

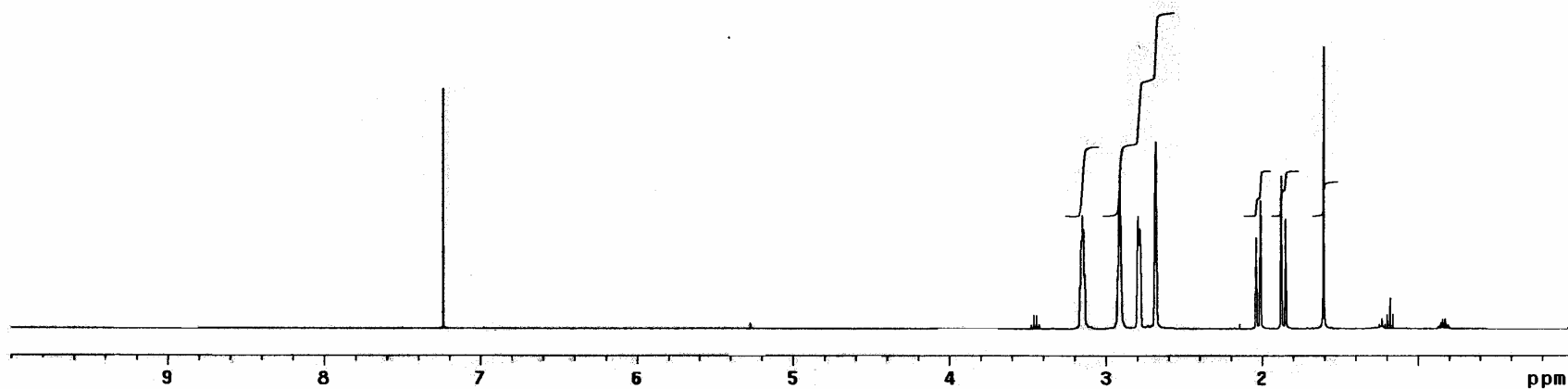
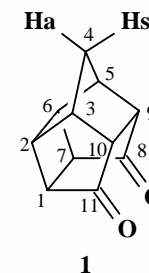
Supplementary material to:

H.G. Kruger and R. Ramdhani, NMR analysis of some pentacycloundecanedione derivatives, *S. Afr. J. Chem.*, 2006, **59**, 71–74.

hdione.dione in cdc13
probe=5mmASW

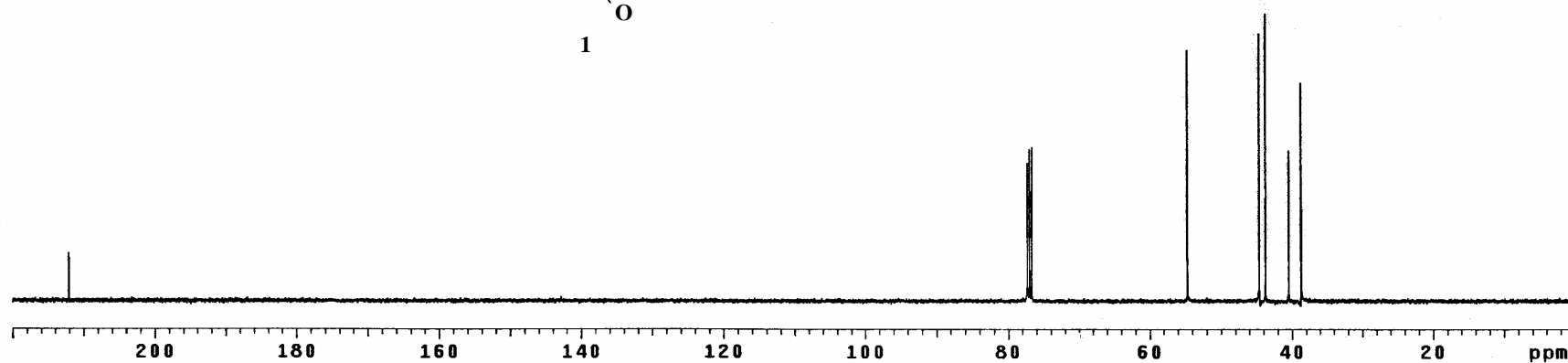
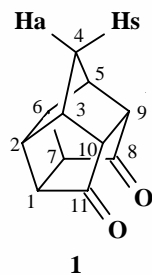
Pulse Sequence: s2pu1

| INDEX | FREQUENCY | PPM | HEIGHT |
|-------|-----------|-------|--------|
| 1 | 2895.544 | 7.240 | 42.4 |
| 2 | 1263.495 | 3.159 | 15.7 |
| 3 | 1262.030 | 3.156 | 15.8 |
| 4 | 1260.198 | 3.151 | 20.1 |
| 5 | 1258.367 | 3.146 | 17.0 |
| 6 | 1256.902 | 3.143 | 17.6 |
| 7 | 1253.972 | 3.135 | 9.8 |
| 8 | 1170.099 | 2.926 | 11.1 |
| 9 | 1167.718 | 2.920 | 20.5 |
| 10 | 1165.887 | 2.915 | 27.4 |
| 11 | 1164.971 | 2.913 | 19.8 |
| 12 | 1164.055 | 2.911 | 26.4 |
| 13 | 1162.224 | 2.906 | 20.0 |
| 14 | 1160.576 | 2.902 | 9.4 |
| 15 | 1159.843 | 2.900 | 11.5 |
| 16 | 1120.654 | 2.802 | 13.9 |
| 17 | 1119.555 | 2.799 | 17.8 |
| 18 | 1118.456 | 2.797 | 20.0 |
| 19 | 1118.090 | 2.796 | 19.8 |
| 20 | 1116.075 | 2.791 | 17.5 |
| 21 | 1114.610 | 2.787 | 15.7 |
| 22 | 1113.878 | 2.785 | 17.6 |
| 23 | 1113.329 | 2.784 | 17.8 |
| 24 | 1112.413 | 2.781 | 17.5 |
| 25 | 1111.131 | 2.778 | 14.8 |
| 26 | 1073.406 | 2.684 | 33.2 |
| 27 | 815.560 | 2.039 | 16.1 |
| 28 | 804.206 | 2.011 | 22.9 |
| 29 | 752.381 | 1.881 | 14.0 |
| 30 | 750.915 | 1.878 | 27.1 |
| 31 | 749.450 | 1.874 | 14.9 |
| 32 | 741.027 | 1.853 | 10.2 |
| 33 | 739.561 | 1.849 | 19.5 |
| 34 | 738.096 | 1.846 | 10.6 |
| 35 | 642.137 | 1.606 | 50.0 |



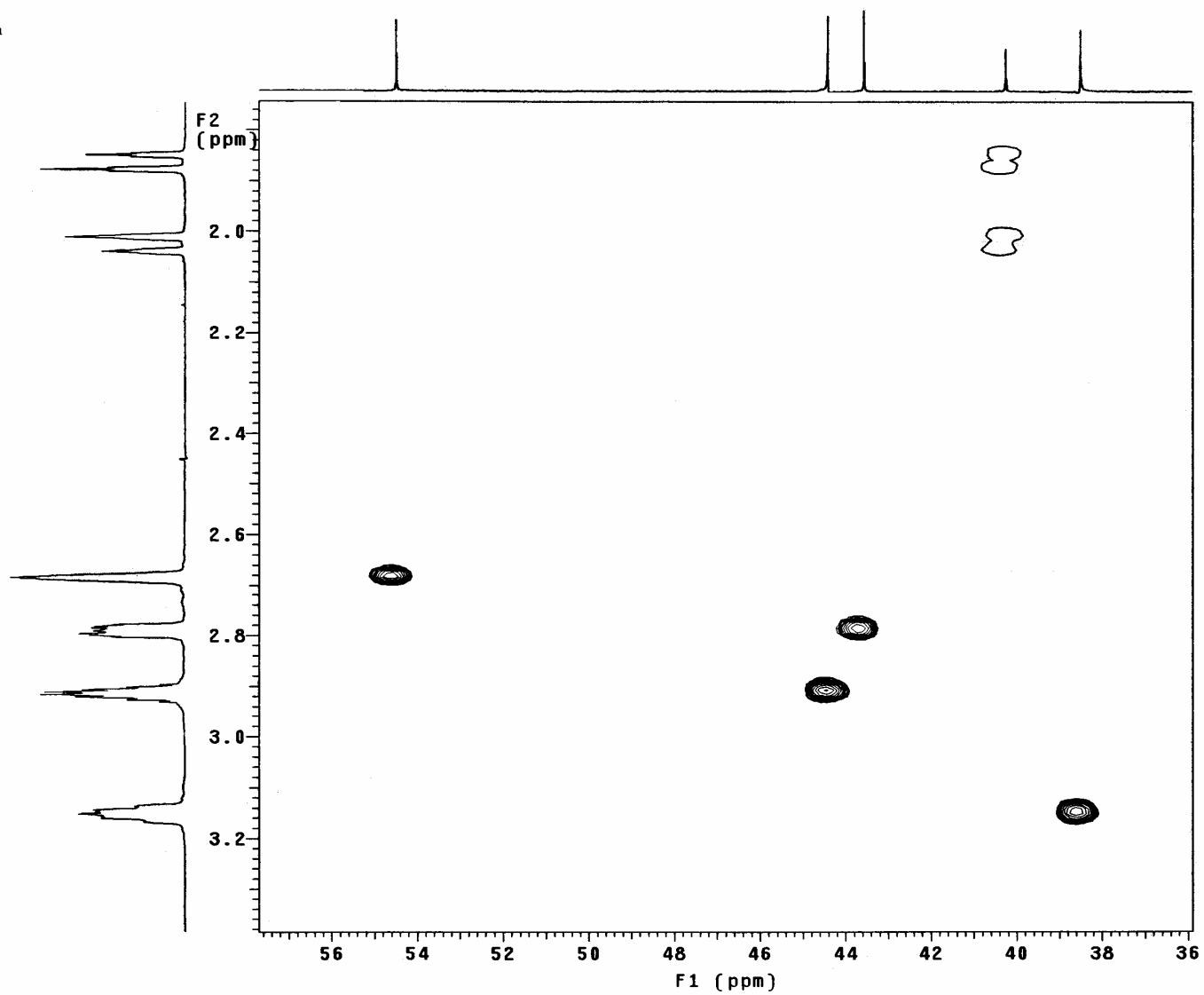
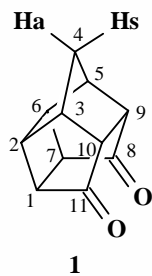
cdione.dione in cdc
probe=5mmASW
Pulse Sequence: s2pu1

| INDEX | FREQUENCY | PPM | HEIGHT |
|-------|-----------|---------|--------|
| 1 | 21328.560 | 212.089 | 8.5 |
| 2 | 7775.581 | 77.320 | 24.3 |
| 3 | 7743.445 | 77.000 | 26.7 |
| 4 | 7711.310 | 76.680 | 27.0 |
| 5 | 5499.722 | 54.689 | 43.9 |
| 6 | 4486.215 | 44.610 | 46.8 |
| 7 | 4400.520 | 43.758 | 50.0 |
| 8 | 4068.452 | 40.456 | 26.4 |
| 9 | 3892.943 | 38.711 | 38.2 |

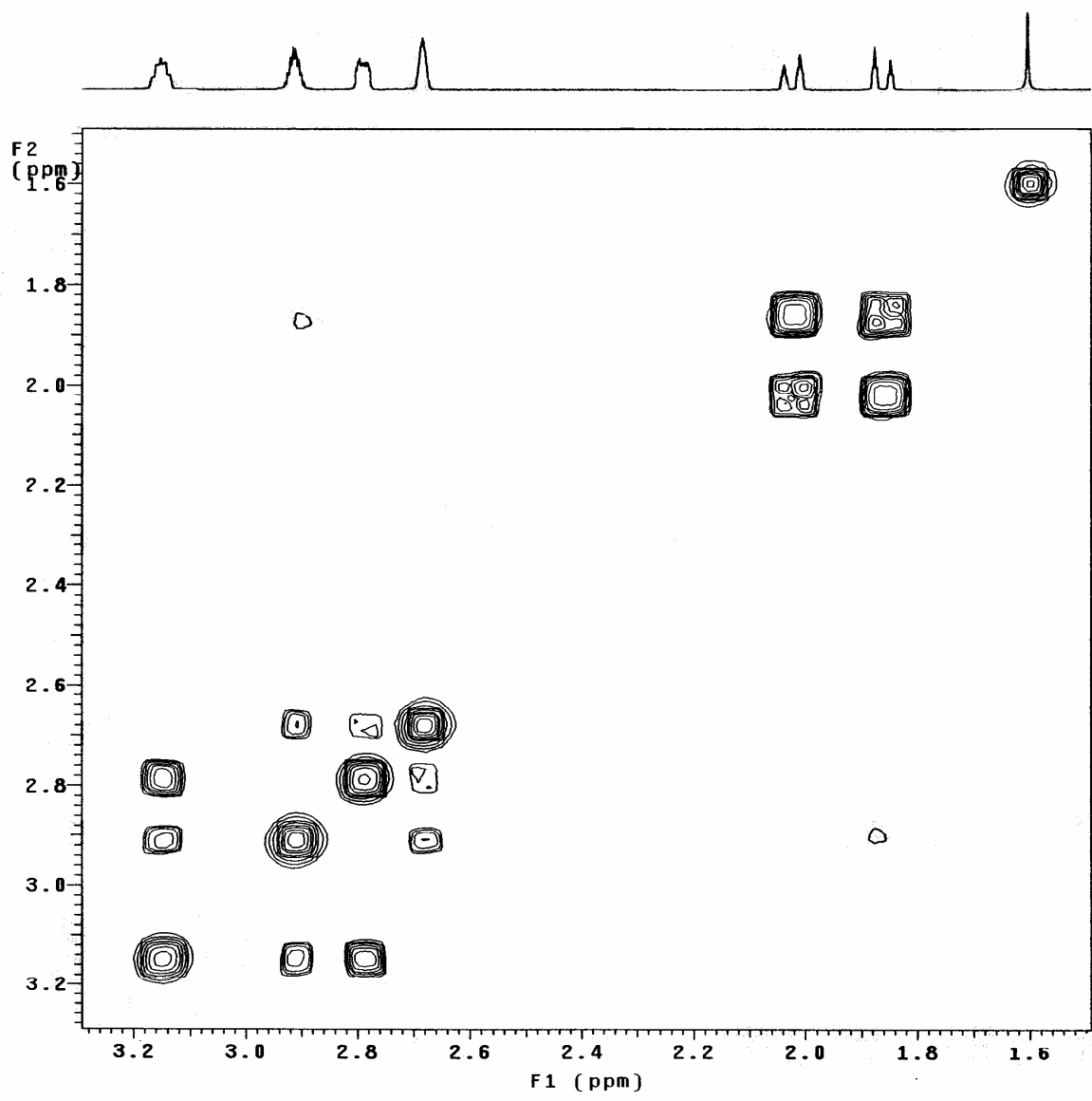
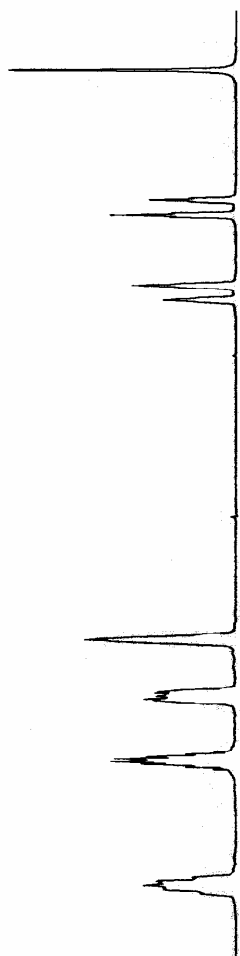
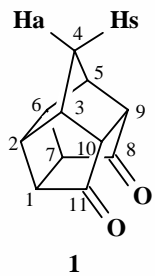


