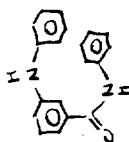


# SUPPORTING INFORMATION

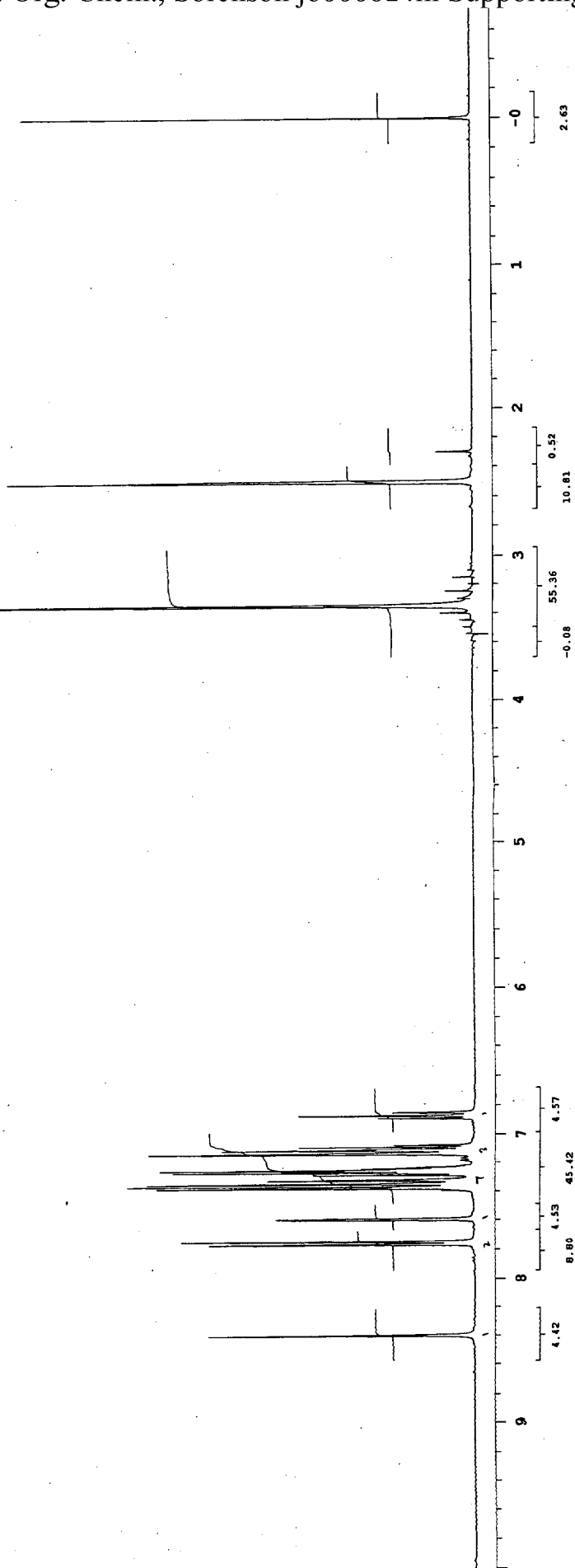


Entry 1

53187X116 /SORENSEN /h1 /DMSO /  
STANDARD 1H OBSERVE

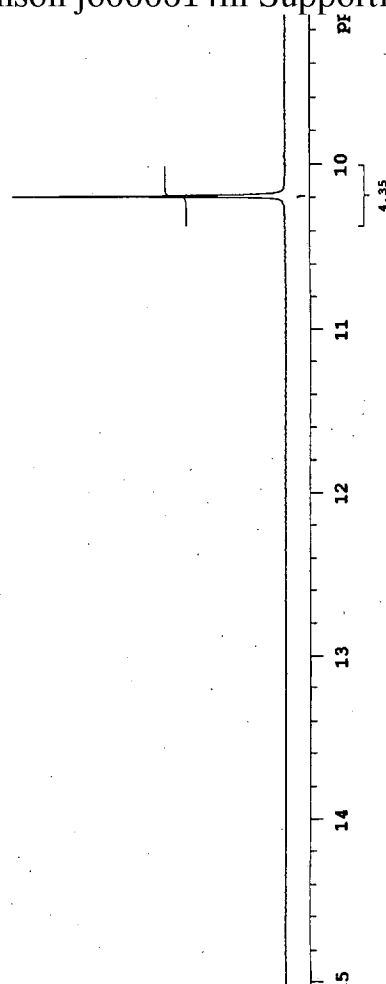
exp2 std1h

SAMPLE  
user cf  
date Jul 31 96  
solvent DMSO  
files /home/cf/-  
vnmrswa/hf/nf96313-  
12701  
ACQUISITION  
freq 399.966  
tn H1  
at 3.001  
sv 7900.5  
pw 4.0  
cl 1.000  
nt 32



| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.191          | 4071.966       | 55.5   |
| 2     | 8.398           | 3351.905       | 65.8   |
| 3     | 7.772           | 3101.822       | 84.6   |
| 4     | 7.772           | 3101.822       | 84.6   |
| 5     | 7.751           | 3099.952       | 72.5   |
| 6     | 7.751           | 3099.952       | 72.5   |
| 7     | 7.595           | 3037.746       | 49.1   |
| 8     | 7.392           | 2955.733       | 8.2    |
| 9     | 7.389           | 2955.266       | 8.2    |
| 10    | 7.379           | 2951.429       | 78.5   |
| 11    | 7.377           | 2950.705       | 78.5   |
| 12    | 7.374           | 2949.259       | 46.1   |
| 13    | 7.370           | 2947.812       | 40.2   |
| 14    | 7.362           | 2944.436       | 85.8   |
| 15    | 7.342           | 2936.480       | 80.9   |
| 16    | 7.321           | 2928.541       | 32.1   |
| 17    | 7.290           | 2915.544       | 37.5   |
| 18    | 7.277           | 2911.770       | 67.5   |
| 19    | 7.269           | 2907.305       | 74.6   |
| 20    | 7.263           | 2905.135       | 34.6   |
| 21    | 7.257           | 2902.483       | 47.6   |
| 22    | 7.251           | 2900.072       | 77.7   |
| 23    | 7.242           | 2896.455       | 28.0   |
| 24    | 7.235           | 2893.562       | 16.8   |
| 25    | 7.223           | 2888.981       | 2.9    |
| 26    | 7.183           | 2872.827       | 3.5    |
| 27    | 7.163           | 2865.111       | 3.4    |
| 28    | 7.139           | 2855.467       | 67.3   |
| 29    | 7.137           | 2854.502       | 60.6   |
| 30    | 7.118           | 2844.376       | 25.4   |
| 31    | 7.102           | 2838.154       | 31.7   |
| 32    | 7.109           | 2843.170       | 43.3   |
| 33    | 7.090           | 2835.696       | 43.3   |
| 34    | 7.074           | 2829.427       | 13.5   |
| 35    | 7.072           | 2828.462       | 19.9   |
| 36    | 6.893           | 2756.853       | 23.8   |
| 37    | 6.875           | 2749.619       | 43.4   |
| 38    | 6.859           | 2743.351       | 13.9   |
| 39    | 6.857           | 2742.386       | 20.3   |
| 40    | 3.543           | 1417.245       | -3.9   |
| 41    | 3.493           | 1398.992       | 2.4    |
| 42    | 3.443           | 1377.703       | 3.2    |
| 43    | 3.394           | 1356.414       | 5.0    |
| 44    | 3.327           | 1338.884       | 2218.6 |
| 45    | 3.302           | 1330.801       | 2.2    |
| 46    | 3.298           | 1319.113       | 3.7    |
| 47    | 3.249           | 1299.583       | 6.7    |
| 48    | 3.152           | 1260.765       | 4.9    |
| 49    | 2.511           | 1004.465       | 40.3   |
| 50    | 2.507           | 1002.777       | 83.9   |
| 51    | 2.502           | 1000.849       | 115.0  |
| 52    | 2.498           | 999.160        | 82.3   |
| 53    | 2.484           | 997.472        | 39.7   |
| 54    | 2.289           | 919.594        | 8.9    |
| 55    | 0.008           | 0.156          | 0.0    |
| 56    | 0.008           | 0.156          | 111.1  |
| 57    | -0.008          | -3.376         | 5.0    |

Entry 1



53167X116 /SORENSEN /h1 /DMSO /  
STANDARD 1H OBSERVE

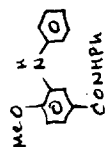
exp2 std1h

SAMPLE

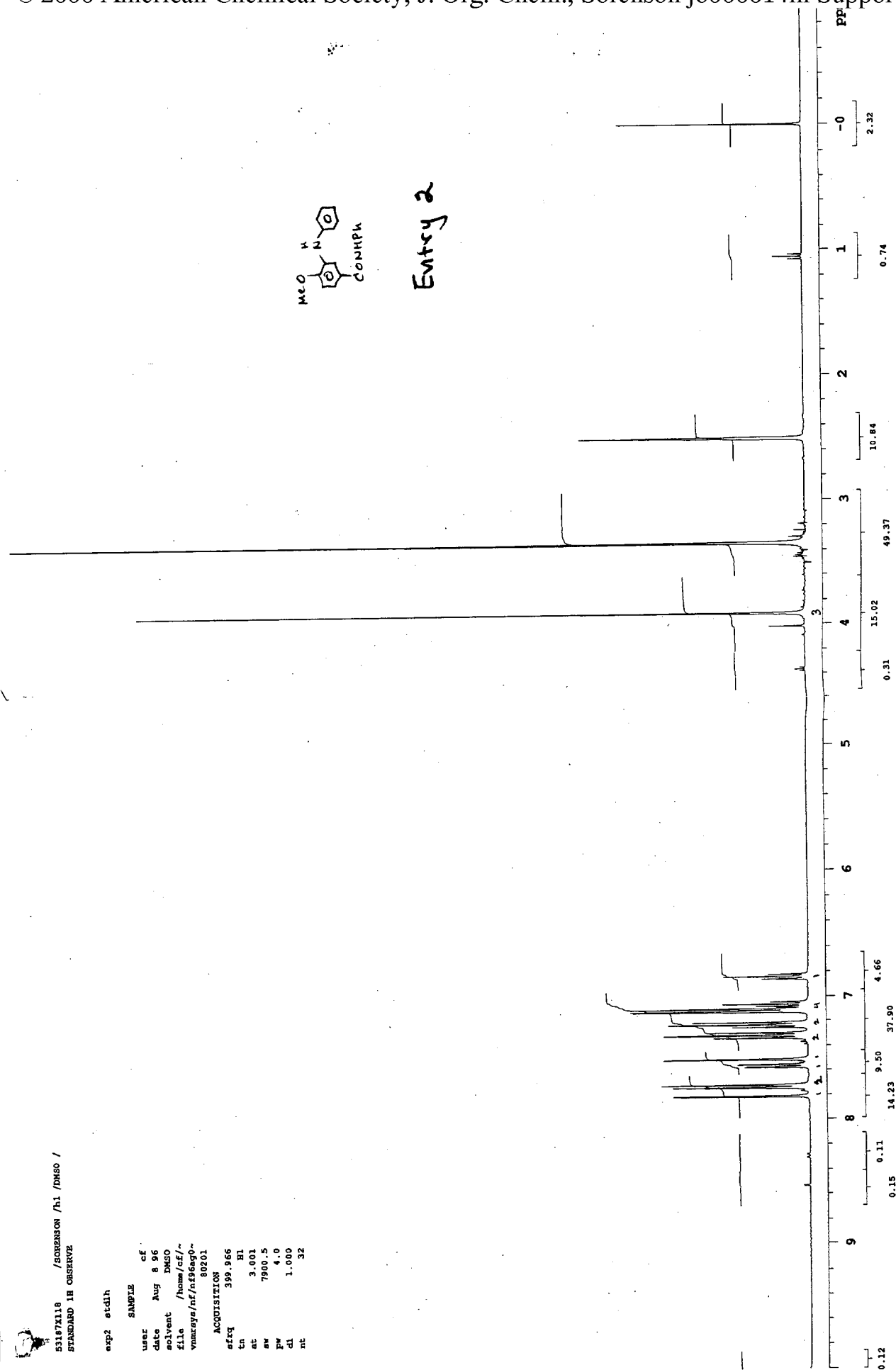
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solvent DMSO  
file /home/cf/~  
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80201

ACQUISITION

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tn h1  
at 3.001  
pw 7900.5  
pc 4.0  
di 1.000  
nt 32



Entry 2



53197118 /SORENSEN /H1 /DMSO /  
STANDARD 1H OBSERVE

exp2 stdlh

user SAMPLE

date Aug 8 96

solvent DMSO

file /home/cf/-

vmwsys/hf/nf56sgb-

80201

ACQUISITION

sfrq 399.966

tn H1

at 3.001

sw 7900.5

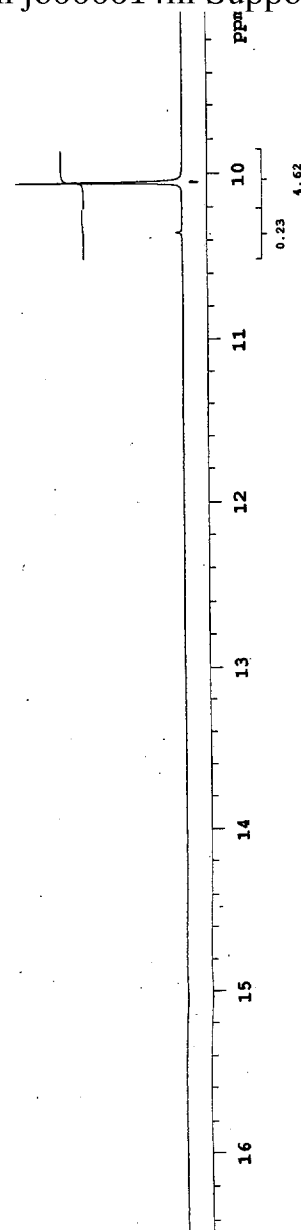
pw 4.0

dl 1.000

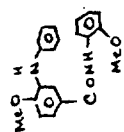
nt 32

Entry 2

| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.047          | 4082.341       | 33.7   |
| 2     | 7.817           | 3124.546       | 36.7   |
| 3     | 7.812           | 3124.546       | 38.8   |
| 4     | 7.767           | 3106.703       | 31.5   |
| 5     | 7.746           | 3098.265       | 31.5   |
| 6     | 7.743           | 3097.059       | 39.0   |
| 7     | 7.725           | 3089.585       | 42.2   |
| 8     | 7.579           | 3031.477       | 18.4   |
| 9     | 7.574           | 3028.307       | 17.9   |
| 10    | 7.558           | 3023.038       | 20.4   |
| 11    | 7.553           | 3020.868       | 20.0   |
| 12    | 7.539           | 3015.323       | 2.8    |
| 13    | 7.514           | 3005.196       | 41.6   |
| 14    | 7.374           | 2947.571       | 2.3    |
| 15    | 7.341           | 2938.998       | 27.2   |
| 16    | 7.321           | 2930.084       | 28.7   |
| 17    | 7.301           | 2920.084       | 41.6   |
| 18    | 7.256           | 2893.562       | 41.6   |
| 19    | 7.235           | 2886.329       | 33.3   |
| 20    | 7.216           | 2886.329       | 50.3   |
| 21    | 7.129           | 2851.368       | 48.4   |
| 22    | 7.127           | 2850.403       | 50.9   |
| 23    | 7.124           | 2849.198       | 51.2   |
| 24    | 7.108           | 2842.929       | 15.0   |
| 25    | 7.084           | 2833.526       | 24.5   |
| 26    | 7.066           | 2826.051       | 10.9   |
| 27    | 7.046           | 2818.818       | 13.3   |
| 28    | 6.859           | 2742.351       | 24.2   |
| 29    | 6.841           | 2728.884       | 11.5   |
| 30    | 6.823           | 2728.884       | 10.4   |
| 31    | 4.368           | 1747.084       | 10.4   |
| 32    | 4.020           | 1607.963       | 192.0  |
| 33    | 3.913           | 1565.046       | 3.2    |
| 34    | 3.457           | 1382.525       | 2.8    |
| 35    | 3.444           | 1377.462       | 2.2    |
| 36    | 3.439           | 1375.533       | 2.2    |
| 37    | 3.426           | 1370.470       | 2.2    |
| 38    | 3.349           | 1339.367       | 1022.8 |
| 39    | 3.266           | 1318.390       | 4.5    |
| 40    | 3.245           | 1297.896       | 3.2    |
| 41    | 2.512           | 1004.106       | 23.2   |
| 42    | 2.508           | 1003.138       | 47.1   |
| 43    | 2.503           | 1001.089       | 64.4   |
| 44    | 2.499           | 999.401        | 84.1   |
| 45    | 2.494           | 997.714        | 22.5   |
| 46    | 1.074           | 429.658        | 4.3    |
| 47    | 1.057           | 422.666        | 8.5    |
| 48    | 1.039           | 415.674        | 4.2    |
| 49    | -0.000          | -0.000         | 52.7   |
| 50    | -0.008          | -3.134         | 2.4    |

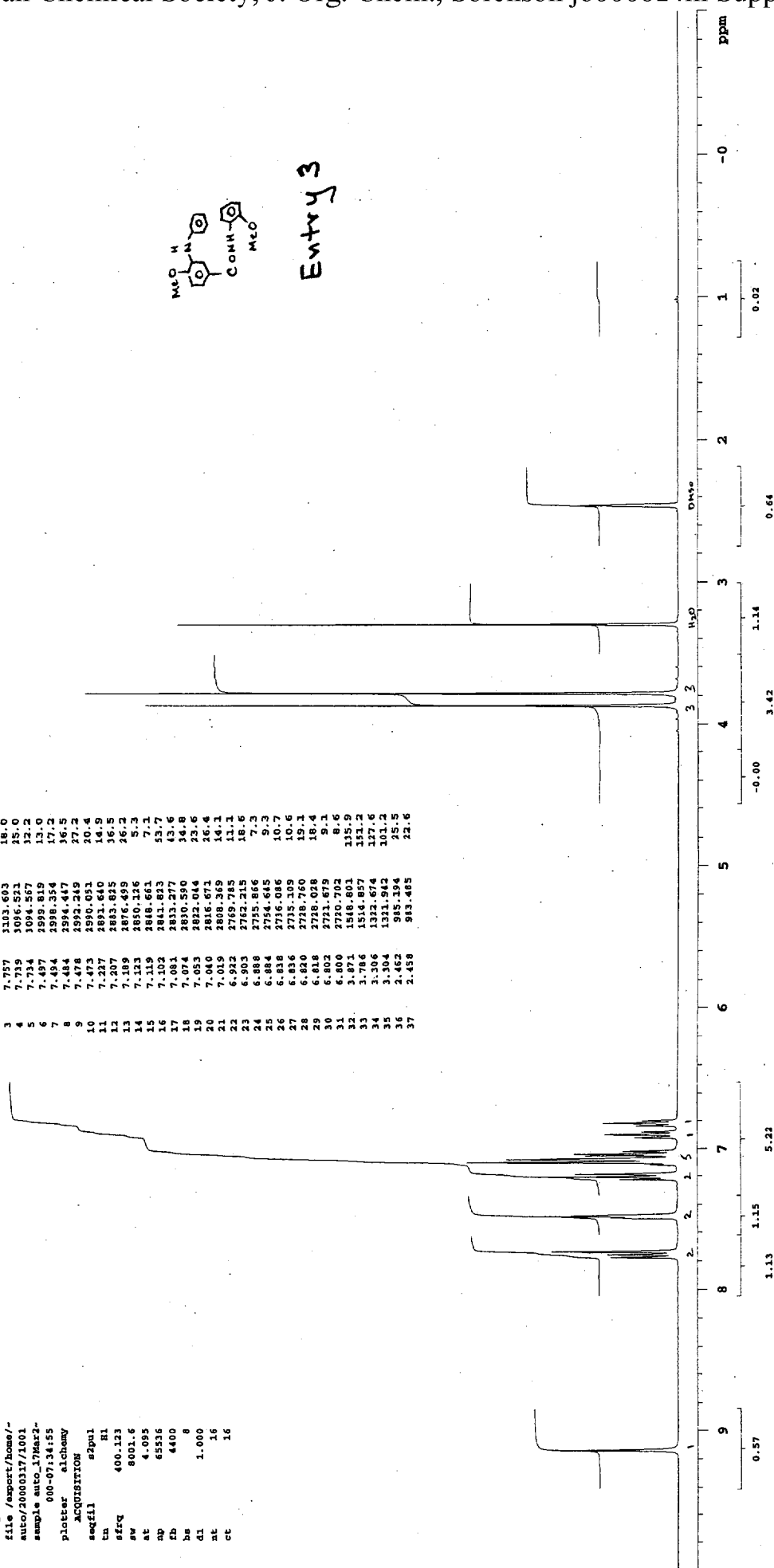


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Entry 3

| INDEX | (PPM) | (Hz)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 9.118 | 1656.220 | 10.0   |
| 2     | 7.776 | 1111.417 | 17.1   |
| 3     | 7.757 | 1103.603 | 18.0   |
| 4     | 7.739 | 1096.521 | 15.0   |
| 5     | 7.734 | 1094.567 | 12.2   |
| 6     | 7.497 | 1099.819 | 13.0   |
| 7     | 7.494 | 1098.354 | 17.2   |
| 8     | 7.484 | 1094.447 | 16.5   |
| 9     | 7.478 | 1092.249 | 17.2   |
| 10    | 7.473 | 1090.051 | 10.4   |
| 11    | 7.287 | 1091.648 | 14.9   |
| 12    | 7.287 | 1088.655 | 16.5   |
| 13    | 7.139 | 1086.499 | 26.2   |
| 14    | 7.133 | 1080.136 | 5.3    |
| 15    | 7.119 | 1080.651 | 7.1    |
| 16    | 7.102 | 1081.823 | 53.7   |
| 17    | 7.081 | 1083.277 | 43.6   |
| 18    | 7.074 | 1080.590 | 34.8   |
| 19    | 7.053 | 1082.014 | 23.6   |
| 20    | 7.040 | 1081.671 | 26.4   |
| 21    | 7.019 | 1080.369 | 14.1   |
| 22    | 6.912 | 1069.785 | 11.1   |
| 23    | 6.903 | 1062.215 | 18.6   |
| 24    | 6.888 | 1055.866 | 6.3    |
| 25    | 6.884 | 1054.645 | 10.7   |
| 26    | 6.838 | 1048.068 | 10.6   |
| 27    | 6.836 | 1047.309 | 19.1   |
| 28    | 6.818 | 1048.760 | 18.4   |
| 29    | 6.802 | 1048.028 | 9.1    |
| 30    | 6.800 | 1047.702 | 8.6    |
| 31    | 3.871 | 1548.601 | 135.9  |
| 32    | 3.786 | 1514.857 | 151.2  |
| 33    | 3.706 | 1322.674 | 127.6  |
| 34    | 3.304 | 1311.942 | 101.2  |
| 35    | 2.462 | 985.194  | 75.5   |
| 36    | 2.458 | 983.485  | 72.6   |
| 37    | 2.458 | 983.485  | 72.6   |

