

Guanylation of Thiosemicarbazones: A New Synthetic Route to Polysubstituted Guanylhydrazones with Antimicrobial Activity

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The spectra were acquired with a Varian Gemini-300 spectrometer operating at 300.069 MHz for ¹H and 75.458 MHz for ¹³C using a 5mm direct probe unless otherwise indicated.

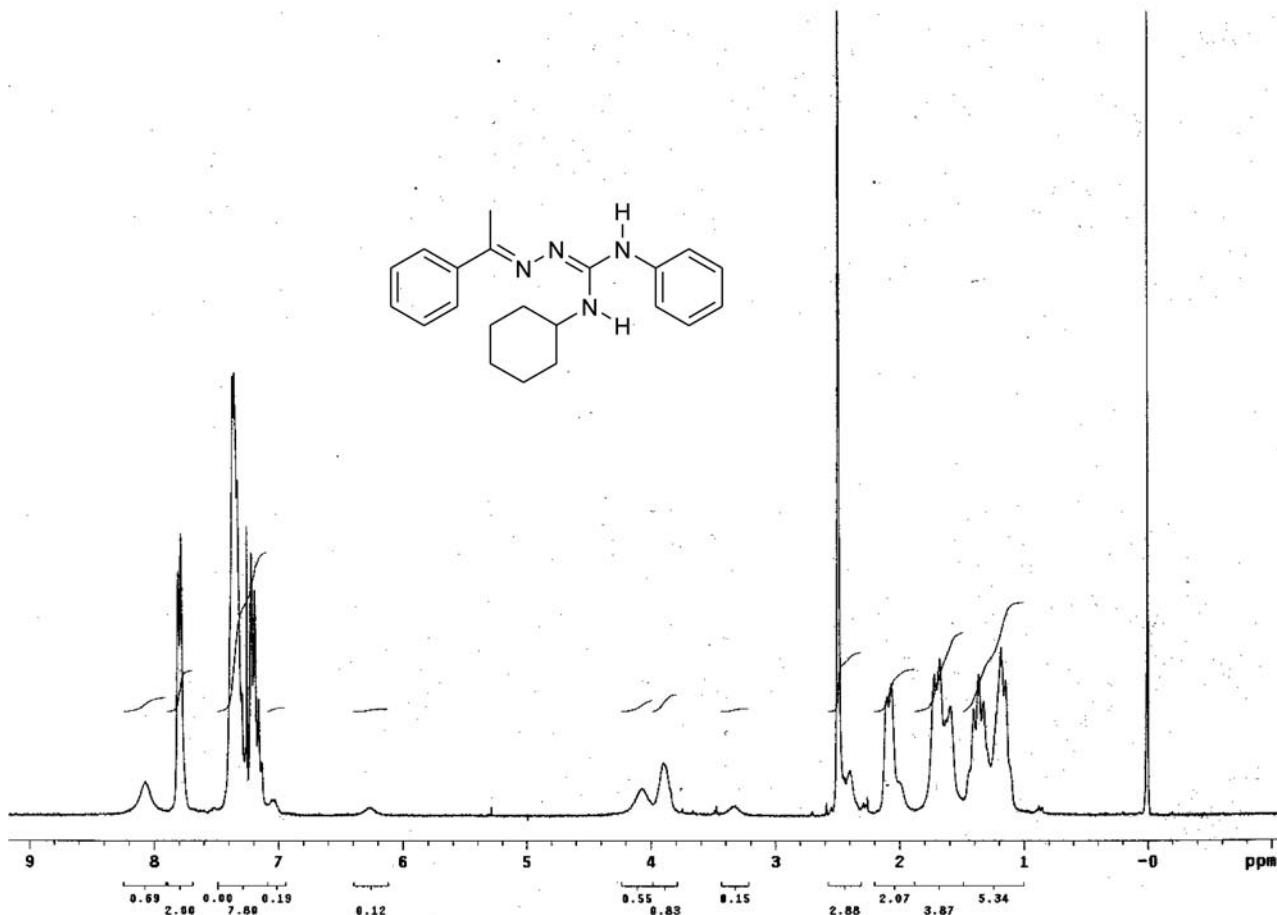


Figure S1. Full ¹H NMR spectrum of compound 2a (CDCl₃).

