

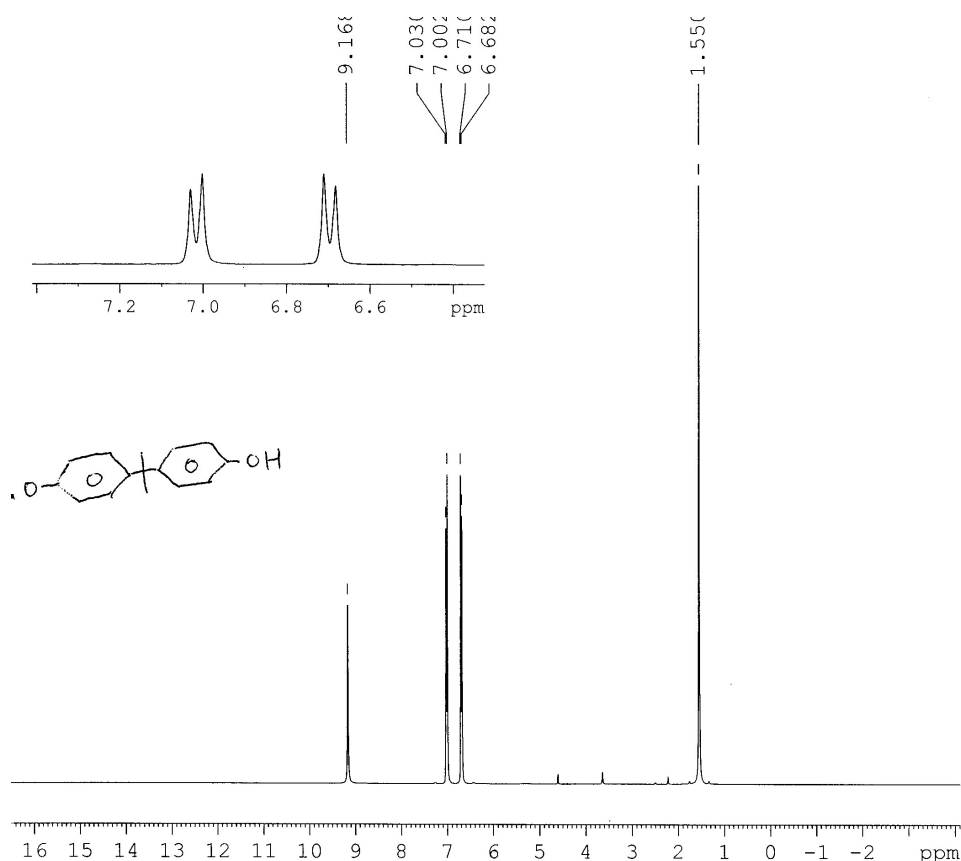
Assignment 1 – Due 10/14/08

- 1. We know that 1-chloroethylene has 12 proton peaks. Then how many proton peaks do 1-chloroethane have? Explain.

- Left is a spectrum of bisphenol-A (leftmost group should be a OH)

- Answer:

- If the 9.1 ppm peak has an area of 2.0, what should be the areas of the 1.55 ppm peak and the 6.6-7.1 ppm peak group? Explain.
- Why is the 1.55 ppm peak a singlet?
- Why are the 6.5 and 7.0 ppm peaks doublets?
- Why does the 6.5 ppm doublet not have a 1:1 ratio?