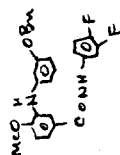


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gain not used  
temp not used  
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plotter alchemy  
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at 16  
ct 16

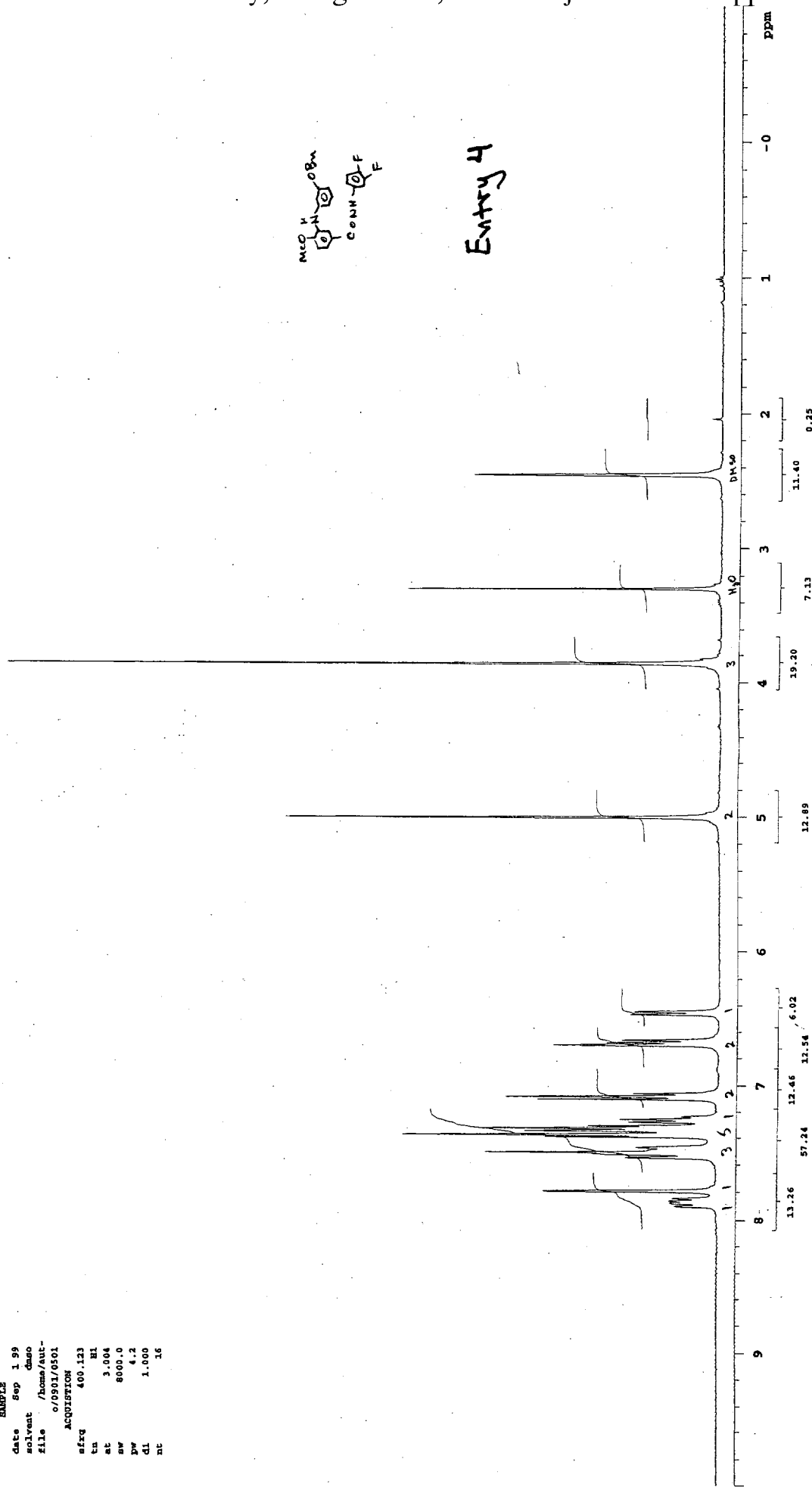
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 so Chem400 1H OBSERVE

exp2 std1h

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Entry 4

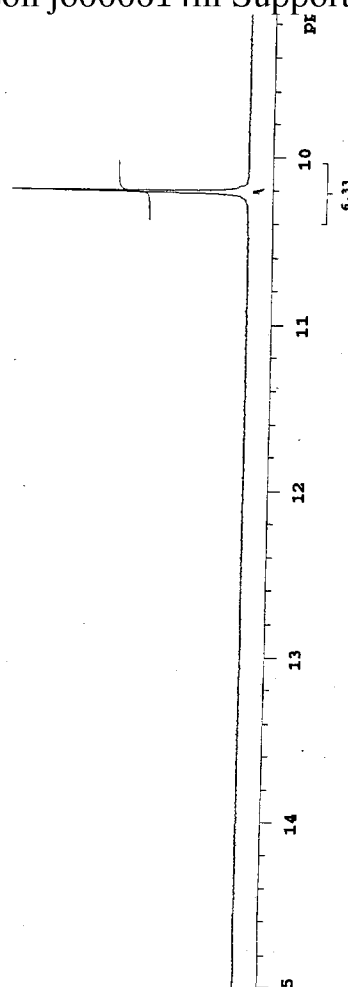


56

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Entry 4

| INDEX | (PPM)  | (Hz)     | HEIGHT |
|-------|--------|----------|--------|
| 1     | 10.212 | 4086.107 | 48.2   |
| 2     | 7.899  | 3160.542 | 11.6   |
| 3     | 7.879  | 3152.729 | 13.0   |
| 4     | 7.870  | 3148.823 | 13.1   |
| 5     | 7.810  | 3111.254 | 12.2   |
| 6     | 7.792  | 3117.836 | 46.8   |
| 7     | 7.540  | 3016.983 | 48.3   |
| 8     | 7.515  | 3006.728 | 33.9   |
| 9     | 7.508  | 3003.310 | 42.6   |
| 10    | 7.465  | 2986.952 | 21.9   |
| 11    | 7.388  | 2956.190 | 46.5   |
| 12    | 7.369  | 2948.377 | 84.8   |
| 13    | 7.342  | 2937.879 | 51.9   |
| 14    | 7.327  | 2931.531 | 63.5   |
| 15    | 7.307  | 2923.718 | 35.0   |
| 16    | 7.275  | 2910.778 | 24.0   |
| 17    | 7.258  | 2903.942 | 26.3   |
| 18    | 7.241  | 2897.106 | 9.9    |
| 19    | 7.130  | 2840.352 | 48.4   |
| 20    | 7.090  | 2825.570 | 37.0   |
| 21    | 7.062  | 2815.570 | 44.8   |
| 22    | 6.694  | 2678.593 | 44.8   |
| 23    | 6.676  | 2671.269 | 30.1   |
| 24    | 6.655  | 2662.968 | 26.1   |
| 25    | 6.467  | 2587.526 | 23.7   |
| 26    | 6.448  | 2579.957 | 22.8   |
| 27    | 5.001  | 2001.082 | 117.1  |
| 28    | 3.862  | 1545.258 | 192.0  |
| 29    | 3.828  | 1531.586 | 5.7    |
| 30    | 3.298  | 1319.665 | 84.3   |
| 31    | 3.264  | 1305.993 | 2.2    |
| 32    | 2.335  | 922.741  | 66.6   |
| 33    | 2.039  | 815.464  | 2.8    |
| 34    | 1.010  | 404.110  | 2.1    |



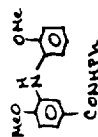
5747116 /SORENSEN /hl /DMSO /  
STANDARD IN OBSERVE

exp2 stdih

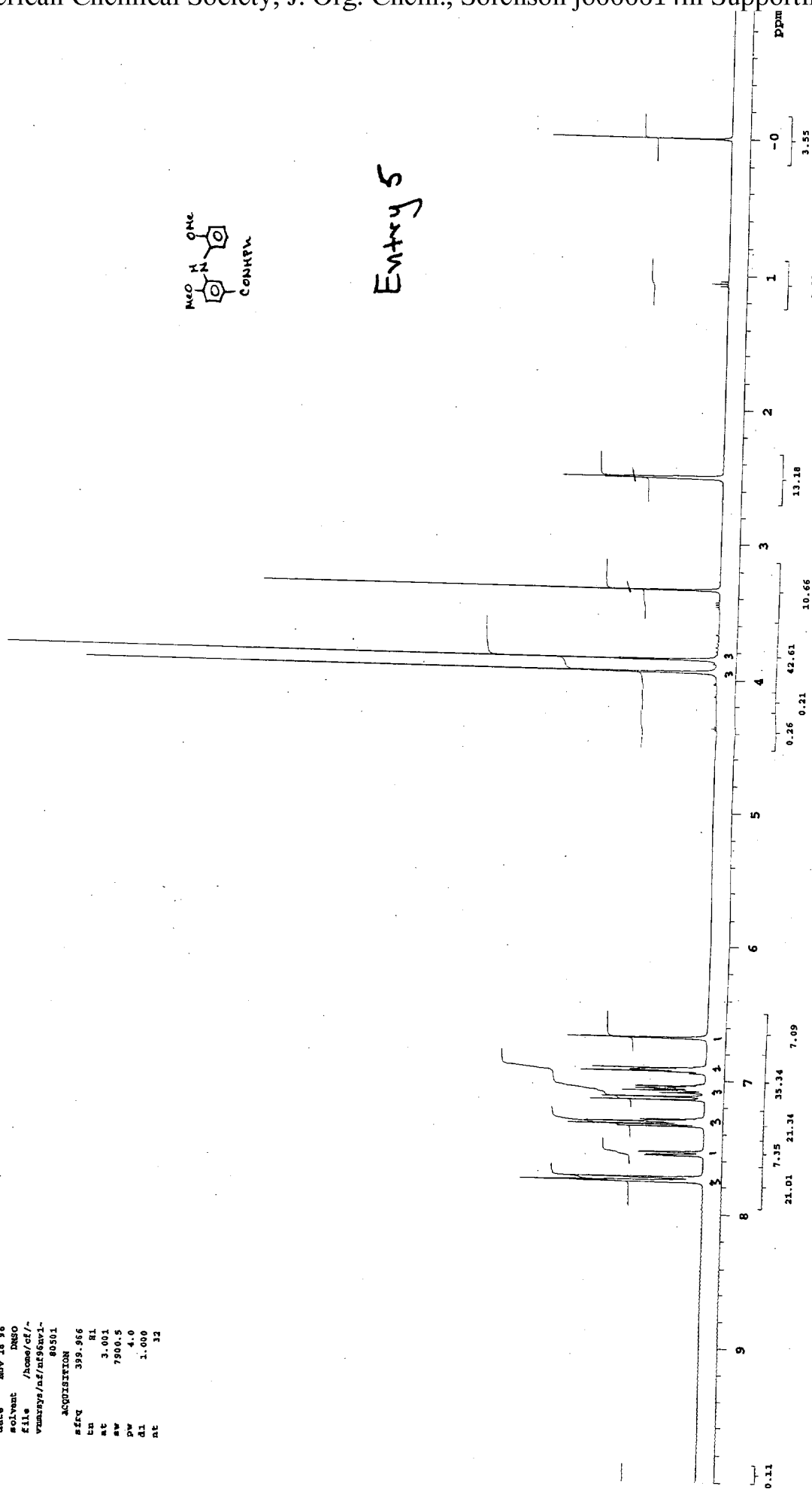
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user  
date Nov 18 96

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80501

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at 32

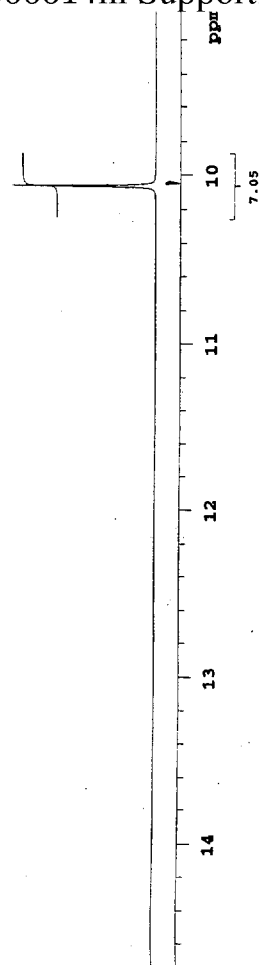


Entry 5



Entry 5

| INDEX | FREQUENCY (SPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.464          | 4025.032       | 29.2   |
| 2     | 7.761           | 3104.051       | 34.1   |
| 3     | 7.755           | 3101.881       | 49.4   |
| 4     | 7.751           | 3100.134       | 37.6   |
| 5     | 7.732           | 3092.478       | 37.1   |
| 6     | 7.561           | 3024.244       | 16.1   |
| 7     | 7.536           | 3022.074       | 15.7   |
| 8     | 7.530           | 3018.805       | 17.9   |
| 9     | 7.523           | 3015.635       | 17.4   |
| 10    | 7.514           | 3012.464       | 23.7   |
| 11    | 7.340           | 2935.716       | 84.6   |
| 12    | 7.326           | 2929.970       | 84.6   |
| 13    | 7.313           | 2925.148       | 17.7   |
| 14    | 7.304           | 2921.531       | 32.5   |
| 15    | 7.300           | 2919.602       | 16.5   |
| 16    | 7.290           | 2915.744       | 17.6   |
| 17    | 7.282           | 2912.369       | 2.6    |
| 18    | 7.136           | 2854.261       | 31.1   |
| 19    | 7.135           | 2845.832       | 28.1   |
| 20    | 7.087           | 2834.711       | 12.6   |
| 21    | 7.069           | 2827.498       | 22.6   |
| 22    | 7.060           | 2823.640       | 14.7   |
| 23    | 7.051           | 2820.024       | 19.1   |
| 24    | 7.041           | 2816.508       | 10.2   |
| 25    | 7.036           | 2814.217       | 13.1   |
| 26    | 7.028           | 2810.861       | 11.1   |
| 27    | 6.945           | 2777.839       | 4.7    |
| 28    | 6.942           | 2776.313       | 3.4    |
| 29    | 6.934           | 2773.248       | 31.9   |
| 30    | 6.926           | 2770.355       | 20.8   |
| 31    | 6.923           | 2768.908       | 20.8   |
| 32    | 6.920           | 2767.703       | 20.7   |
| 33    | 6.917           | 2766.477       | 18.5   |
| 34    | 6.910           | 2763.604       | 30.9   |
| 35    | 6.901           | 2760.228       | 3.0    |
| 36    | 6.891           | 2758.023       | 3.5    |
| 37    | 6.876           | 2670.824       | 37.9   |
| 38    | 3.945           | 1577.824       | 172.0  |
| 39    | 3.852           | 1540.693       | 123.6  |
| 40    | 3.341           | 1336.232       | 15.2   |
| 41    | 2.511           | 1004.465       | 31.9   |
| 42    | 2.507           | 1002.536       | 43.4   |
| 43    | 2.502           | 1000.848       | 30.7   |
| 44    | 2.498           | 999.160        | 2.3    |
| 45    | 1.075           | 430.140        | 4.6    |
| 46    | 1.058           | 423.148        | 2.2    |
| 47    | 1.040           | 416.256        | 48.6   |
| 48    | 0.000           | 0.000          | 2.1    |
| 49    | -0.008          | -3.376         | 2.1    |

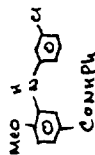


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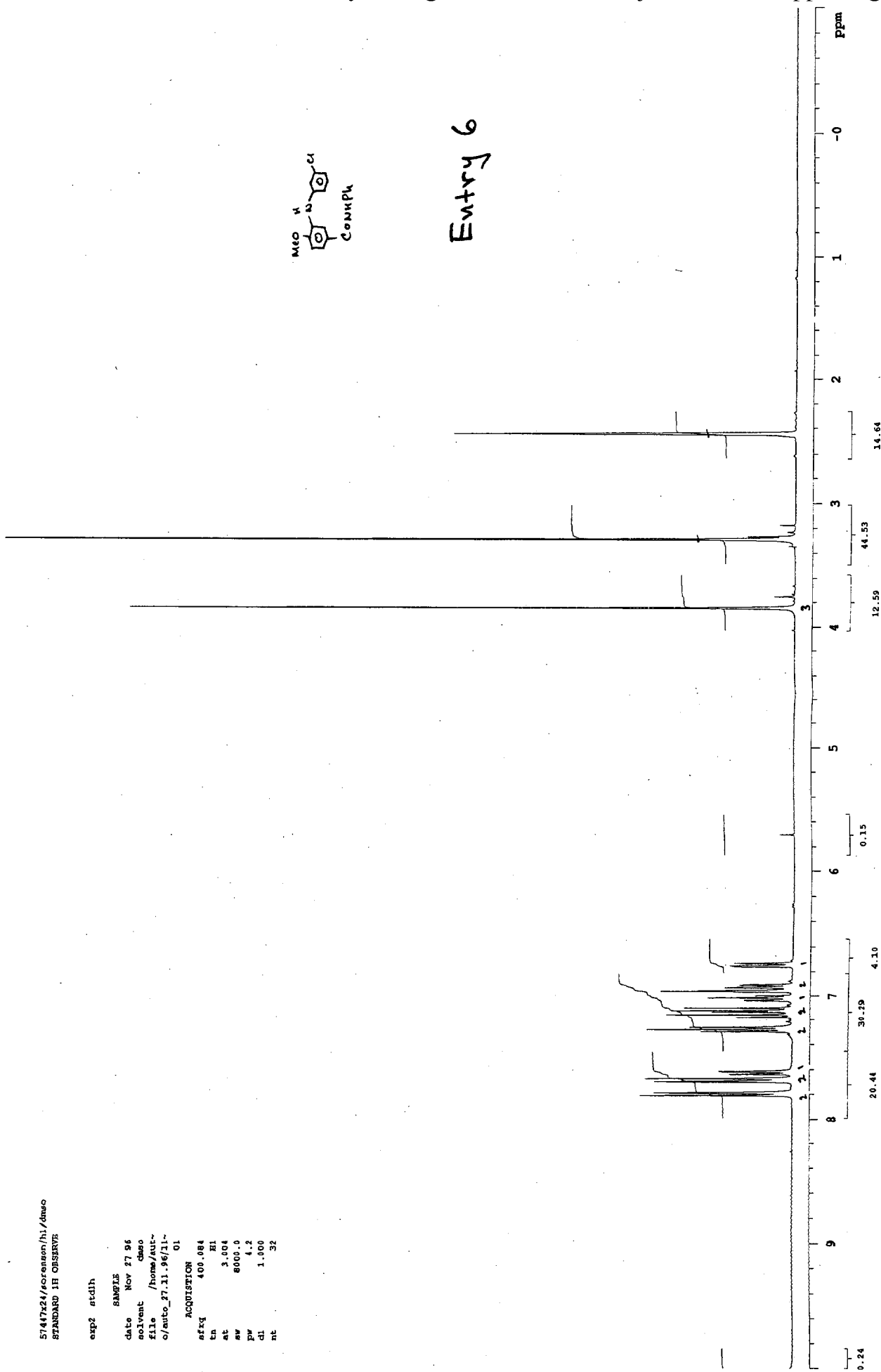
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STANDARD 1H OBSERVE

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tn H1  
at 3.004  
sw 8000.0  
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di 1.000  
nt 32