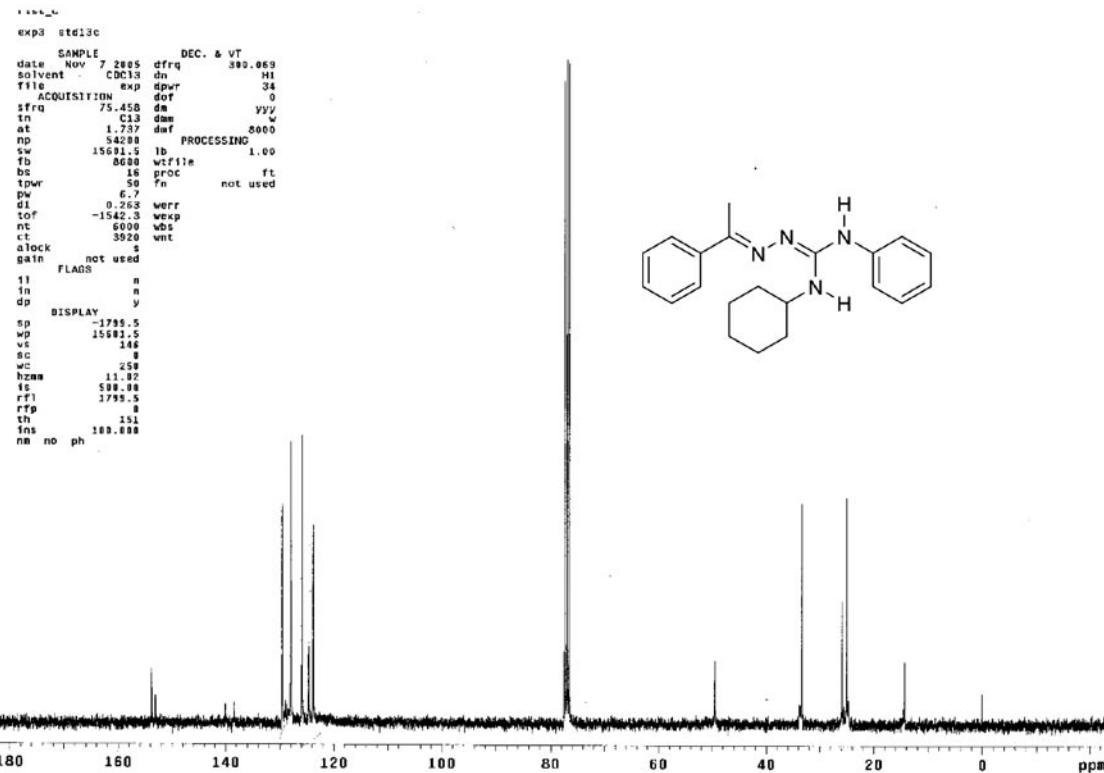


Figure S2. Full ¹³C NMR spectrum of compound 2a (CDCl₃).

