

Cyclochiral conformers of resorcin[4]arenes stabilized by hydrogen bonds

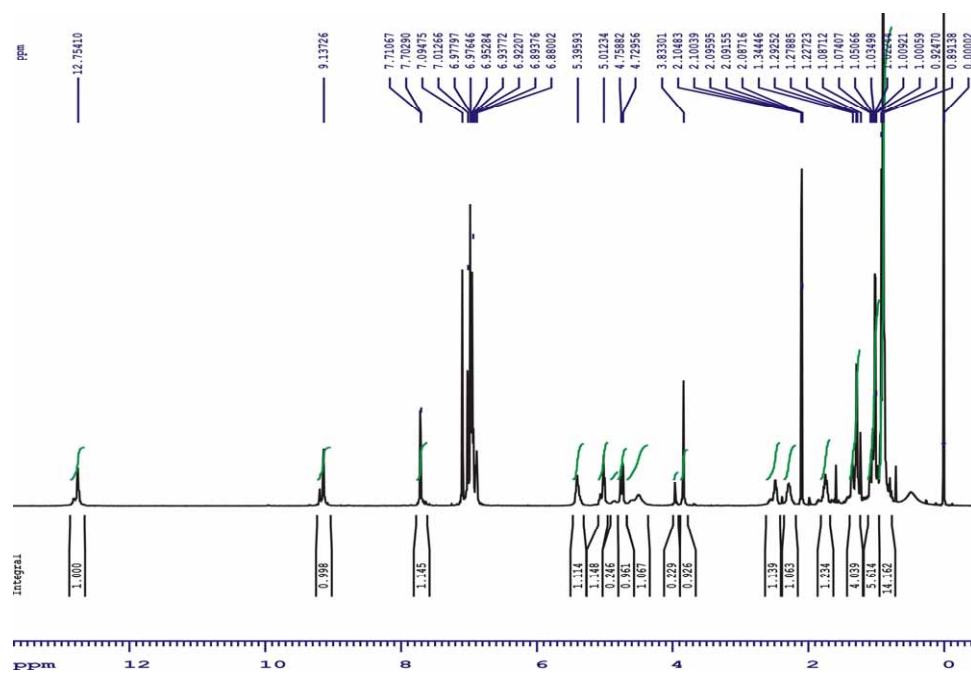
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