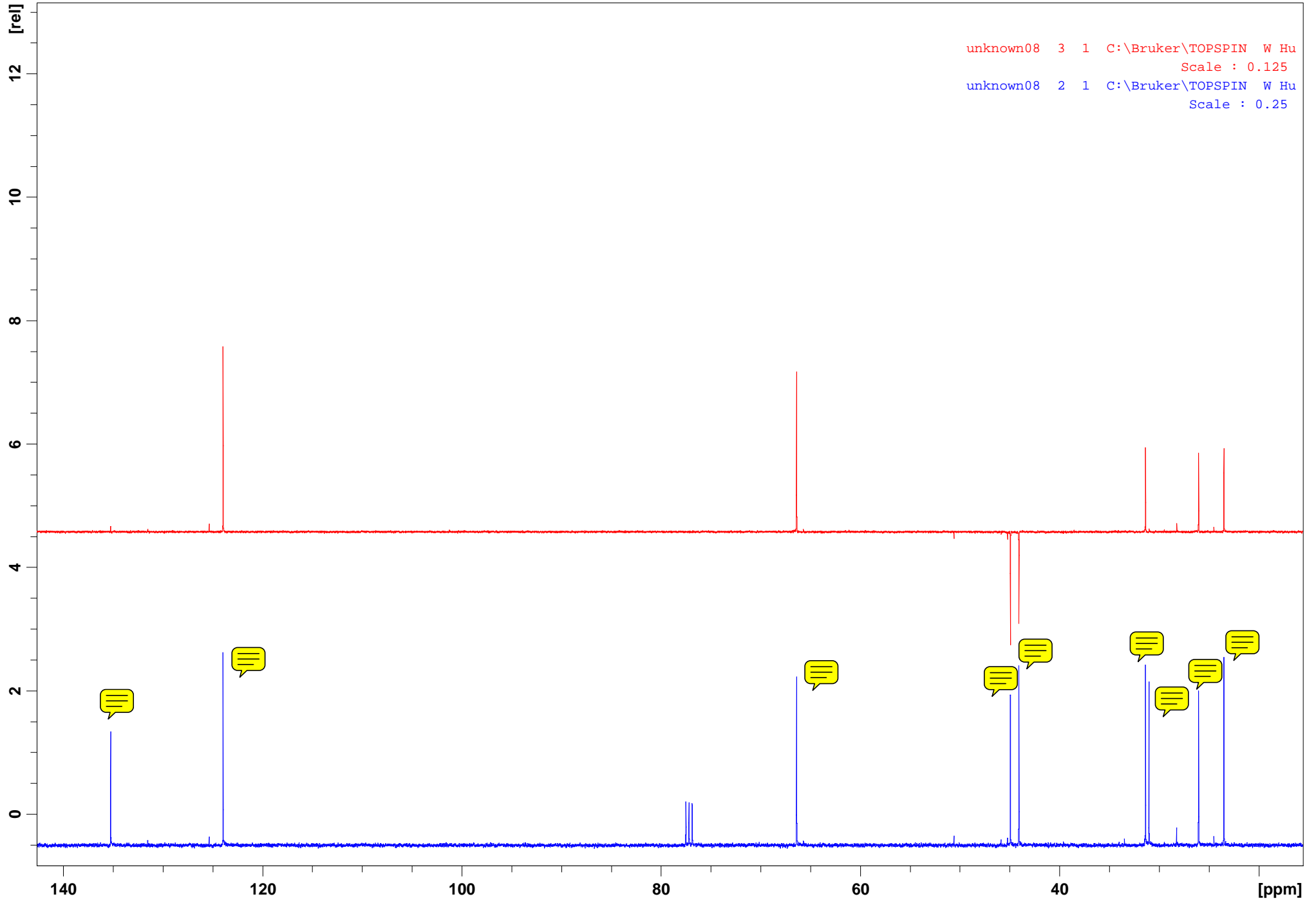


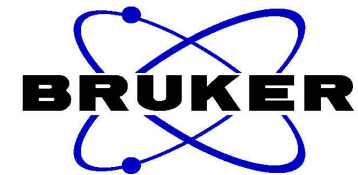
Assignment 2 – Due 10/22/08

- Solve the structure of the unknown molecule according to the spectra provided
 - Draw the molecular structure, label carbon and proton groups according to my numbering of peaks on the spectra.
 - Measure the J coupling constant between protons 4 and 6. Is it a 2J , 3J or 4J ?
- Notes:
 - Unlabeled small peaks on 1D spectra are due to impurity;
 - On COSY spectrum, the several peaks on the horizontal 3.5 ppm line are “center glitches” (artifacts)
 - The molecular formula is $C_9H_{16}O$.

unknown08 2 1 C:\Bruker\TOPSPIN W Hu

unknown08 3 1 C:\Bruker\TOPSPIN W Hu
Scale : 0.125
unknown08 2 1 C:\Bruker\TOPSPIN W Hu
Scale : 0.25