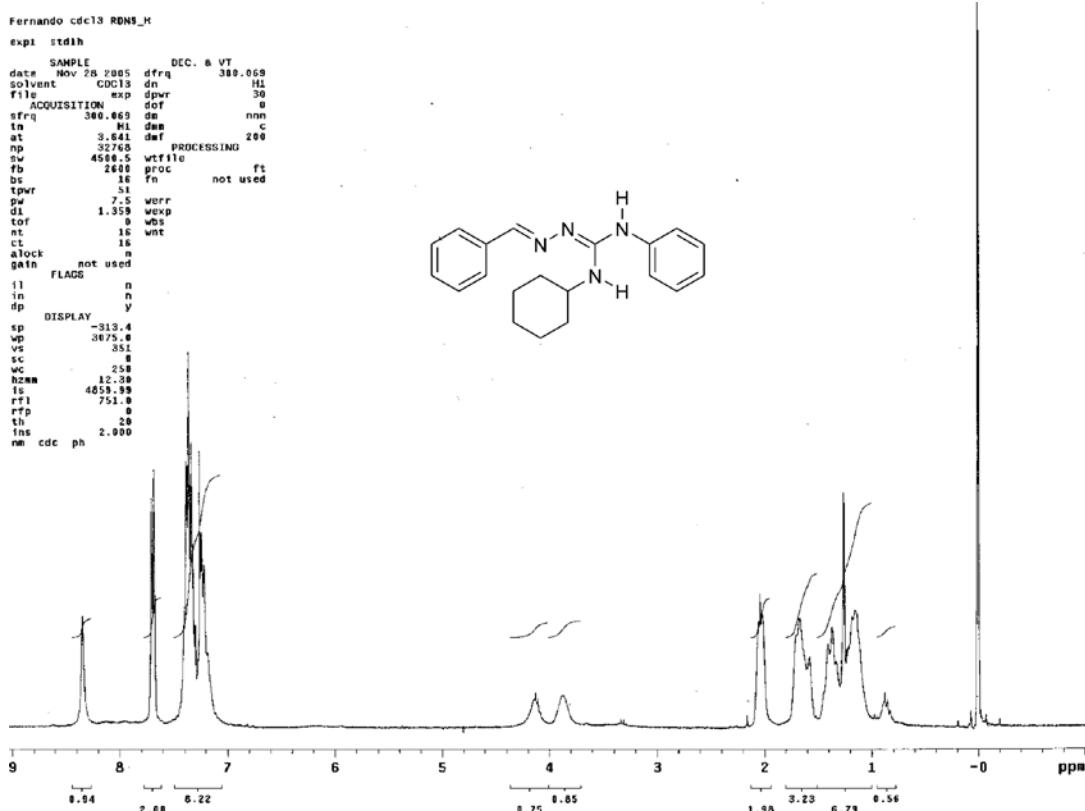
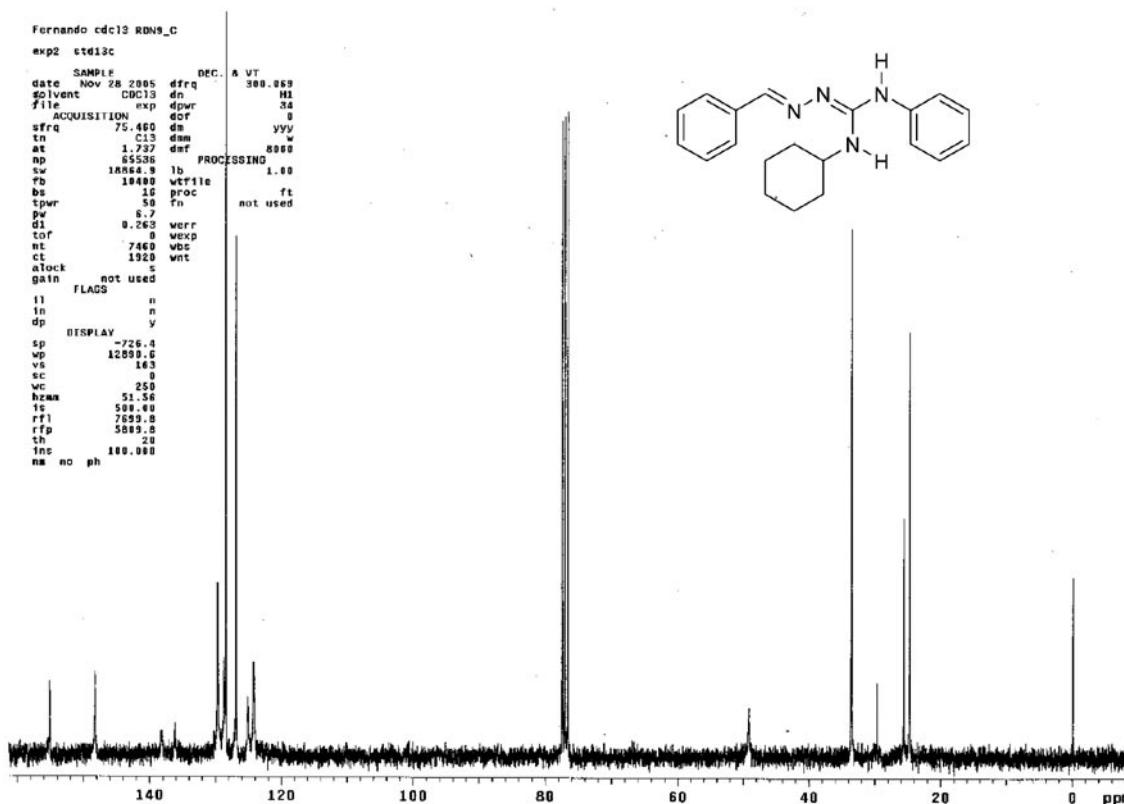
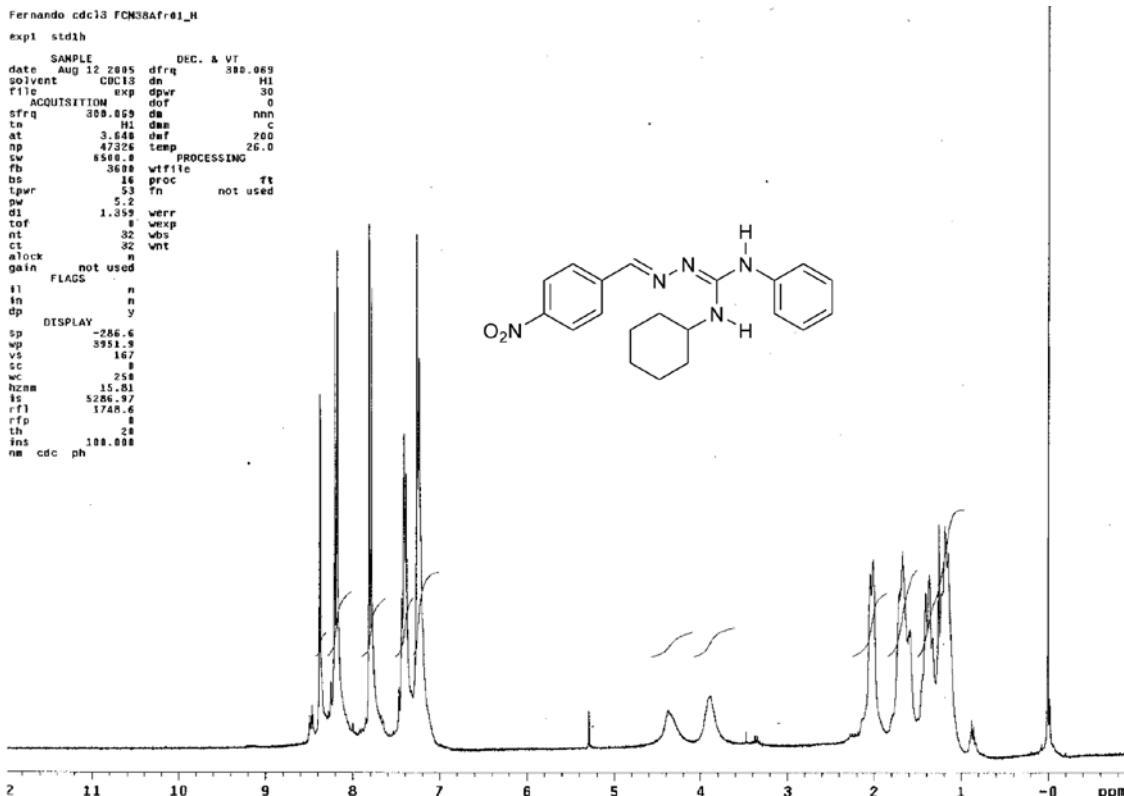


Figure S3. Full ¹H NMR spectrum of compound 2b (CDCl₃).

**Figure S4.** Full ¹³C NMR spectrum of compound **2b** (CDCl₃).**Figure S5.** Full ¹H NMR spectrum of compound **2c** (CDCl₃).