HQdione.dione in cdc13
Gradient HSQC expt.
with mult.editing
probe=5mmASW

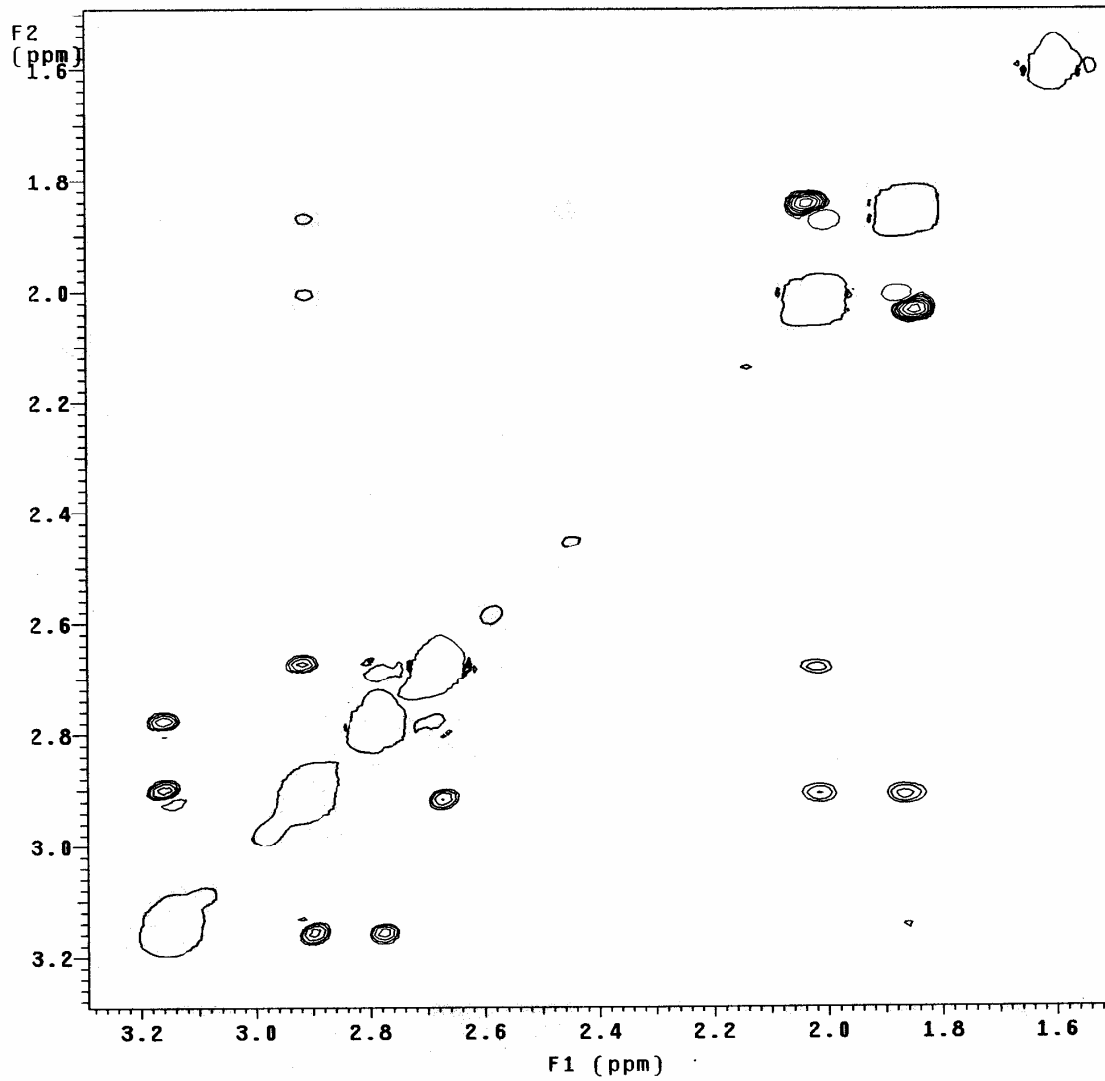
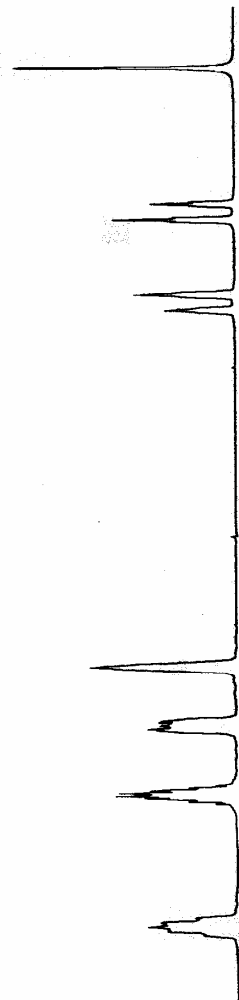
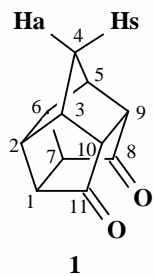
Pulse Sequence: ghsqc_da



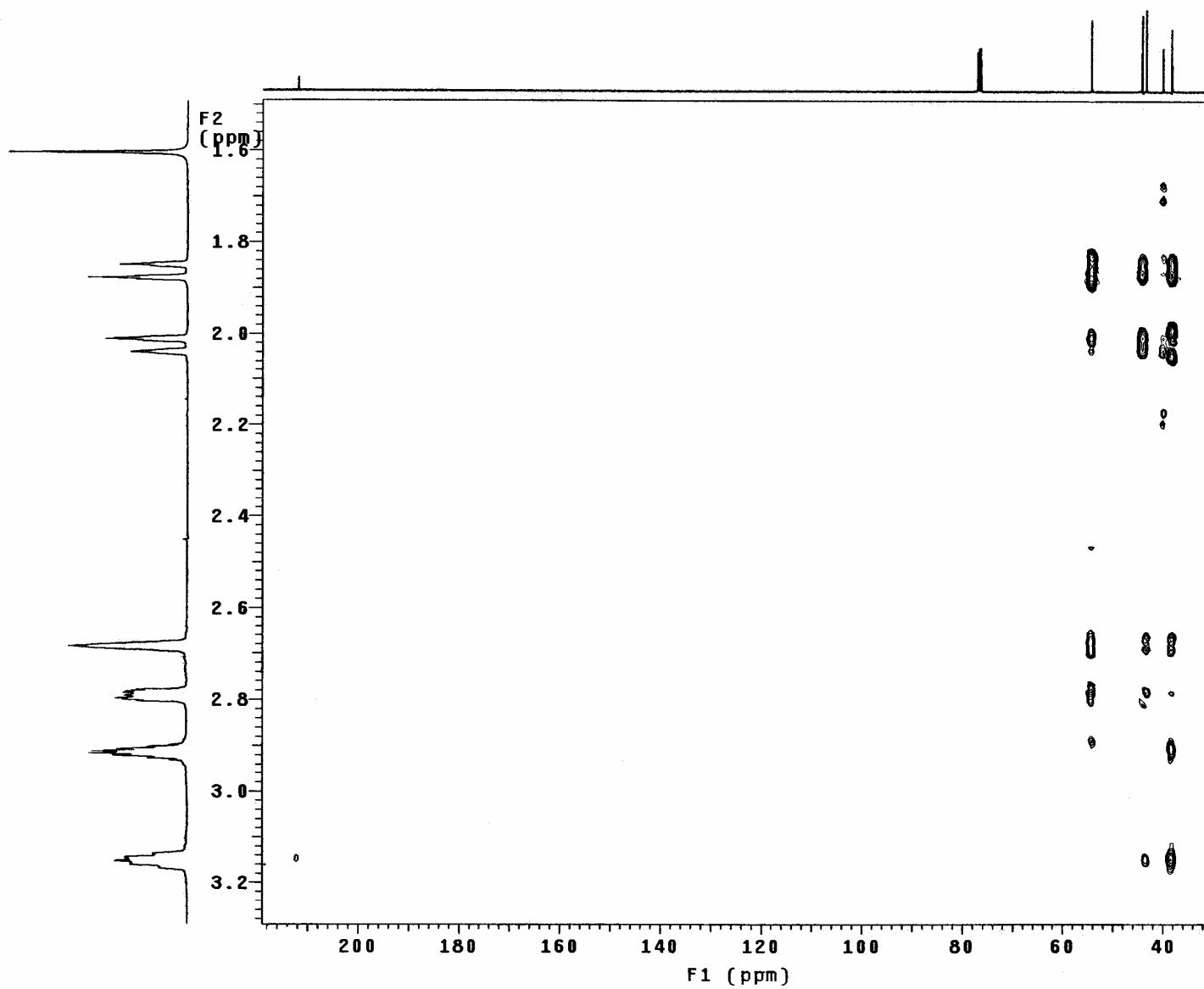
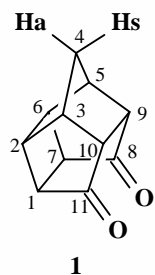
cydione.dione in cdc13
1H Cosy-90
probe=5mmASW
Pulse Sequence: relayh



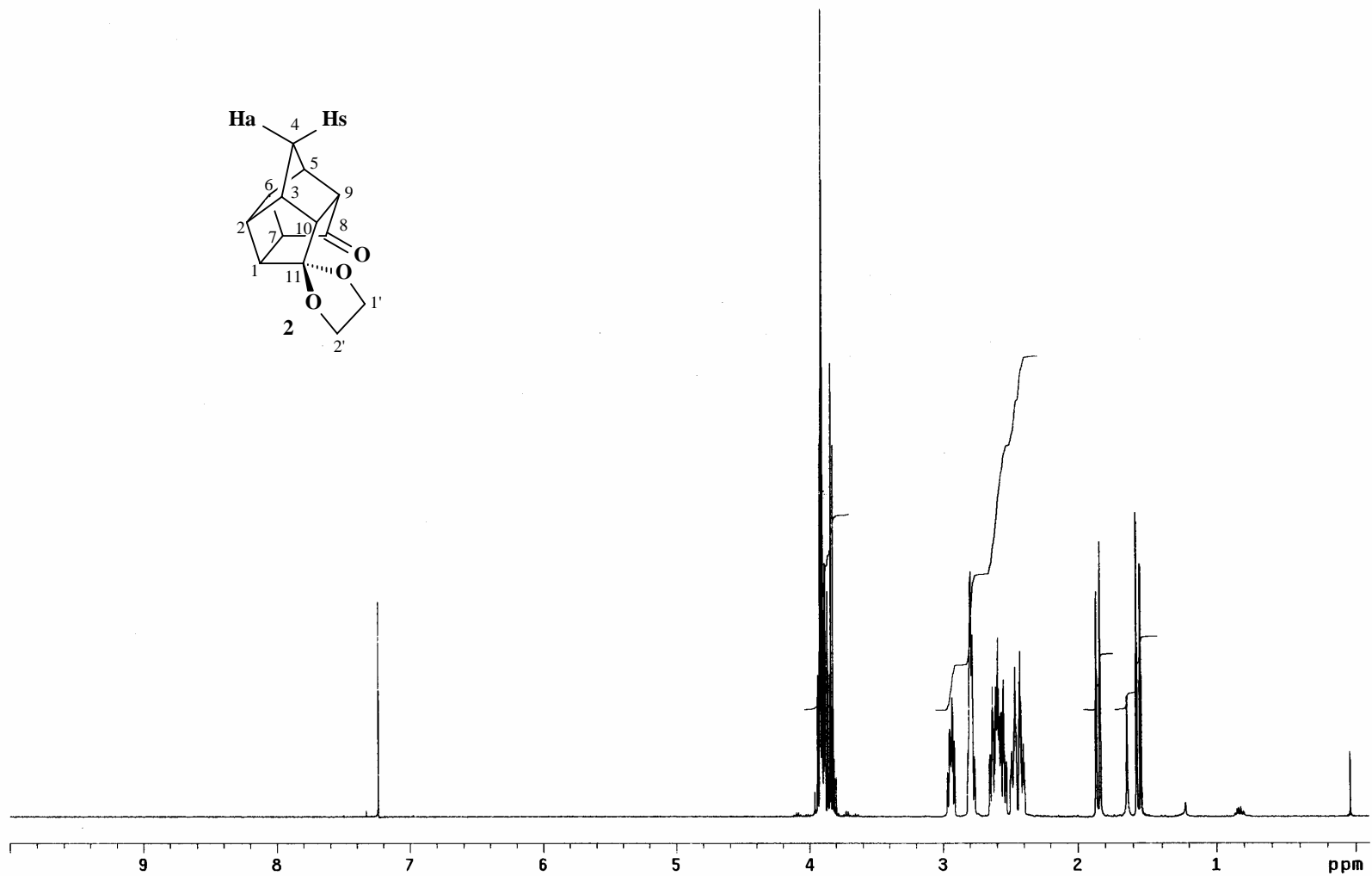
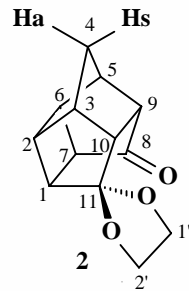
N0dione.dione in cdc13
NOESY expt.
mix=1sec
probe=5mmASW
Pulse Sequence: noesy_da