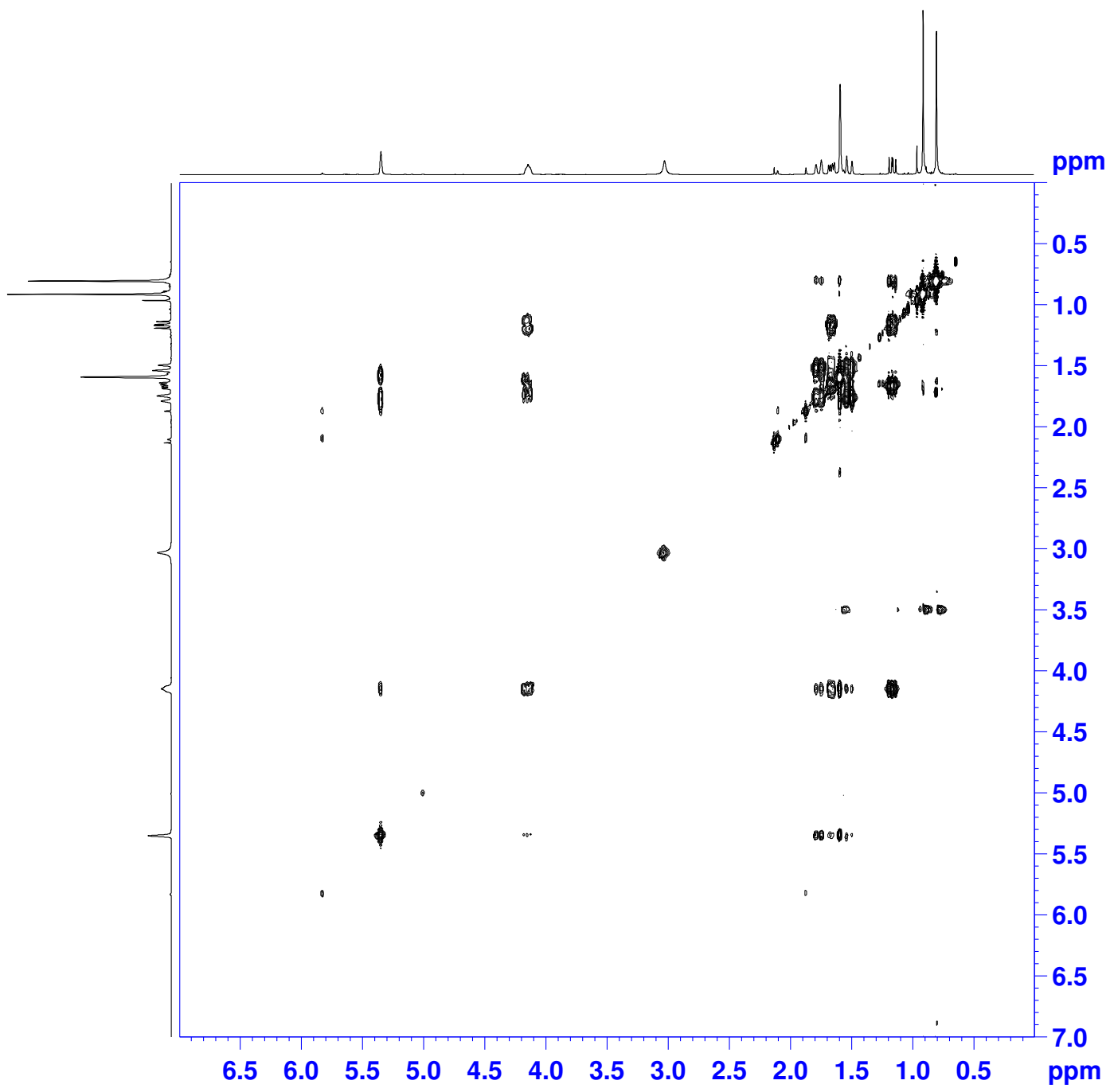


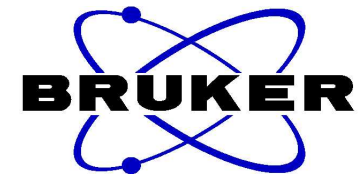


NAME unknown08
EXPNO 6
PROCNO 1
Date_ 20081001
Time 11.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG cosygpgf
TD 2048
SOLVENT DMSO
NS 1
DS 8
SWH 2796.421 Hz
FIDRES 1.365440 Hz
AQ 0.3662324 sec
RG 25.4
DW 178.800 usec
DE 6.00 usec
TE 296.1 K
d0 0.00000300 sec
D1 1.48689198 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00035703 sec
MCREST 0.00000000 sec
MCWRK 1.48689198 sec