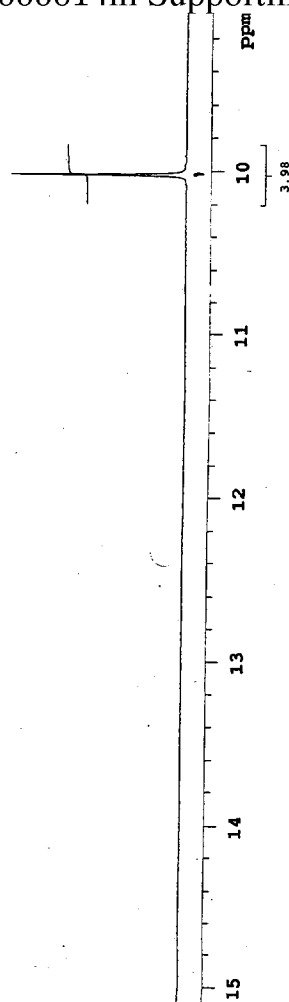
Entry 6



S10

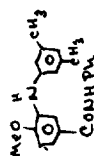
Entry 6

| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | BRIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.023          | 4010.164       | 35.4   |
| 2     | 7.809           | 3124.151       | 44.0   |
| 3     | 7.792           | 3117.559       | 35.5   |
| 4     | 7.787           | 3115.361       | 39.9   |
| 5     | 7.694           | 3078.251       | 39.8   |
| 6     | 7.675           | 3070.682       | 42.5   |
| 7     | 7.635           | 3054.813       | 18.0   |
| 8     | 7.610           | 3032.615       | 18.3   |
| 9     | 7.600           | 3024.267       | 20.3   |
| 10    | 7.599           | 3023.979       | 21.2   |
| 11    | 7.292           | 2907.544       | 26.6   |
| 12    | 7.272           | 2901.488       | 42.1   |
| 13    | 7.252           | 2901.488       | 42.1   |
| 14    | 7.172           | 2869.504       | 12.8   |
| 15    | 7.152           | 2861.447       | 16.4   |
| 16    | 7.132           | 2853.390       | 23.4   |
| 17    | 7.123           | 2849.728       | 35.0   |
| 18    | 7.101           | 2840.939       | 31.4   |
| 19    | 7.036           | 2814.815       | 14.2   |
| 20    | 7.017           | 2807.491       | 24.5   |
| 21    | 6.999           | 2800.166       | 11.0   |
| 22    | 6.954           | 2786.005       | 17.2   |
| 23    | 6.954           | 2786.005       | 38.1   |
| 24    | 6.954           | 2786.005       | 27.3   |
| 25    | 6.934           | 2775.019       | 12.8   |
| 26    | 6.932           | 2773.310       | 15.2   |
| 27    | 6.917           | 2767.206       | 14.4   |
| 28    | 6.912           | 2765.253       | 14.4   |
| 29    | 6.759           | 2703.972       | 17.1   |
| 30    | 6.755           | 2702.751       | 18.2   |
| 31    | 6.741           | 2696.891       | 15.2   |
| 32    | 6.739           | 2696.159       | 15.1   |
| 33    | 6.736           | 2694.938       | 17.1   |
| 34    | 6.703           | 2681.596       | 4.2    |
| 35    | 3.742           | 1538.409       | 192.0  |
| 36    | 3.742           | 1538.409       | 6.0    |
| 37    | 3.742           | 1538.409       | 936.7  |
| 38    | 3.268           | 1304.445       | 13.8   |
| 39    | 3.236           | 1294.505       | 2.3    |
| 40    | 3.233           | 1293.284       | 2.3    |
| 41    | 3.177           | 1271.067       | 4.5    |
| 42    | 2.467           | 986.878        | 3.9    |
| 43    | 2.462           | 985.169        | 5.3    |
| 44    | 2.449           | 978.798        | 72.8   |
| 45    | 2.445           | 978.089        | 98.8   |
| 46    | 2.440           | 976.380        | 74.3   |

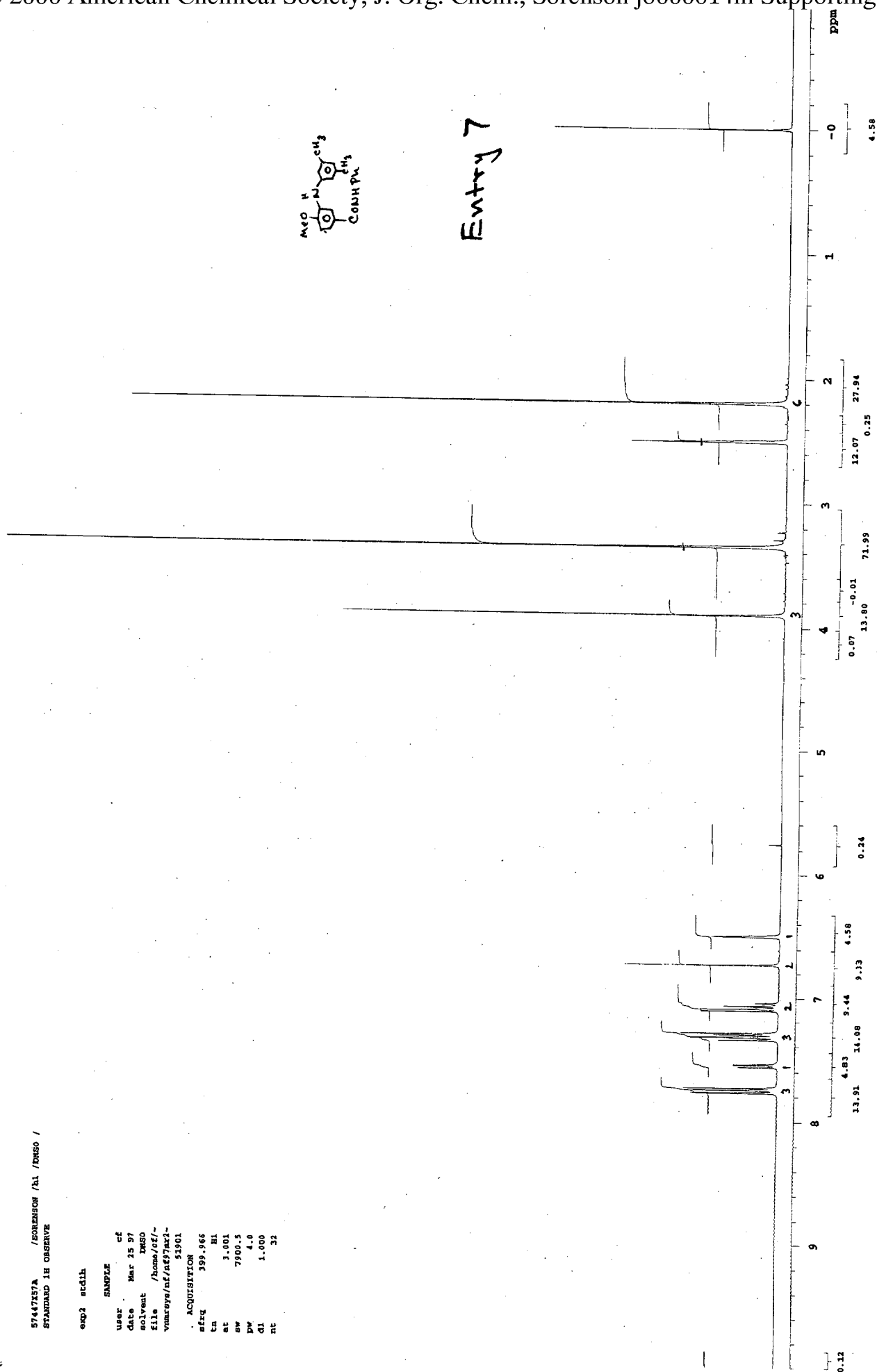


S11

| SAMPLE      |  | user    | date                  | cf |
|-------------|--|---------|-----------------------|----|
|             |  | solvent | Mar 25 97             |    |
|             |  | file    | WMSO                  |    |
|             |  |         | /home/cf/~            |    |
|             |  |         | vnuar05a/nf/nf2/nf22- |    |
|             |  |         | 51901                 |    |
| ACQUISITION |  |         |                       |    |
|             |  | strq    | 399.966               |    |
|             |  | tn      | H1                    |    |
|             |  | at      | 3.001                 |    |
|             |  | sw      | 7900.5                |    |
|             |  | pw      | 4.0                   |    |
|             |  | dl      | 1.000                 |    |
|             |  | nt      | 32                    |    |

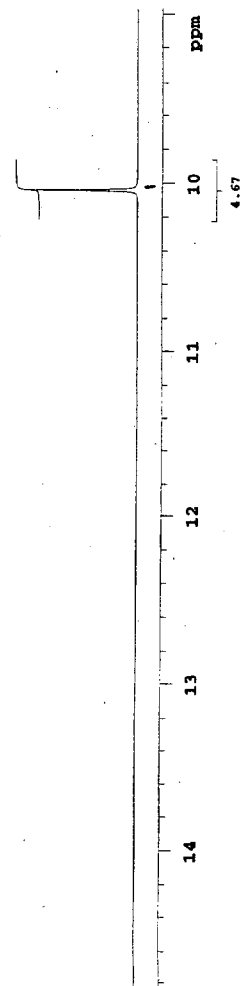


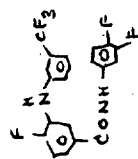
Entry 7



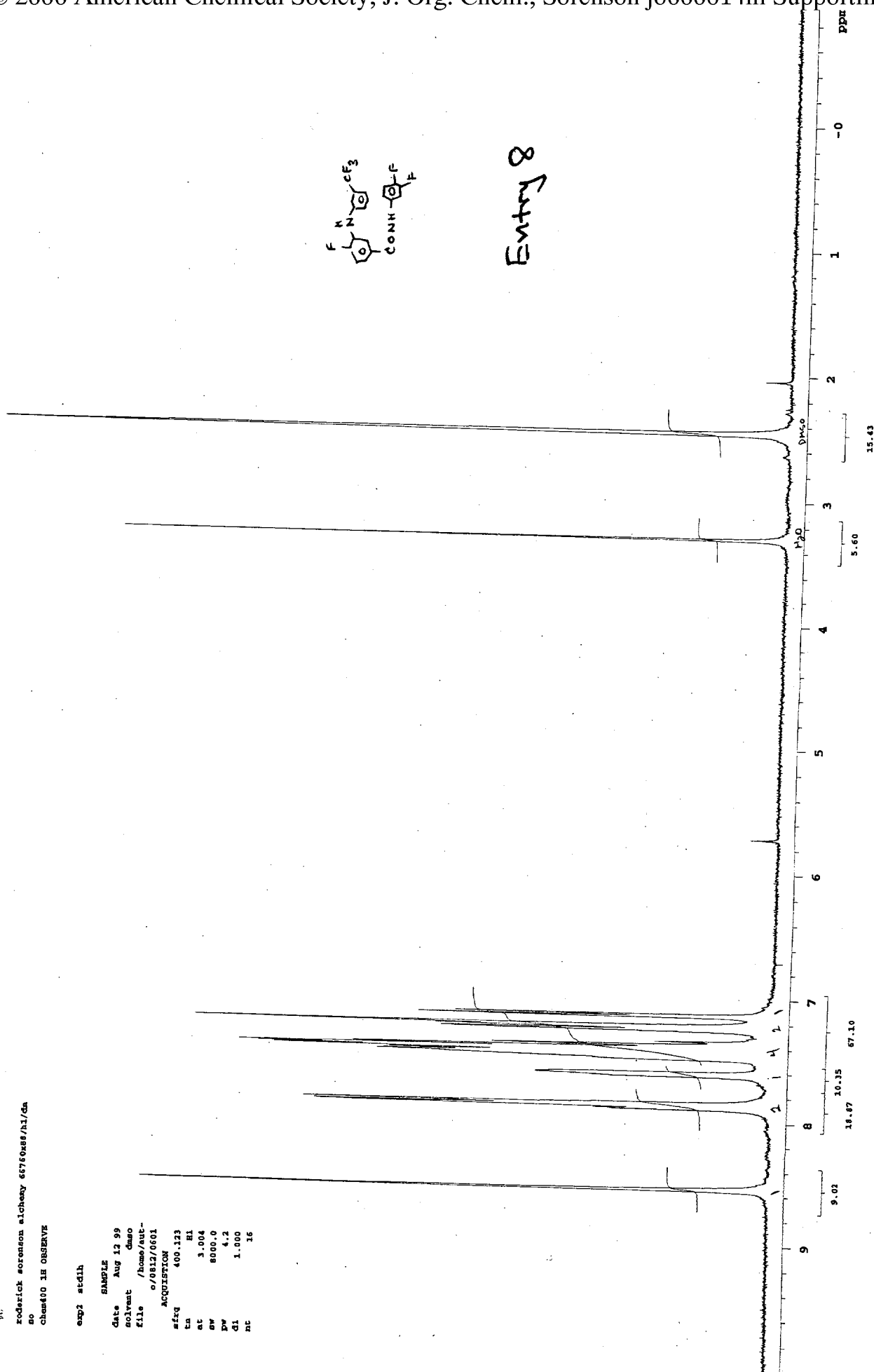
Entry 7

| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | BRIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.043          | 4016.894       | 21.9   |
| 2     | 7.773           | 3108.871       | 23.9   |
| 3     | 7.767           | 3106.701       | 25.4   |
| 4     | 7.749           | 3099.470       | 20.4   |
| 5     | 7.746           | 3098.506       | 23.4   |
| 6     | 7.728           | 3090.790       | 27.4   |
| 7     | 7.539           | 3023.521       | 12.0   |
| 8     | 7.554           | 3021.351       | 11.6   |
| 9     | 7.538           | 3015.082       | 13.2   |
| 10    | 7.533           | 3012.913       | 13.0   |
| 11    | 7.341           | 2936.239       | 17.6   |
| 12    | 7.337           | 2934.551       | 6.4    |
| 13    | 7.323           | 2928.764       | 26.6   |
| 14    | 7.302           | 2920.567       | 19.1   |
| 15    | 7.297           | 2918.397       | 4.9    |
| 16    | 7.288           | 2913.021       | 28.7   |
| 17    | 7.110           | 2863.893       | 23.3   |
| 18    | 7.089           | 2855.455       | 22.8   |
| 19    | 7.084           | 2854.021       | 11.2   |
| 20    | 7.048           | 2836.051       | 16.0   |
| 21    | 6.724           | 2689.342       | 45.3   |
| 22    | 6.724           | 2689.342       | 45.3   |
| 23    | 6.498           | 2598.926       | 20.1   |
| 24    | 5.758           | 2303.084       | 3.7    |
| 25    | 3.899           | 1559.500       | 129.5  |
| 26    | 3.350           | 1339.849       | 994.3  |
| 27    | 3.290           | 1315.738       | 3.7    |
| 28    | 3.228           | 1291.145       | 2.5    |
| 29    | 2.512           | 1004.706       | 15.4   |
| 30    | 2.508           | 1003.018       | 32.9   |
| 31    | 2.503           | 1001.089       | 45.6   |
| 32    | 2.499           | 999.701        | 12.9   |
| 33    | 2.197           | 878.605        | 182.0  |
| 34    | -0.000          | -0.000         | 69.7   |
| 35    | -0.000          | -0.000         | 3.3    |
| 36    | -0.008          | -3.134         | 3.3    |





Entry 8



6.  
6.  
roderick\_sorenson\_alchey 4676088/h1/ds  
no  
chem400 1H OBSERVE

exp2 std1h

## SAMPLE

Date Aug 12 99  
Solvent DMSO  
File o/0812/0601

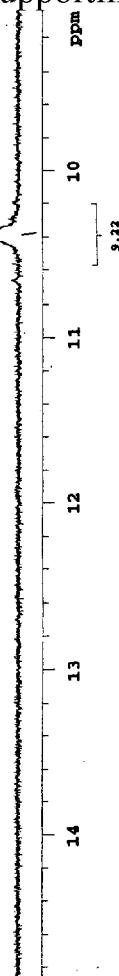
## ACQUISITION

freq 400.123  
t1 H1  
t2 H1  
at 3.004  
sw 8000.0  
pw 4.2  
d1 1.000  
nt 16

514

| INDEX | (PPM)  | (Hz)     | HEIGHT |
|-------|--------|----------|--------|
| 1     | 10.386 | 415.412  | 171.6  |
| 2     | 9.785  | 3419.094 | 182.2  |
| 3     | 7.985  | 3158.813 | 46.7   |
| 4     | 7.889  | 3156.615 | 51.3   |
| 5     | 7.876  | 3151.264 | 130.8  |
| 6     | 7.871  | 3149.555 | 132.5  |
| 7     | 7.856  | 3143.451 | 135.7  |
| 8     | 7.622  | 3049.698 | 52.6   |
| 9     | 7.616  | 3047.501 | 58.4   |
| 10    | 7.607  | 3043.595 | 68.6   |
| 11    | 7.601  | 3041.353 | 68.4   |
| 12    | 7.480  | 2992.812 | 51.9   |
| 13    | 7.449  | 2980.360 | 114.6  |
| 14    | 7.439  | 2976.698 | 111.1  |
| 15    | 7.428  | 2972.553 | 144.5  |
| 16    | 7.418  | 2965.397 | 149.5  |
| 17    | 7.413  | 2965.467 | 154.8  |
| 18    | 7.396  | 2959.364 | 132.0  |
| 19    | 7.372  | 2949.598 | 41.3   |
| 20    | 7.349  | 2940.310 | 34.0   |
| 21    | 7.253  | 2901.989 | 96.3   |
| 22    | 7.231  | 2893.199 | 98.1   |
| 23    | 7.216  | 2887.340 | 167.6  |
| 24    | 7.144  | 2858.286 | 103.0  |
| 25    | 7.125  | 2850.962 | 92.3   |
| 26    | 6.701  | 2681.279 | -2.6   |
| 27    | 5.718  | 2287.956 | 8.0    |
| 28    | 3.300  | 1320.398 | 192.0  |
| 29    | 2.812  | 894.581  | 233.0  |
| 30    | 2.042  | 816.964  | 7.5    |

Entry 8

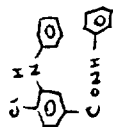


S15

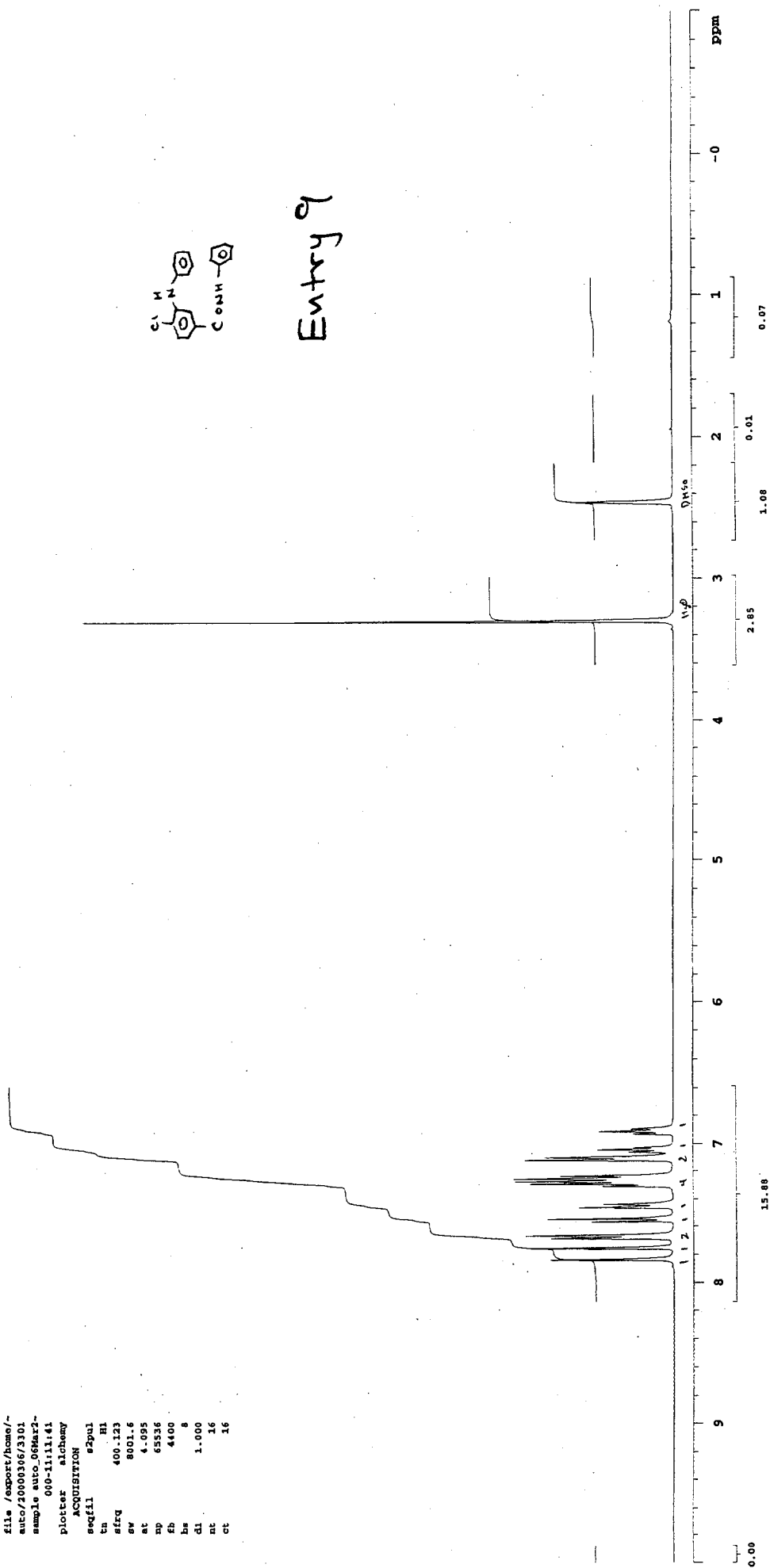
Ref: 732736/HI/dmsc  
 barton: HI OBSERVE

exp2 s2pul

NAME  
 user: rodrick sore-  
 nson  
 date: Mar 6 2000  
 solvent: dmsc  
 spin: not used  
 gain: not used  
 temp: not used  
 file: /export/home/~  
 auto/20000306/3301  
 sample: auto\_06Mar2-  
 000-11111.41  
 plotter: alchemy  
 ACQUISITION  
 seqfil s2pul  
 tn HI  
 sfreq 400.123  
 gw 8001.6  
 at 4.095  
 zp 65536  
 fs 4400  
 bs 8  
 dl 1.000  
 nt 16  
 ct 16