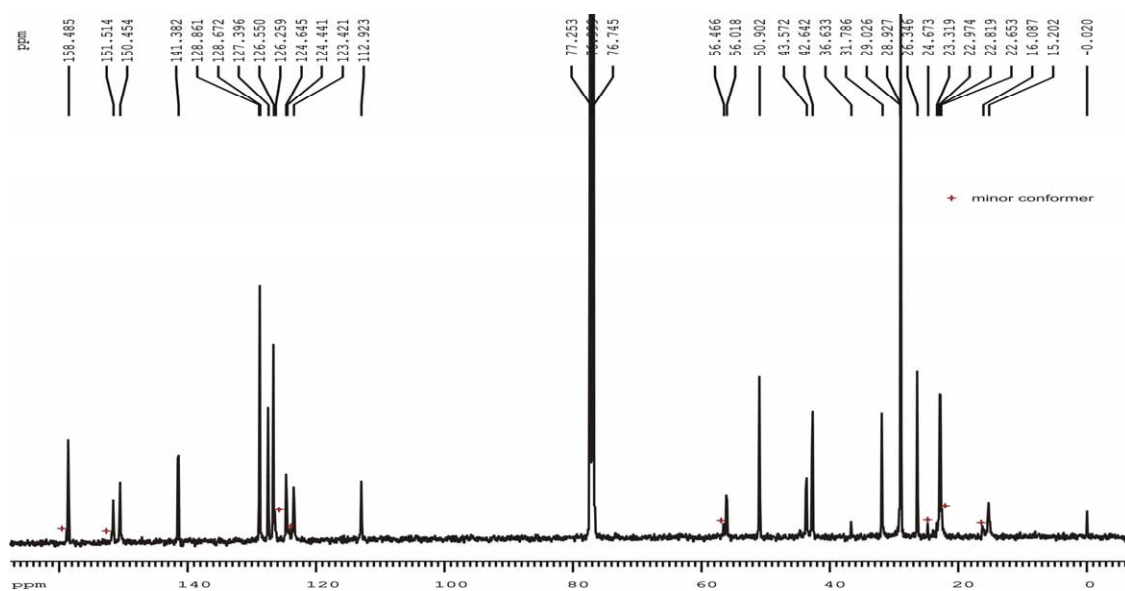
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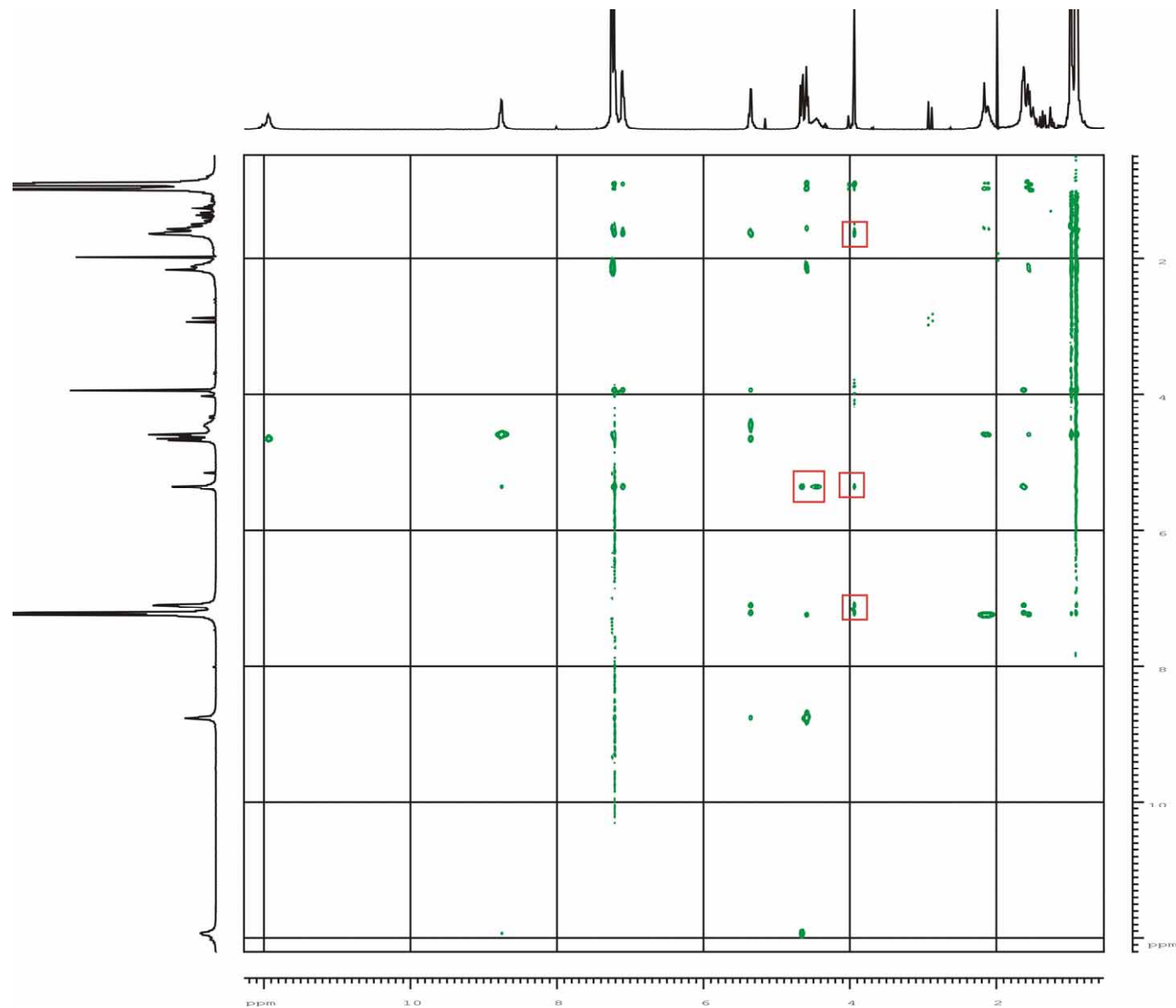
¹H NMR spectrum of 4i