===== CHANNEL f1 =====
NUC1 1H
P0 8.85 usec
P1 8.85 usec
PL1 0.00 dB
SFO1 400.1314005 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec
ND0 1
TD 128
SFO1 400.1314 MHz
FIDRES 21.882221 Hz
SW 7.000 ppm
FnMODE QF
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

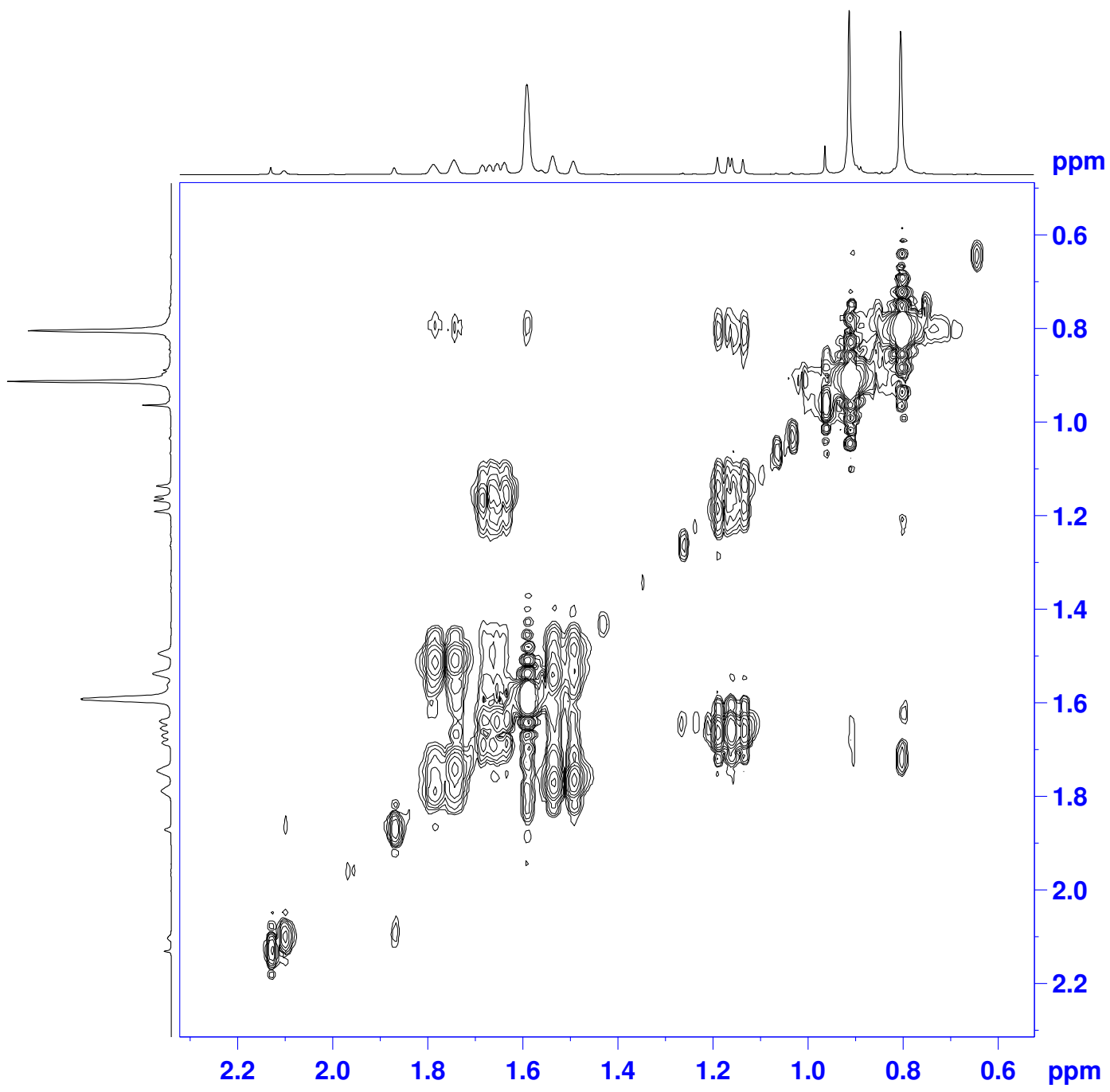


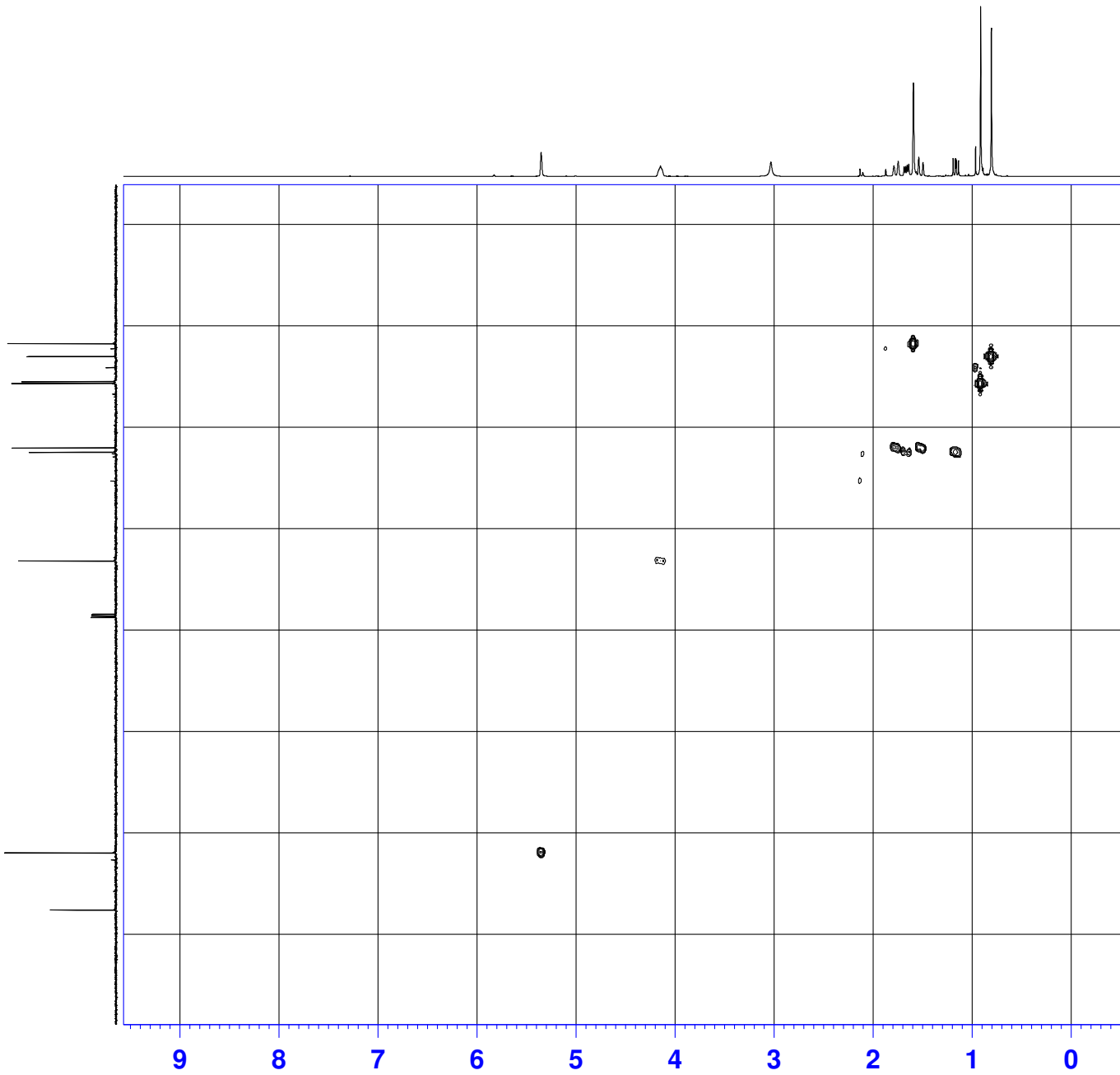
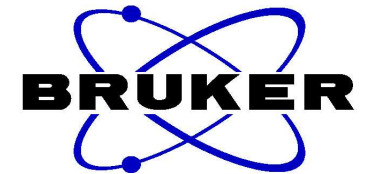