Resolution: 1000 MHz
Gradient HMBC expt.
probe=5mmASW
Pulse Sequence: ghmqc_da

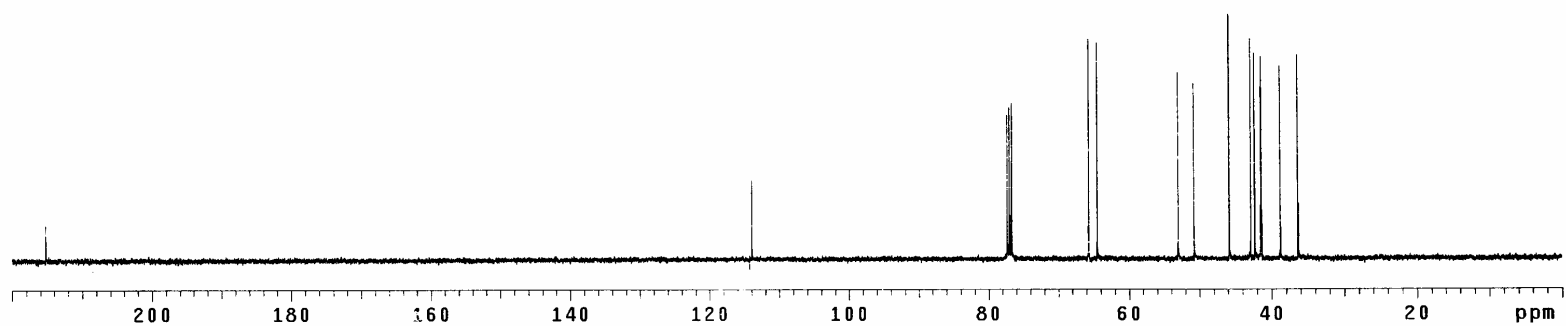
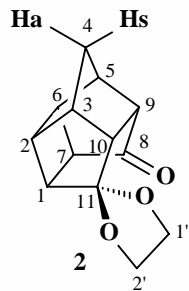


hketal.ketal in cdc13
probe=5mmASW
Pulse Sequence: s2pu1

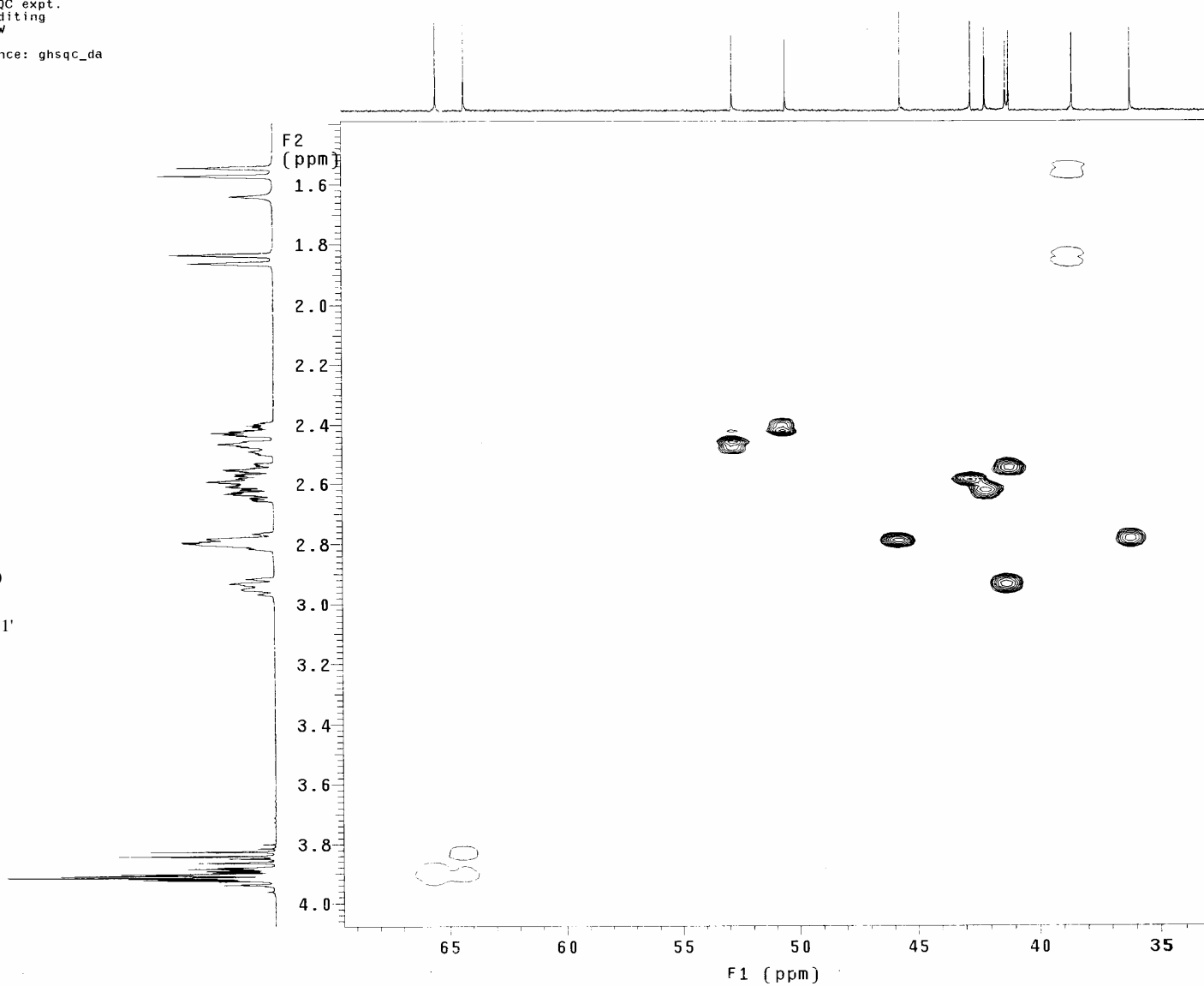
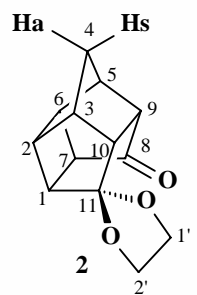


cketal.ketal in cdc13
probe=5mmASW
Pulse Sequence: s2pu1

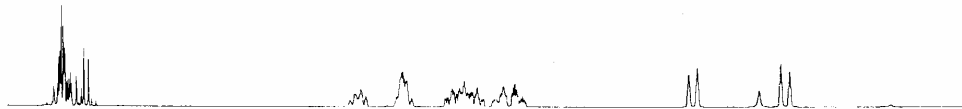
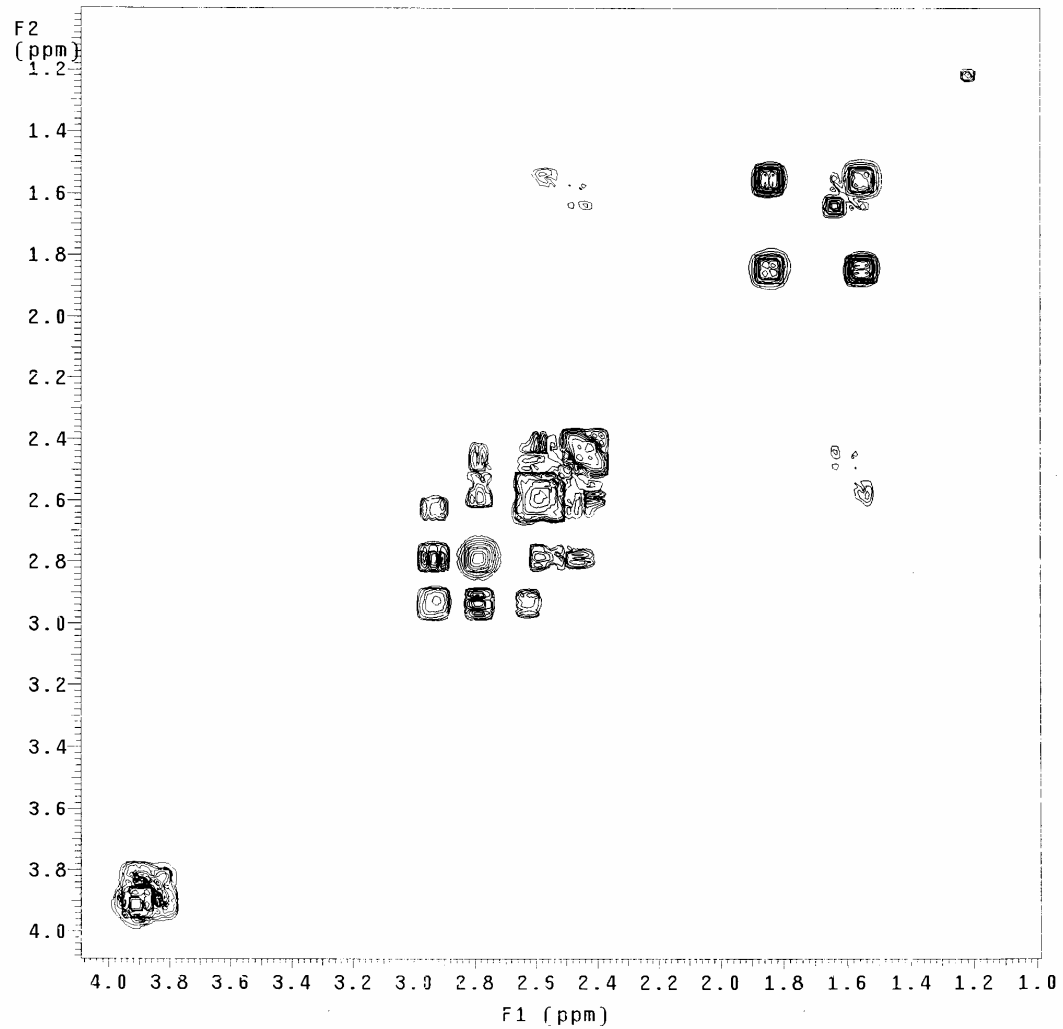
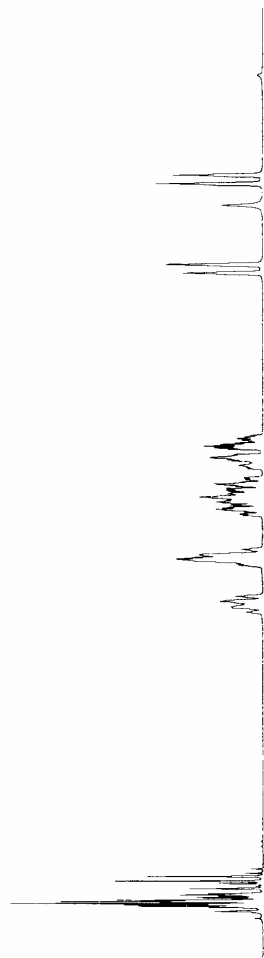
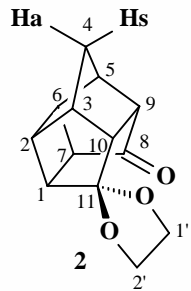
| INDEX | FREQUENCY | PPM | HEIGHT |
|-------|-----------|---------|--------|
| 1 | 21644.148 | 215.227 | 5.5 |
| 2 | 11456.342 | 113.921 | 12.9 |
| 3 | 7774.757 | 77.311 | 23.5 |
| 4 | 7743.446 | 77.000 | 24.7 |
| 5 | 7711.310 | 76.680 | 25.4 |
| 6 | 6607.164 | 65.701 | 35.9 |
| 7 | 6486.862 | 64.505 | 35.1 |
| 8 | 5331.628 | 53.017 | 30.4 |
| 9 | 5101.735 | 50.731 | 28.7 |
| 10 | 4608.990 | 45.831 | 40.0 |
| 11 | 4309.881 | 42.857 | 35.9 |
| 12 | 4253.026 | 42.292 | 33.4 |
| 13 | 4168.979 | 41.456 | 28.1 |
| 14 | 4155.795 | 41.325 | 32.9 |
| 15 | 3893.767 | 38.719 | 31.4 |
| 16 | 3653.986 | 36.335 | 33.2 |