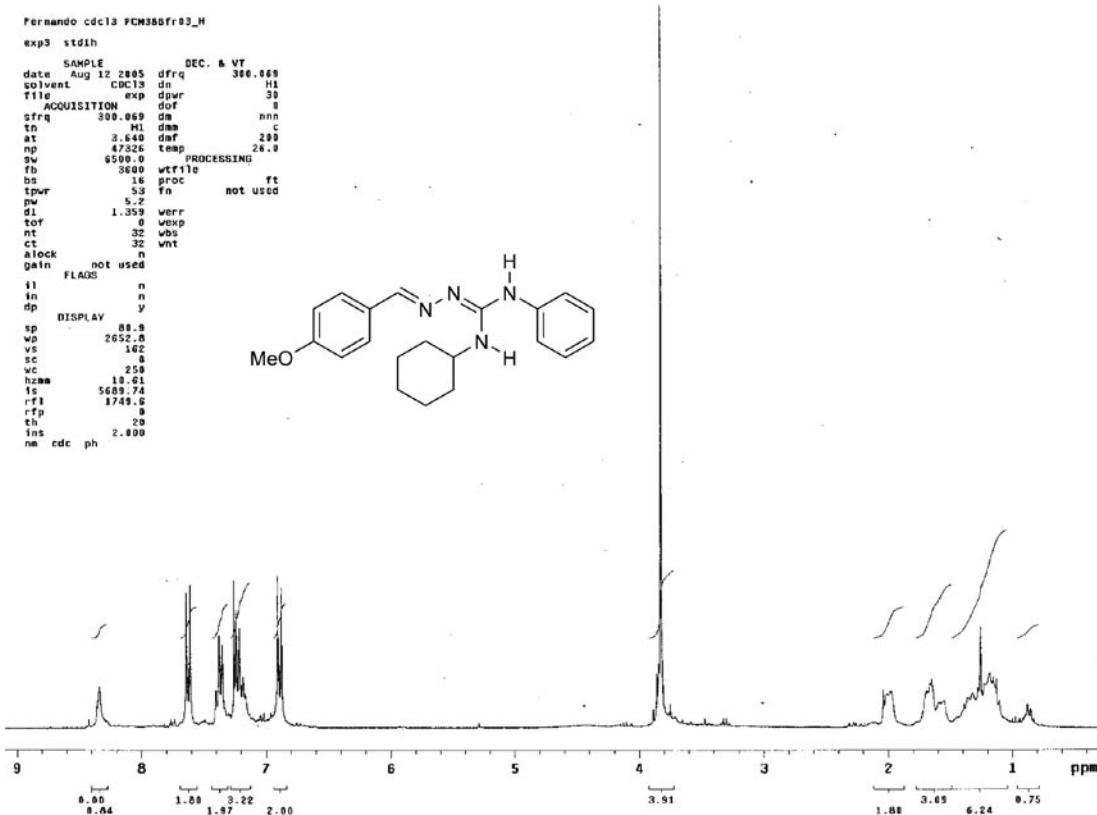
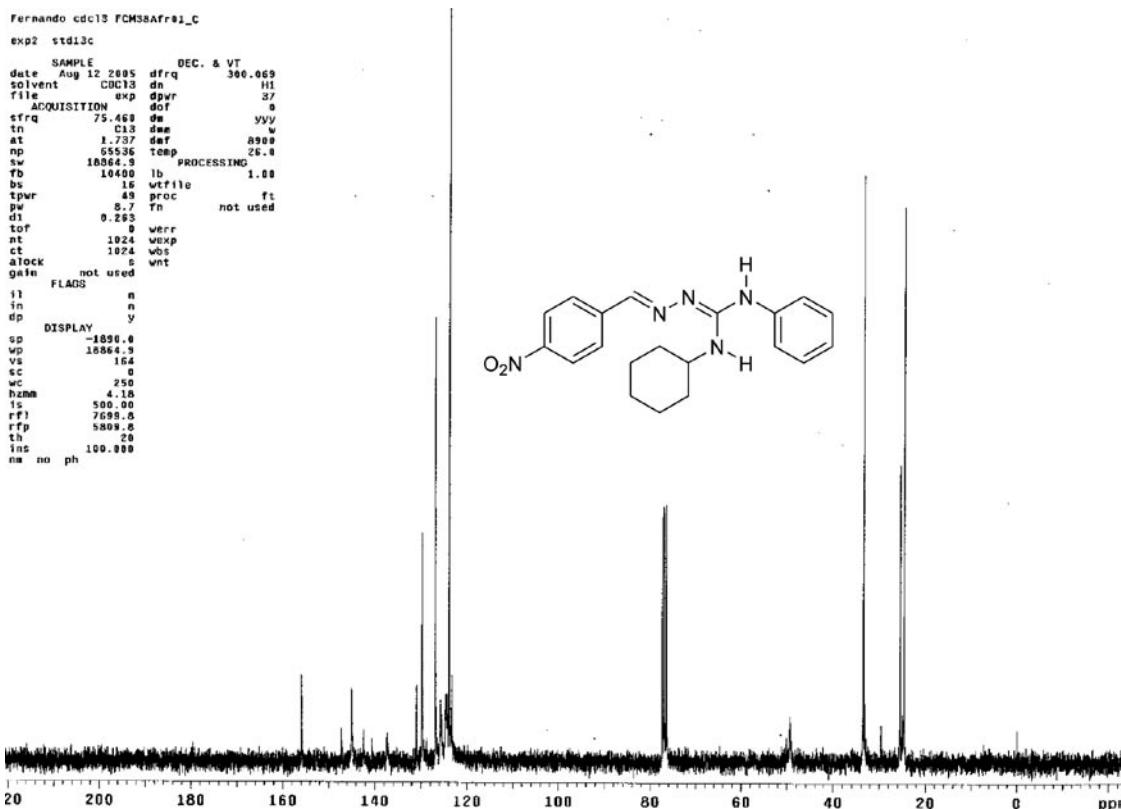