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NAME unknown08
EXPNO 6
PROCNO 1
Date_ 20081001
Time 11.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG cosygpgf
TD 2048
SOLVENT DMSO
NS 1
DS 8
SWH 2796.421 Hz
FIDRES 1.365440 Hz
AQ 0.3662324 sec
RG 25.4
DW 178.800 usec
DE 6.00 usec
TE 296.1 K
d0 0.00000300 sec
D1 1.48689198 sec
d13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00035703 sec
MCREST 0.00000000 sec
MCWRK 1.48689198 sec
```

```
===== CHANNEL f1 =====
NUC1 1H
P0 8.85 usec
P1 8.85 usec
PL1 0.00 dB
SFO1 400.1314005 MHz
```

```
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 10.00 %
GPZ2 10.00 %
P16 1000.00 usec
ND0 1
TD 128
SFO1 400.1314 MHz
FIDRES 21.882221 Hz
SW 7.000 ppm
FnMODE QF
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 400.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
```





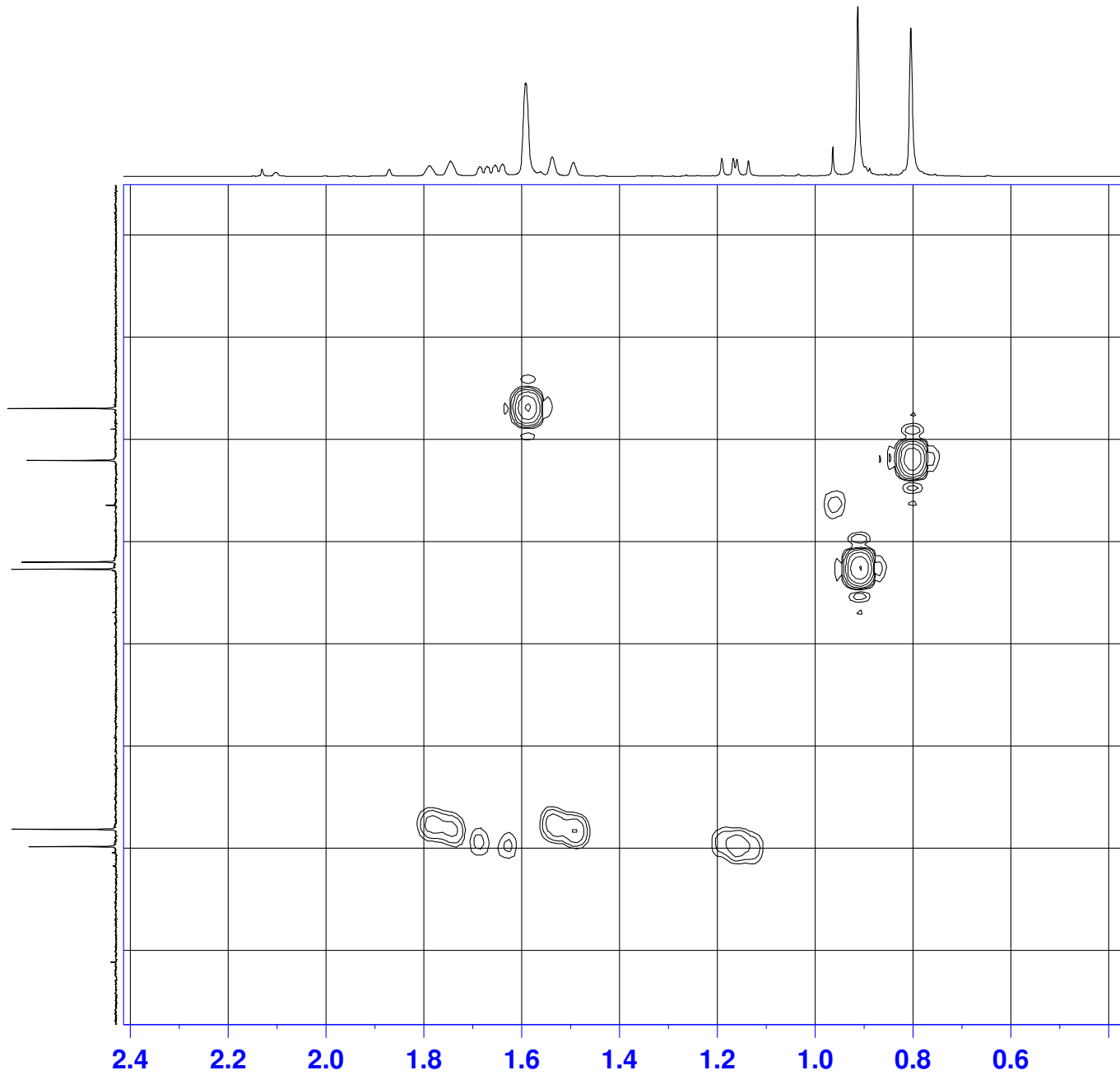
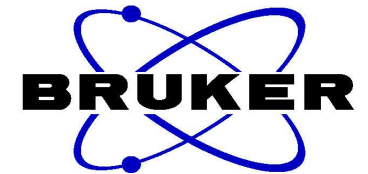
ppm
0
20
40
60
80
100
120
140
ppm