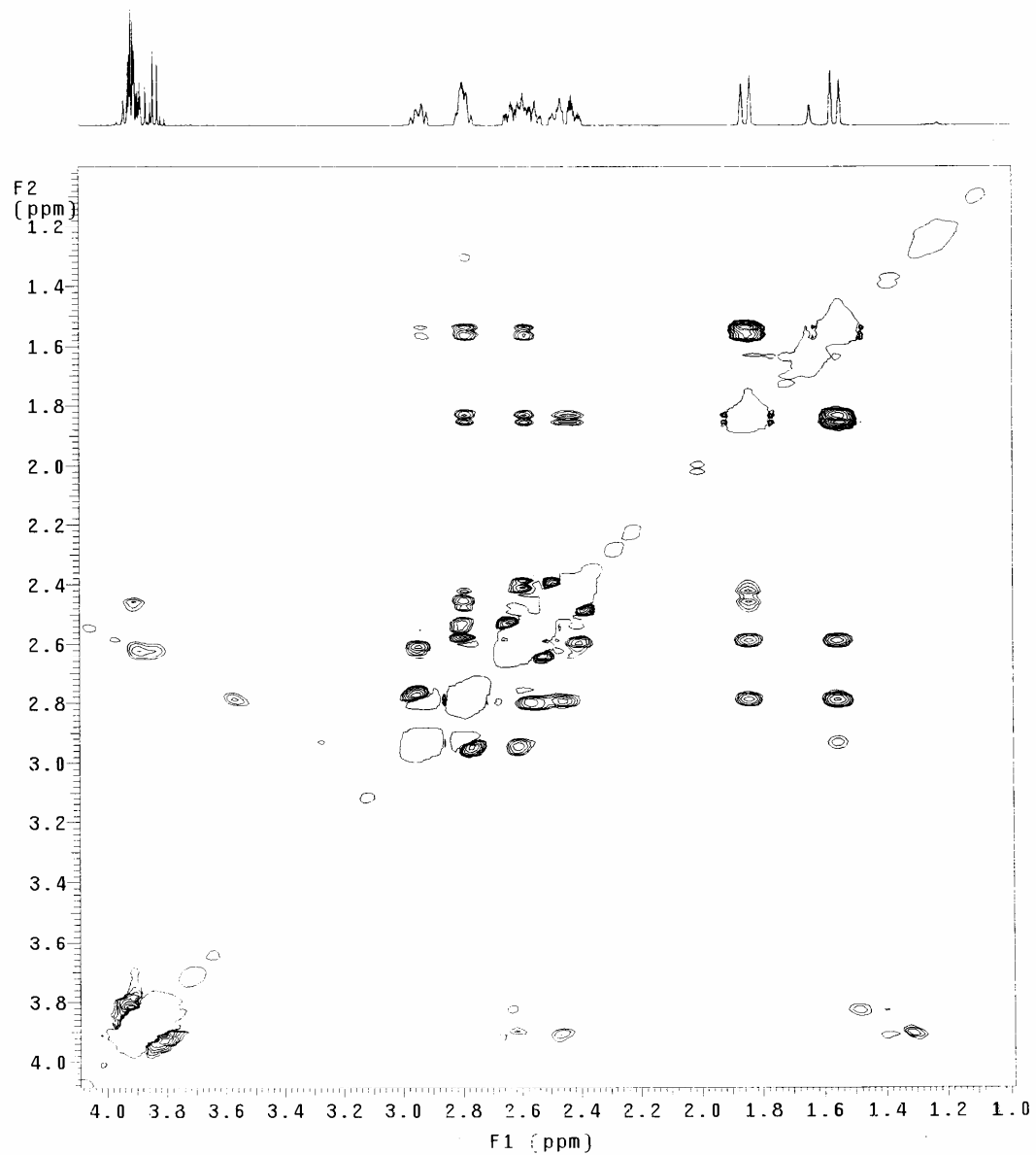
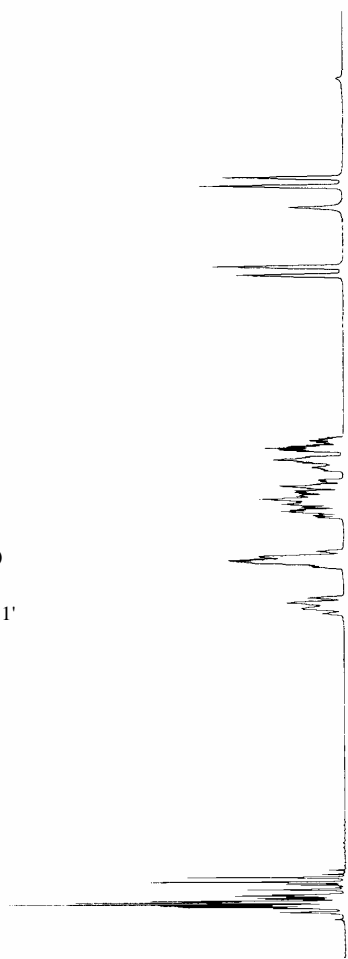
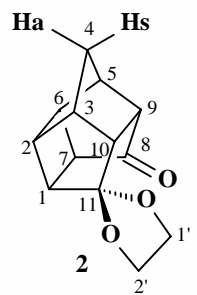
HQketal.ketal in cdc13
Gradient HSQC expt.
with mult.editing
probe=5mmASW
Pulse Sequence: ghsqc_da



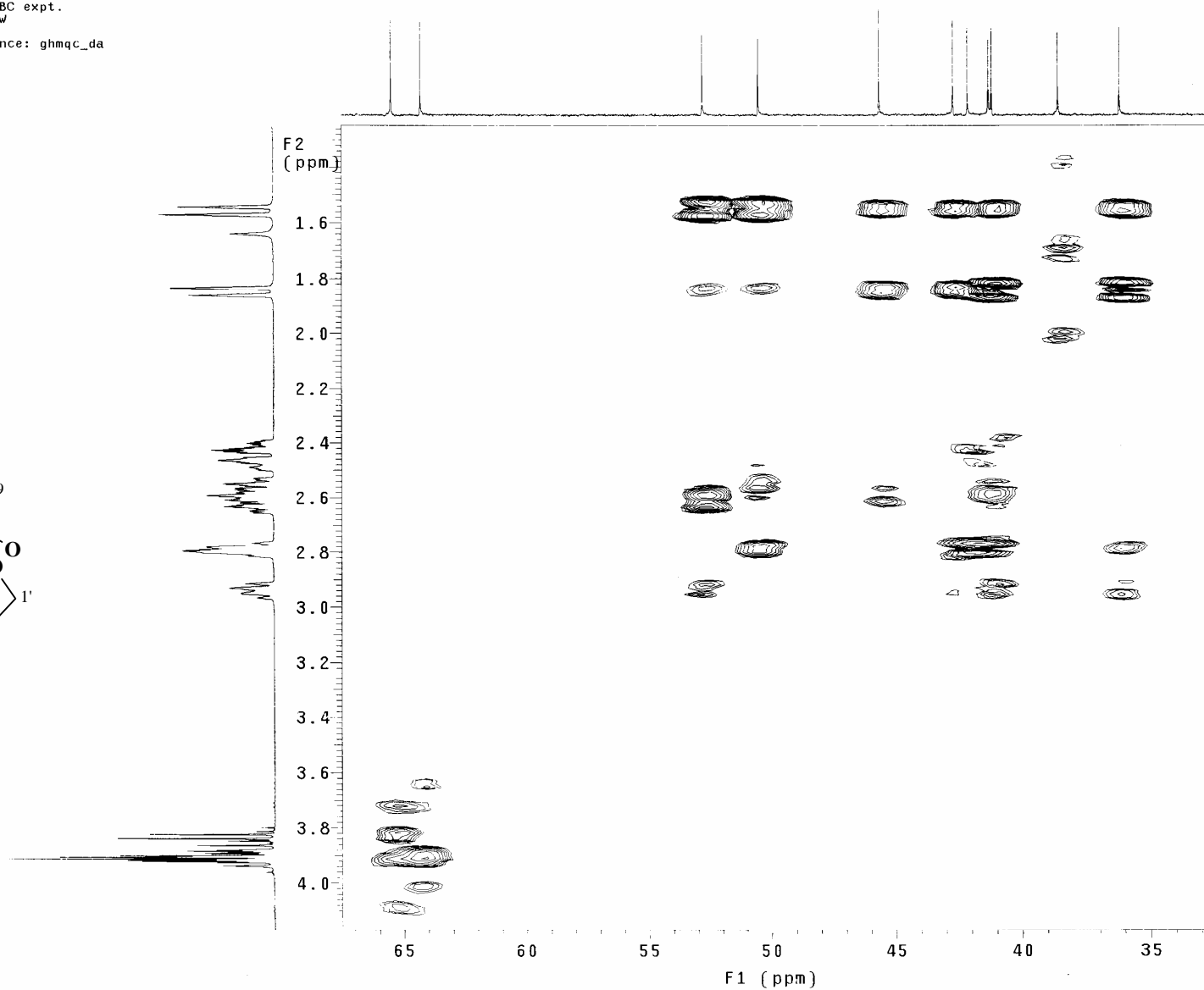
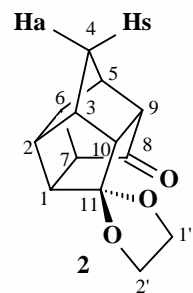
cyketal.ketal in cdc13
1H Cosy-90
probe=5mmASW
Pulse Sequence: relayh



NOketal.ketal in cdc13
NOESY expt.
mix=190C
probe=5mmASW
Pulse Sequence: noesy_da

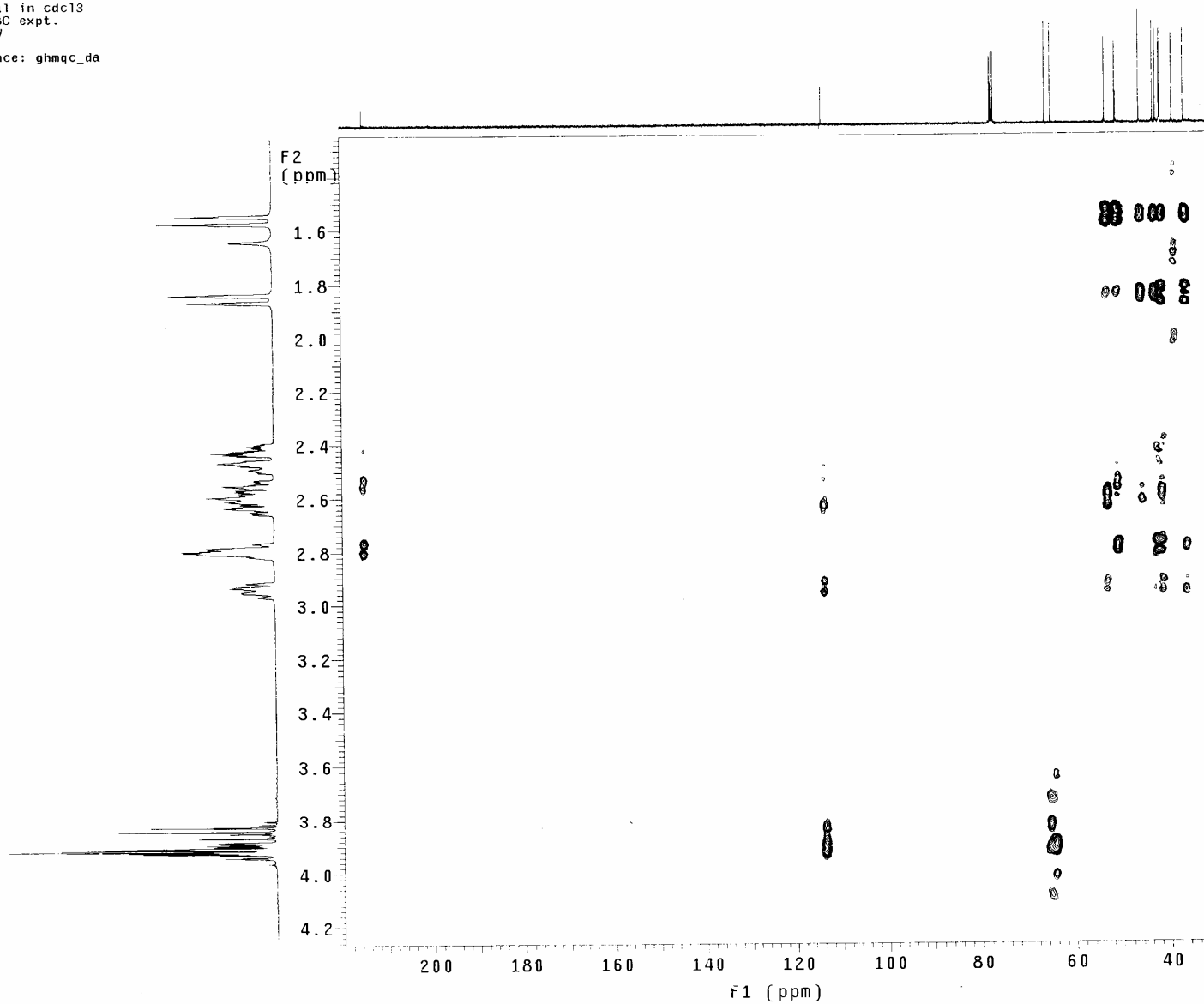
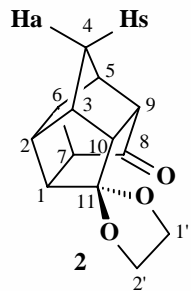