¹³C NMR spectrum of 4i



ROESY spectrum of 4i □ - most relevant ROESY cross-peaks



```
Current Data Parameters
NAME      R217a
EXPNO     4
PROCNO    1

F2 - Acquisition Parameters
Date_     20060928
Time      19.05
INSTRUM   spect
PROBHD    5 mm TBI 1H/1
PULPROG   zgpg30
TD         2048
SOLVENT   D2O
NS         32
DS         16
SWH        6510.417 Hz
FIDRES     3.179914 Hz
AQ         0.1979364 sec
RG         64
CW         76.400 usec
DE         4.00 usec
TE         300.0 K
DQ         0.0000000 sec
D1         1.5000000 sec
d11        0.0300000 sec
D12        0.0002000 sec
RG         0.0019360 sec
L3         45

----- CHANNEL f1 -----
NUC1       1H
P1         8.80 usec
PL1        250000.00 usec
PL2        3.00 dB
PL11       25.00 dB
RF01       500.133809 MHz

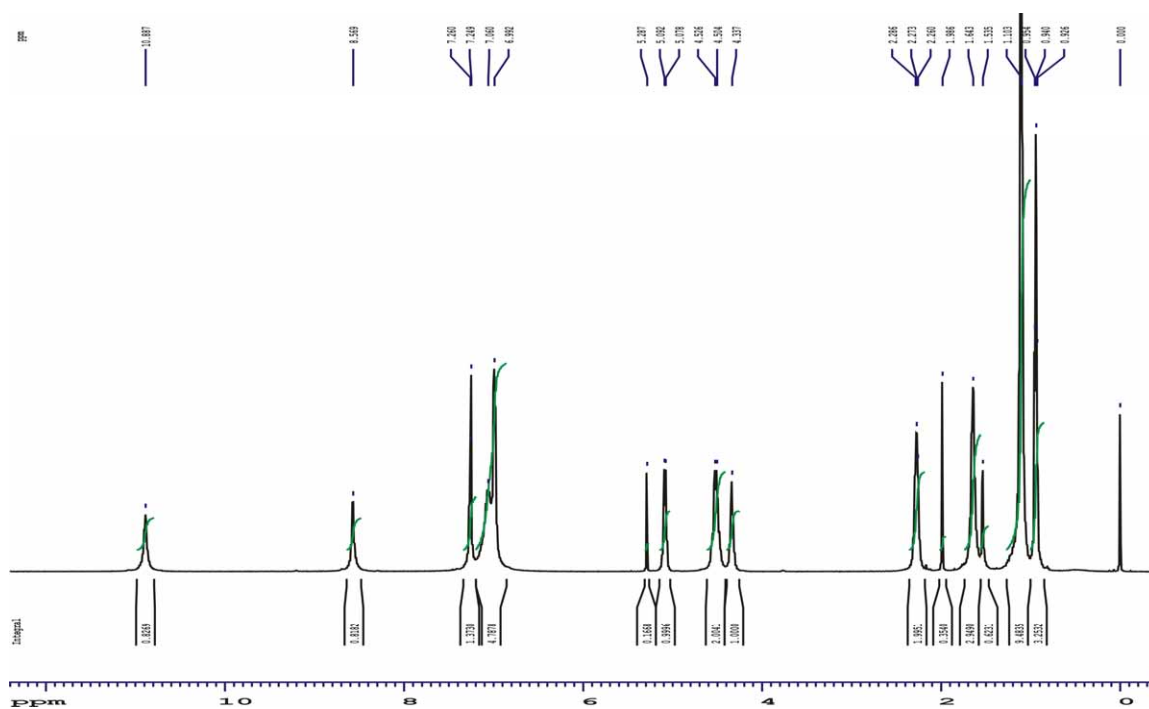
