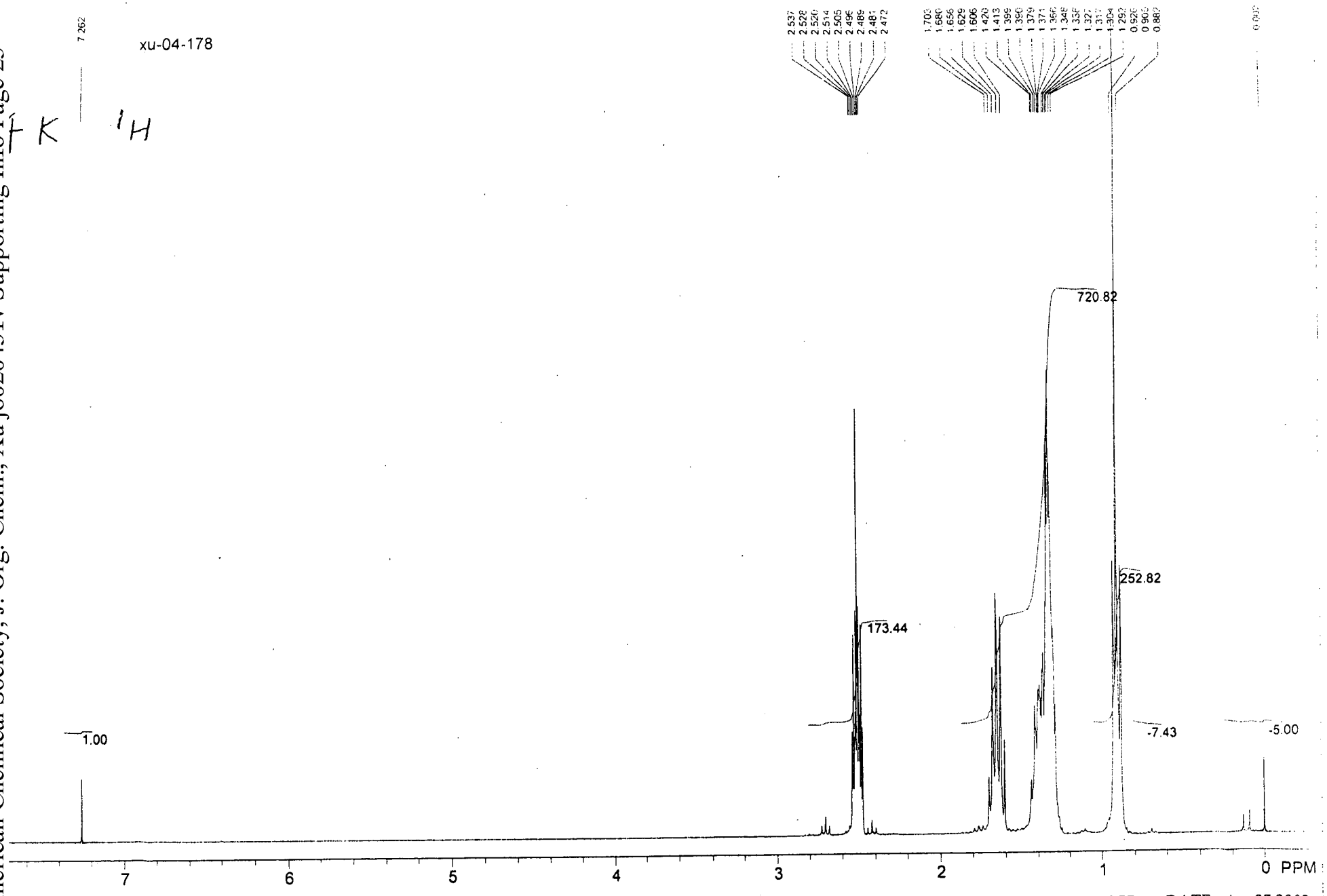
xu-04-178

FK $^1$H

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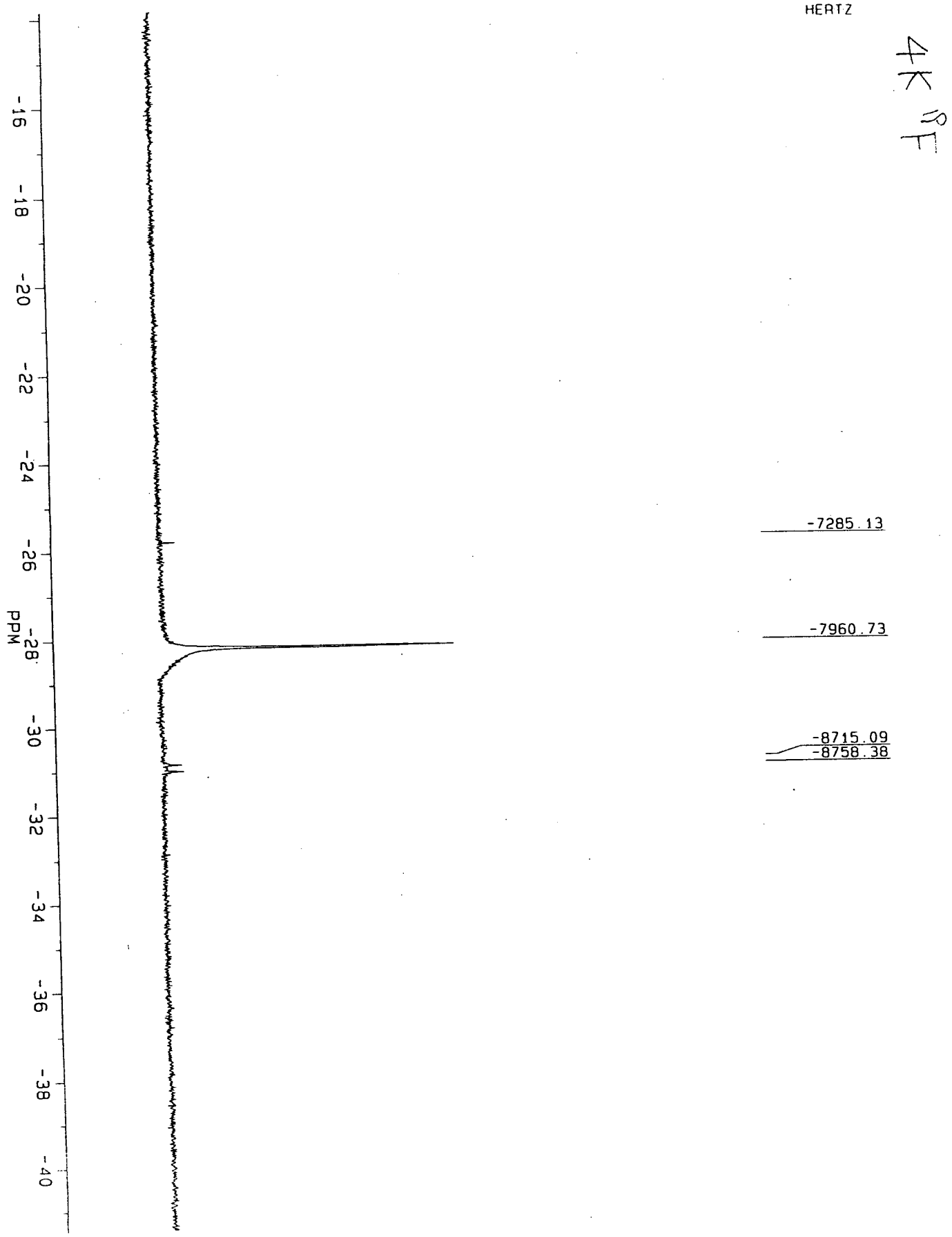
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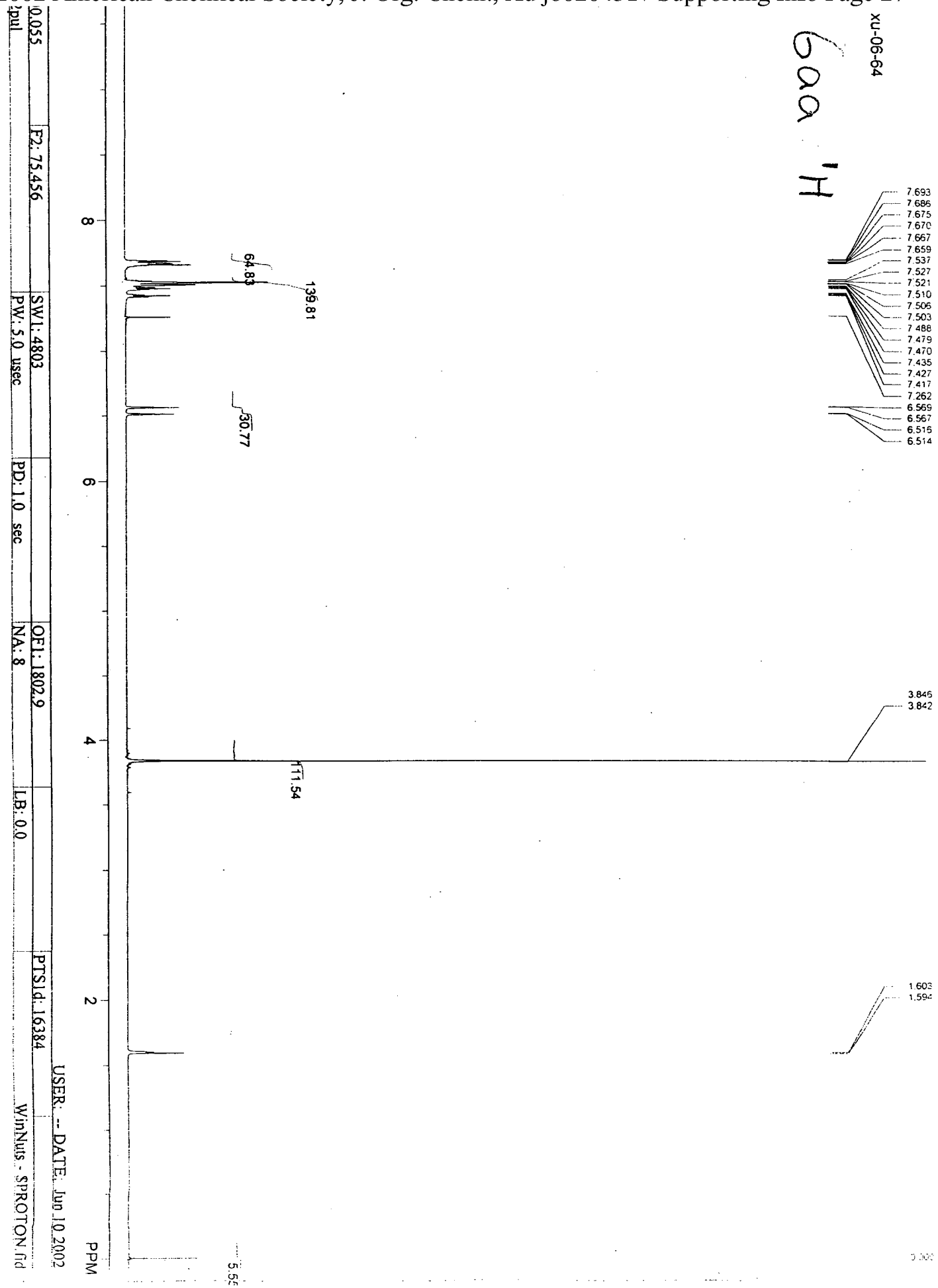
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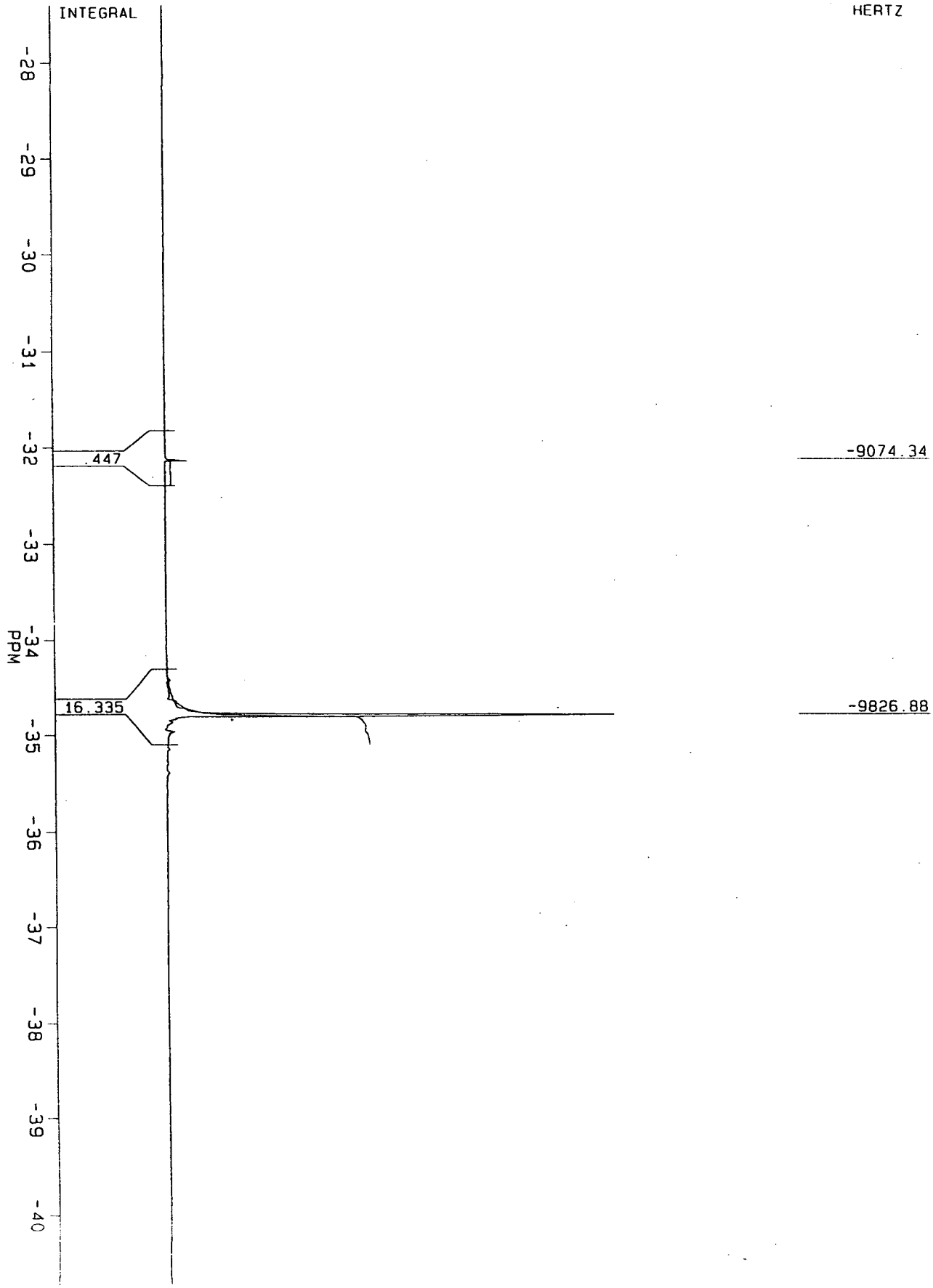
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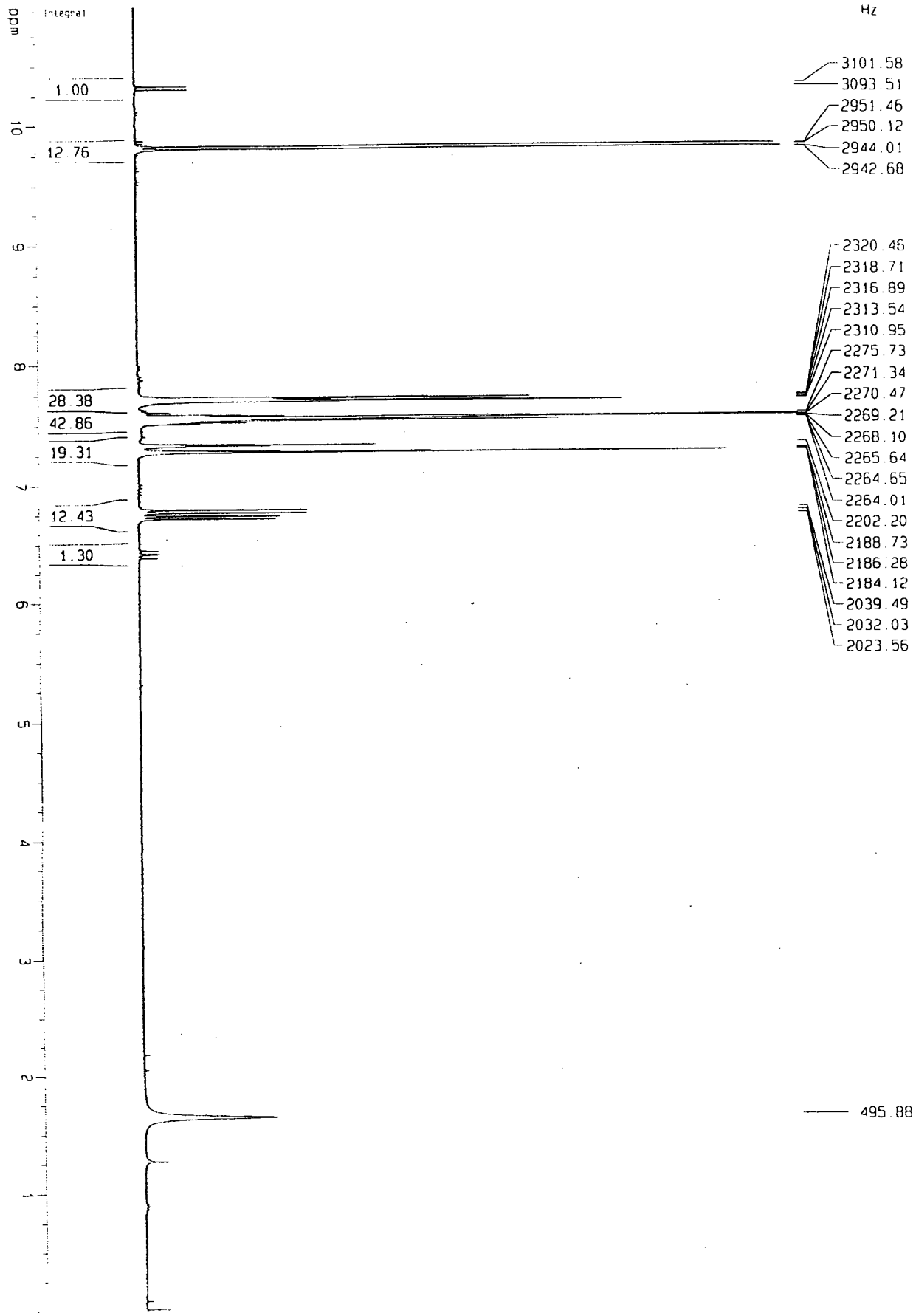