Entry 9



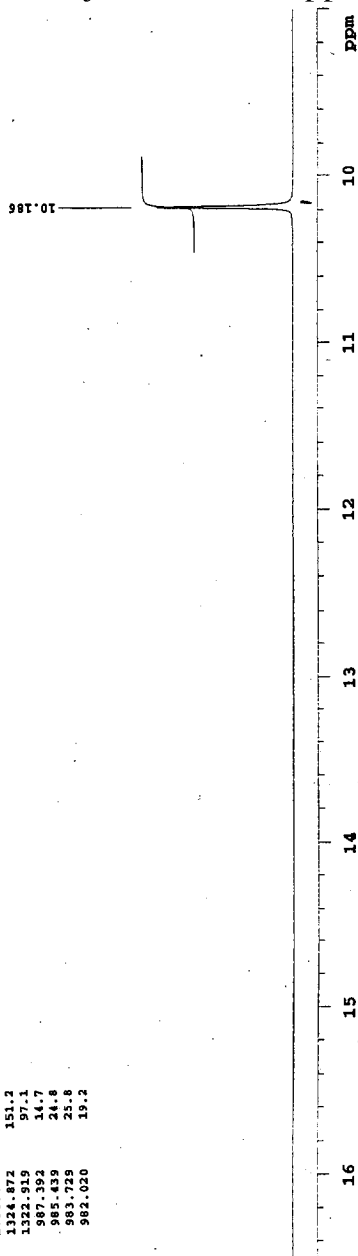
S16

(1)

Rod 73127a36/HI/dmsc  
 bartoni HI OBSERVE  
 exp2 s2pul  
 SAMPLE  
 user roderick more-  
 nson  
 date Mar 6 2000  
 solvent dmsc  
 spin not used  
 gain not used  
 temp not used  
 file /export/home/-  
 auto/20000306/3301  
 sample auto 06a2-  
 000-111141  
 Plotter alchemy  
 ACQUISITION  
 seqfil s2pul  
 tn HI  
 tn 400.123  
 sw 8001.6  
 at 4.095  
 xp 65536  
 fb 4400  
 bs 8  
 d1 1.000  
 nt 16  
 ct 16

| INDEX | (PPM) | (HZ)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 7.837 | 3133.837 | 31.6   |
| 2     | 7.837 | 3133.837 | 31.6   |
| 3     | 7.755 | 3103.114 | 37.6   |
| 4     | 7.688 | 3076.253 | 31.5   |
| 5     | 7.668 | 3068.194 | 38.1   |
| 6     | 7.563 | 3025.948 | 21.0   |
| 7     | 7.558 | 3023.994 | 14.9   |
| 8     | 7.542 | 3017.645 | 32.3   |
| 9     | 7.537 | 3015.692 | 21.9   |
| 10    | 7.458 | 2984.190 | 15.4   |
| 11    | 7.453 | 2982.237 | 24.3   |
| 12    | 7.437 | 2975.888 | 13.3   |
| 13    | 7.433 | 2973.934 | 18.1   |
| 14    | 7.312 | 2925.583 | 18.1   |
| 15    | 7.307 | 2923.629 | 16.9   |
| 16    | 7.290 | 2915.624 | 27.9   |
| 17    | 7.277 | 2909.710 | 40.6   |
| 18    | 7.272 | 2907.756 | 41.0   |
| 19    | 7.266 | 2905.802 | 15.0   |
| 20    | 7.244 | 2897.745 | 15.0   |
| 21    | 7.237 | 2895.791 | 29.1   |
| 22    | 7.233 | 2894.082 | 20.9   |
| 23    | 7.133 | 2849.882 | 38.1   |
| 24    | 7.102 | 2841.579 | 33.0   |
| 25    | 7.068 | 2828.148 | 11.4   |
| 26    | 7.066 | 2827.172 | 11.6   |
| 27    | 7.050 | 2820.823 | 19.5   |
| 28    | 7.032 | 2813.497 | 10.4   |
| 29    | 7.029 | 2812.476 | 8.9    |
| 30    | 6.932 | 2771.653 | 10.4   |
| 31    | 6.930 | 2770.629 | 10.4   |
| 32    | 6.931 | 2769.605 | 15.1   |
| 33    | 6.911 | 2765.367 | 15.1   |
| 34    | 6.896 | 2759.285 | 10.9   |
| 35    | 6.893 | 2758.064 | 9.9    |
| 36    | 3.311 | 1324.872 | 151.2  |
| 37    | 3.306 | 1322.919 | 97.1   |
| 38    | 2.468 | 987.392  | 14.7   |
| 39    | 2.463 | 985.439  | 24.8   |
| 40    | 2.459 | 983.729  | 25.8   |
| 41    | 2.454 | 982.020  | 19.2   |

Entry 9



S17

sorenson alchemy 61477x31a  
STANDARD IN OBSERVE

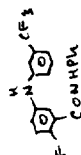
exp2 stdih

SAMPLE

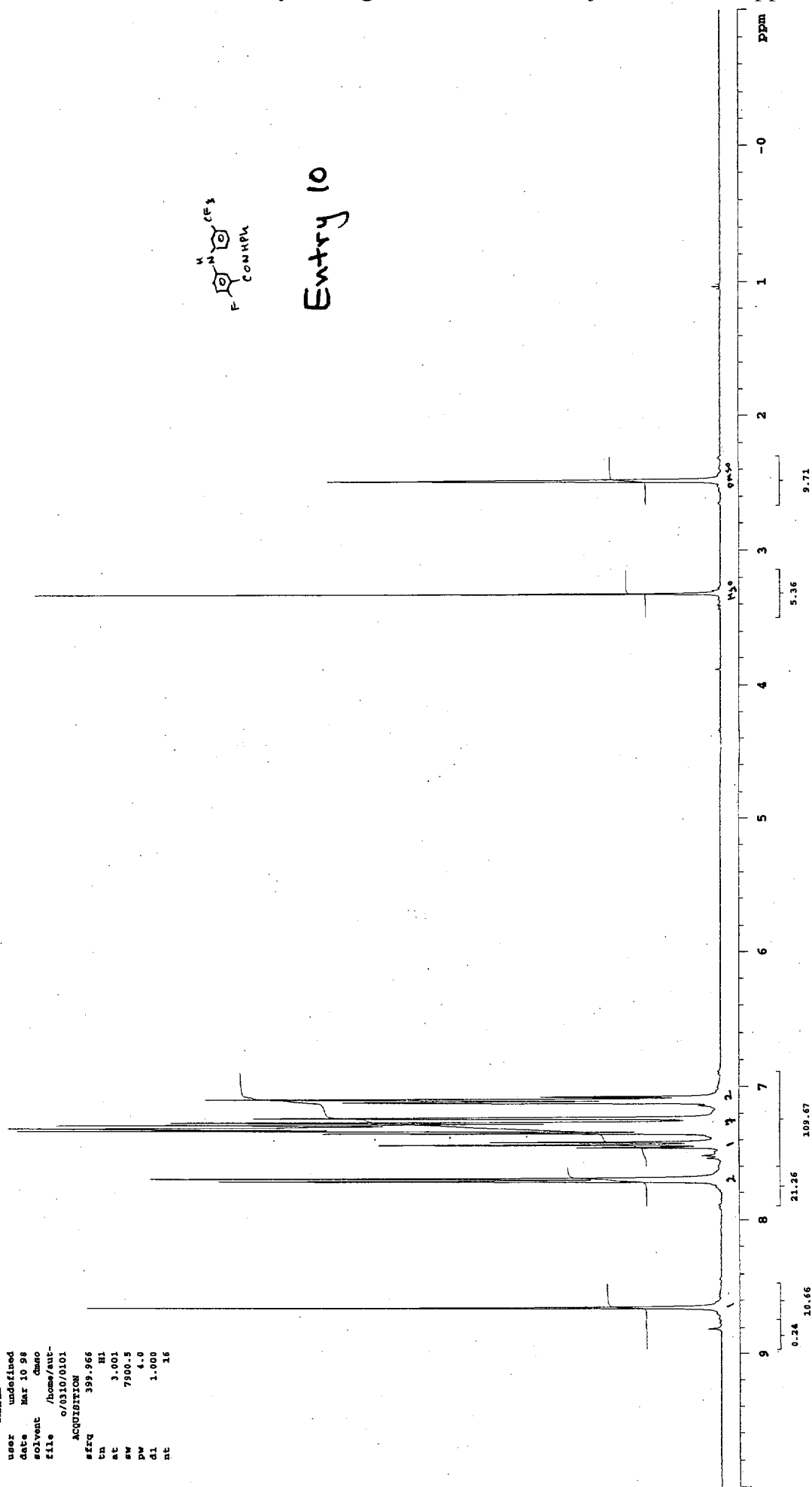
user undefined  
date Mar 10 98  
solvent chmo  
file /home/aut-  
o/0310/0101

ACQUISITION

sfreq 399.966  
tn H1  
at 3.001  
sw 7900.5  
pw 4.0  
gi 1.000  
nt 16



Entry 10



exp1 stdth  
 sorenson alchemy 61477211a  
 STANDARD IN OBSERVE

exp1 stdth

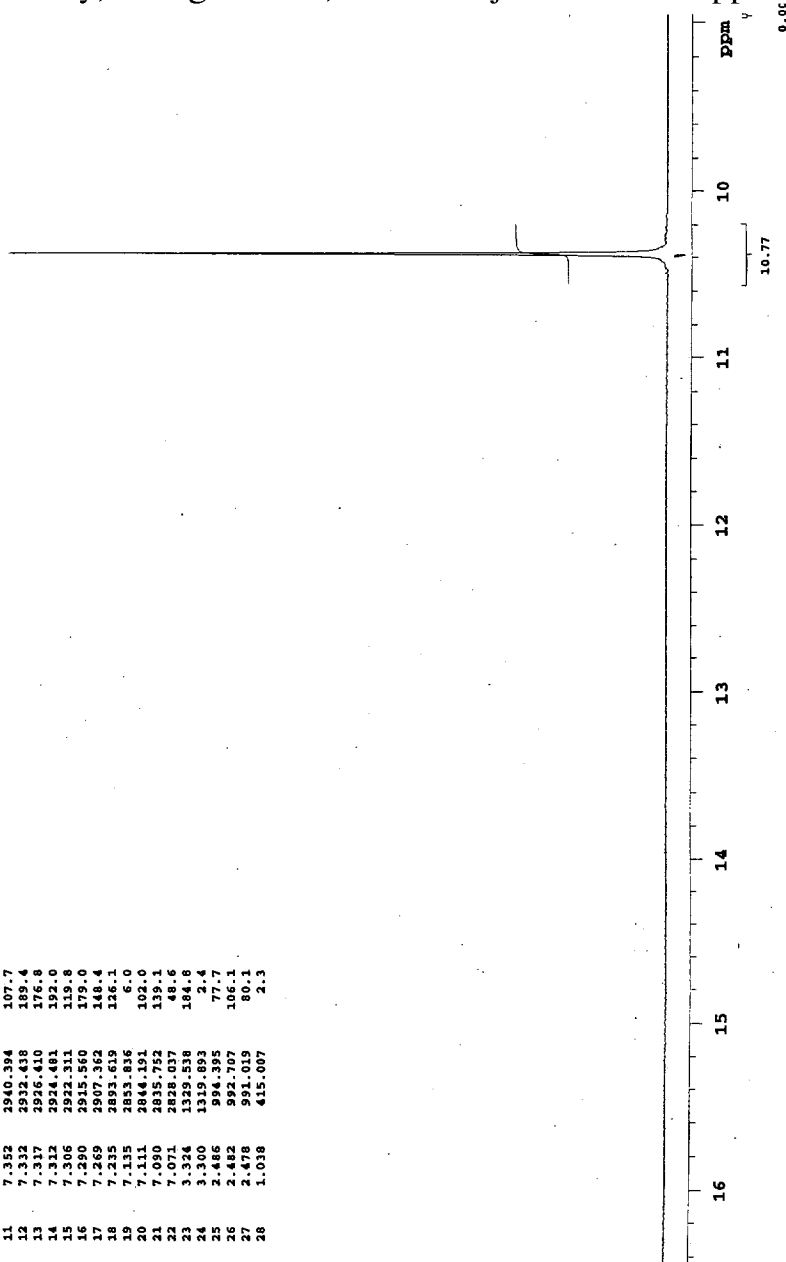
SAMPLE  
 user undefined  
 date Mar 10 98  
 solvent dmsc  
 file c:/home/aut-

ACQUISITION

sfreq 399.966  
 tn H1  
 at 3.001  
 sw 7900.5  
 pw 4.0  
 d1 1.000  
 nt 16

| INDEX | PPM    | (HZ)     | HEIGHT |
|-------|--------|----------|--------|
| 1     | 10.380 | 4151.490 | 134.1  |
| 2     | 8.807  | 3522.434 | 3.7    |
| 3     | 8.656  | 3462.156 | 171.1  |
| 4     | 7.711  | 3084.096 | 135.7  |
| 5     | 7.692  | 3076.380 | 134.0  |
| 6     | 7.534  | 3013.451 | 3.8    |
| 7     | 7.513  | 3004.771 | 5.1    |
| 8     | 7.432  | 2980.660 | 38.8   |
| 9     | 7.432  | 2972.703 | 62.3   |
| 10    | 7.342  | 2948.762 | 67.1   |
| 11    | 7.342  | 2940.394 | 107.7  |
| 12    | 7.312  | 2932.438 | 189.4  |
| 13    | 7.312  | 2926.410 | 176.8  |
| 14    | 7.312  | 2924.481 | 192.0  |
| 15    | 7.306  | 2922.311 | 119.8  |
| 16    | 7.290  | 2915.560 | 179.0  |
| 17    | 7.269  | 2907.362 | 148.4  |
| 18    | 7.235  | 2893.619 | 126.1  |
| 19    | 7.135  | 2853.836 | 6.0    |
| 20    | 7.111  | 2844.191 | 102.0  |
| 21    | 7.090  | 2835.752 | 139.1  |
| 22    | 7.071  | 2828.037 | 48.6   |
| 23    | 3.324  | 1329.538 | 184.6  |
| 24    | 3.306  | 1324.395 | 14.4   |
| 25    | 2.406  | 964.395  | 77.7   |
| 26    | 2.482  | 982.707  | 106.1  |
| 27    | 2.478  | 981.019  | 80.1   |
| 28    | 1.038  | 415.007  | 2.3    |

Entry 10

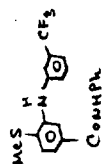


57447X115 /SORENSEN /H1 /DMSO /  
STANDARD IN OBSERVE

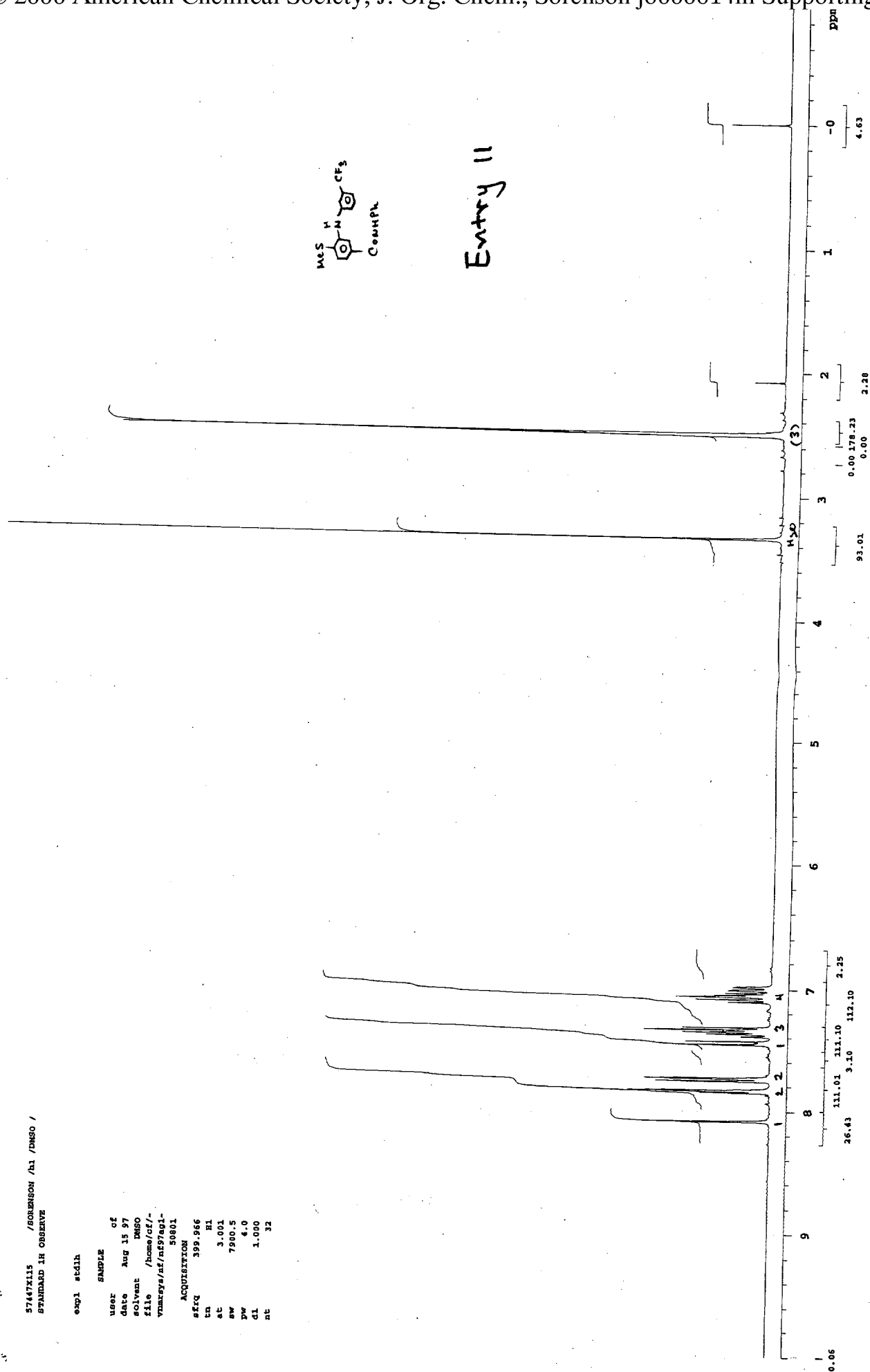
exp1 stdkh

user of  
date Aug 15 97  
solvent DMSO  
file /home/cf/-  
vnmrpy/mf/mf9/agl-  
50801

ACQUISITION  
sfreq 399.966  
tn H1  
at 3.001  
sw 7980.5  
pw 4.0  
cl 1.000  
nt 32