```
NAME unknown08
EXPNO 5
PROCNO 1
Date_ 20081001
Time 10.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG hmqcpgpgf
TD 1024
SOLVENT DMSO
NS 2
DS 16
SWH 4032.255 Hz
FIDRES 3.937752 Hz
AQ 0.1270260 sec
RG 2580.3
DW 124.000 usec
DE 6.00 usec
TE 296.1 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.50000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
d13 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00003000 sec
MCREST 0.00000000 sec
MCWRK 1.50000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.85 usec
p2 17.70 usec
PL1 0.00 dB
SFO1 400.1318130 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 6.85 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 27.60 dB
SFO2 100.6203140 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE,100
GPNAM2 SINE,100
GPNAM3 SINE,100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
PI6 1000.00 usec
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FnMODE QF
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 1
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MCZ QF
SF 100.6127690 MHz
WDW SINE
SSB 1
LB 0.00 Hz
GB 0
```



NAME unknown08
EXPNO 5
PROCNO 1
Date_ 20081001
Time 10.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG hmqcpgpgf
TD 1024
SOLVENT DMSO
NS 2
DS 16
SWH 4032.258 Hz
FIDRES 3.937752 Hz
AQ 0.1270260 sec
RG 2580.3
DW 124.000 usec
DE 6.00 usec
TE 296.1 K
CNST2 145.0000000
d0 0.00000300 sec
D1 1.50000000 sec
d2 0.00344828 sec
dI2 0.00002000 sec
dI3 0.00000400 sec
D16 0.00020000 sec
DELTA1 0.00222428 sec
IN0 0.00003000 sec
MCREST 0.00000000 sec
MCWRK 1.50000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.85 usec
p2 17.70 usec
PL1 0.00 dB
SFO1 400.1318130 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 6.85 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 27.60 dB
SFO2 100.6203140 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPX3 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPY3 0.00 %
GPZ1 50.00 %
GPZ2 30.00 %
GPZ3 40.10 %
P16 1000.00 usec
ND0 2
TD 128
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FnMODE QF
SI 1024
SF 400.1300000 MHz
WDW SINE
SSB 1
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MCZ QF
SF 100.6127690 MHz
WDW SINE
SSB 1
LB 0.00 Hz
GB 0