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2944.01
2942.68
2320.46
2318.71
2316.89
2313.54
2310.95
2275.73
2271.34
2270.47
2269.21
2268.10
2265.64
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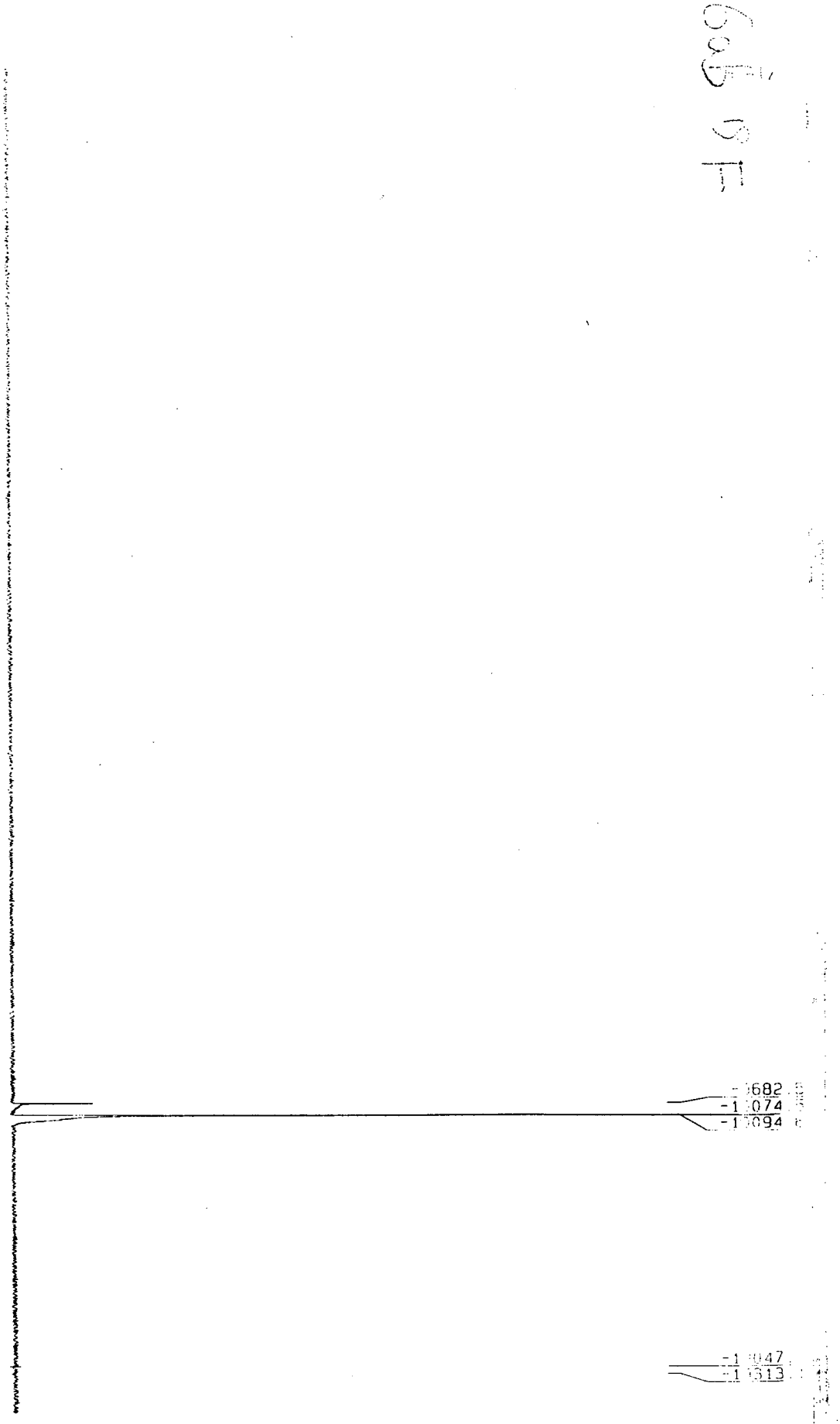
2184.12
2039.49
2032.03
2023.56
495.88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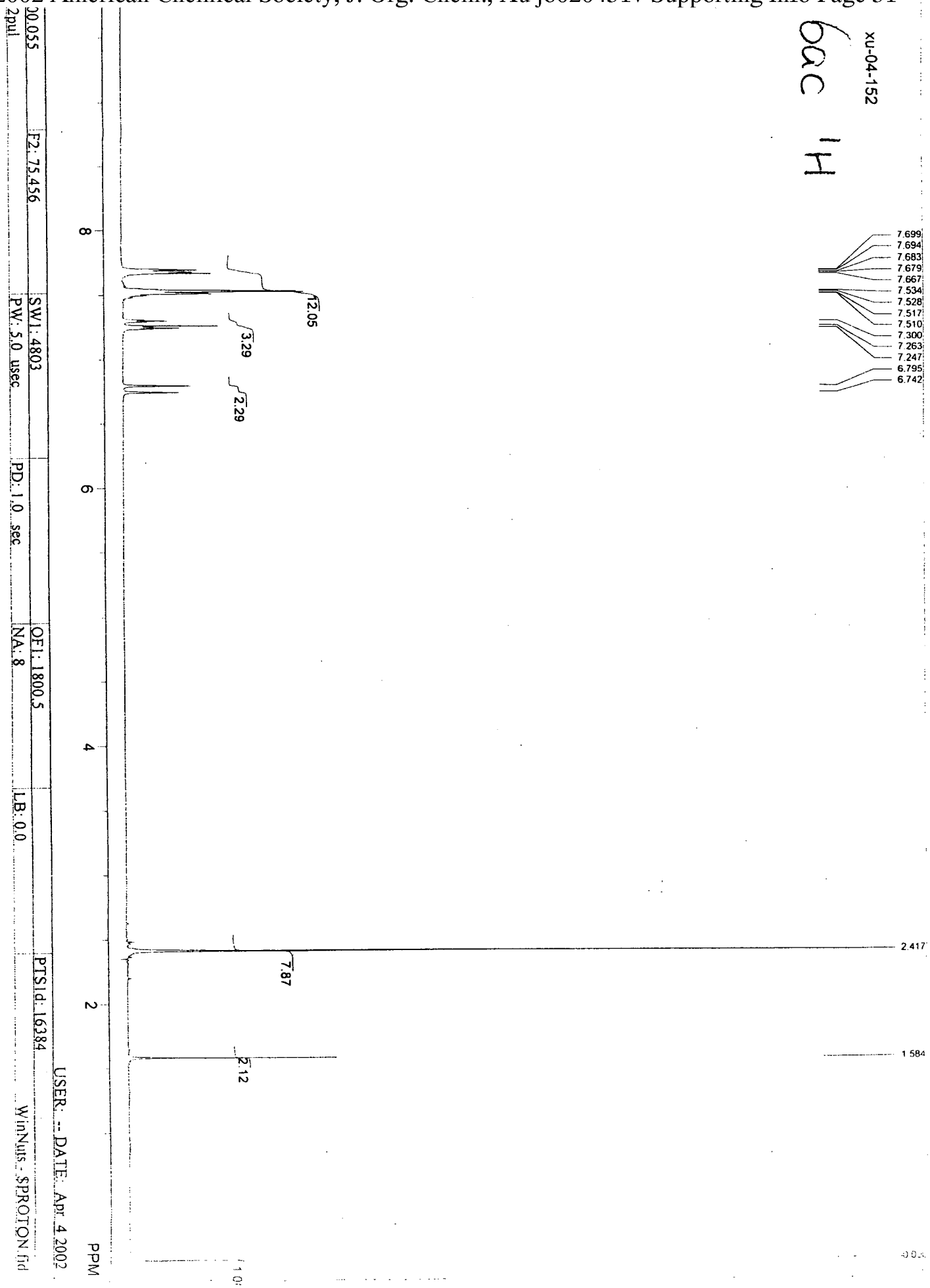