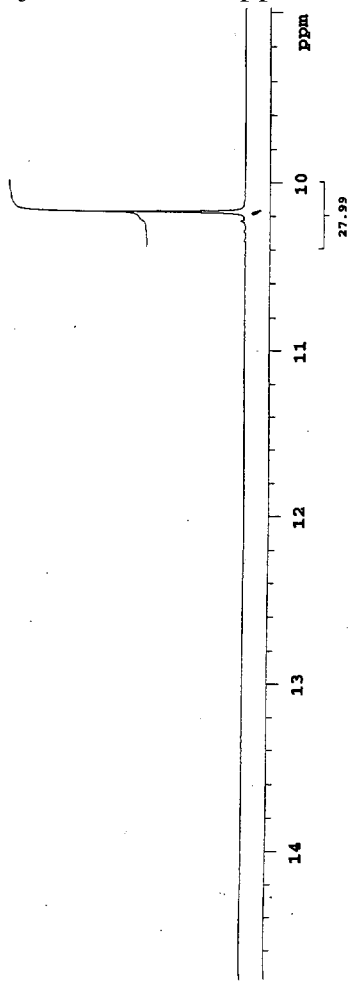
Entry 11



574

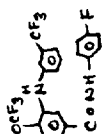
| INDEX | FREQUENCY (CPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.175          | 4069.697       | 29.9   |
| 2     | 8.085           | 3233.527       | 37.6   |
| 3     | 7.848           | 3139.012       | 11.5   |
| 4     | 7.843           | 3137.583       | 20.7   |
| 5     | 7.834           | 3133.226       | 28.4   |
| 6     | 7.830           | 3131.538       | 41.6   |
| 7     | 7.755           | 3101.861       | 11.6   |
| 8     | 7.753           | 3100.517       | 36.8   |
| 9     | 7.734           | 3093.478       | 32.4   |
| 10    | 7.732           | 3092.291       | 27.4   |
| 11    | 7.656           | 2979.156       | 5.1    |
| 12    | 7.642           | 2976.504       | 4.7    |
| 13    | 7.642           | 2973.370       | 24.9   |
| 14    | 7.634           | 2955.527       | 8.8    |
| 15    | 7.389           | 2947.571       | 18.8   |
| 16    | 7.370           | 2942.508       | 26.0   |
| 17    | 7.357           | 2940.338       | 27.9   |
| 18    | 7.351           | 2935.013       | 37.3   |
| 19    | 7.338           | 2926.394       | 26.1   |
| 20    | 7.317           | 2883.652       | 8.1    |
| 21    | 7.310           | 2882.682       | 21.1   |
| 22    | 7.107           | 2835.214       | 8.1    |
| 23    | 7.106           | 2827.719       | 21.3   |
| 24    | 7.089           | 2826.534       | 24.2   |
| 25    | 7.067           | 2820.265       | 16.9   |
| 26    | 7.051           | 2812.067       | 11.7   |
| 27    | 7.031           | 2802.905       | 11.9   |
| 28    | 6.987           | 2794.707       | 11.6   |
| 29    | 6.983           | 2793.019       | 10.8   |
| 30    | 3.339           | 1335.509       | 311.3  |
| 31    | 2.512           | 1004.706       | 22.1   |
| 32    | 2.508           | 1003.018       | 21.0   |
| 33    | 2.503           | 1001.081       | 92.8   |
| 34    | 2.499           | 997.231        | 76.8   |
| 35    | 2.493           | 989.516        | 194.2  |
| 36    | 2.472           | 980.624        | 5.5    |
| 37    | 2.077           | 830.624        | 9.0    |
| 38    | 0.000           | 0.000          | 17.4   |

Entry =

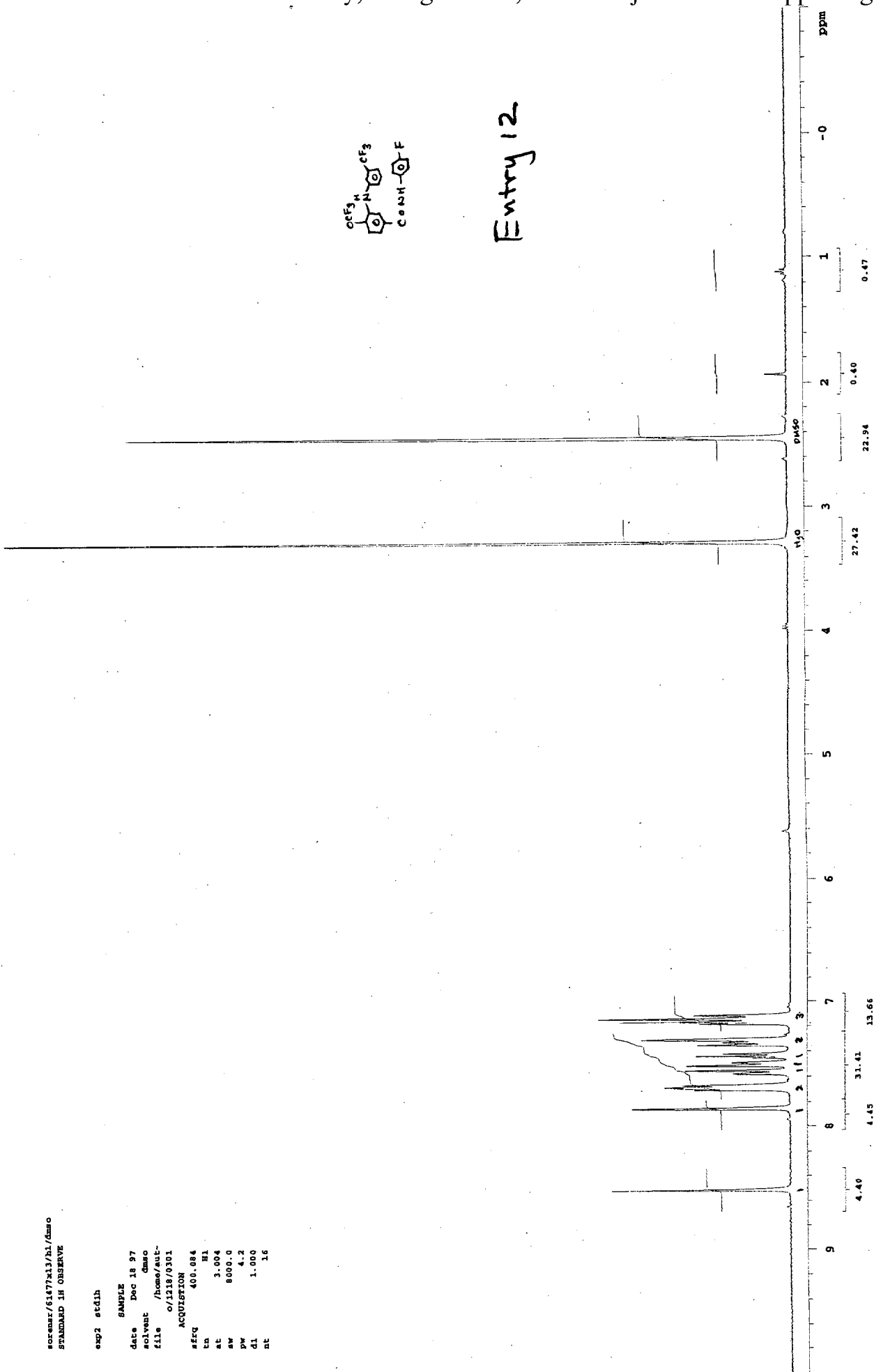


521

S22



Entry 12



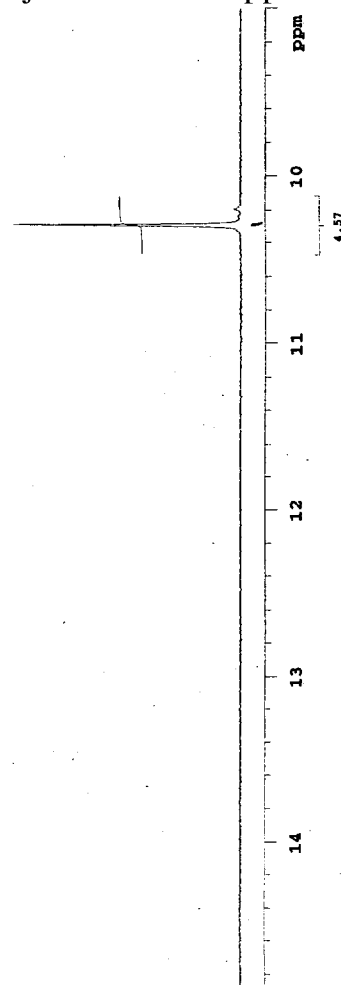
sorenson/61477013/bl/dmsd  
STANDARD IN OBSERVE

exp2 stdih

SAMPLE  
date Dec 18 97  
solvent dmsd  
file /home/aut-  
o/1218/0301  
ACQUISITION  
freq 400.084  
in H1  
at 3.004  
sw 8000.0  
pw 4.2  
d1 1.000  
nt 16

Entry 12

| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.295          | 4119.054       | 46.2   |
| 2     | 8.514           | 3406.142       | 52.2   |
| 3     | 7.854           | 3142.218       | 46.2   |
| 4     | 7.702           | 3081.425       | 28.0   |
| 5     | 7.689           | 3076.298       | 34.1   |
| 6     | 7.681           | 3073.124       | 36.7   |
| 7     | 7.668           | 3067.997       | 31.3   |
| 8     | 7.582           | 3033.572       | 16.8   |
| 9     | 7.561           | 3025.026       | 30.8   |
| 10    | 7.512           | 3005.495       | 30.3   |
| 11    | 7.490           | 2996.705       | 17.1   |
| 12    | 7.434           | 2975.061       | 21.3   |
| 13    | 7.434           | 2974.264       | 21.3   |
| 14    | 7.415           | 2966.675       | 18.6   |
| 15    | 7.344           | 2938.354       | 27.1   |
| 16    | 7.323           | 2929.609       | 19.9   |
| 17    | 7.305           | 2922.728       | 41.2   |
| 18    | 7.181           | 2872.922       | 26.6   |
| 19    | 7.160           | 2864.621       | 49.6   |
| 20    | 7.137           | 2855.588       | 56.0   |
| 21    | 7.115           | 2846.798       | 28.3   |
| 22    | 5.619           | 2248.147       | 2.2    |
| 23    | 3.287           | 1335.013       | 461.0  |
| 24    | 2.447           | 978.821        | 192.0  |
| 25    | 1.934           | 773.727        | 6.4    |
| 26    | 1.117           | 447.067        | 3.1    |

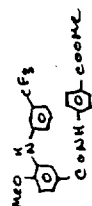


S23

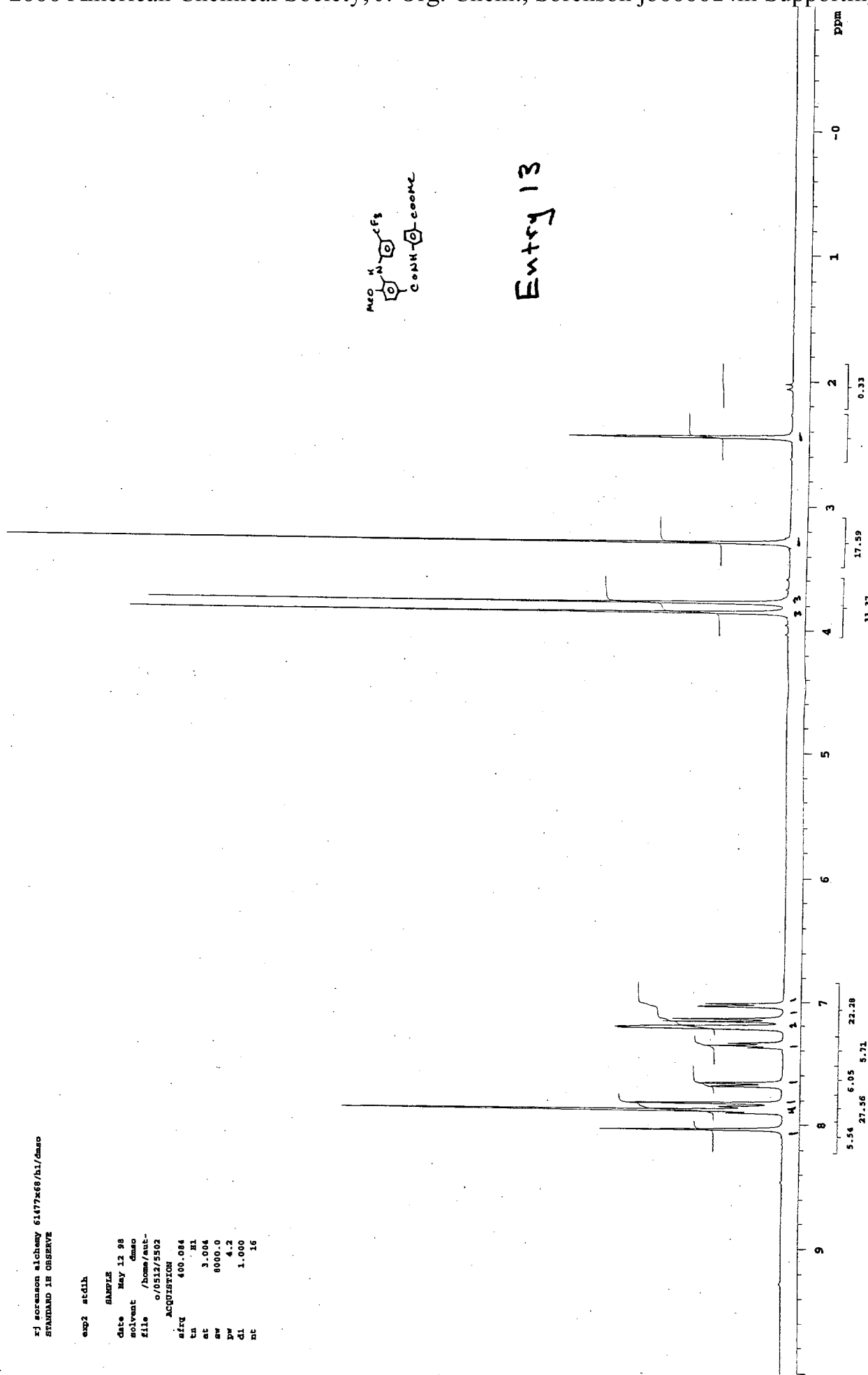
rj sorenson alchemy 61477x68/h1/dmsd  
STANDARD 1H OBSERVE

exp2 std1h

SAMPLE  
date May 12 98  
solvent dmsd  
file o/0512/5502  
ACQUISITION  
sfrq 400.084  
t1 11  
t2 3.004  
sw 8000.0  
pw 4.2  
d1 1.000  
nt 16



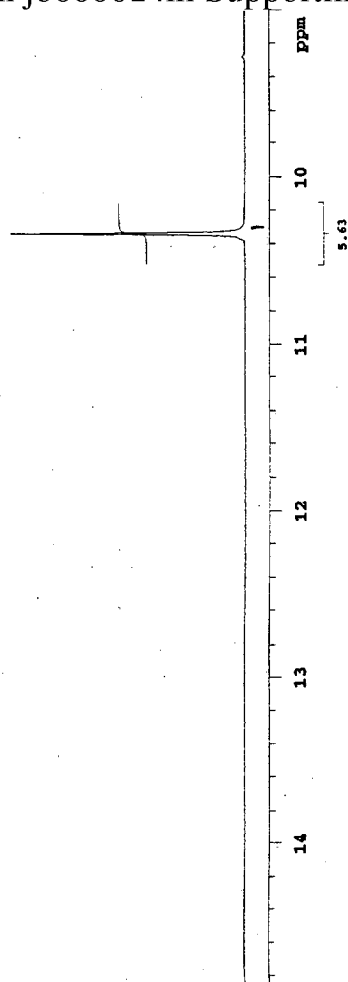
Entry 13



524

Entry 13

| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.342          | 4137.409       | 47.8   |
| 2     | 8.036           | 3115.118       | 53.0   |
| 3     | 7.903           | 3161.994       | 16.7   |
| 4     | 7.881           | 3152.960       | 128.6  |
| 5     | 7.873           | 3150.030       | 122.9  |
| 6     | 7.850           | 3140.753       | 18.7   |
| 7     | 7.836           | 3131.331       | 44.4   |
| 8     | 7.822           | 3123.278       | 44.9   |
| 9     | 7.687           | 3075.965       | 31.9   |
| 10    | 7.682           | 3073.612       | 20.8   |
| 11    | 7.666           | 3067.020       | 24.5   |
| 12    | 7.661           | 3065.967       | 24.6   |
| 13    | 7.312           | 2820.405       | 13.4   |
| 14    | 7.305           | 2814.361       | 13.2   |
| 15    | 7.313           | 2837.448       | 16.2   |
| 16    | 7.216           | 2687.983       | 48.3   |
| 17    | 7.211           | 2685.130       | 49.1   |
| 18    | 7.164           | 2664.086       | 35.1   |
| 19    | 7.142           | 2657.297       | 32.4   |
| 20    | 7.039           | 2616.036       | 25.1   |
| 21    | 7.019           | 2608.223       | 22.9   |
| 22    | 3.853           | 1541.339       | 192.0  |
| 23    | 3.774           | 1510.088       | 186.8  |
| 24    | 3.289           | 1315.746       | 266.0  |
| 25    | 2.445           | 978.333        | 64.9   |
| 26    | 2.020           | 806.162        | 2.3    |



S25

Rod 57447x63sm/H1/dmsd  
barton: H1 OBSERVE

exp2 s2pul

SAMPLE

user roderick sore~

date Mar 3 2000

solvent dmsd

spin not used

gain not used

temp not used

file /export/home/~

auto/20000303/2201

sample auto\_03Mar2~

000-09:45:13

plotter alchemyl

ACQUISITION

seqf11 s2pul

tn H1

sfreq 400.123

sw 8001.6

at 4.095

np 65536

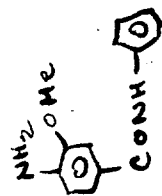
fb 4400

bs 8

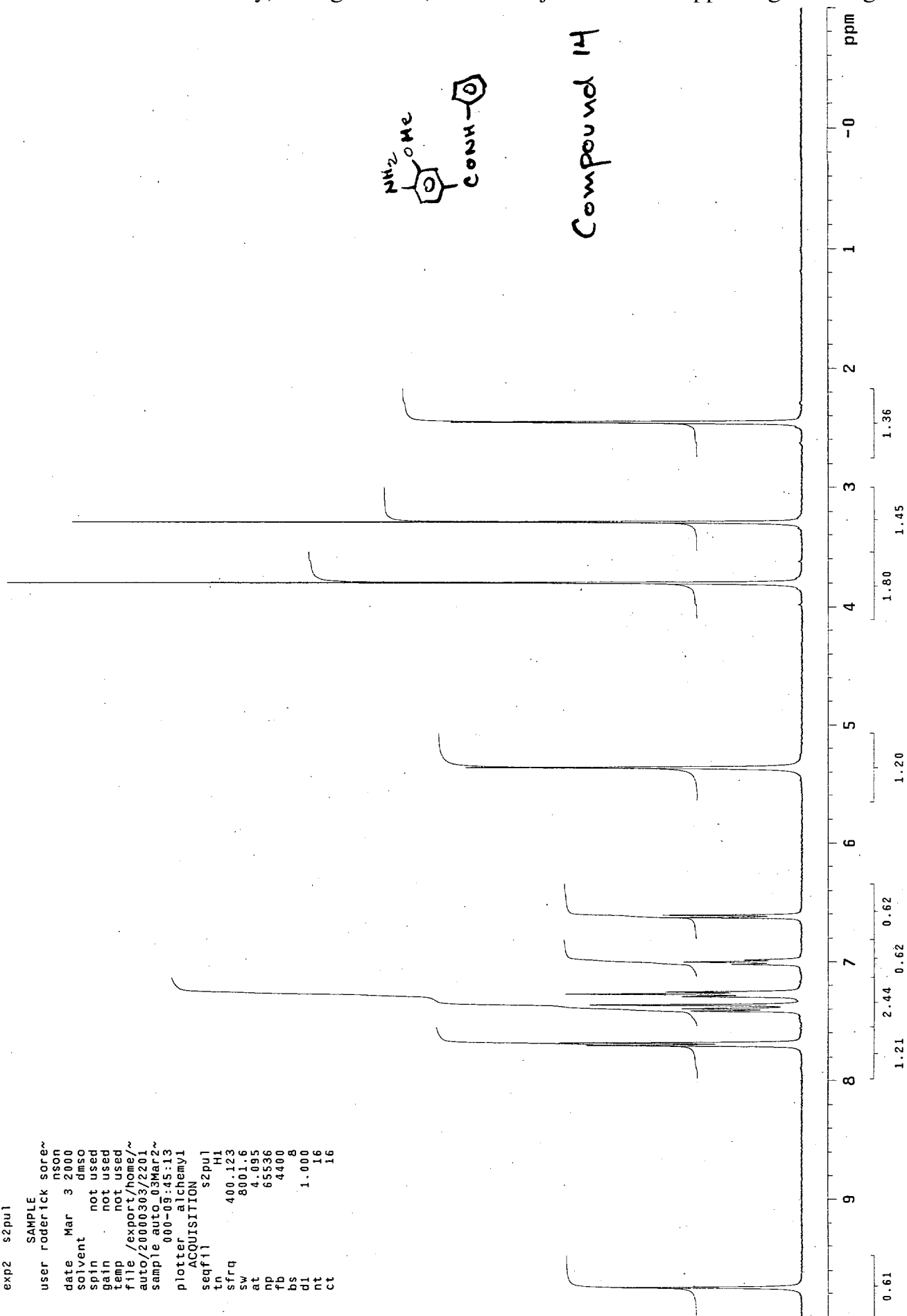
dl 1.000

nt 16

ct 16



Compound 14



574

Rod 57447x63sm/H1/dmsd  
barton: H1 OBSERVE

exp2 s2pul

SAMPLE

user roderick sore~

date Mar 3 2000

solvent dmsd

spin not used

gain not used

temp not used

file /export/home/~

auto/20000303/2201

sample auto\_03Mar2~

000-05:45:13

plotter alchemyl

ACQUISITION

seqf11 s2pul

tn H1

sfrq 400.123

sw 8001.6

at 4.095

np 65536

fb 4400

bs 8

dl 1.000

nt 16

ct 16

| INDEX | (PPM) | (H2)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 9.754 | 3902.615 | 34.3   |
| 2     | 7.706 | 3083.334 | 41.1   |
| 3     | 7.685 | 3075.032 | 46.3   |
| 4     | 7.417 | 2967.829 | 21.2   |
| 5     | 7.397 | 2959.771 | 22.9   |
| 6     | 7.365 | 2947.072 | 40.5   |
| 7     | 7.295 | 2918.746 | 22.9   |
| 8     | 7.275 | 2910.931 | 45.1   |
| 9     | 7.256 | 2903.361 | 26.0   |
| 10    | 7.021 | 2809.345 | 13.5   |
| 11    | 7.004 | 2802.264 | 22.6   |
| 12    | 6.986 | 2795.182 | 11.0   |
| 13    | 6.634 | 2654.524 | 27.1   |
| 14    | 6.615 | 2646.710 | 26.5   |
| 15    | 5.367 | 2147.327 | 64.1   |
| 16    | 3.806 | 1522.672 | 151.2  |
| 17    | 3.299 | 1319.988 | 138.7  |
| 18    | 2.461 | 984.706  | 66.9   |