HBketal.ketal in cdc13
Gradient HMBC expt.
probe=5mmASW
Pulse Sequence: ghmqc_da

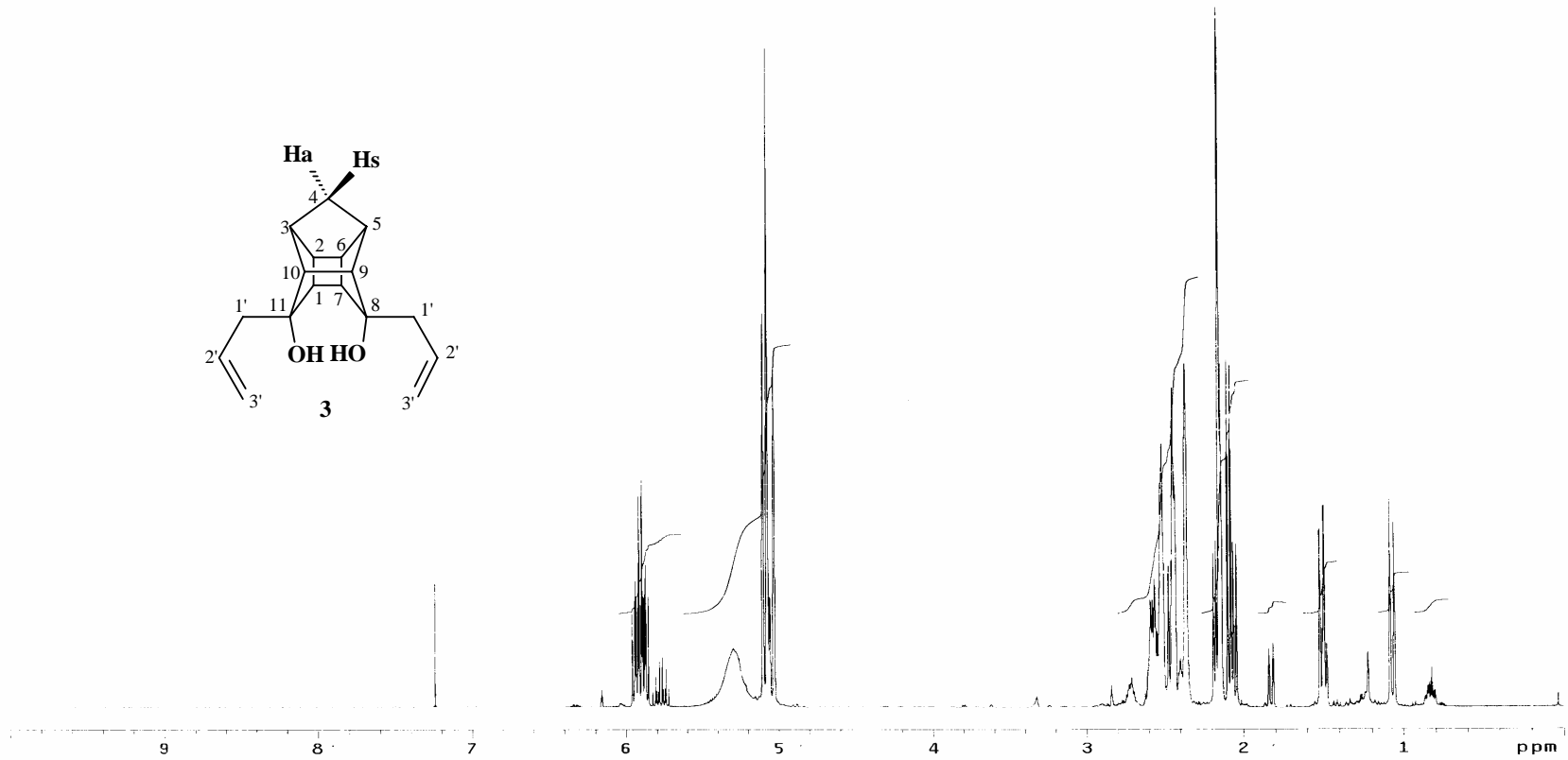
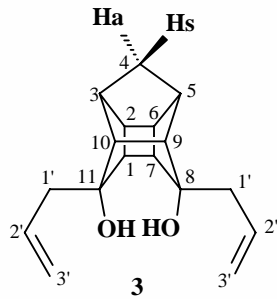


HBketal.ketal in cdc13
Gradient HMBC expt.
probe=5mmASW

Pulse Sequence: ghmqc_da

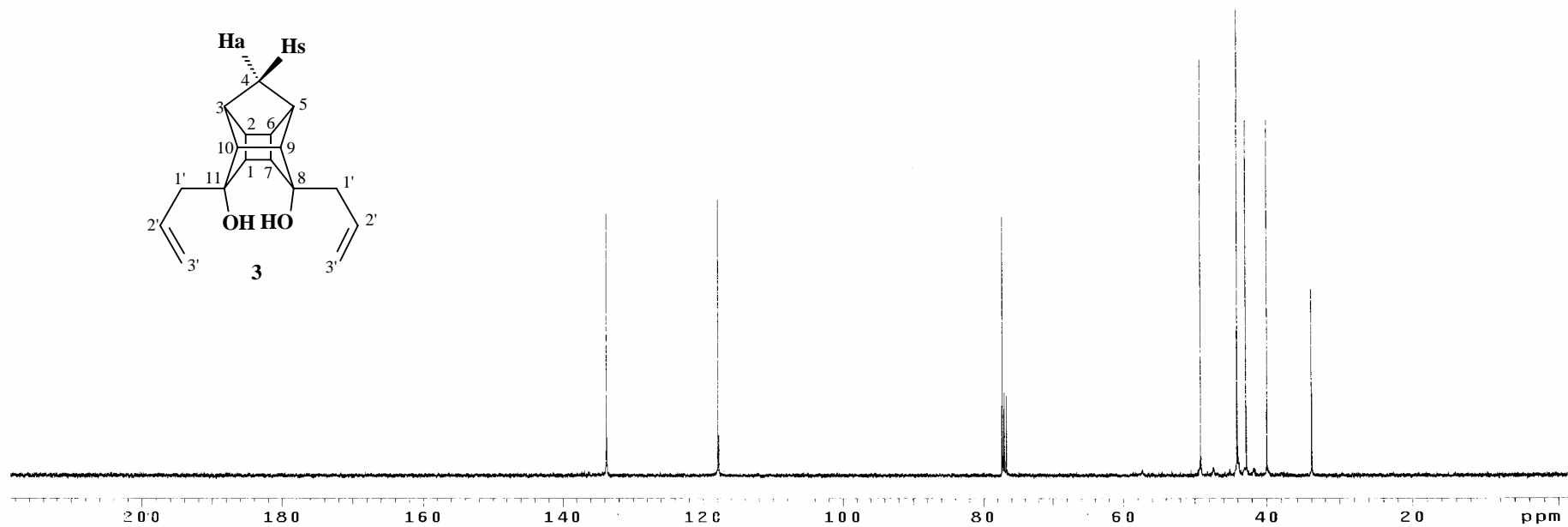
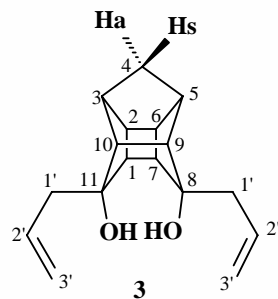


hediol_endo_endo_diol_in_cdc13
probe=5mmASW
Pulse Sequence: s2pu1



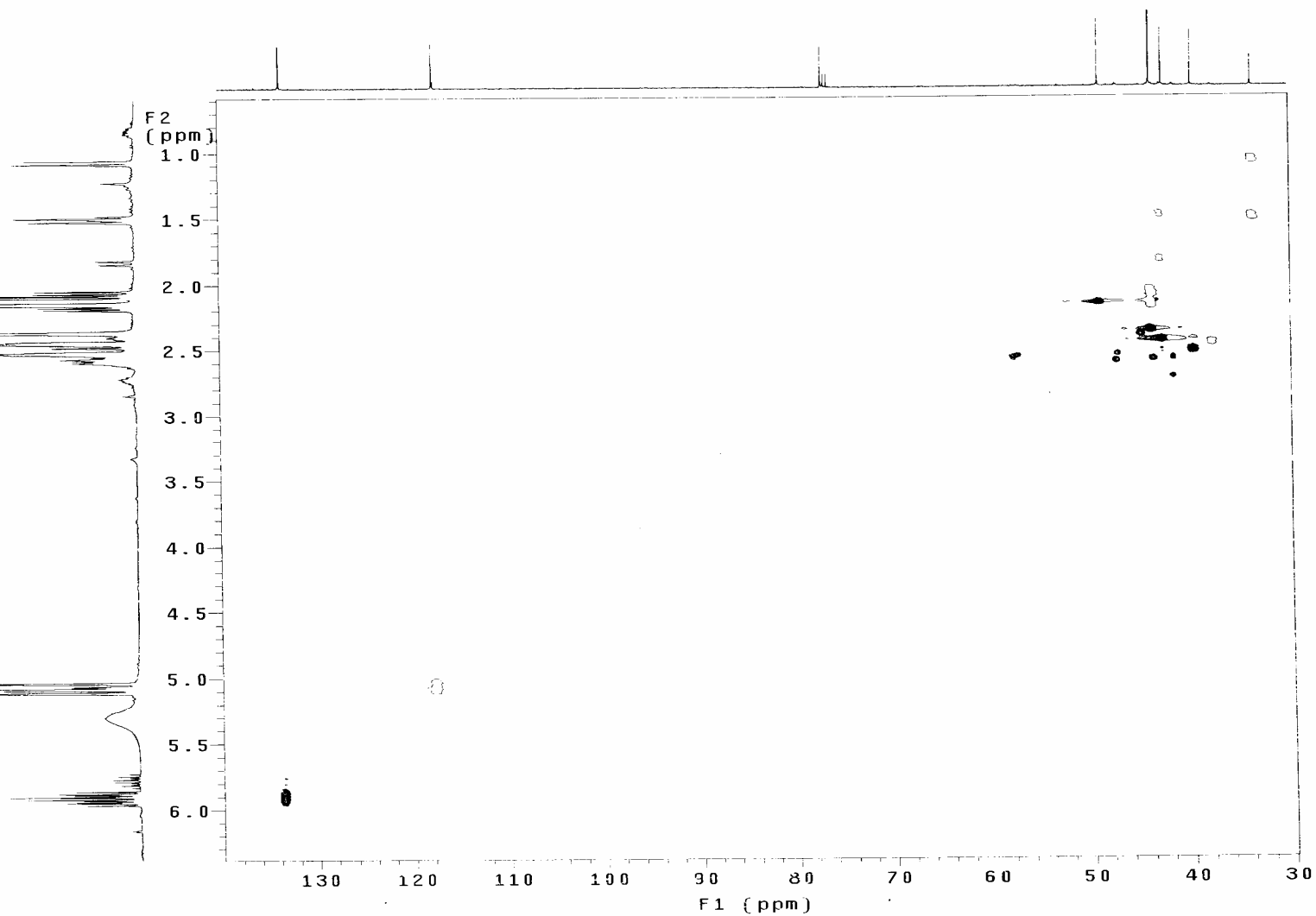
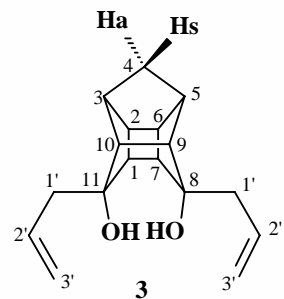
cediol_endo_endo diol in cdcl3
 probe=5mmASW
 Pulse Sequence: s2pul

| INDEX | FREQUENCY | PPM | HEIGHT |
|-------|-----------|---------|--------|
| 1 | 13450.407 | 133.749 | 55.6 |
| 2 | 13440.488 | 133.651 | 8.3 |
| 3 | 11852.000 | 117.855 | 58.8 |
| 4 | 11835.978 | 117.696 | 8.8 |
| 5 | 7775.490 | 77.319 | 15.0 |
| 6 | 7771.675 | 77.281 | 55.0 |
| 7 | 7743.446 | 77.000 | 17.9 |
| 8 | 7711.401 | 76.681 | 17.2 |
| 9 | 5815.439 | 57.828 | 9.4 |
| 10 | 4941.846 | 49.141 | 88.9 |
| 11 | 4767.128 | 47.404 | 11.4 |
| 12 | 4530.609 | 45.052 | 11.0 |
| 13 | 4426.847 | 44.020 | 100.0 |
| 14 | 4424.558 | 43.997 | 99.2 |
| 15 | 4397.091 | 43.724 | 10.6 |
| 16 | 4302.484 | 42.783 | 75.8 |
| 17 | 4195.669 | 41.721 | 13.2 |
| 18 | 4014.084 | 39.916 | 75.9 |
| 19 | 3408.291 | 33.892 | 35.8 |

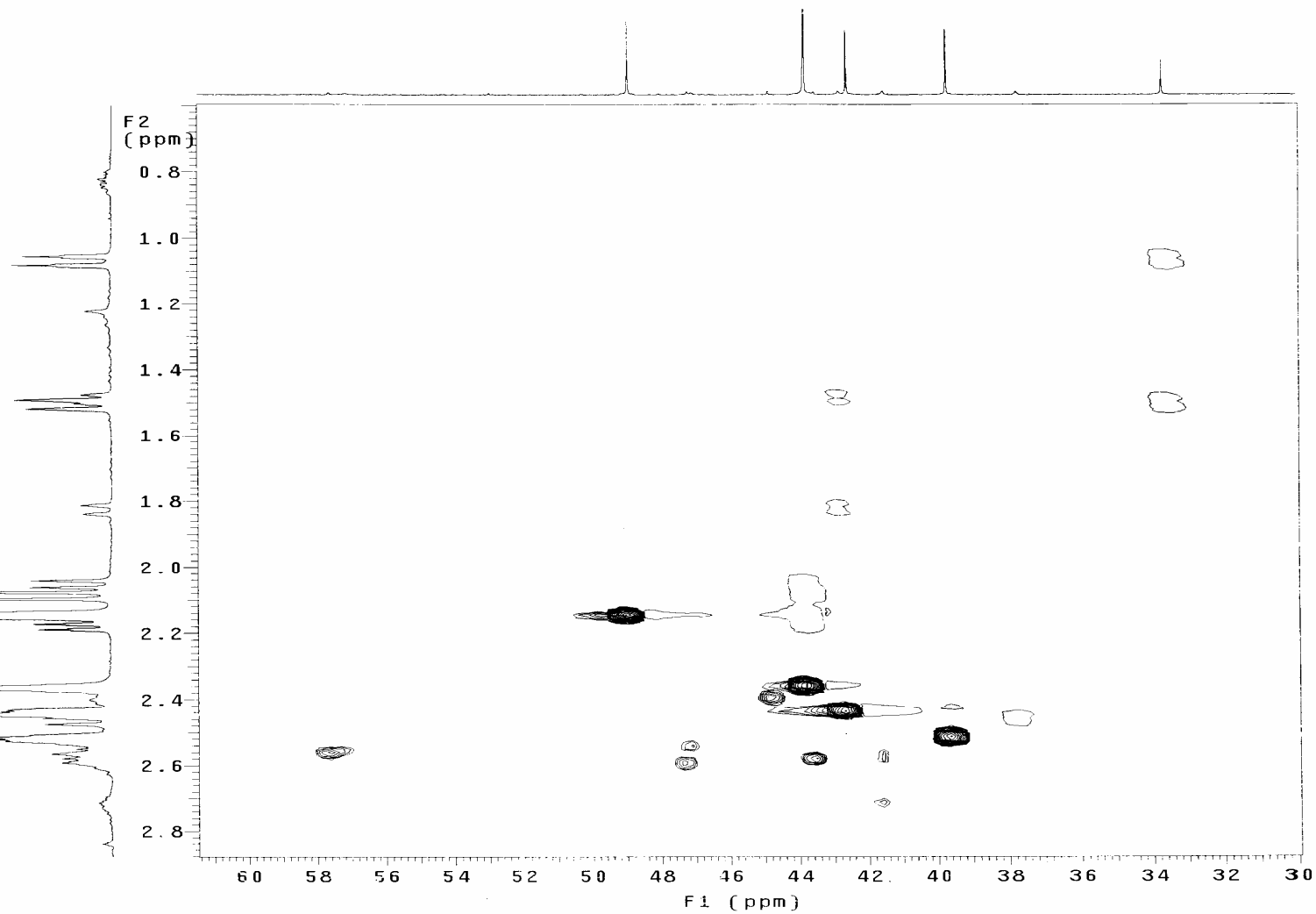
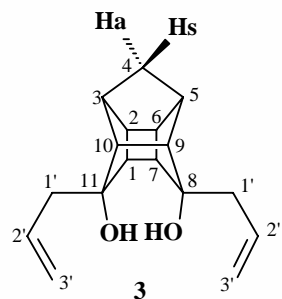