xu-04-152
6aC 1H
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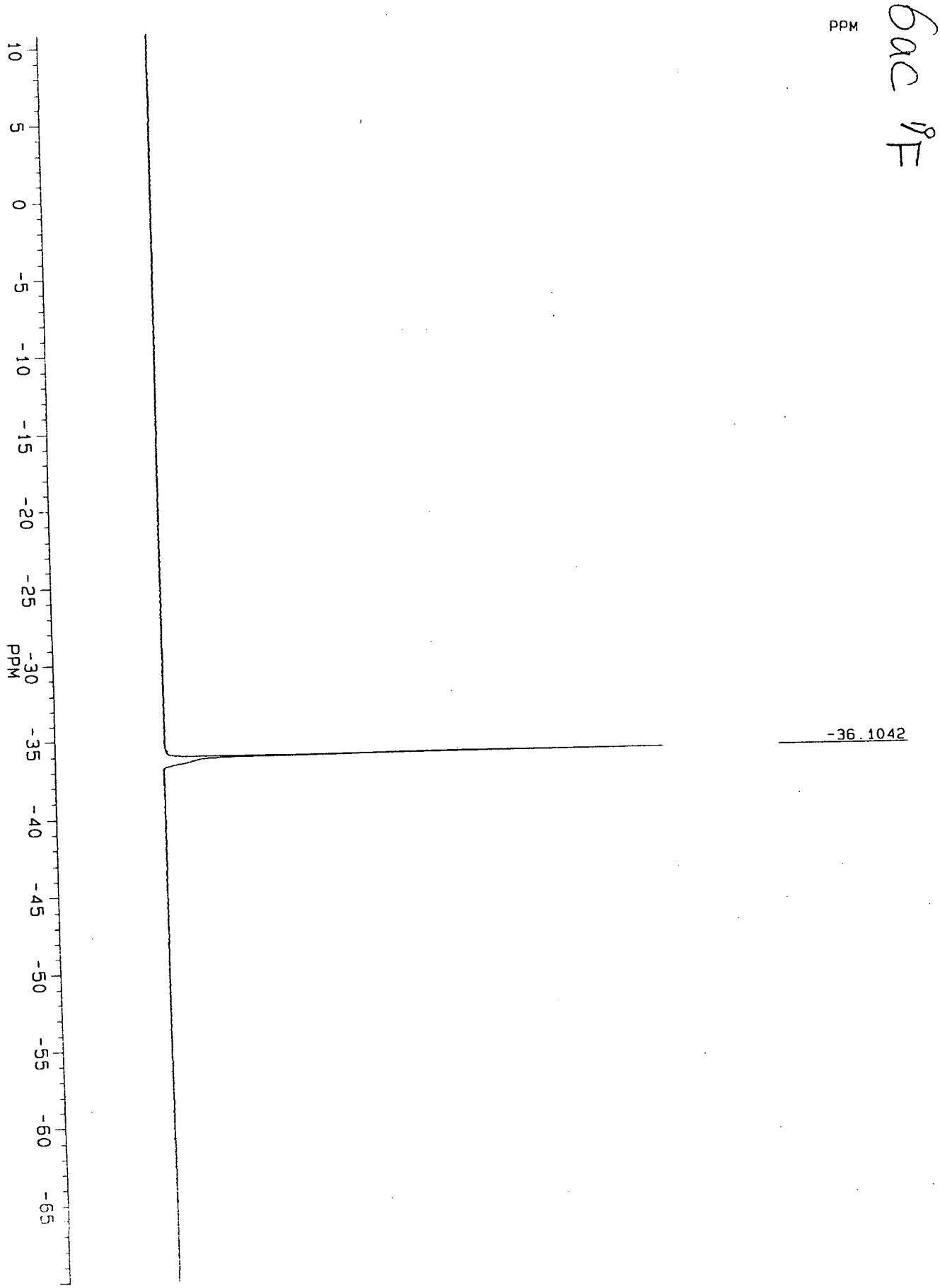
7.694
7.683
7.679
7.667
7.534
7.528
7.517
7.510
7.300
7.263
7.247
6.795
6.742
2.417
1.584
12.05
3.29
2.29
7.87
2.12
PPM
10
8
6
4
2
0
F1: 300.055
F2: 75.456
SW1: 4803
PW: 5.0 usec
PD: 1.0 sec
OF1: 1800.5
NA: 8
LB: 0.0
PTS1d: 16384
2pul
USER: -- DATE: Apr 4 2002
WinNuts: $PROTON.fid