Compound 14

9.754

16 15 14 13 12 11 10 ppm

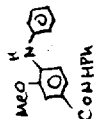
S27

57447X63 /SORENSEN /H1 /DMSO /  
STANDARD 1H OBSERVE

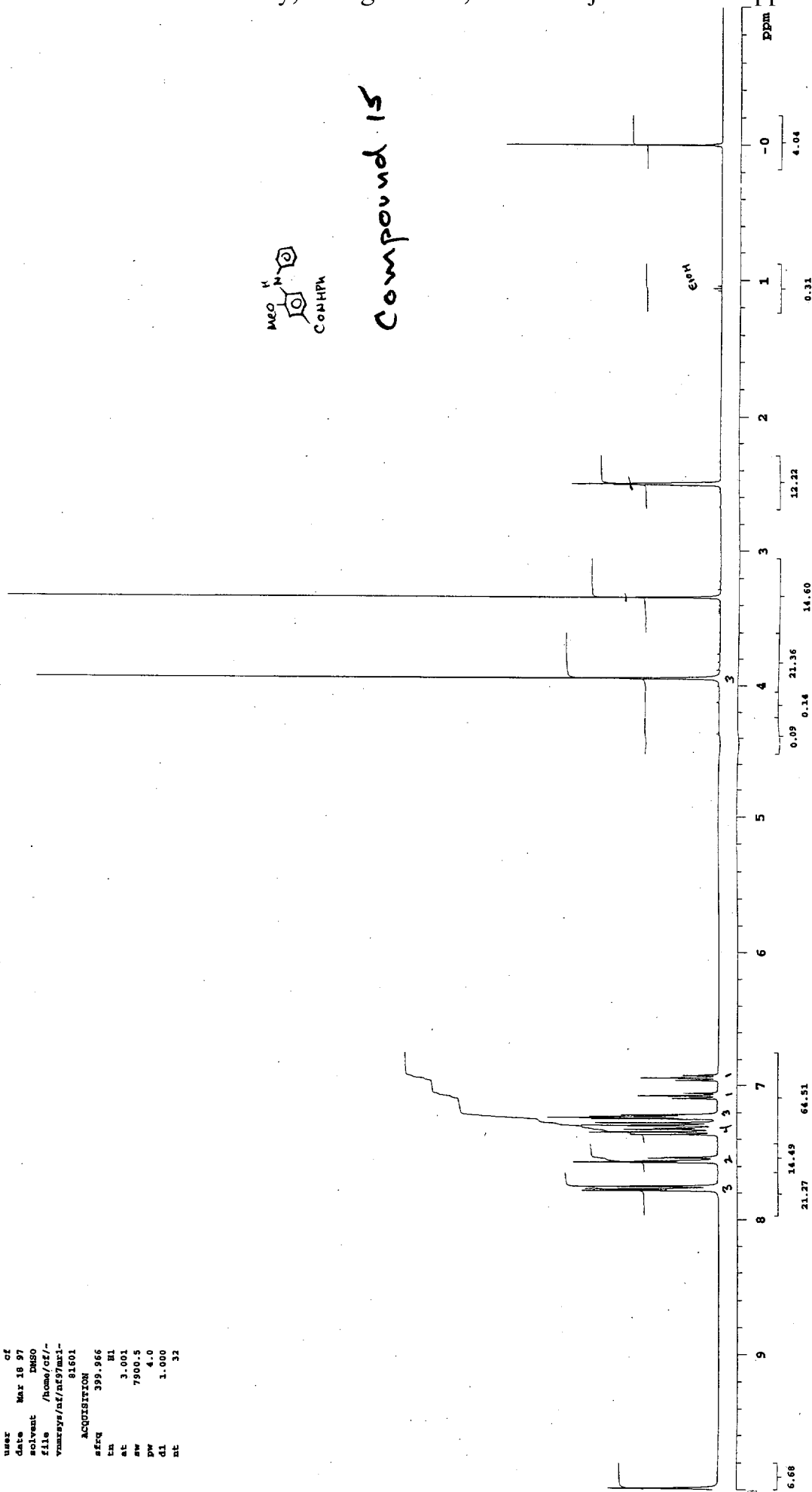
exp2 std1h

SAMPLE  
user cf  
date Mar 18 97  
solvent DMSO  
file /home/cf/-  
vnmrpy/mf/mf97mcl-  
81601

ACQUISITION  
sfreq 399.966  
tn H1  
at 3.001  
sw 7900.5  
pw 4.0  
d1 3.000  
nt 32



Compound 15



578

5747X63 /SORENSEN /h1 /DMISO /  
STANDARD IN OBSERVE

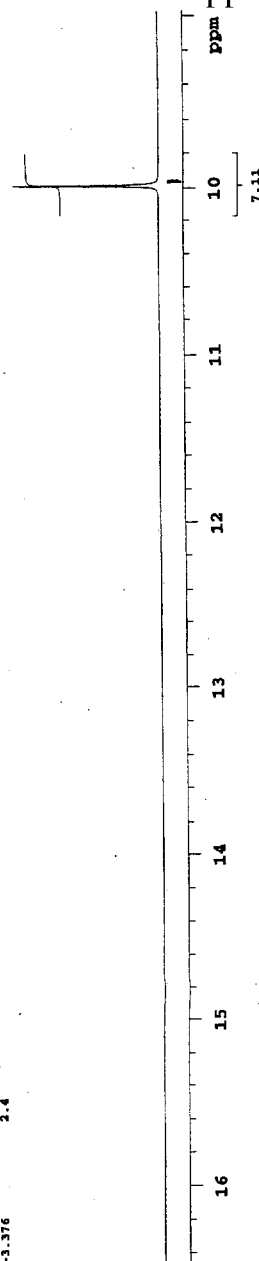
exp2 stdlh

SAMPLE

user cf  
date Mar 18 97  
solvent DMISO  
file /home/cf/-  
vname/sr/mf/mf/mf-  
81601  
ACQUISITION  
sfrq 399.966  
ta H1  
at 3.001  
sw 7900.5  
pw 4.0  
d1 1.000  
nt 32

| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 9.988           | 3994.712       | 29.7   |
| 2     | 7.781           | 3112.249       | 37.0   |
| 3     | 7.772           | 3108.632       | 30.1   |
| 4     | 7.769           | 3107.427       | 36.0   |
| 5     | 7.731           | 3099.352       | 31.6   |
| 6     | 7.710           | 3095.514       | 24.0   |
| 7     | 7.676           | 3087.619       | 39.3   |
| 8     | 7.565           | 3025.912       | 21.9   |
| 9     | 7.558           | 3023.038       | 11.2   |
| 10    | 7.553           | 3021.109       | 19.0   |
| 11    | 7.538           | 3014.841       | 15.4   |
| 12    | 7.533           | 3012.912       | 21.9   |
| 13    | 7.362           | 2944.436       | 8.4    |
| 14    | 7.357           | 2942.508       | 9.8    |
| 15    | 7.342           | 2936.721       | 23.6   |
| 16    | 7.326           | 2930.211       | 10.6   |
| 17    | 7.322           | 2928.523       | 17.3   |
| 18    | 7.317           | 2926.594       | 7.3    |
| 19    | 7.312           | 2924.665       | 37.0   |
| 20    | 7.296           | 2918.778       | 9.8    |
| 21    | 7.291           | 2916.207       | 33.2   |
| 22    | 7.279           | 2911.163       | 34.3   |
| 23    | 7.273           | 2908.993       | 37.5   |
| 24    | 7.244           | 2897.179       | 46.2   |
| 25    | 7.235           | 2893.803       | 34.8   |
| 26    | 7.232           | 2892.598       | 26.3   |
| 27    | 7.223           | 2888.981       | 20.5   |
| 28    | 7.213           | 2885.123       | 12.6   |
| 29    | 7.211           | 2884.159       | 7.6    |
| 30    | 7.097           | 2838.589       | 21.8   |
| 31    | 7.095           | 2837.625       | 6.1    |
| 32    | 7.092           | 2836.419       | 5.6    |
| 33    | 7.066           | 2831.881       | 6.9    |
| 34    | 7.066           | 2831.881       | 11.7   |
| 35    | 7.057           | 2822.676       | 6.9    |
| 36    | 7.055           | 2821.711       | 21.0   |
| 37    | 6.963           | 2784.822       | 5.9    |
| 38    | 6.960           | 2783.616       | 5.9    |
| 39    | 6.957           | 2782.410       | 5.9    |
| 40    | 6.942           | 2776.383       | 5.9    |
| 41    | 6.927           | 2770.596       | 5.4    |
| 42    | 6.923           | 2769.149       | 184.5  |
| 43    | 6.920           | 2767.944       | 133.6  |
| 44    | 3.945           | 1577.824       | 13.8   |
| 45    | 3.941           | 1576.518       | 28.8   |
| 46    | 2.811           | 1092.214       | 40.2   |
| 47    | 2.807           | 1092.536       | 28.5   |
| 48    | 2.802           | 1090.607       | 13.7   |
| 49    | 2.498           | 998.919        | 2.3    |
| 50    | 2.491           | 996.990        | 58.3   |
| 51    | 1.057           | 422.666        | -0.000 |
| 52    | -0.000          | -0.000         | -3.376 |
| 53    | -0.008          | -3.376         | 2.4    |

Compound 15



C19

Rod 72327x29sm/H1/dmsd  
barton: H1 OBSERVE

exp2 s2pul

user roderick sore~

date Mar 3 2000  
solvent dmsd  
spin not used  
gain not used  
temp not used  
file /export/home/~  
auto/20000303/2101  
sample auto\_03Mar2~  
000-09:40:23

plotter alchemyl

ACQUISITION

seqf11 s2pul

tn H1

sfreq 400.123

sw 8001.6

at 4.095

np 65536

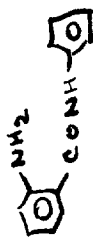
fb 4400

bs 8

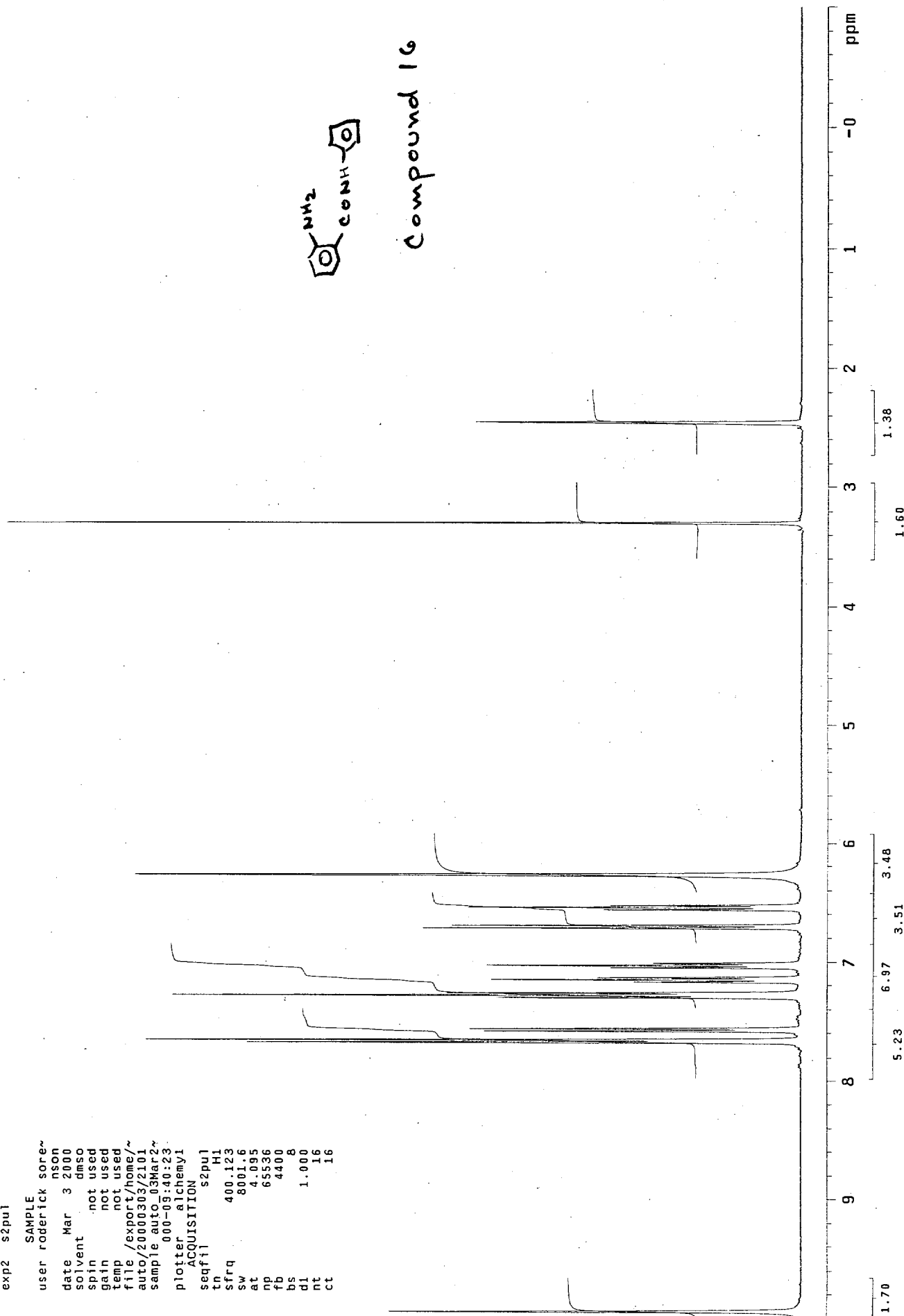
dl 1.000

nt 16

ct 16



Compound 16



Rod 72327x29sm/H1/dmsd  
barton: H1 OBSERVE

exp2 s2pul

SAMPLE  
user roderick sore~  
date Mar 3 2000  
solvent dmsd  
spin not used  
gain not used  
temp not used  
file /export/home/~  
auto/20000303/2101  
sample auto\_03Mar2~  
000-09:40:23  
plotter alchemyl  
ACQUISITION  
seqfil s2pul  
tn H1  
strq 400.123  
sw 8001.6  
at 4.095  
np 65536  
fb 4400  
bs 8  
dl 1.000  
nt 16  
ct 16

| INDEX | (PPM) | (HZ)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 9.952 | 3982.223 | 78.7   |
| 2     | 7.679 | 3072.590 | 105.5  |
| 3     | 7.658 | 3064.287 | 124.8  |
| 4     | 7.586 | 3035.227 | 60.4   |
| 5     | 7.566 | 3027.169 | 63.2   |
| 6     | 7.303 | 2922.164 | 58.0   |
| 7     | 7.285 | 2914.838 | 119.7  |
| 8     | 7.271 | 2909.466 | 28.1   |
| 9     | 7.267 | 2907.757 | 67.5   |
| 10    | 7.177 | 2871.860 | 31.9   |
| 11    | 7.160 | 2864.778 | 52.2   |
| 12    | 7.157 | 2863.557 | 59.1   |
| 13    | 7.143 | 2857.940 | 24.5   |
| 14    | 7.139 | 2856.475 | 39.0   |
| 15    | 7.052 | 2821.799 | 33.0   |
| 16    | 7.049 | 2820.578 | 36.3   |
| 17    | 7.034 | 2814.473 | 56.8   |
| 18    | 7.030 | 2813.008 | 60.0   |
| 19    | 7.018 | 2808.124 | 15.1   |
| 20    | 7.016 | 2807.148 | 27.0   |
| 21    | 7.013 | 2805.927 | 28.2   |
| 22    | 6.720 | 2688.712 | 72.1   |
| 23    | 6.699 | 2680.409 | 66.5   |
| 24    | 6.571 | 2629.128 | 21.5   |
| 25    | 6.568 | 2627.907 | 37.7   |
| 26    | 6.548 | 2620.093 | 63.6   |
| 27    | 6.534 | 2614.232 | 23.6   |
| 28    | 6.531 | 2613.011 | 36.5   |
| 29    | 6.277 | 2511.669 | 126.8  |
| 30    | 3.307 | 1323.163 | 151.2  |
| 31    | 3.303 | 1321.698 | 140.0  |
| 32    | 2.467 | 987.148  | 34.0   |
| 33    | 2.463 | 985.439  | 57.9   |
| 34    | 2.459 | 983.729  | 62.1   |

Compound 16

9.956.6

16 15 14 13 12 11 10 ppm

Mod 7232723A/HL/dmsd  
 Barton: H1 OBSERVE

exp2 s2pul

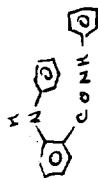
# SAMPLE

user roderick sore-  
 nson  
 date Mar 15 2000  
 solvent dmsd  
 spin not used  
 gain not used  
 temp not used  
 file /export/home/~  
 auto/20000315/0601  
 sample auto\_15mar2-  
 000-08:47:57

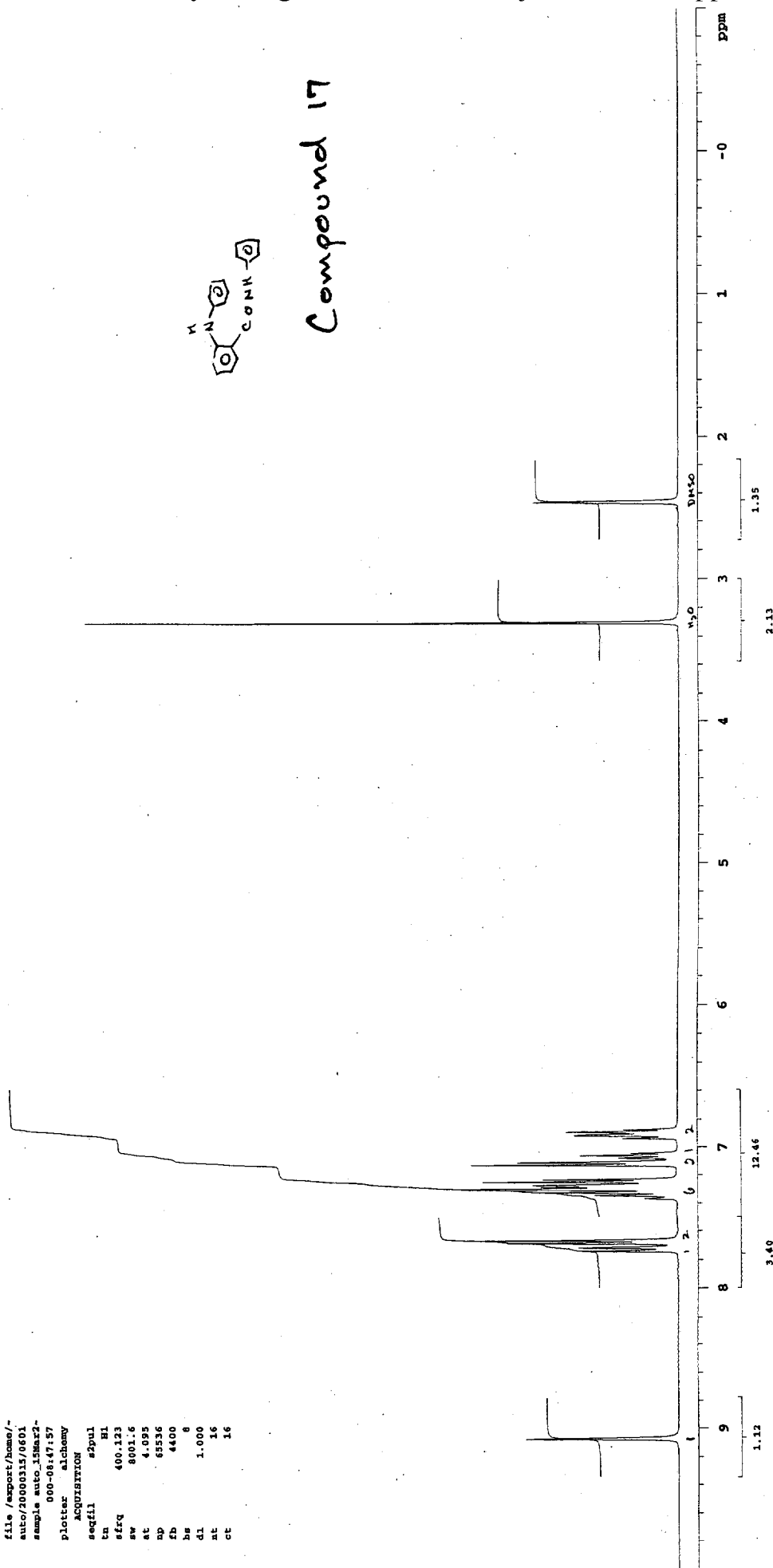
Plotter alchemy

# ACQUISITION

seqfil s2pul  
 tn H1  
 sfreq 400.123  
 sw 8001.6  
 at 4.095  
 xp 65536  
 fb 4400  
 bs 8  
 di 1.000  
 at 16  
 ct 16