HQendoendo diol in cdc13
Gradient HSQC expt.
with mult. editing
probe=5mmASW

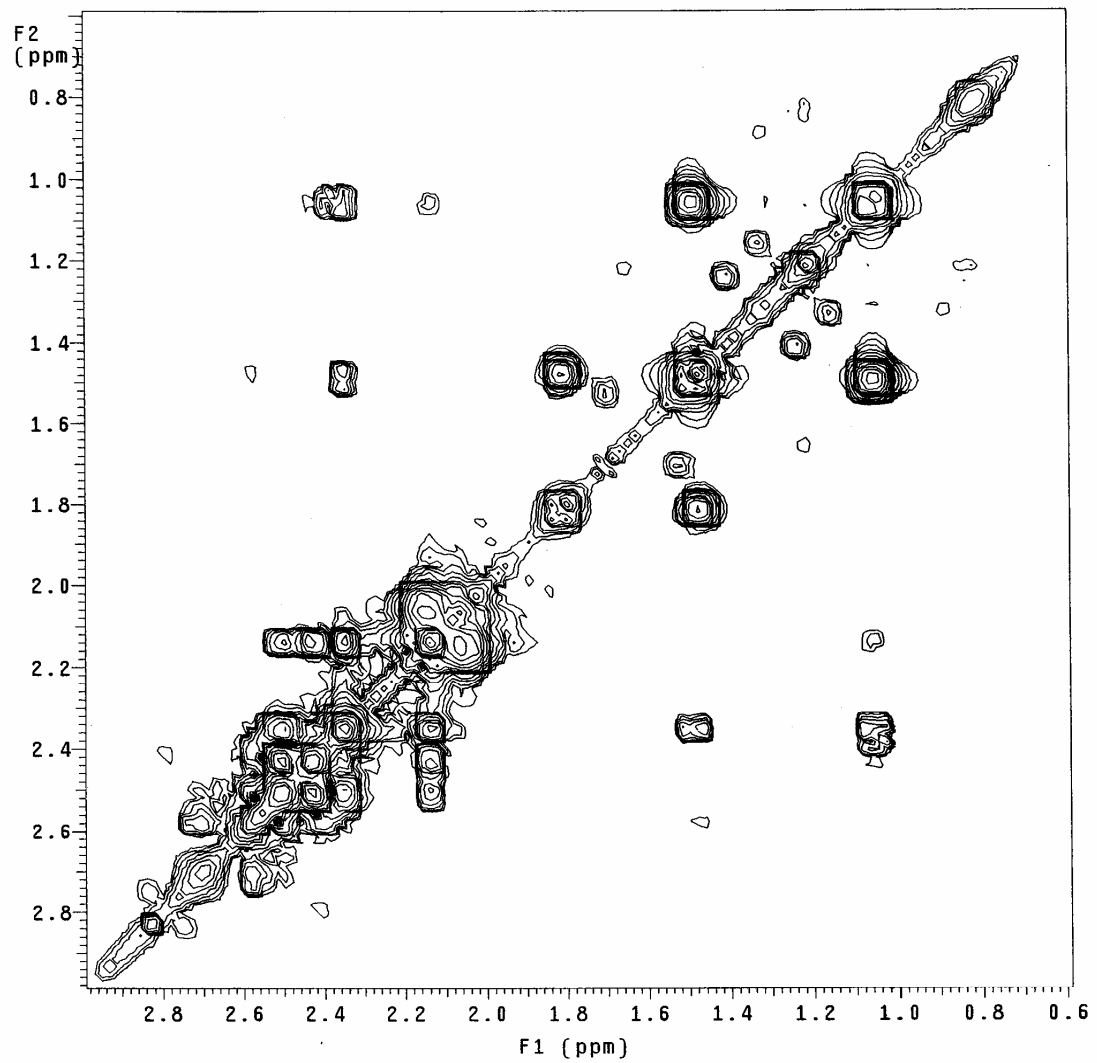
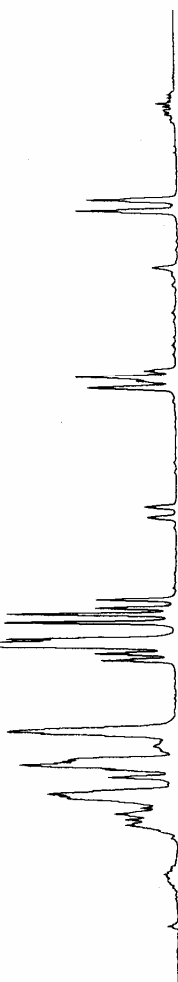
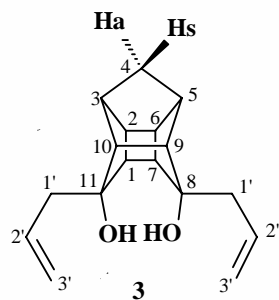
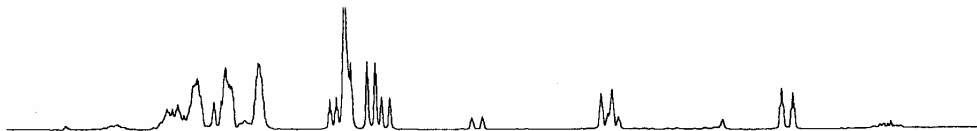
Pulse Sequence: ghsqc_da



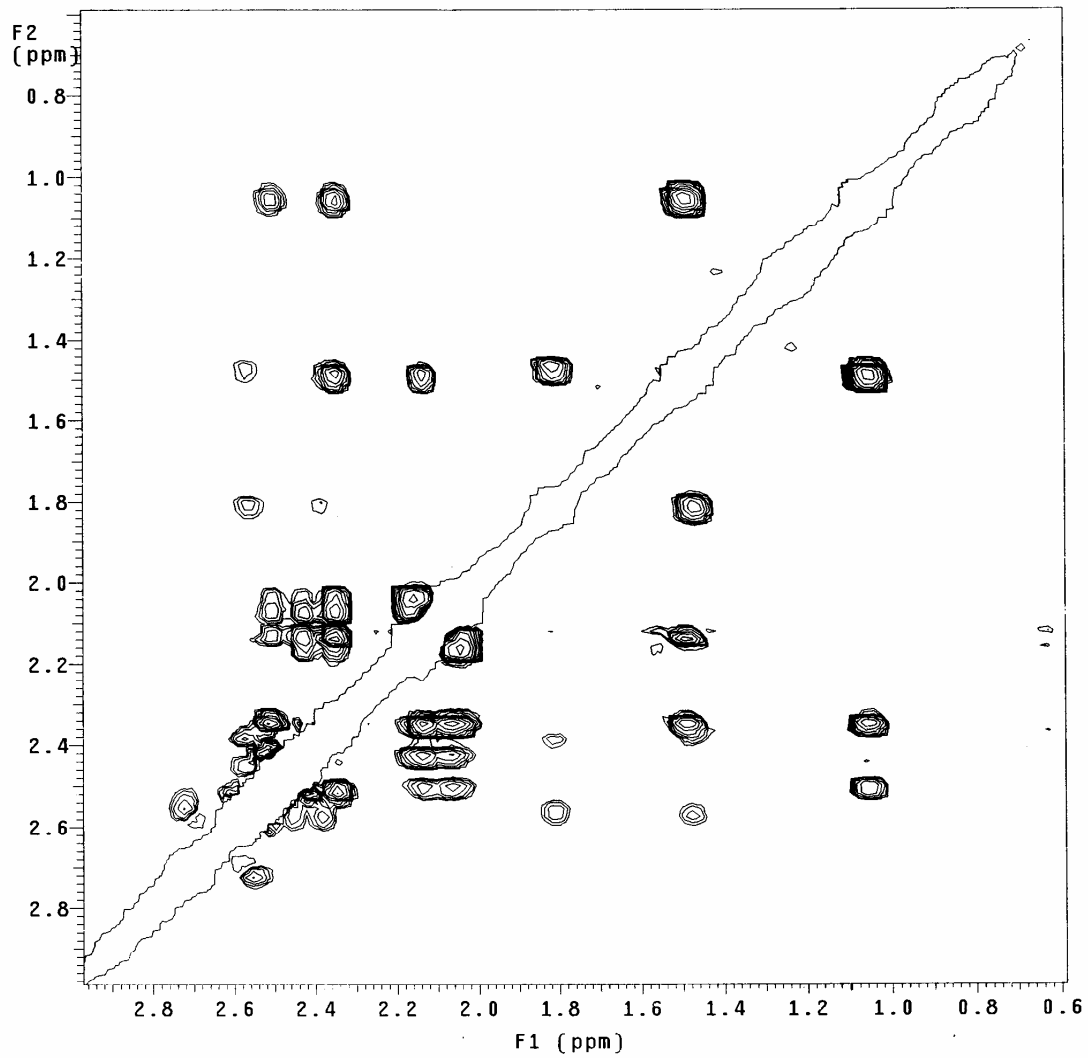
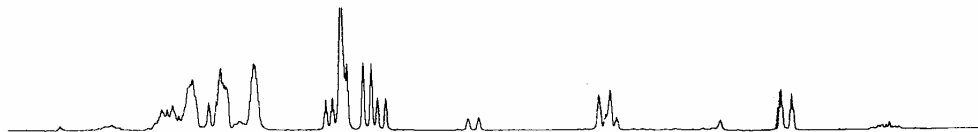
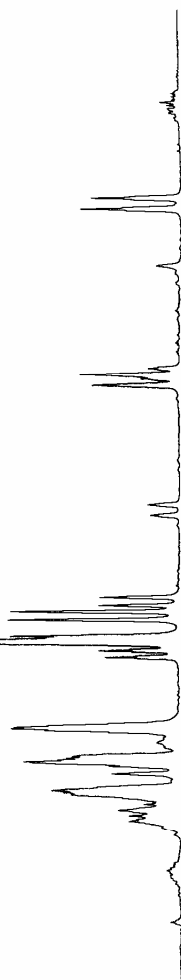
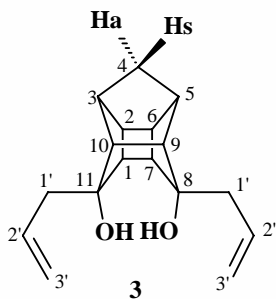
H0edio1.endo endo diol in cdc13
Gradient HSQC expt.
with mult.editing
probe=5mmASW
Pulse Sequence: ghsqc_da



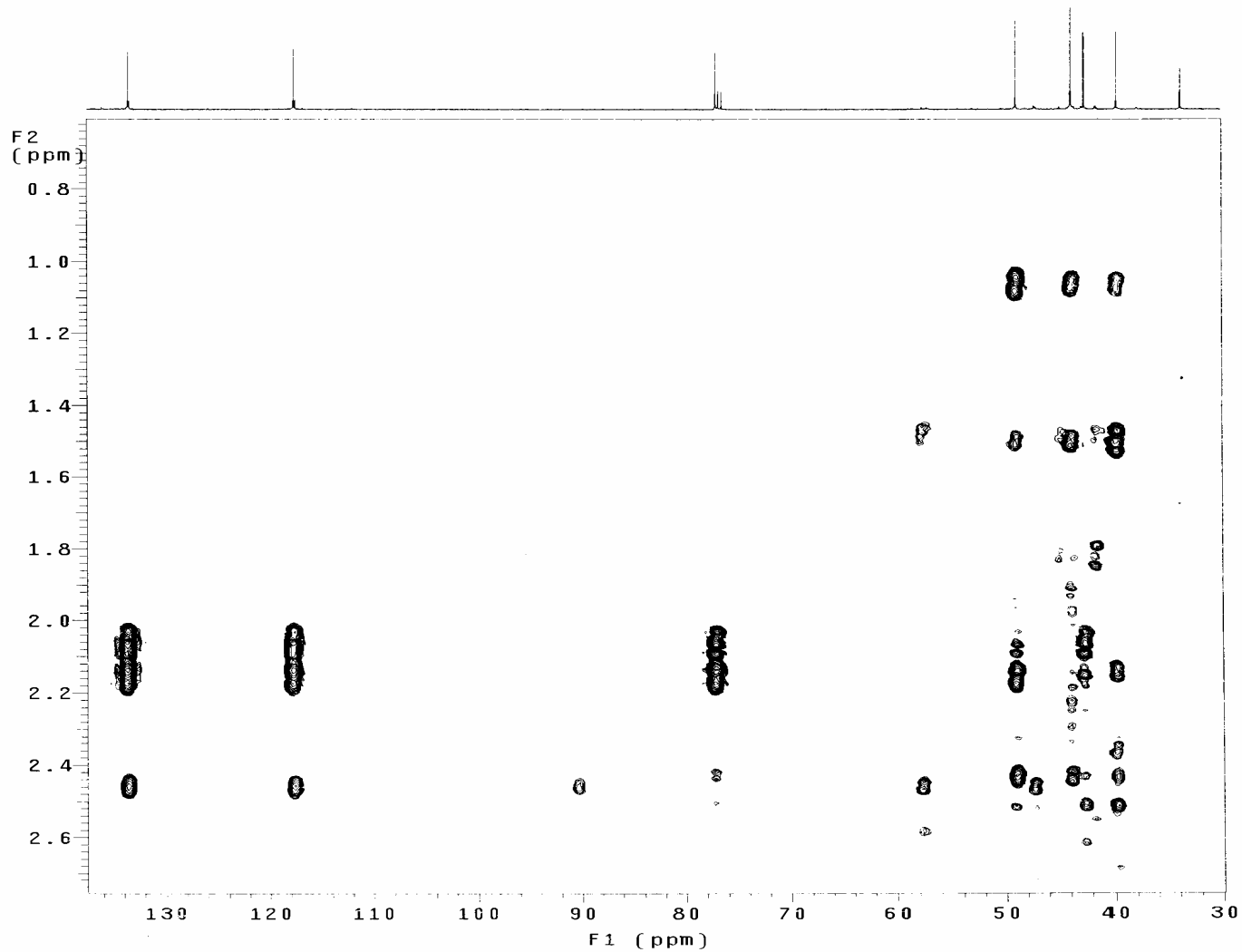
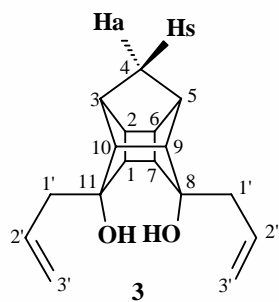
cyediol.endo endo diol in cdc13
1H Cosy-30
probe=5mmASW
Pulse Sequence: relayh