6ac 19F
PPM
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10
5
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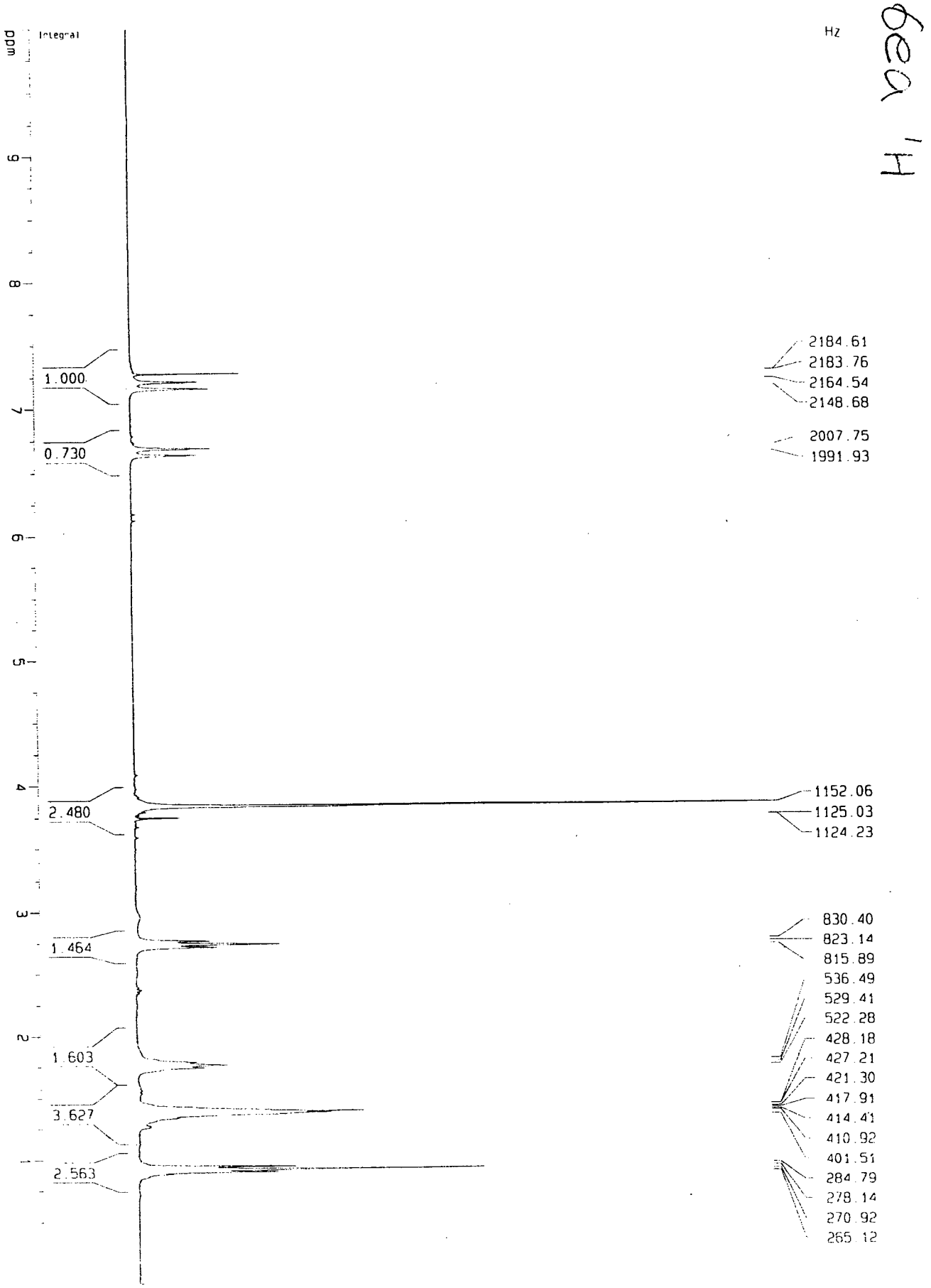
-25
-30
PPM
-35
-40
-45
-50
-55
-60
-65