Compound 17



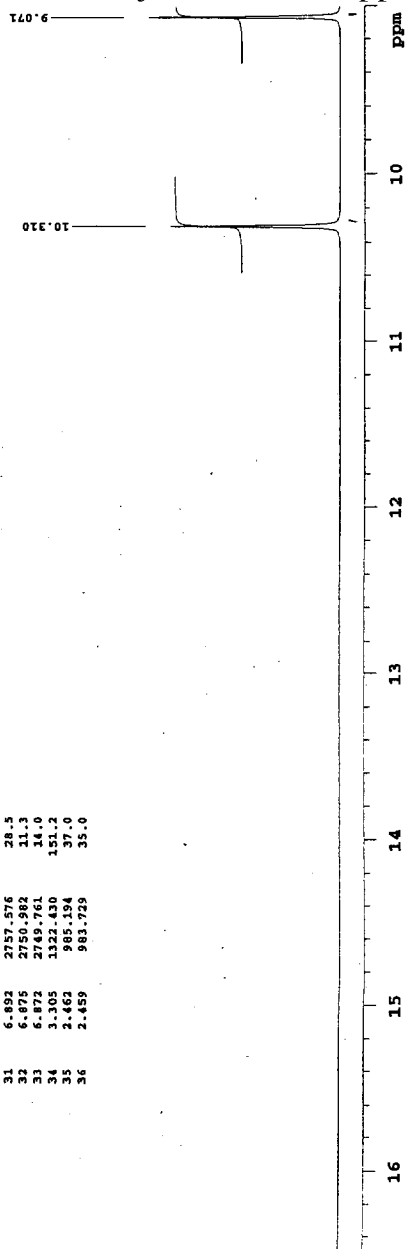
Red 7237429A/H1/dmsd  
 Barton: H1 OBSERVE  
 exp2 s2pul

SAMPLE  
 user roderick sore-  
 nson  
 date Mar 15 2000  
 solvent dmsd  
 spin not used  
 gain not used  
 temp not used  
 file /export/home/-  
 auto/20000315/0601  
 sample auto\_13mar21-  
 000-08:47:57  
 plotter alchemy

ACQUISITION  
 seqfil s2pul  
 tn H1  
 sw 400.123  
 sr 8001.6  
 at 4.095  
 up 65536  
 zb 4400  
 bs 8  
 cl 1.000  
 nc 16  
 cc 16

| INDEX | (PPM) | (Hz)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 9.071 | 3629.159 | 38.9   |
| 2     | 7.733 | 3086.775 | 23.7   |
| 3     | 7.713 | 3086.265 | 23.2   |
| 4     | 7.685 | 3075.032 | 43.5   |
| 5     | 7.664 | 3066.485 | 50.2   |
| 6     | 7.367 | 2947.805 | 8.7    |
| 7     | 7.346 | 2939.502 | 21.3   |
| 8     | 7.326 | 2931.200 | 36.7   |
| 9     | 7.304 | 2922.653 | 53.4   |
| 10    | 7.301 | 2921.187 | 55.2   |
| 11    | 7.298 | 2920.311 | 54.7   |
| 12    | 7.291 | 2917.280 | 24.1   |
| 13    | 7.286 | 2915.327 | 35.0   |
| 14    | 7.275 | 2910.931 | 37.1   |
| 15    | 7.254 | 2902.384 | 49.7   |
| 16    | 7.235 | 2895.056 | 34.4   |
| 17    | 7.131 | 2823.501 | 40.6   |
| 18    | 7.111 | 2814.998 | 40.6   |
| 19    | 7.084 | 2834.198 | 15.2   |
| 20    | 7.081 | 2833.277 | 15.0   |
| 21    | 7.065 | 2826.927 | 25.0   |
| 22    | 7.063 | 2826.195 | 23.5   |
| 23    | 7.047 | 2819.602 | 12.1   |
| 24    | 7.044 | 2818.625 | 11.1   |
| 25    | 6.936 | 2775.158 | 14.2   |
| 26    | 6.933 | 2774.181 | 13.8   |
| 27    | 6.917 | 2767.832 | 26.3   |
| 28    | 6.915 | 2766.855 | 26.5   |
| 29    | 6.910 | 2764.901 | 24.0   |
| 30    | 6.899 | 2760.506 | 16.4   |
| 31    | 6.896 | 2759.526 | 16.3   |
| 32    | 6.875 | 2750.781 | 11.4   |
| 33    | 6.872 | 2749.761 | 14.0   |
| 34    | 3.105 | 1322.430 | 151.2  |
| 35    | 2.462 | 985.194  | 37.0   |
| 36    | 2.459 | 983.729  | 35.0   |

Compound 17

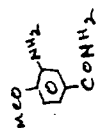


Mod 7132757/HL/duuo  
Barton: H1 OHSRVS

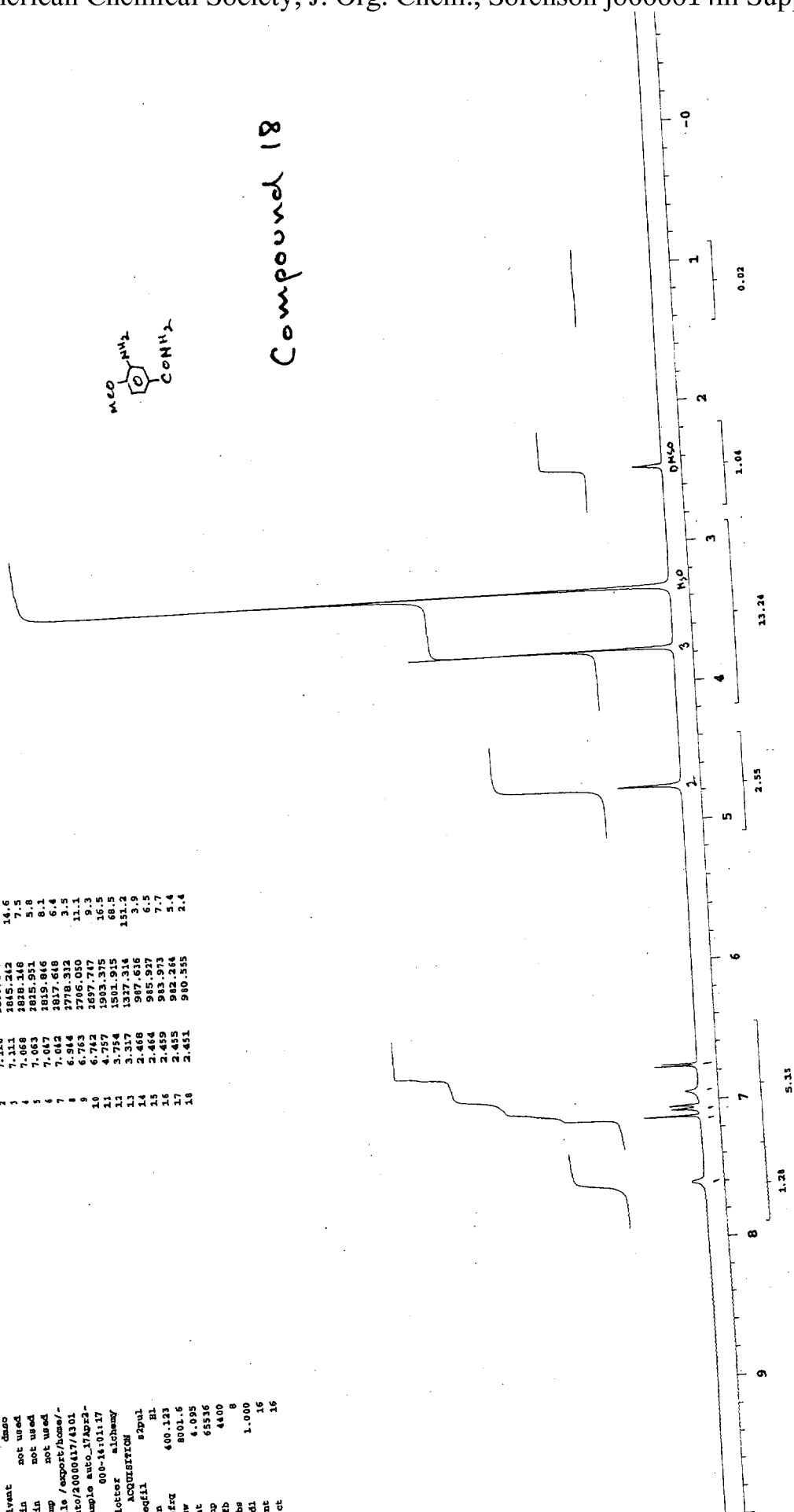
exp2 s2pul

SAMPLE  
user roderick sore-  
Date Apr 17 2000  
solvent dmsu  
spin not used  
gain not used  
temp not used  
file /export/home/-  
auto/2000417/4301  
sample auto.17Apr2-  
000-1810117  
plotter alchemy  
ACQUISITION  
seqfil s2pul  
tn H1  
sw 400.123  
sfreq 8001.6  
at 4.095  
ap 65536  
z0 4400  
hs 1.000  
dl 16  
nt 16  
ct

| INDEX | (PPM) | (Hz)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 7.595 | 1877.890 | 3.5    |
| 2     | 7.114 | 1817.440 | 14.1   |
| 3     | 7.058 | 1845.242 | 14.6   |
| 4     | 7.053 | 1828.118 | 7.5    |
| 5     | 7.053 | 1825.931 | 5.8    |
| 6     | 7.047 | 1819.846 | 8.1    |
| 7     | 7.042 | 1817.648 | 6.4    |
| 8     | 6.944 | 1778.312 | 3.5    |
| 9     | 6.763 | 1706.050 | 11.1   |
| 10    | 6.742 | 1697.747 | 9.3    |
| 11    | 4.757 | 1983.375 | 10.5   |
| 12    | 3.754 | 1501.915 | 18.5   |
| 13    | 3.317 | 1327.314 | 131.2  |
| 14    | 2.468 | 597.600  | 3.9    |
| 15    | 2.464 | 585.929  | 6.5    |
| 16    | 2.439 | 583.973  | 7.7    |
| 17    | 2.431 | 582.264  | 5.4    |
| 18    | 2.431 | 580.555  | 2.4    |



Compound 18



c 2d

william patt hockey 66934x57B  
auto400 STANDARD 1H OBSERVE

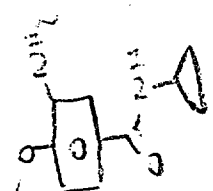
exp2 stdlh

SAMPLE

user undefined  
date Apr 23 99  
solvent dms  
file /home/aut-  
o/0423/0301

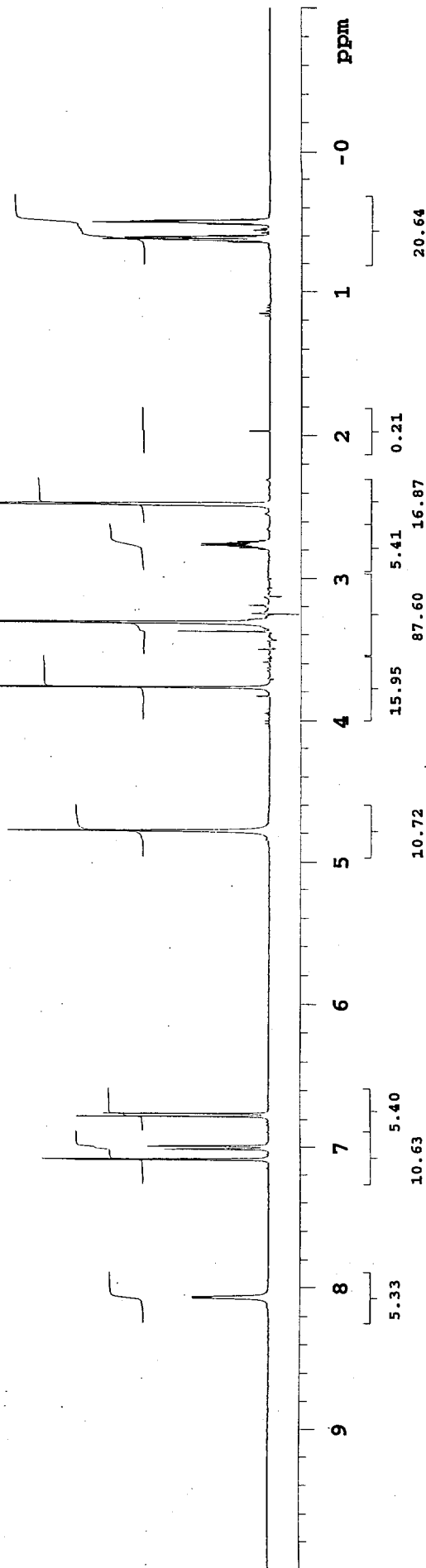
ACQUISITION

sfrq 399.966  
tn H1  
at 3.001  
sw 7900.5  
pw 6.9  
d1 1.000  
nt 16



Compound 19

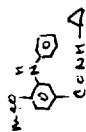
| INDEX | (PPM) | (HZ)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 8.073 | 3228.762 | 12.1   |
| 2     | 8.063 | 3224.904 | 12.2   |
| 3     | 7.093 | 2836.958 | 32.1   |
| 4     | 7.088 | 2834.788 | 36.1   |
| 5     | 7.018 | 2806.819 | 16.6   |
| 6     | 7.012 | 2804.649 | 14.6   |
| 7     | 6.997 | 2798.621 | 19.2   |
| 8     | 6.992 | 2796.452 | 17.4   |
| 9     | 6.778 | 2711.099 | 30.5   |
| 10    | 6.758 | 2702.901 | 26.2   |
| 11    | 4.784 | 1913.265 | 41.6   |
| 12    | 3.772 | 1508.683 | 192.0  |
| 13    | 3.377 | 1350.755 | 14.6   |
| 14    | 3.316 | 1326.162 | 1293.6 |
| 15    | 3.292 | 1316.759 | 3.5    |
| 16    | 3.254 | 1301.569 | -4.7   |
| 17    | 3.251 | 1300.122 | 2.9    |
| 18    | 3.192 | 1276.735 | 3.4    |
| 19    | 3.127 | 1250.695 | -2.1   |
| 20    | 2.784 | 1113.503 | 4.9    |
| 21    | 2.774 | 1103.645 | 6.8    |
| 22    | 2.766 | 1106.270 | 11.0   |
| 23    | 2.756 | 1102.171 | 10.9   |
| 24    | 2.748 | 1099.036 | 6.9    |
| 25    | 2.738 | 1094.938 | 5.1    |
| 26    | 2.492 | 996.565  | 25.1   |
| 27    | 2.487 | 994.877  | 53.0   |
| 28    | 2.483 | 992.948  | 71.7   |
| 29    | 2.478 | 991.260  | 50.8   |
| 30    | 2.474 | 989.572  | 23.1   |
| 31    | 1.970 | 788.004  | 3.3    |
| 32    | 0.646 | 258.527  | 6.8    |
| 33    | 0.634 | 253.463  | 17.1   |
| 34    | 0.628 | 251.293  | 26.7   |
| 35    | 0.617 | 246.712  | 23.1   |
| 36    | 0.610 | 244.060  | 20.0   |
| 37    | 0.599 | 239.720  | 10.1   |
| 38    | 0.560 | 224.048  | 2.7    |
| 39    | 0.520 | 208.135  | 10.1   |
| 40    | 0.510 | 204.036  | 28.3   |
| 41    | 0.502 | 200.901  | 22.3   |
| 42    | 0.493 | 197.285  | 18.4   |
| 43    | 0.482 | 192.704  | 6.4    |



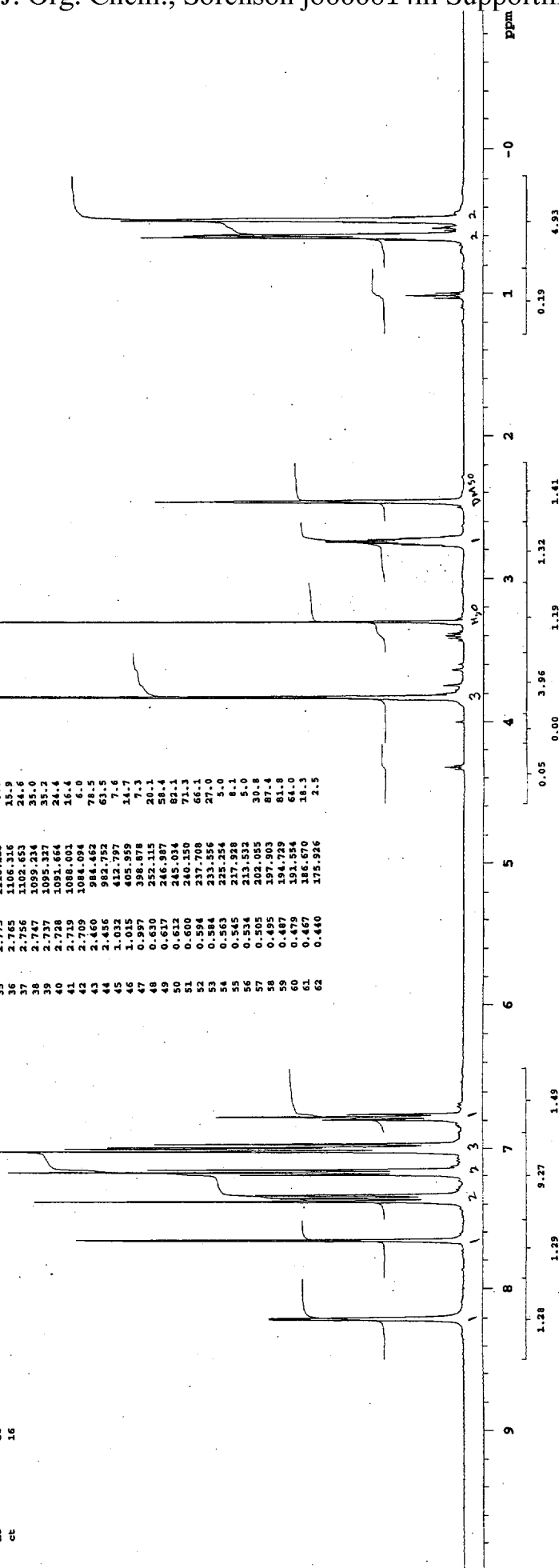
S35

Rod 71317216/H1/dmsd  
 bartoni: H1 OBSERVE  
 exp2 a2pul  
 SAMPLEX  
 user rodarich score-  
 mon  
 date Feb 16 2000  
 solvent dmsd  
 spin not used  
 gain not used  
 temp not used  
 file /export/home/-  
 auto/20000216/0701  
 sample auto\_16Feb2-  
 000-0910138  
 plotter alchemy  
 ACQUISITION  
 seqfil a2pul  
 tn H1  
 sw 400.123  
 at 8001.6  
 mp 4.095  
 fb 65536  
 4400  
 bs 8  
 dl 1.000  
 nt 16  
 ct 16

| INDEX | (PPM) | (HZ)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 8.200 | 3280.797 | 49.3   |
| 2     | 7.664 | 3066.729 | 90.0   |
| 3     | 7.660 | 3064.775 | 98.6   |
| 4     | 7.379 | 2952.445 | 109.3  |
| 5     | 7.357 | 2943.898 | 46.5   |
| 6     | 7.353 | 2941.944 | 46.9   |
| 7     | 7.336 | 2935.351 | 50.3   |
| 8     | 7.331 | 2933.397 | 52.8   |
| 9     | 7.173 | 2877.963 | 56.7   |
| 10    | 7.173 | 2877.963 | 135.8  |
| 11    | 7.173 | 2877.963 | 80.3   |
| 12    | 7.134 | 2852.356 | 125.6  |
| 13    | 7.129 | 2850.302 | 101.4  |
| 14    | 7.022 | 2807.331 | 90.6   |
| 15    | 6.980 | 2786.891 | 78.5   |
| 16    | 6.980 | 2786.891 | 35.7   |
| 17    | 6.980 | 2786.891 | 62.8   |
| 18    | 6.777 | 2711.657 | 29.5   |
| 19    | 6.777 | 2711.657 | 2.5    |
| 20    | 6.759 | 2704.341 | 2.5    |
| 21    | 4.338 | 1735.611 | 4.9    |
| 22    | 4.325 | 1730.483 | 2.3    |
| 23    | 4.312 | 1725.355 | 2.6    |
| 24    | 4.001 | 1600.815 | 466.7  |
| 25    | 3.823 | 1529.509 | 7.2    |
| 26    | 3.804 | 1521.939 | 5.3    |
| 27    | 3.774 | 1510.218 | 5.3    |
| 28    | 3.746 | 1498.700 | 3.2    |
| 29    | 3.634 | 1458.032 | 4.1    |
| 30    | 3.601 | 1446.084 | 4.3    |
| 31    | 3.401 | 1361.013 | 4.6    |
| 32    | 3.397 | 1359.060 | 4.1    |
| 33    | 3.384 | 1353.932 | 151.2  |
| 34    | 3.302 | 1321.209 | 5.8    |
| 35    | 2.775 | 1110.223 | 15.9   |
| 36    | 2.765 | 1106.316 | 24.6   |
| 37    | 2.756 | 1102.653 | 35.0   |
| 38    | 2.747 | 1099.234 | 35.2   |
| 39    | 2.737 | 1095.327 | 15.4   |
| 40    | 2.728 | 1092.664 | 6.0    |
| 41    | 2.719 | 1089.094 | 78.5   |
| 42    | 2.710 | 1085.484 | 61.5   |
| 43    | 2.460 | 984.462  | 7.6    |
| 44    | 2.456 | 982.752  | 14.7   |
| 45    | 1.032 | 412.797  | 7.3    |
| 46    | 1.015 | 405.959  | 20.1   |
| 47    | 0.997 | 398.878  | 58.4   |
| 48    | 0.630 | 252.115  | 82.1   |
| 49    | 0.617 | 246.397  | 71.3   |
| 50    | 0.612 | 245.034  | 27.0   |
| 51    | 0.600 | 240.130  | 6.1    |
| 52    | 0.594 | 237.708  | 30.8   |
| 53    | 0.584 | 233.526  | 81.8   |
| 54    | 0.583 | 233.156  | 64.0   |
| 55    | 0.534 | 213.928  | 18.3   |
| 56    | 0.534 | 213.928  | 2.5    |
| 57    | 0.505 | 202.055  |        |
| 58    | 0.495 | 197.903  |        |
| 59    | 0.487 | 194.729  |        |
| 60    | 0.479 | 191.554  |        |
| 61    | 0.467 | 186.670  |        |
| 62    | 0.440 | 175.926  |        |