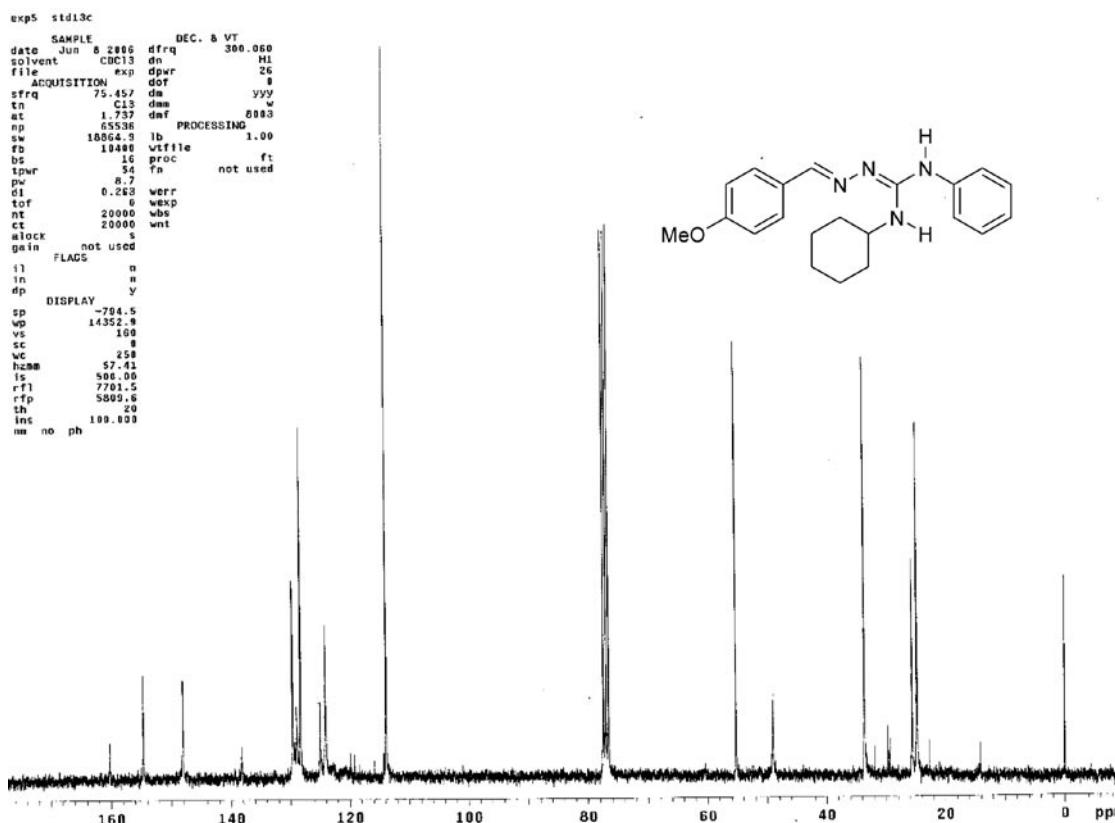
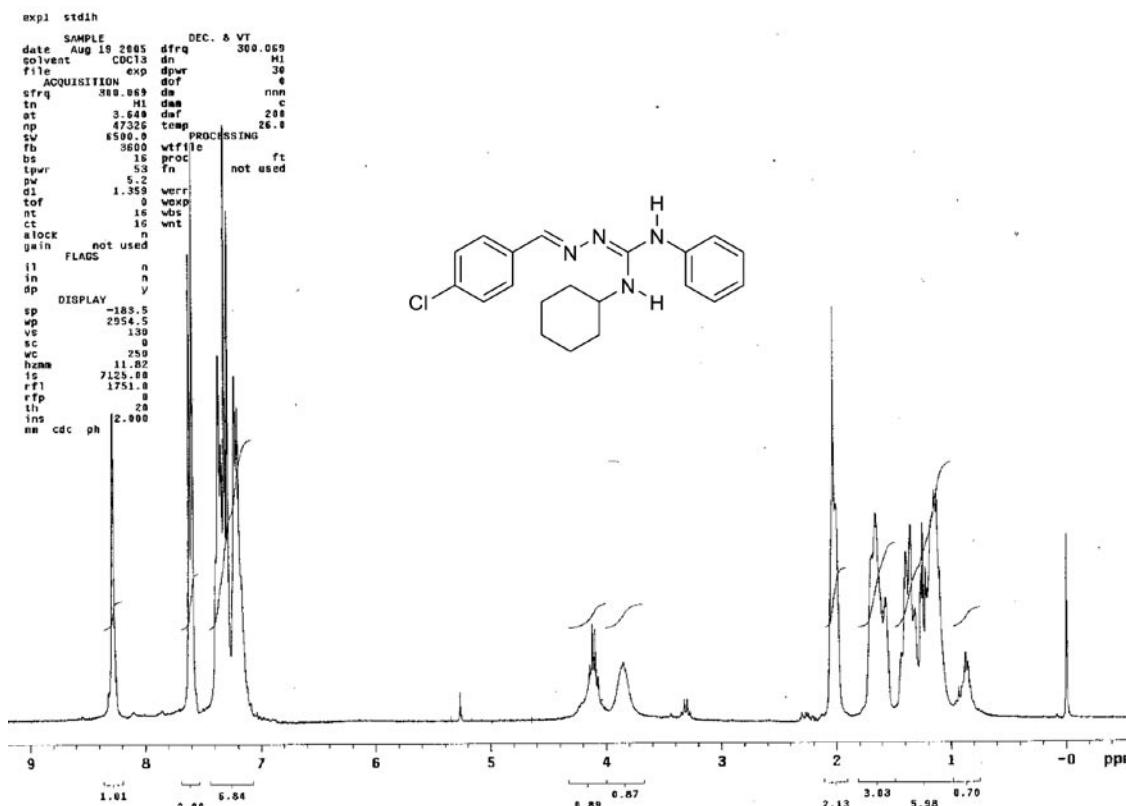