ppm
Integral
Hz
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2007.75
1991.93
1152.06
1125.03
1124.23
830.40
823.14
815.89
536.49
529.41
522.28
428.18
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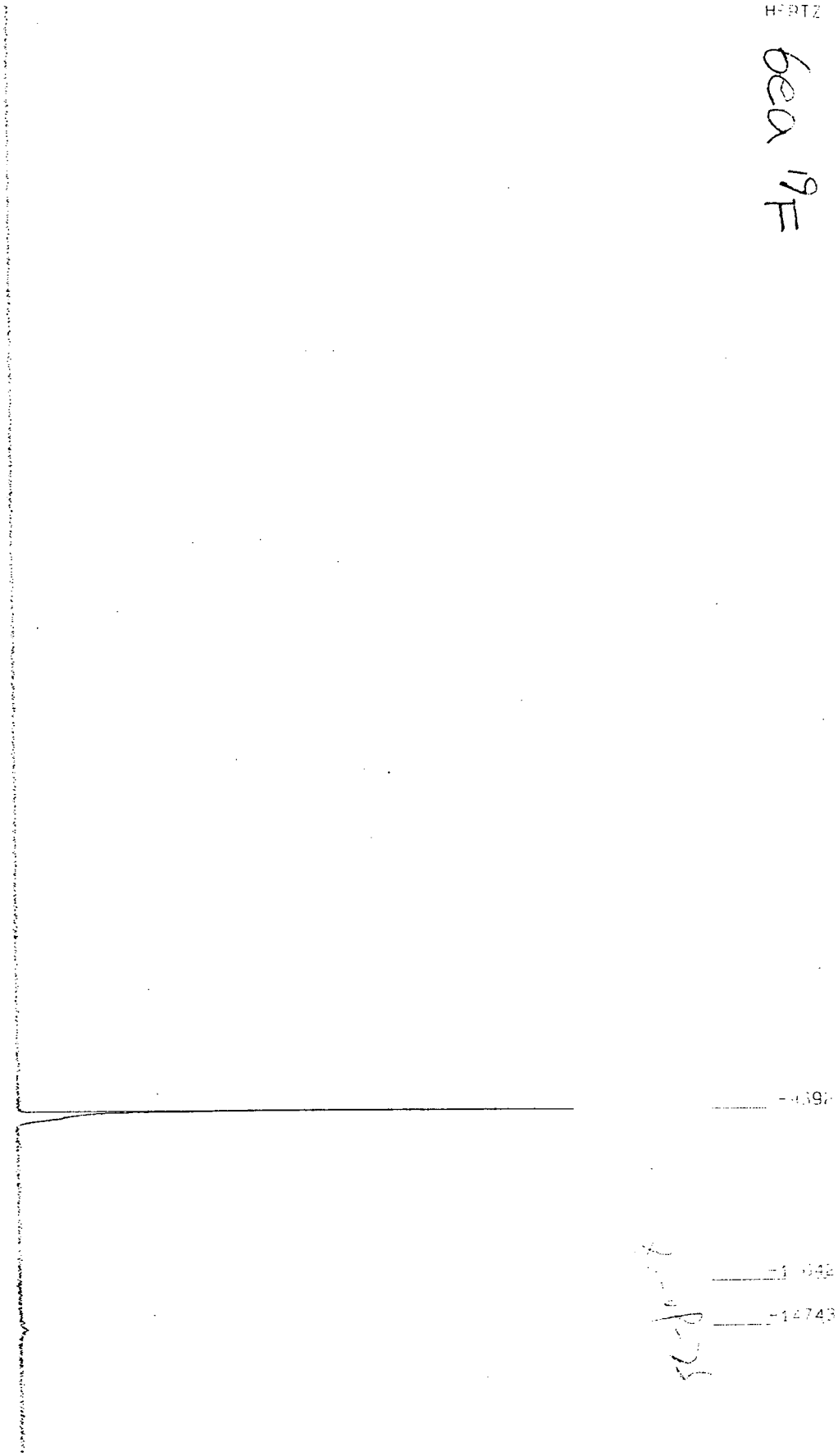
417.91
414.41
410.92
401.51
284.79
278.14
270.92
265.12

$^1$H


HERTZ
6ea 19F
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-14.742
-14.743