Compound 20



S 36

Pod 7437455M/HI/dmsd  
 barton: HI OBSERVE

exp2 s2pul

user rcdrick score-

date Mar 17 2000

solvent dmsd

spin not used

gain not used

temp not used

file /export/home/-

auto/2000317/2101

sample auto.17mar2-

000-09.10.46

Plotter alchemy

ACQUISITION

seqfil s2pul

tn HI

sfreq 400.123

sw 8001.6

at 4.095

up 65536

fb 4400

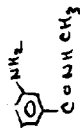
bm 8

dl 1.000

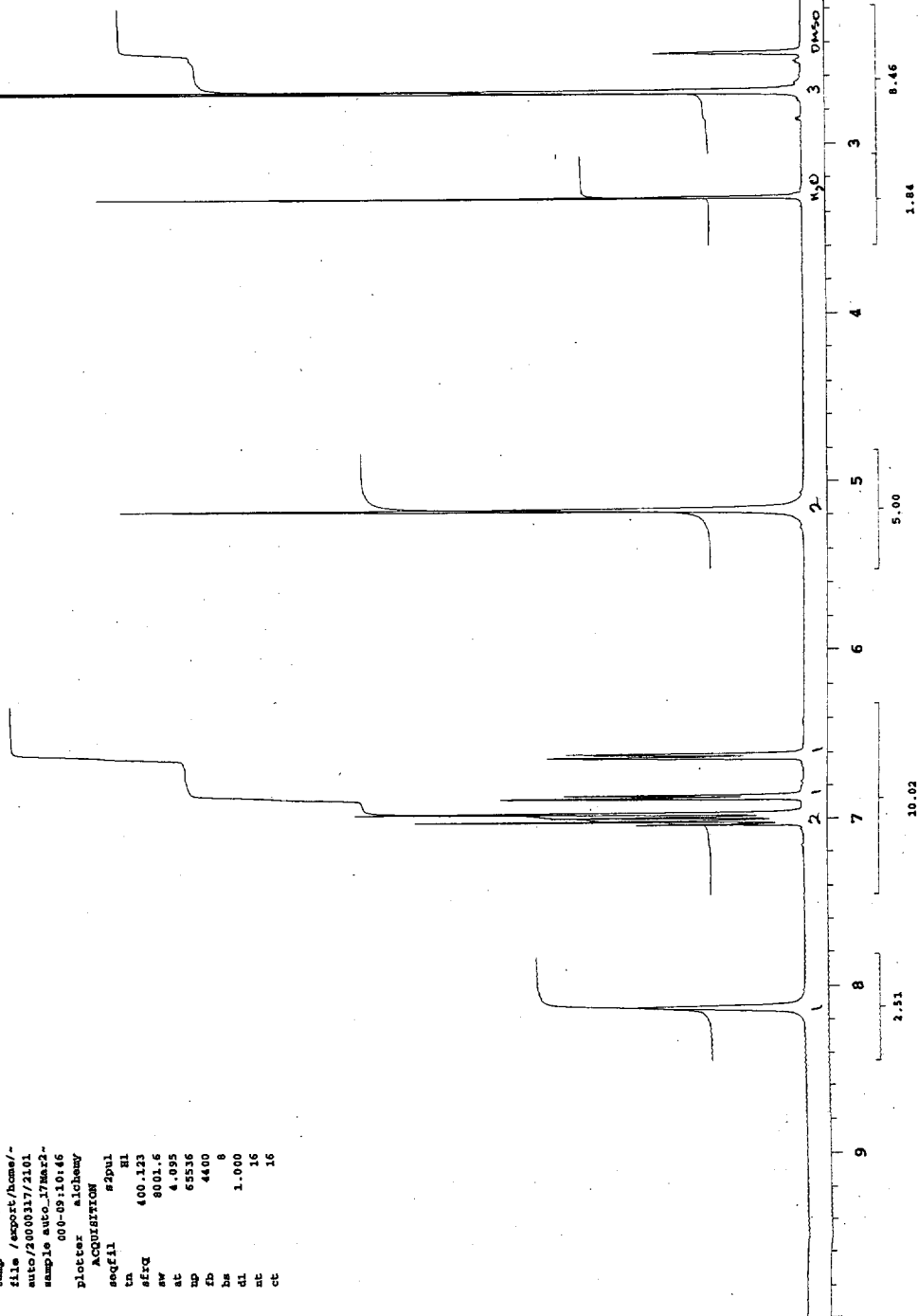
zc 16

ct 16

| INDEX | (PPM) | (HZ)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 8.140 | 3256.938 | 13.4   |
| 2     | 8.130 | 3252.807 | 36.0   |
| 3     | 7.033 | 2814.229 | 35.9   |
| 4     | 7.014 | 2806.659 | 43.3   |
| 5     | 6.995 | 2798.845 | 54.4   |
| 6     | 6.974 | 2790.298 | 96.3   |
| 7     | 6.970 | 2788.833 | 89.0   |
| 8     | 6.884 | 2754.645 | 43.6   |
| 9     | 6.882 | 2753.668 | 45.0   |
| 10    | 6.866 | 2747.073 | 51.4   |
| 11    | 6.863 | 2746.098 | 51.0   |
| 12    | 6.834 | 2634.280 | 47.2   |
| 13    | 6.831 | 2633.059 | 47.1   |
| 14    | 6.828 | 2632.042 | 55.0   |
| 15    | 6.814 | 2624.466 | 44.9   |
| 16    | 6.810 | 2624.001 | 47.1   |
| 17    | 6.808 | 2624.024 | 50.9   |
| 18    | 5.173 | 2069.673 | 146.5  |
| 19    | 3.317 | 1337.070 | 151.2  |
| 20    | 2.695 | 1078.233 | 245.7  |
| 21    | 2.684 | 1073.838 | 275.9  |
| 22    | 2.463 | 985.439  | 11.7   |
| 23    | 2.459 | 983.729  | 10.1   |



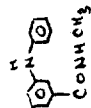
Compound 21



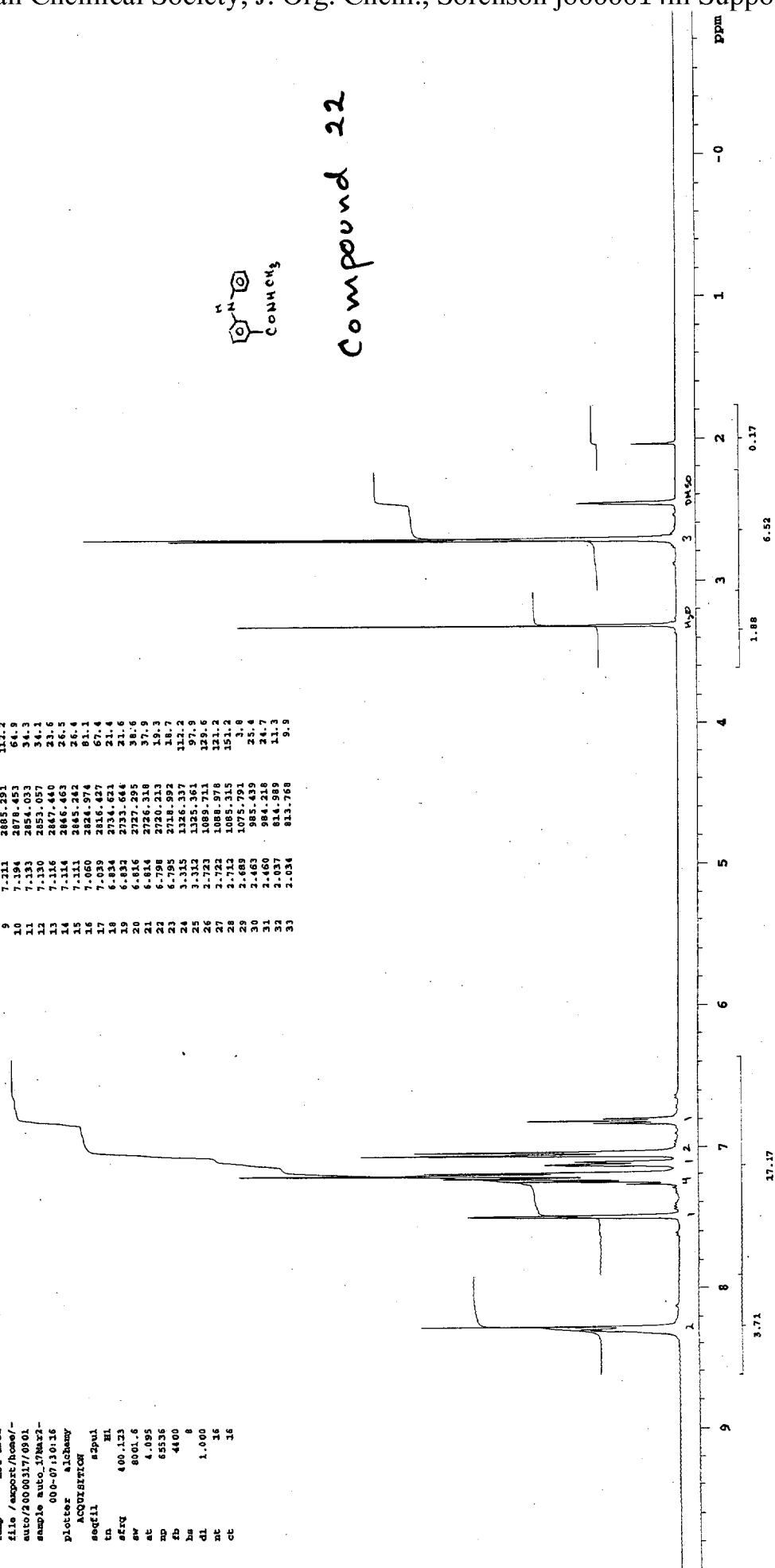
527

Rod 72375256/H1/dmsc  
 Barton: H1 OBSERVE  
 exp2 s2pul  
 user rodrick exte-  
 son  
 Date Mar 17 2000  
 solvent dmsc  
 spin not used  
 gain not used  
 temp not used  
 file /export/home/-  
 auto/20000317/0901  
 sample auto\_17Mar2-  
 000-0713015  
 plotter alchemy  
 ACQUISITION  
 seqfil s2pul  
 tn H1  
 atqy 400.123  
 sw 8001.6  
 at 4.095  
 mp 65536  
 fb 4400  
 ha 8  
 dl 1.000  
 at 15  
 ct 15

| INDEX | (PPM) | (HZ)     | HEIGHT |
|-------|-------|----------|--------|
| 1     | 8.310 | 3324.845 | 22.7   |
| 2     | 8.299 | 3320.694 | 21.3   |
| 3     | 8.275 | 3311.370 | 65.9   |
| 4     | 7.501 | 3001.284 | 51.8   |
| 5     | 7.265 | 2907.024 | 12.1   |
| 6     | 7.256 | 2903.361 | 11.6   |
| 7     | 7.246 | 2899.864 | 41.8   |
| 8     | 7.227 | 2885.984 | 59.9   |
| 9     | 7.194 | 2878.453 | 112.2  |
| 10    | 7.183 | 2854.033 | 64.9   |
| 11    | 7.130 | 2853.057 | 34.1   |
| 12    | 7.116 | 2847.440 | 23.6   |
| 13    | 7.114 | 2846.463 | 26.5   |
| 14    | 7.111 | 2845.342 | 26.4   |
| 15    | 7.060 | 2824.974 | 81.1   |
| 16    | 7.039 | 2816.427 | 67.4   |
| 17    | 6.934 | 2734.621 | 21.4   |
| 18    | 6.932 | 2733.644 | 21.6   |
| 19    | 6.916 | 2727.295 | 38.6   |
| 20    | 6.914 | 2726.319 | 37.9   |
| 21    | 6.798 | 2720.430 | 19.3   |
| 22    | 6.795 | 2719.492 | 18.7   |
| 23    | 6.715 | 1326.337 | 112.2  |
| 24    | 6.712 | 1325.361 | 97.9   |
| 25    | 6.723 | 1089.711 | 129.6  |
| 26    | 6.722 | 1088.978 | 121.2  |
| 27    | 6.712 | 1085.315 | 151.2  |
| 28    | 6.689 | 1075.791 | 3.8    |
| 29    | 6.683 | 985.439  | 25.4   |
| 30    | 2.463 | 984.218  | 24.7   |
| 31    | 2.460 | 814.989  | 11.3   |
| 32    | 2.037 | 813.768  | 9.5    |
| 33    | 2.034 |          |        |



Compound 22



538

57447188 /SORENSEN /H1 /TMSO /  
STANDARD 1H OBSERVE

exp3 std1h

SAMPLE

user cf  
date Dec 3 96  
solvent DMSO  
file /home/rs/-  
vmaraya/nf/nf96d40-

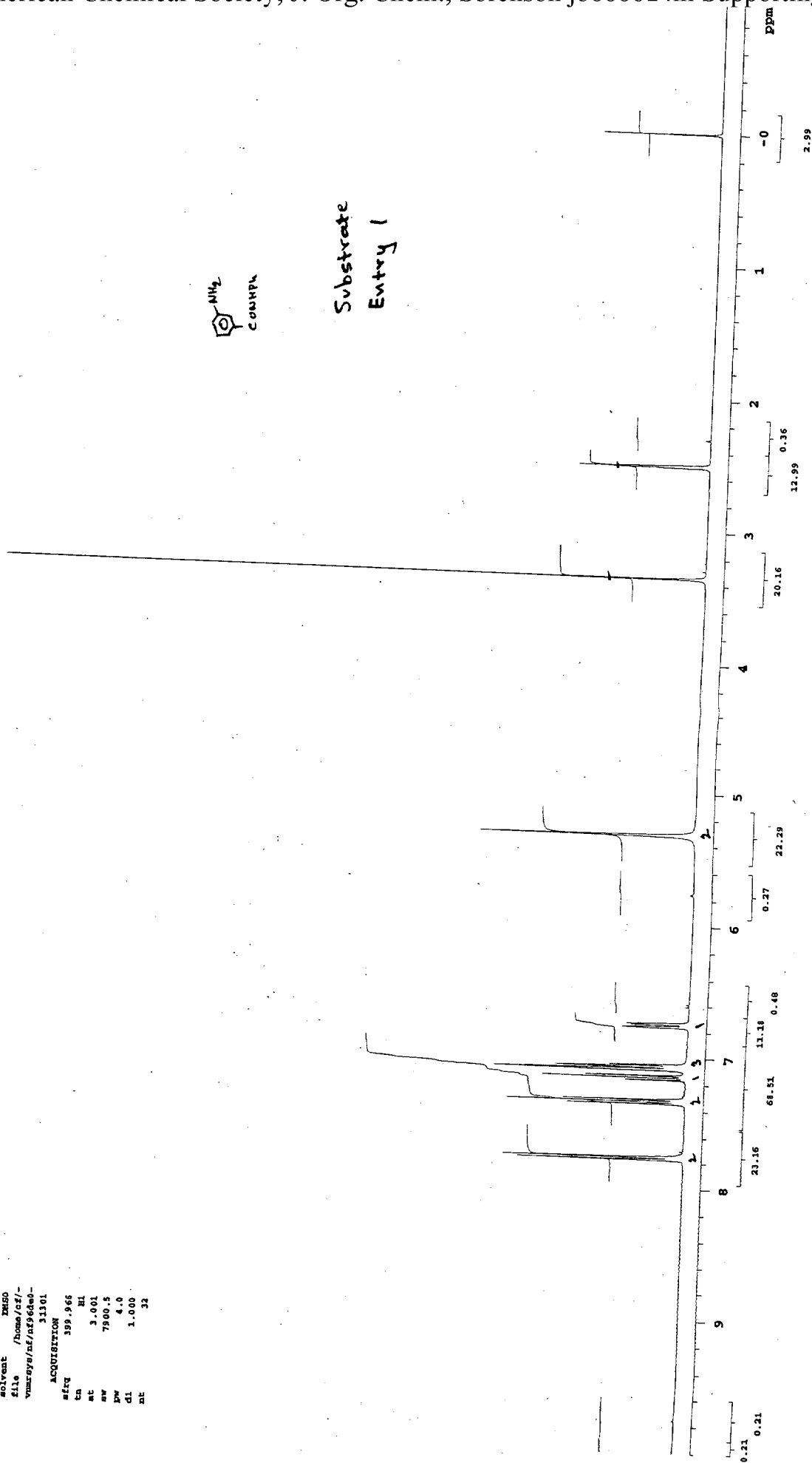
11101

ACQUISITION

freq 399.965  
tn  
at 3.001  
sw 7500.5  
pr 4.0  
d1 1.000  
re 32

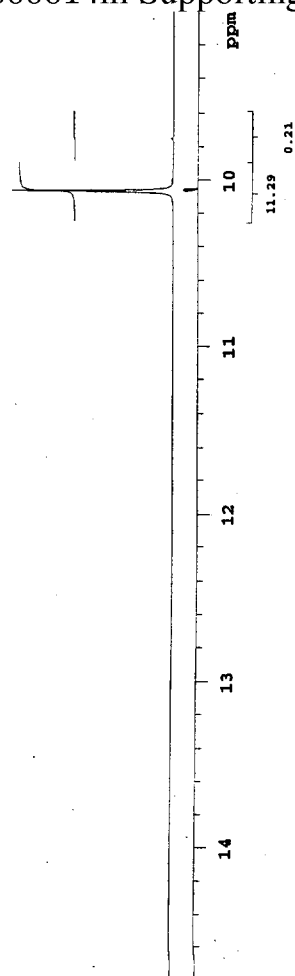


Substrate  
Entry 1



| INDEX | FREQUENCY (PPM) | FREQUENCY (Hz) | HEIGHT |
|-------|-----------------|----------------|--------|
| 1     | 10.065          | 4025.815       | 12.9   |
| 2     | 7.771           | 3108.130       | 37.5   |
| 3     | 7.769           | 3107.188       | 45.6   |
| 4     | 7.765           | 3098.160       | 49.6   |
| 5     | 7.345           | 2935.460       | 12.3   |
| 6     | 7.342           | 2935.480       | 11.3   |
| 7     | 7.327           | 2930.593       | 49.2   |
| 8     | 7.307           | 2922.495       | 13.6   |
| 9     | 7.163           | 2865.111       | 16.8   |
| 10    | 7.144           | 2857.395       | 19.6   |
| 11    | 7.125           | 2849.680       | 27.8   |
| 12    | 7.093           | 2836.650       | 30.9   |
| 13    | 7.089           | 2835.214       | 53.0   |
| 14    | 7.083           | 2833.044       | 31.6   |
| 15    | 7.071           | 2827.980       | 34.9   |
| 16    | 7.068           | 2827.016       | 16.2   |
| 17    | 7.065           | 2825.910       | 12.9   |
| 18    | 7.052           | 2821.711       | 11.1   |
| 19    | 7.049           | 2820.560       | 11.1   |
| 20    | 7.046           | 2819.306       | 21.3   |
| 21    | 7.044           | 2818.336       | 19.2   |
| 22    | 6.758           | 2702.944       | 16.9   |
| 23    | 6.755           | 2701.880       | 18.1   |
| 24    | 6.752           | 2700.674       | 17.9   |
| 25    | 6.750           | 2699.710       | 16.0   |
| 26    | 6.738           | 2694.887       | 16.0   |
| 27    | 6.735           | 2693.923       | 15.7   |
| 28    | 6.732           | 2692.717       | 17.1   |
| 29    | 6.730           | 2691.753       | 14.2   |
| 30    | 5.320           | 2127.797       | 19.2   |
| 31    | 3.347           | 1328.894       | 192.0  |
| 32    | 2.511           | 1004.516       | 16.7   |
| 33    | 2.507           | 1000.536       | 35.9   |
| 34    | 2.503           | 1000.848       | 25.4   |
| 35    | 2.498           | 998.919        | 12.3   |
| 36    | 2.491           | 997.231        | 32.5   |
| 37    | 0.000           | 0.000          |        |

Substrate  
Entry 1



540