Figure S7. Full ^1H NMR spectrum of compound **2d** (CDCl_3).

Figure S8. Full ¹³C NMR spectrum of compound 2d (CDCl₃).Figure S9. Full ¹H NMR spectrum of compound 2e (CDCl₃).

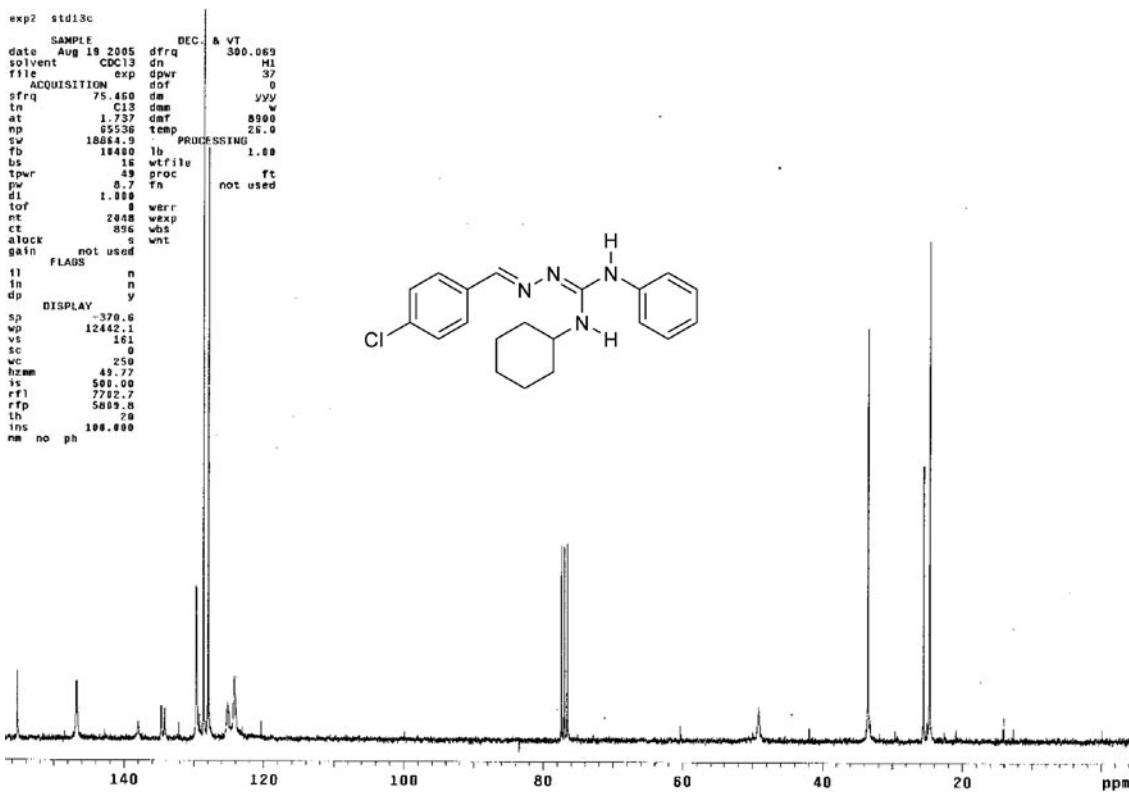


Figure S10. Full ^{13}C NMR spectrum of compound **2e** (CDCl_3).