F1 - Acquisition parameters
RG         1
TD         512
RF01       500.1334 MHz
FIDRES     12.715457 Hz
AQ         13.017 ppm

F2 - Processing parameters
SI         2048
SF         500.1300173 MHz
WDW        SINE
SSB        2
LB         0.00 Hz
GB         0
PC         1.00

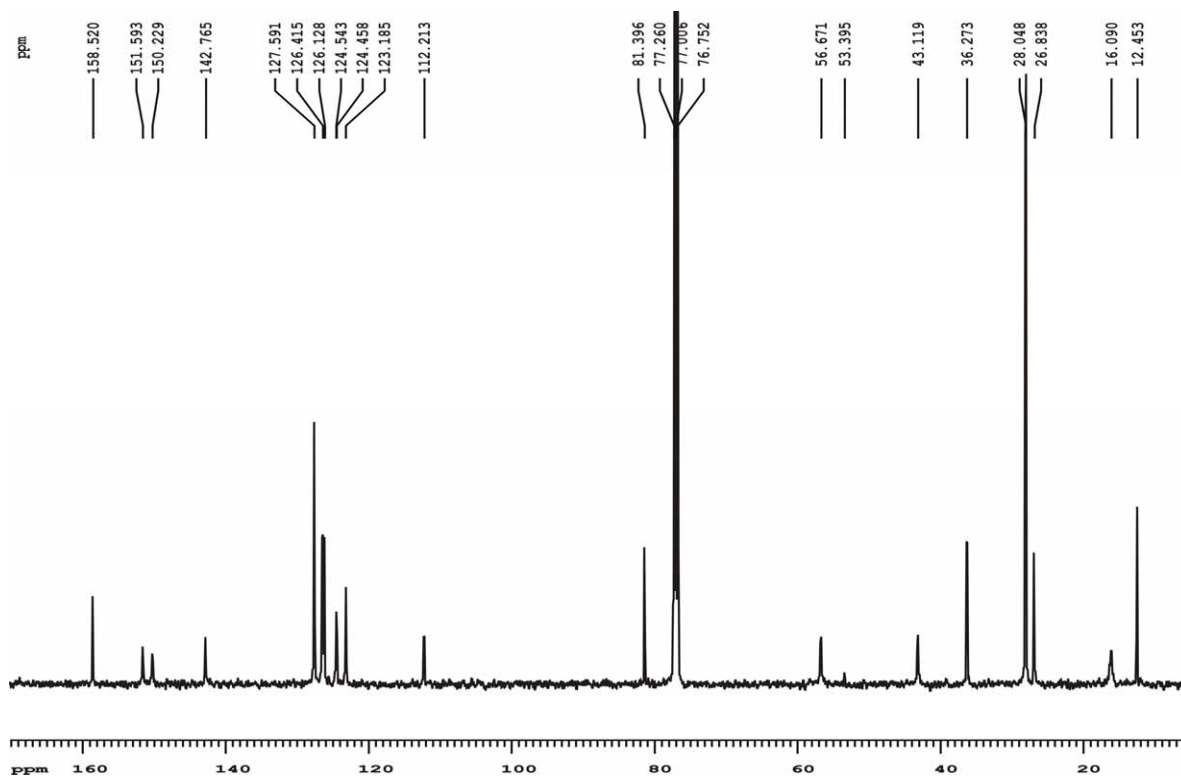
F1 - Processing parameters
SI         2048
MC2        Sine-EMFI
SF         500.1300173 MHz
WDW        SINE
SSB        2
LB         0.00 Hz
GB         0

2D NMR plot parameters
CX2        19.00 cm
CY1        19.00 cm
F2FLO      12.272 ppm
F2SLO      4137.36 Hz
F2PHI      0.592 ppm
F2H1       245.91 Hz
F1FLO      12.202 ppm
F1SLO      4109.36 Hz
F1PHI      0.481 ppm
F1H1       240.48 Hz
F2FPHICH   0.78266 ppm/cm
F2H1CH     291.43020 Hz/cm
F1FPHICH   0.78139 ppm/cm
F1H1CH     390.79483 Hz/cm
```