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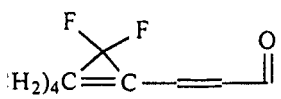
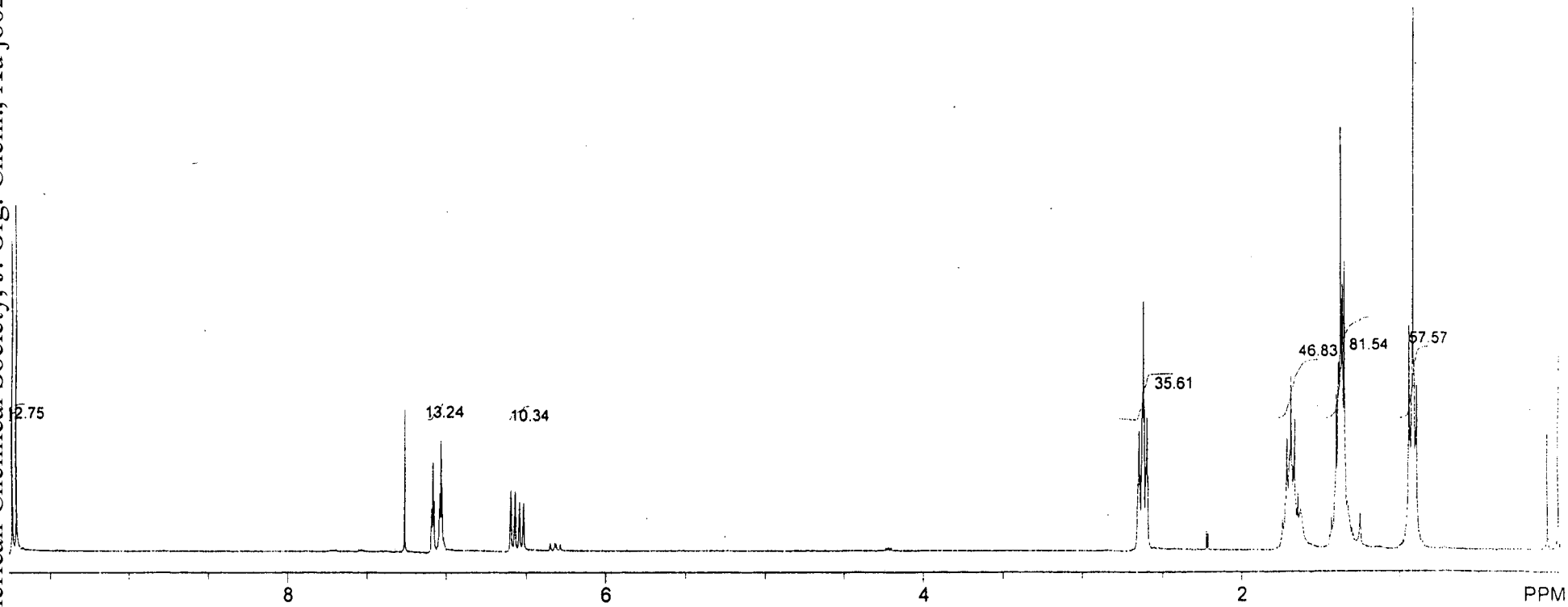
6eb $^1$H




USER: -- DATE: Dec 24 2001

| | | | | | | |
|---|---|---|---|---|---|---|
| 0.054 | F2: 75.456 | SW1: 9009 | | OF1: 1503.2 | | PTS1d: 32768 |
| 2pul | | PW: 8.8 usec | PD: 1.0 sec | NA: 8 | LB: 0.0 | WinNuts - $PROTON.fid |

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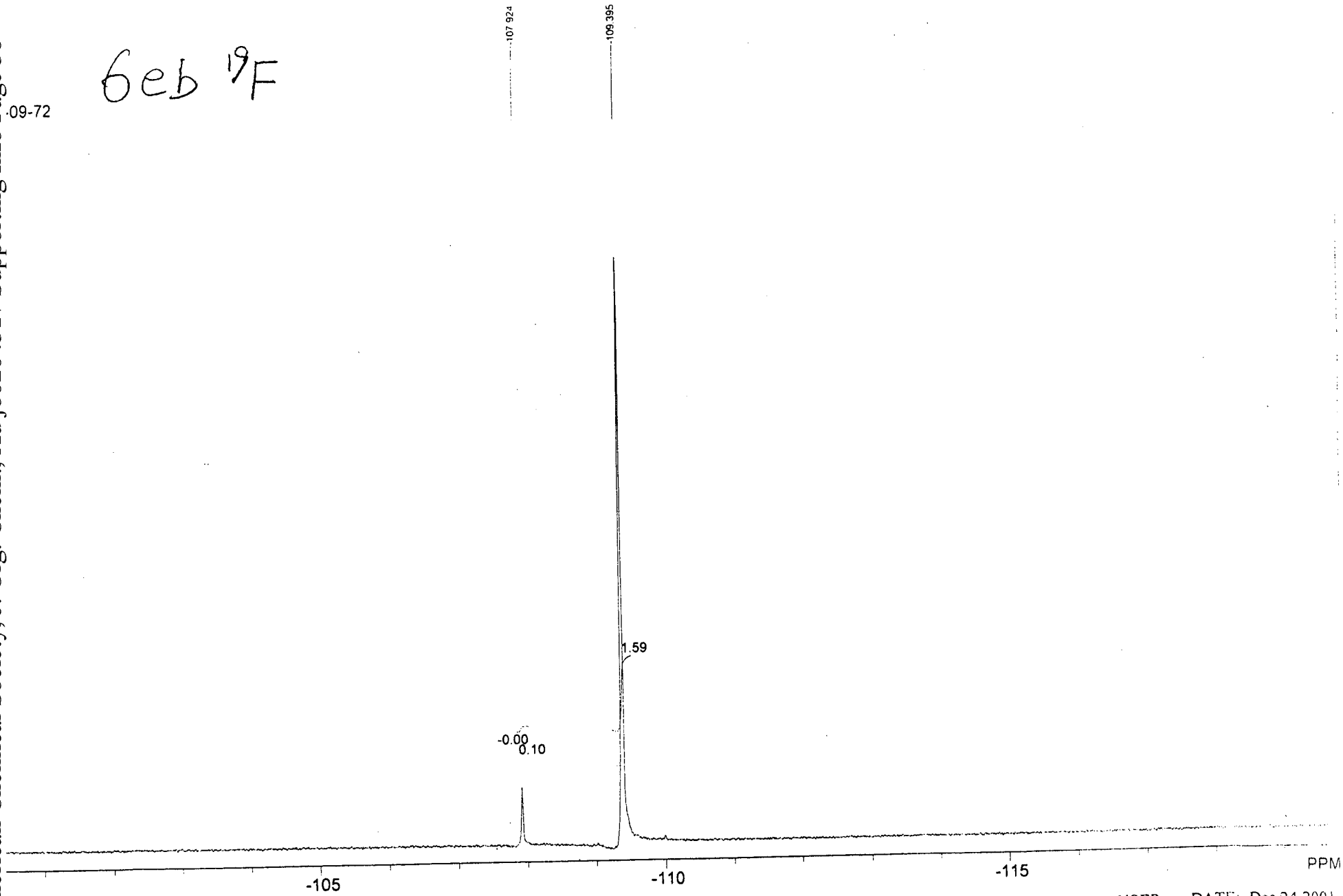
6eb $^{19}F$

-09-72




USER: -- DATE: Dec 24 2001

| | | | | | | |
|---|---|---|---|---|---|---|
| 82.325 | F2: 300.054 | SW1: 99010 | | OF1: -7058.3 | | PTS1d: 32768 |
| s2pul | | PW: 4.4 usec | PD: 1.5 sec | NA: 16 | LB: 0.0 | WinNuts - $FLUORINE.fid |