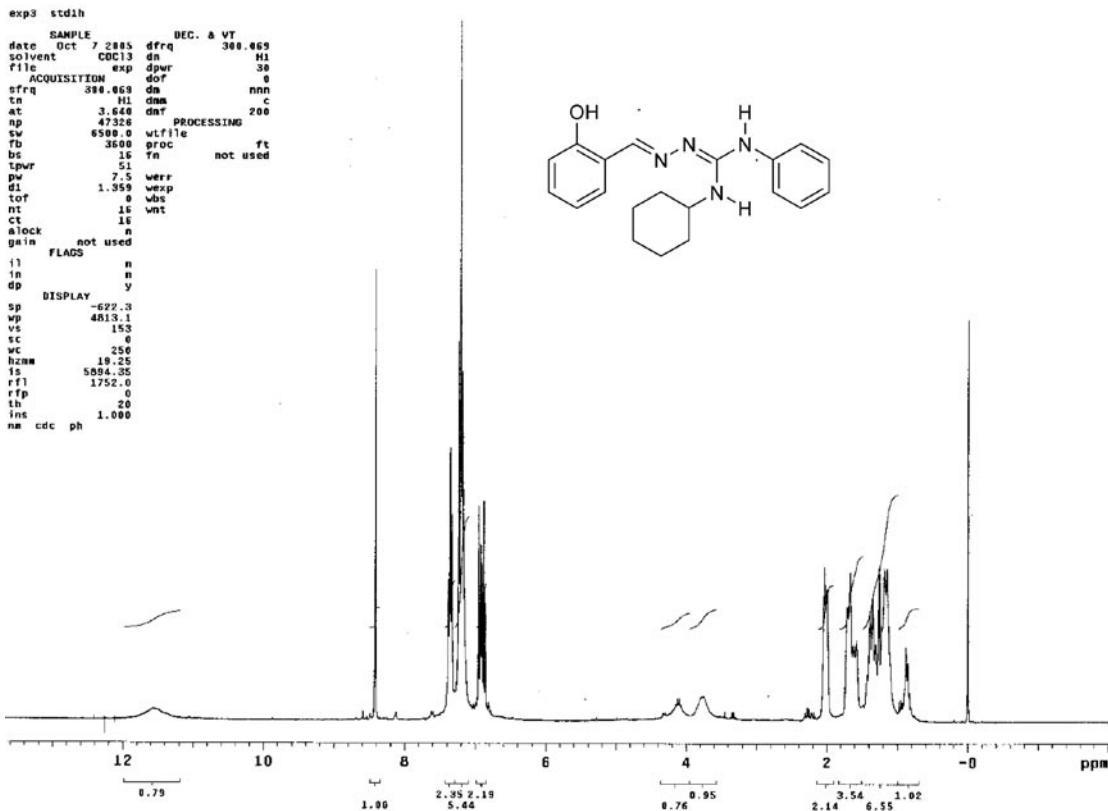
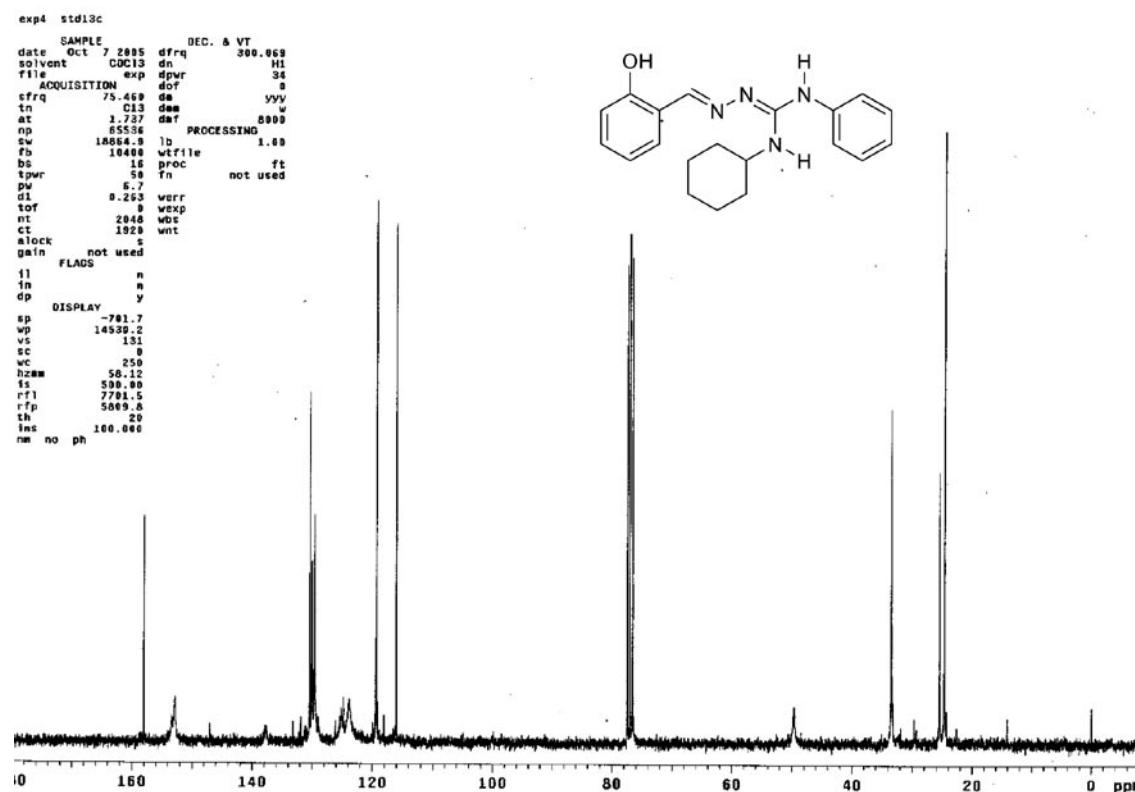
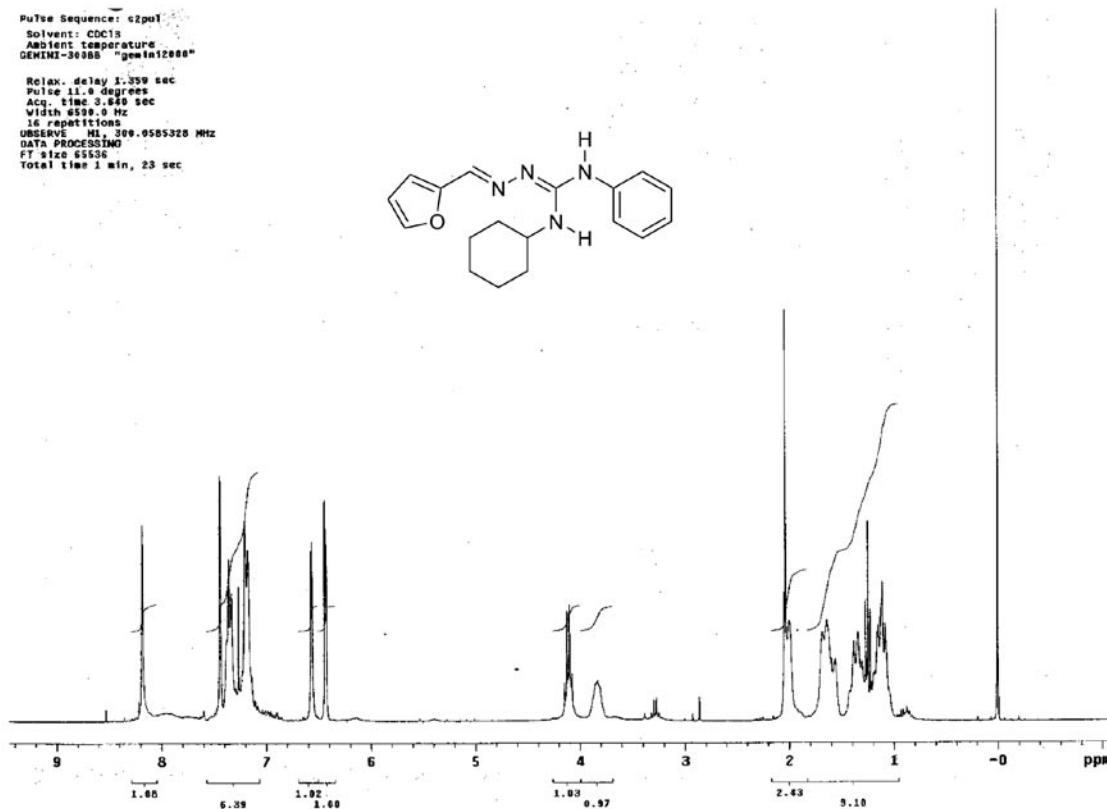