N0ediol.endo endo diol in cdc13
NOESY expt.
mix=1sec
probe=5mmASW
Pulse Sequence: noesy_da

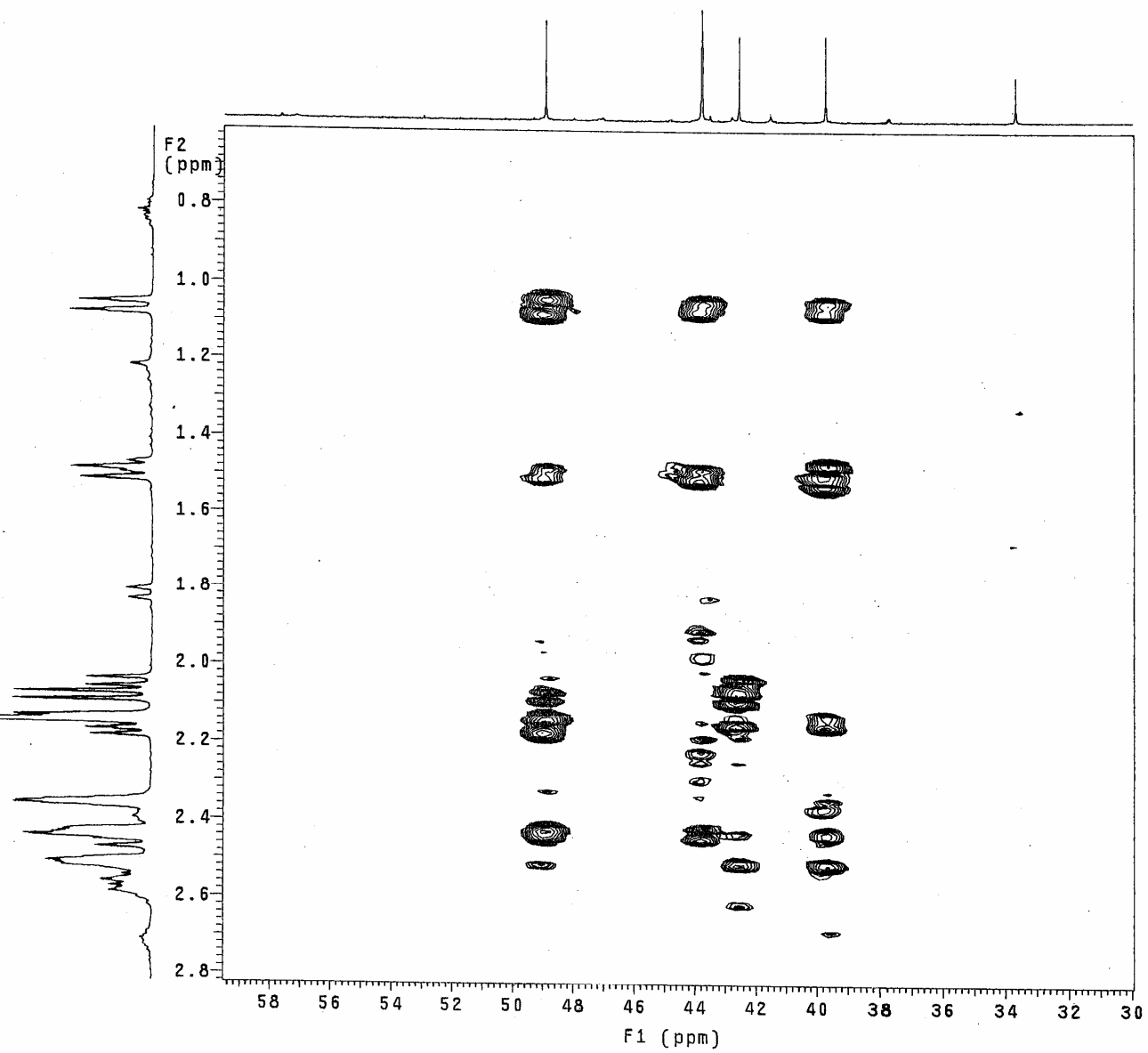
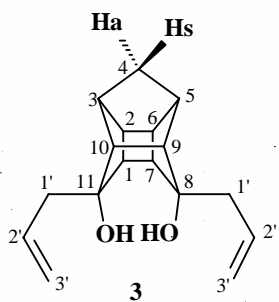


HBediol.endo endo diol in cdcl3
Gradient HMBC expt.
probe=5mmASW
Pulse Sequence: ghmqc_da

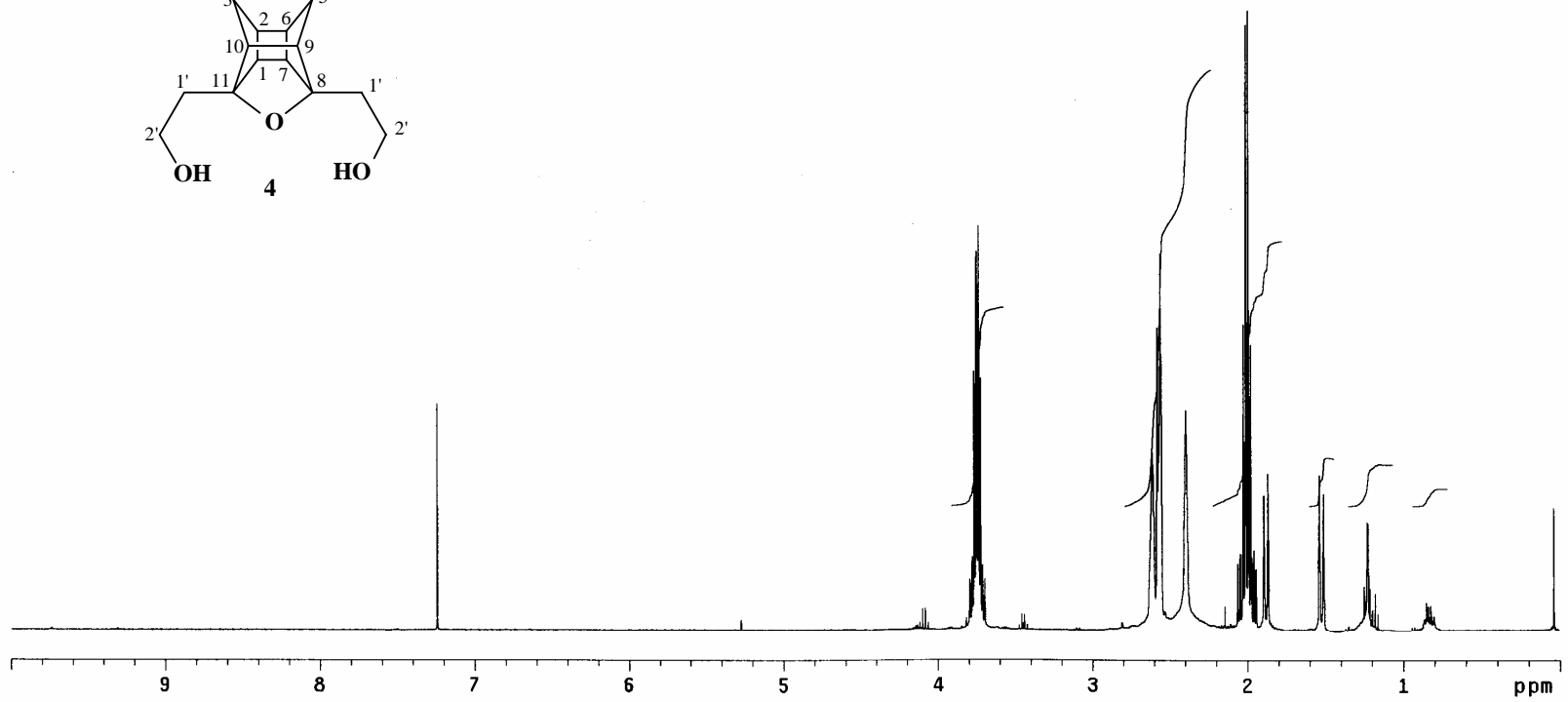
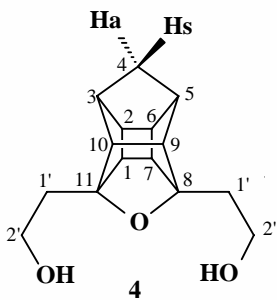


H β diol.endo endo diol in cdc13
Gradient HHBC expt.
probe=5mmASW

Pulse Sequence: ghmqc_da

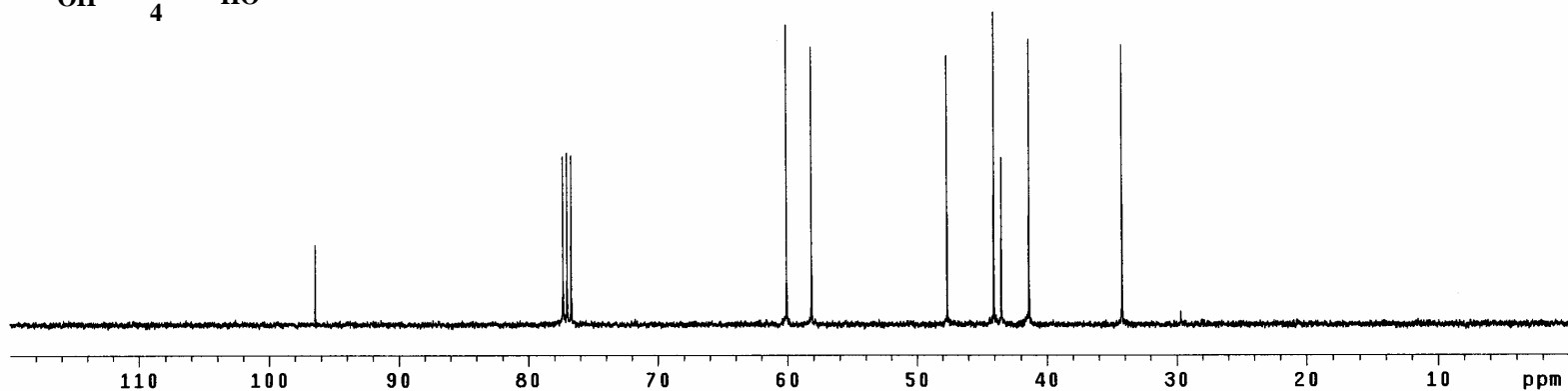
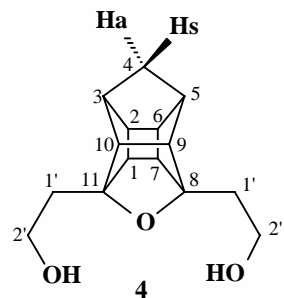