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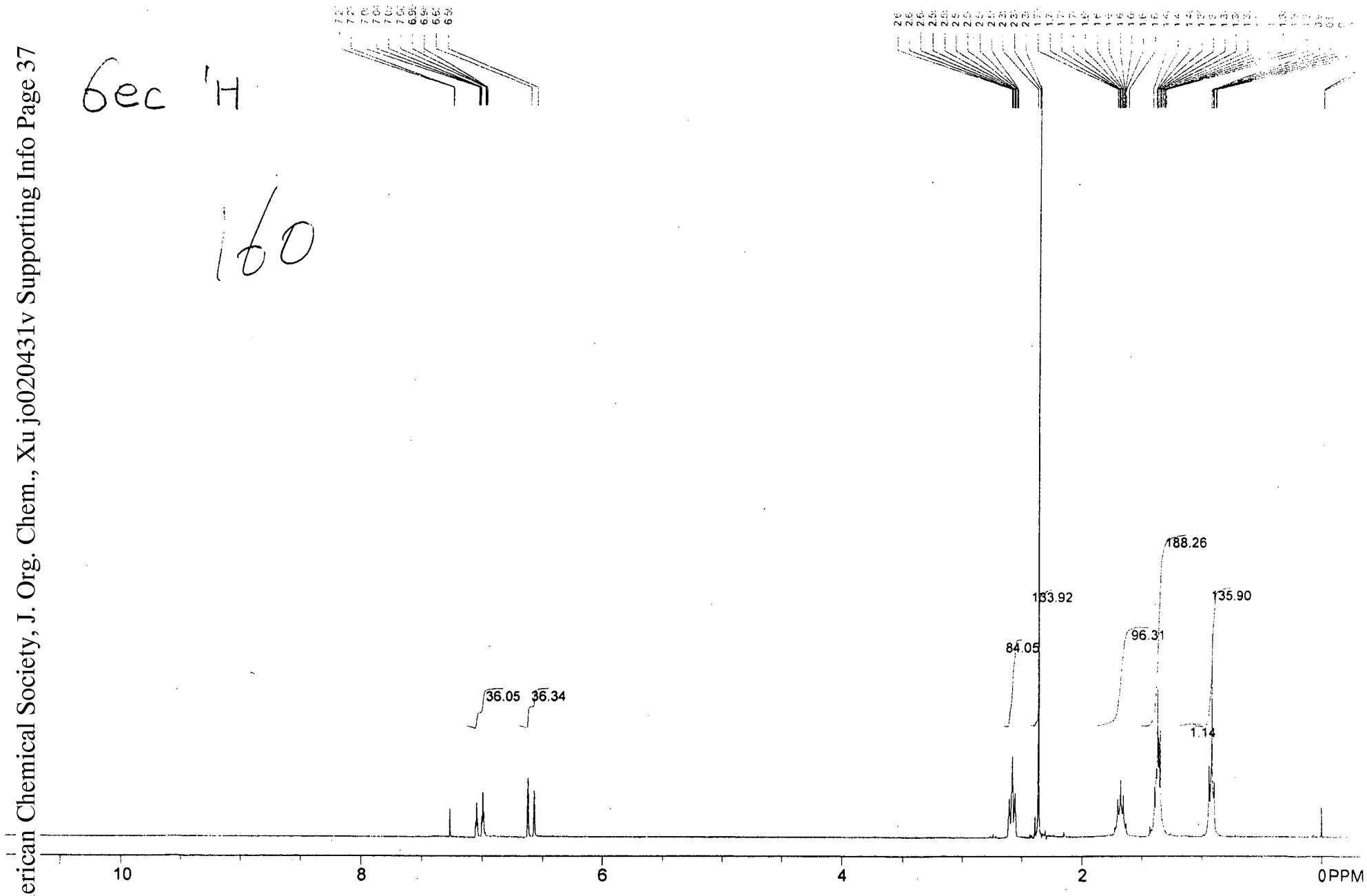
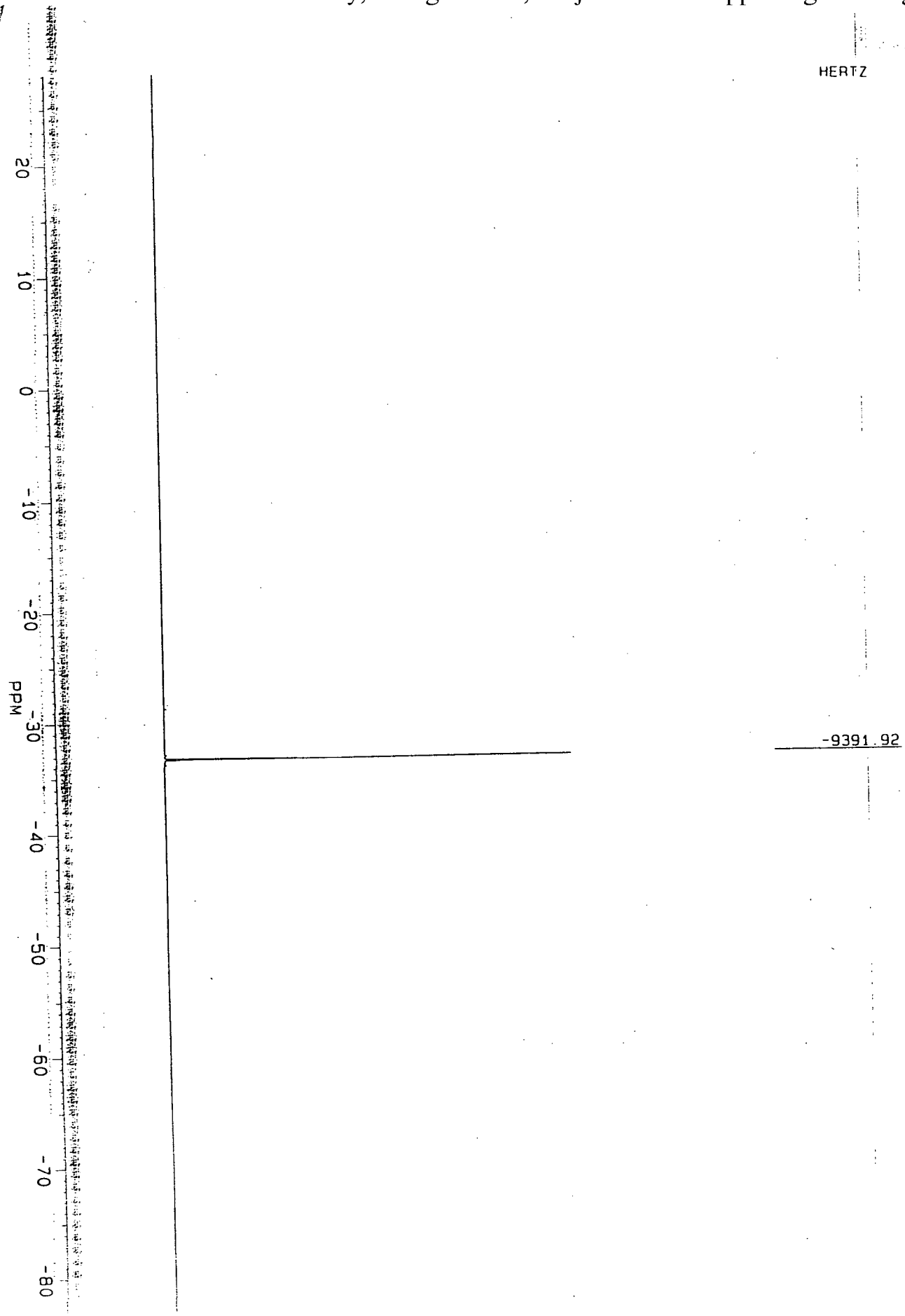
6ec 1H