^1H NMR spectrum of 4e

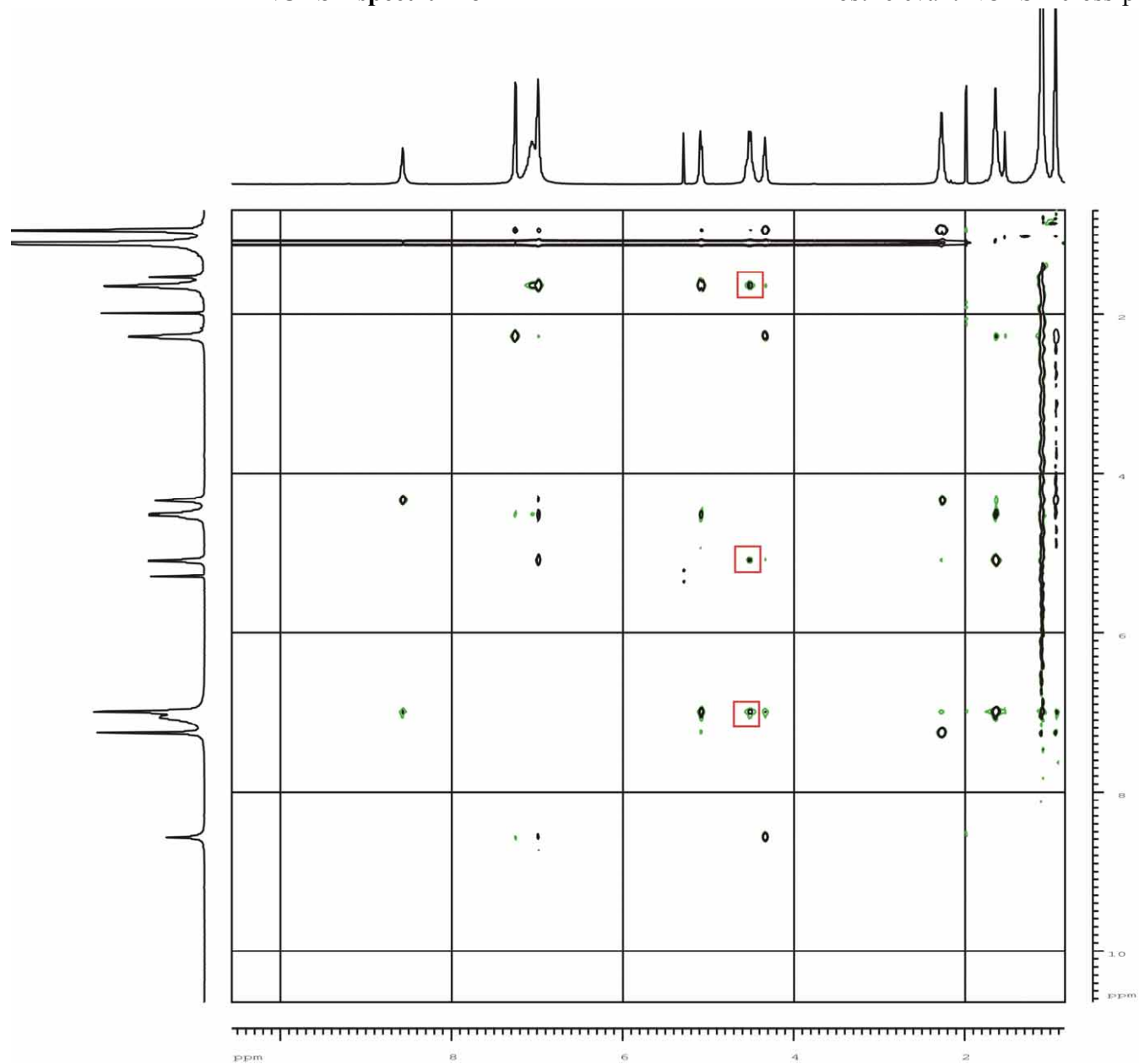


^{13}C NMR spectrum of 4e



NOESY spectrum of 4i

□ - most relevant NOESY cross-peaks



```
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EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20061204
Time      19.23
INSTRUM   spect
PROBHD    5 mm TBI LH/1
PULPROG   nosyvtc
TD         2048
SOLVENT   CDCl3
NS        32
DS         16
SFO1      600.615 MHz
FIDRES    2.934382 Hz
AQ         0.1704436 sec
RG         64
DM         83.200 usec
DE         4.50 usec
TE         303.0 K
D0         0.0000000 sec
D1         1.5000000 sec
D8         0.2500000 sec
D11        0.0300000 sec
EN0        0.00016640 sec
L3         12#

----- CHANNEL f1 -----
NUC1       1H
P1         8.95 usec
PL1        3.00 dB
SFO1      500.1331008 MHz

F1 - Acquisition parameters
MDO        1
TD         400
SFO1      500.1331 MHz
FIDRES    15.024038 Hz
SW         12.016 ppm

F2 - Processing parameters
SI         2048
SF         500.1300197 MHz
WDW        GAUSS
SSB        2
LA         0.00 Hz
GB         0
PC         0.30

F1 - Processing parameters
SI         1024
MC2        States-TPPI
SF         500.1300197 MHz
WDW        GAUSS
SSB        2
LA         0.00 Hz
GB         0

2D NMR plot parameters
CX2        15.00 cm
CX1        15.00 cm
F2PLO     10.567 ppm
F2LO      5284.87 Hz
F2PHI     0.833 ppm
F2HE      416.73 Hz
F1PLO     10.643 ppm
F1LO      5323.01 Hz
F1PHI     0.696 ppm
F1HE      346.30 Hz
F2FREQCM  0.64892 ppm/cm
F2FREQHz  324.54269 Hz/cm
F1FREQCM  0.66339 ppm/cm
F1FREQHz  331.78085 Hz/cm
```