hdio1.dio1 in cdc13
probe=5mmASW
Pulse Sequence: s2pu1

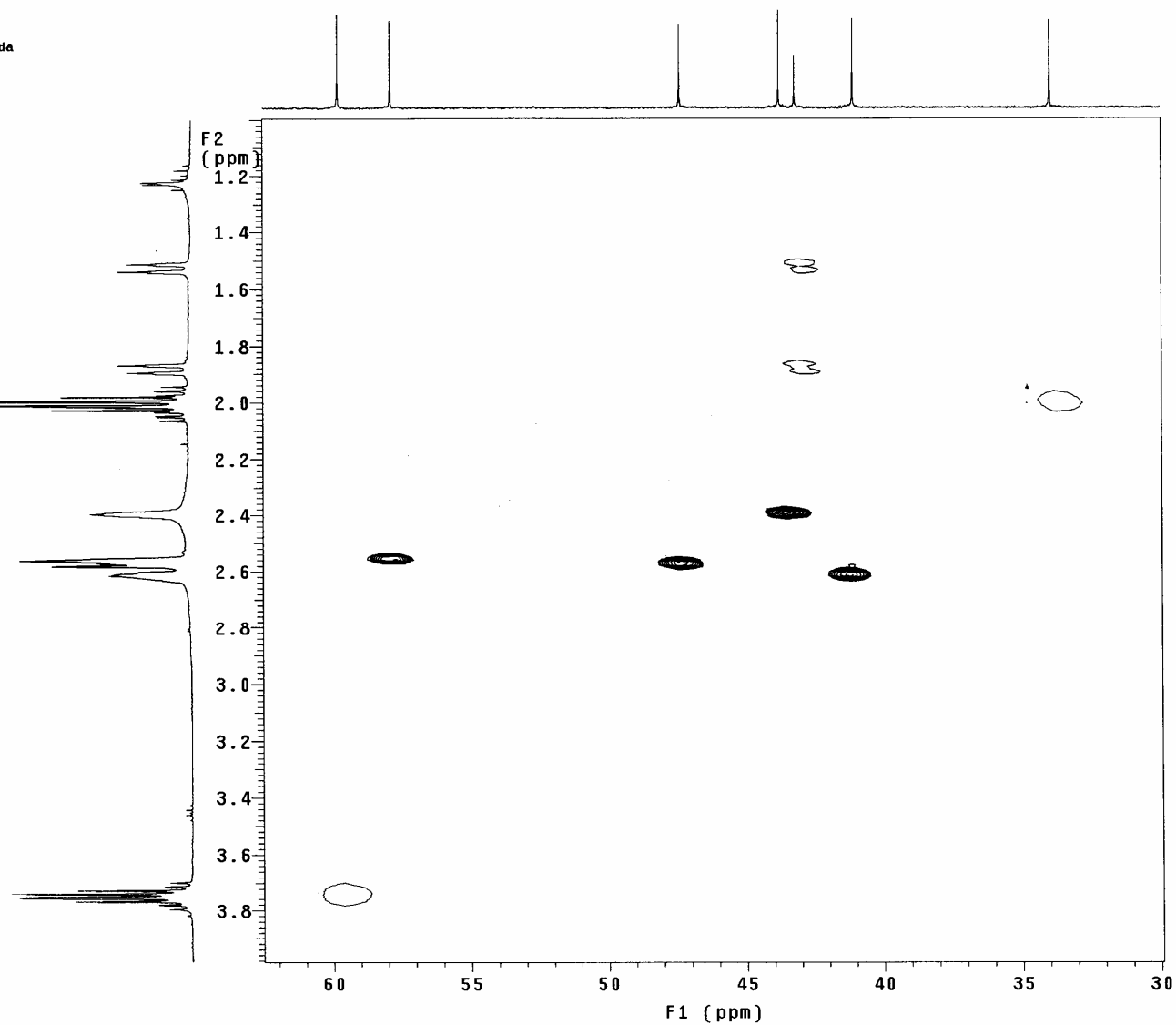
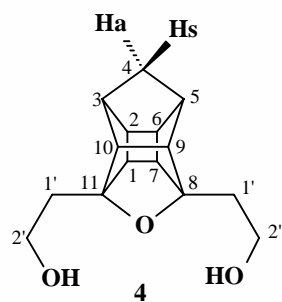


cd1o1.d1o1 in cdc13
probe=5mmASW
Pulse Sequence: s2pu1

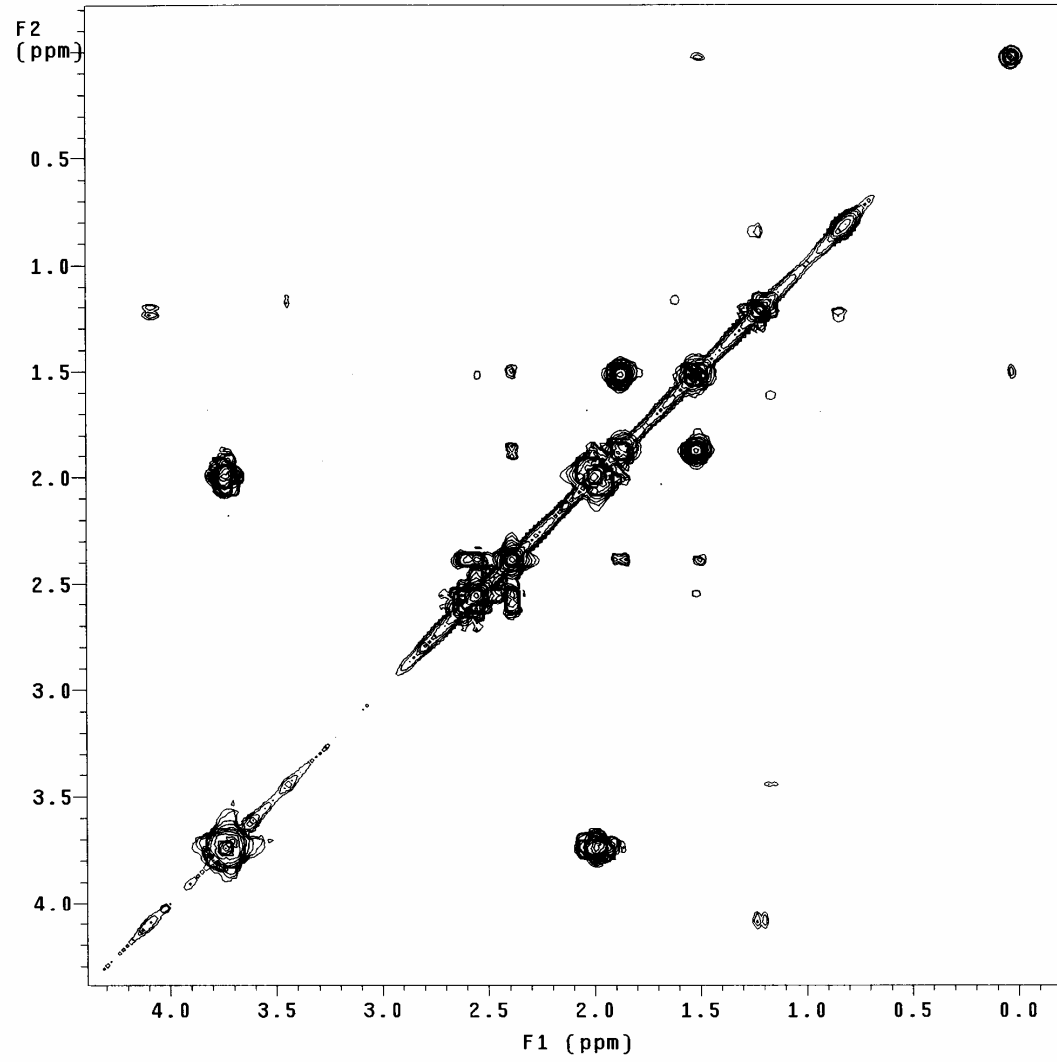
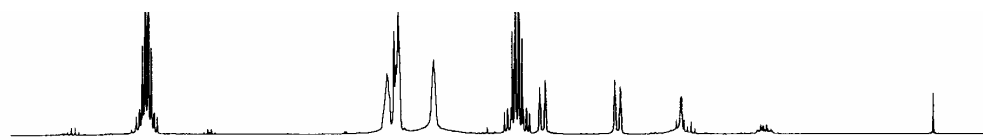
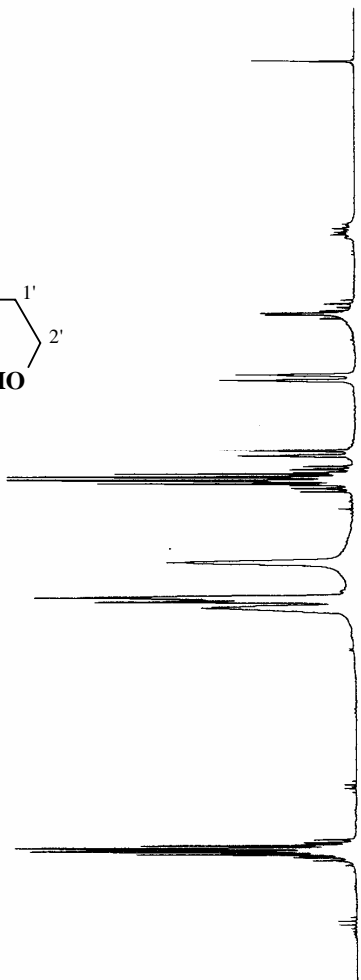
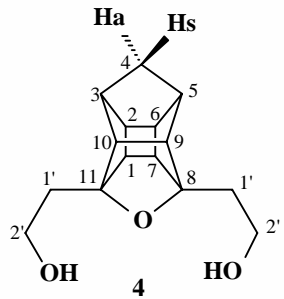
| INDEX | FREQUENCY | PPM | HEIGHT |
|-------|-----------|--------|--------|
| 1 | 9695.867 | 96.415 | 12.9 |
| 2 | 7775.490 | 77.319 | 27.1 |
| 3 | 7743.445 | 77.000 | 27.7 |
| 4 | 7711.401 | 76.681 | 27.2 |
| 5 | 6040.513 | 60.066 | 48.0 |
| 6 | 5847.483 | 58.147 | 44.5 |
| 7 | 4790.780 | 47.639 | 43.2 |
| 8 | 4429.898 | 44.050 | 50.0 |
| 9 | 4372.676 | 43.481 | 26.9 |
| 10 | 4159.809 | 41.365 | 45.8 |
| 11 | 3440.336 | 34.210 | 44.9 |



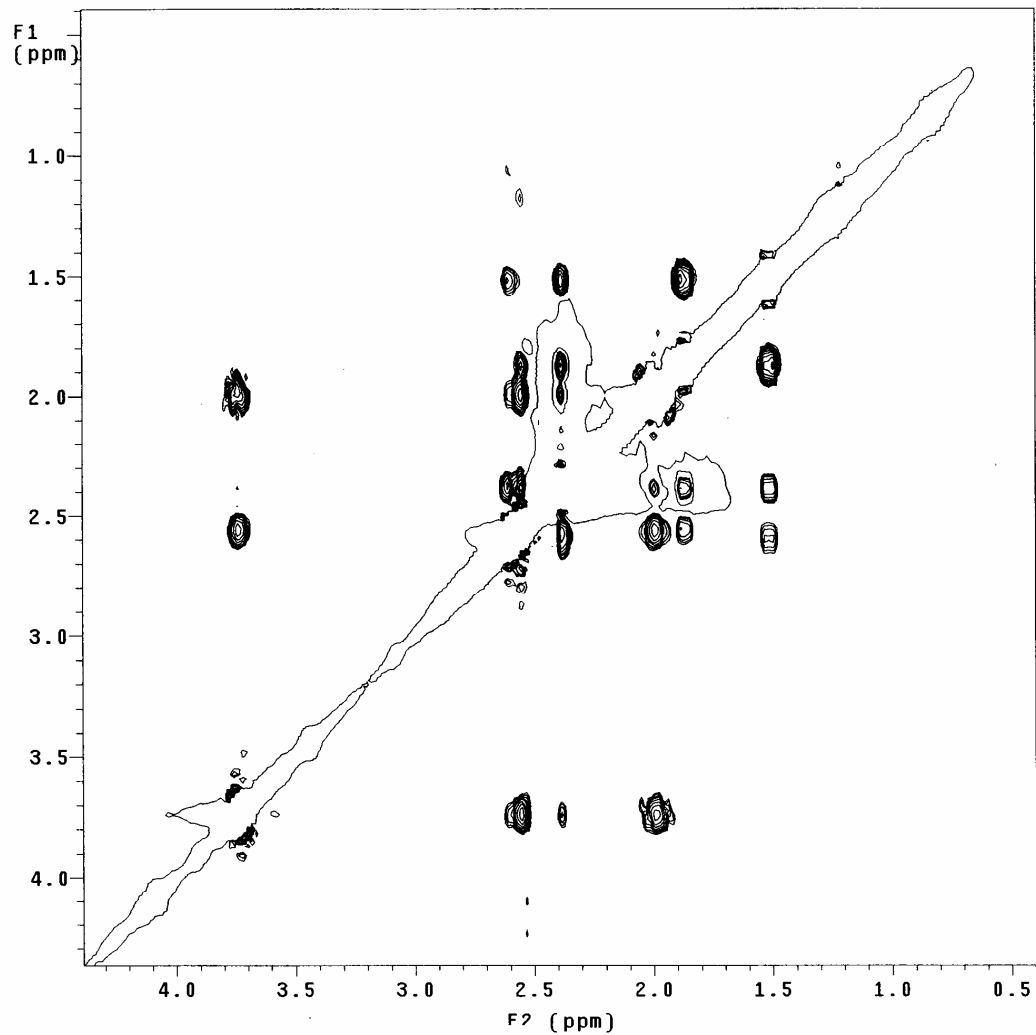
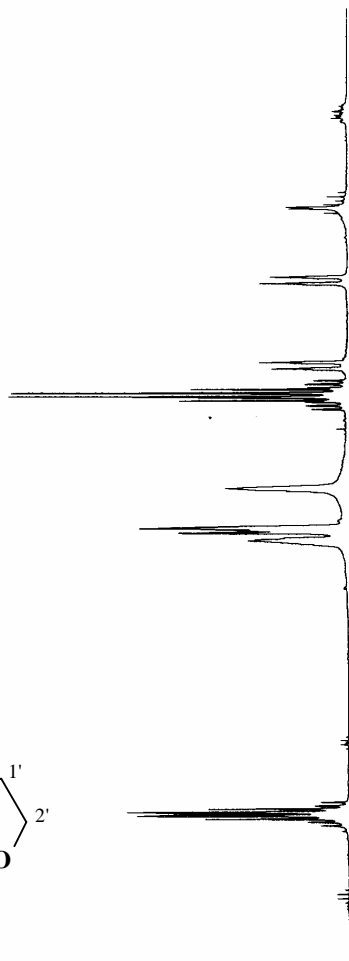
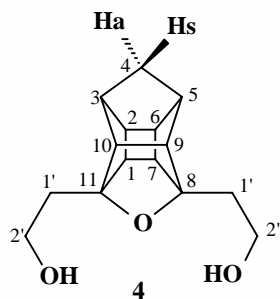
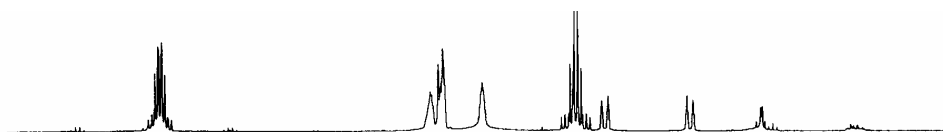
HQdio1.dio1 in cdc13
Gradient HSQC expt.
with mult.editing
probe=5mmASW
Pulse Sequence: ghsqc_da



cydio1.diol in cdcl3
1H Cosy-90
probe=5mmASW
Pulse Sequence: relayh



N0d101.d101 in cdc13
NOESY expt.
mix=1sec
probe=5mmASW
Pulse Sequence: noesy_da



HBdlol.d1o1 in cdcl3
Gradient HNBC expt.
probe=5mmASW
Pulse Sequence: ghmqc_da