160




USER: -- DATE: May 9 2002

| | | | | | | |
|---|---|---|---|---|---|---|
| L: ).055 | F2: 75.456 | SW1: 4803 | | OF1: 1804.6 | | PTS1d: 16384 |
| X: ɔul | | PW: 5.0 usec | PD: 1.0 sec | NA: 8 | LB: 0.0 | WinNuts - $PROTON.fid |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20
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-50
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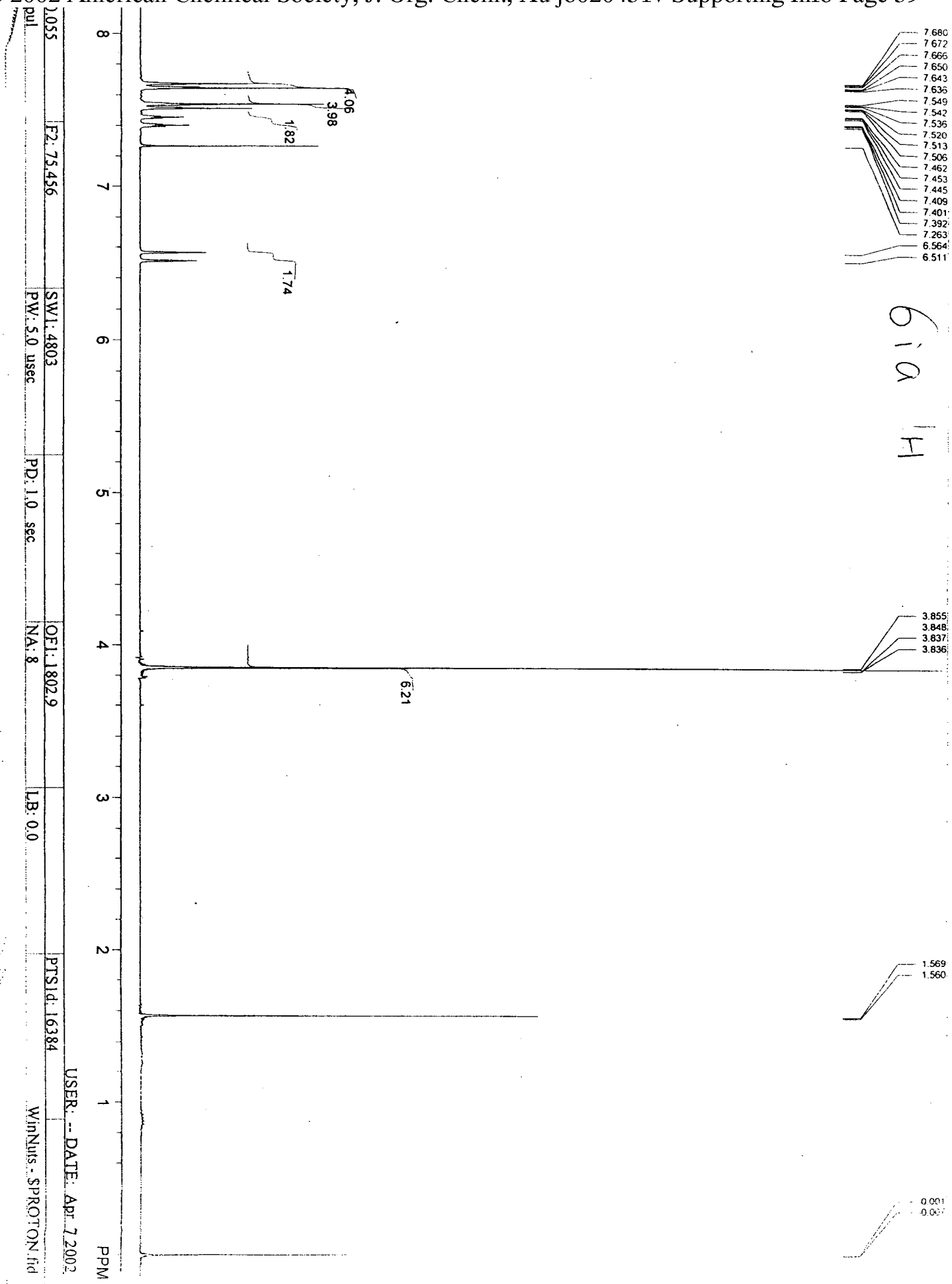
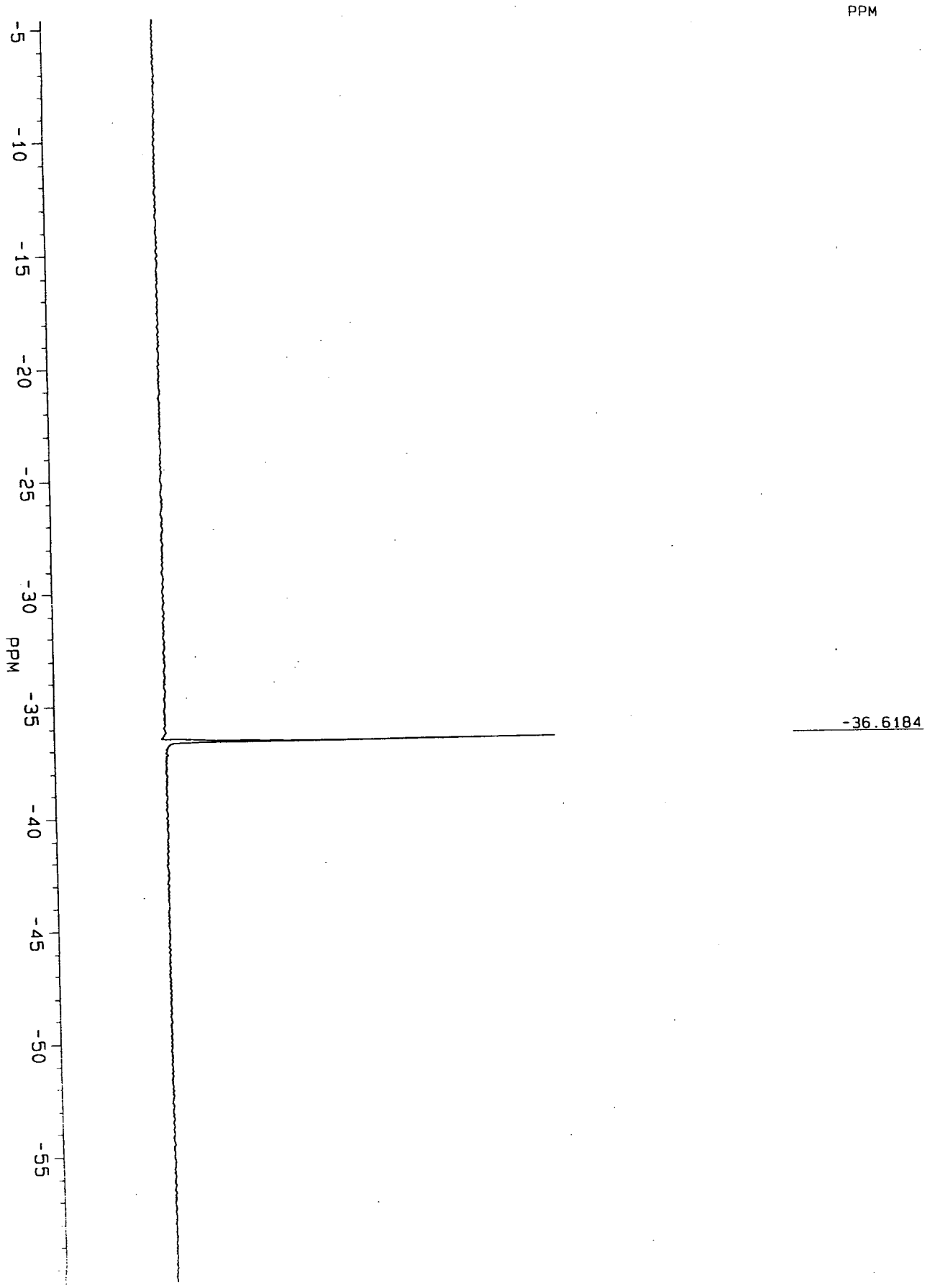
-70
-80
PPM


6ia H
7.680
7.672
7.666
7.650
7.643
7.636
7.549
7.542
7.536
7.520
7.513
7.506
7.462
7.453
7.445
7.409
7.401
7.392
7.263
6.564
6.511
3.855
3.848
3.837
3.836
1.569
1.560
0.001
4.06
3.98
1.82
1.74
6.21
8
7
6
5
4
3
2
1
PPM
USER: -- DATE: Apr 7 2002
PTS1d: 16384
LB: 0.0
OF1: 1802.9
NA: 8
PD: 1.0 sec
PW: 5.0 usec
SW1: 4803
F2: 75.456
1.055
pul
WinNuts - $PROTON.fid




6ia $^{19}$F