Figure S11. Full ^1H NMR spectrum of compound **2f** (CDCl_3).

Figure S12. Full ¹³C NMR spectrum of compound 2f (CDCl₃).Figure S13. Full ¹H NMR spectrum of compound 2g (CDCl₃).

```

SAMPLE      DEC. & VT
date       Jun 12 2006 dfreq   300.068
solvent    CDCl3  dn      H1
file       exp  dpvr    25
          ACQUISITION dof      8
          t0      75.457  vyy
          te      1.737  dme  8003
          n1      C13  dme   w
          np      65536  PROCESSING
          nv      168400 1b      1.00
          tb      16400  wfile
          ts      16      proc   tt
          tppr    54      tn      not used
          pw      8.7
          rf      8.260  werr
          tof     6      wexp
          nt      1624  wbs
          ct      352  wnt
          alock   s
          gain   not used
          flags
          fl     n
          fm     n
          dp     y
DISPLAY
sp      -506.7
wp      12713.2
vt      101
sc      0
wc      259
hzme   50.05
is      50000
rf1    7706.7
rf2    5069.6
th      20
ins    100.000
nm no ph

```

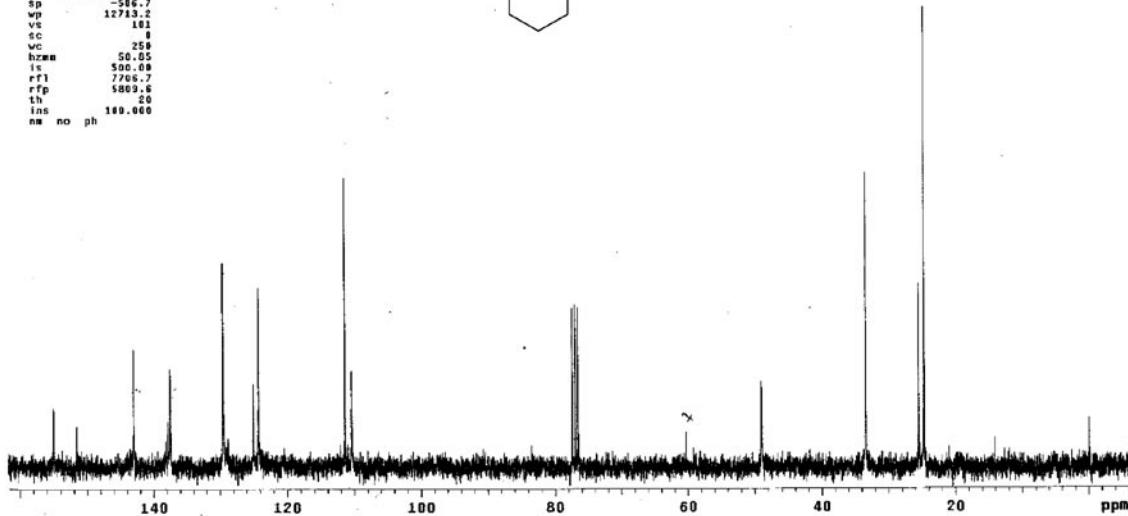
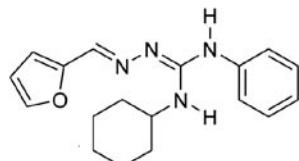


Figure S14. Full ^{13}C NMR spectrum of compound **2g** (CDCl_3).

```

Solvent: CDCl3
Ambient Temperature
DEMINI-300BB "gemini2000"
Relax.: delay 1.359 sec
Pulse: 45.0 degrees
Acq. time: 3.640 sec
V1000: 53500.0 Hz
16 repetitions
OBSERVE: H1, 300.0585378 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 32 sec

```

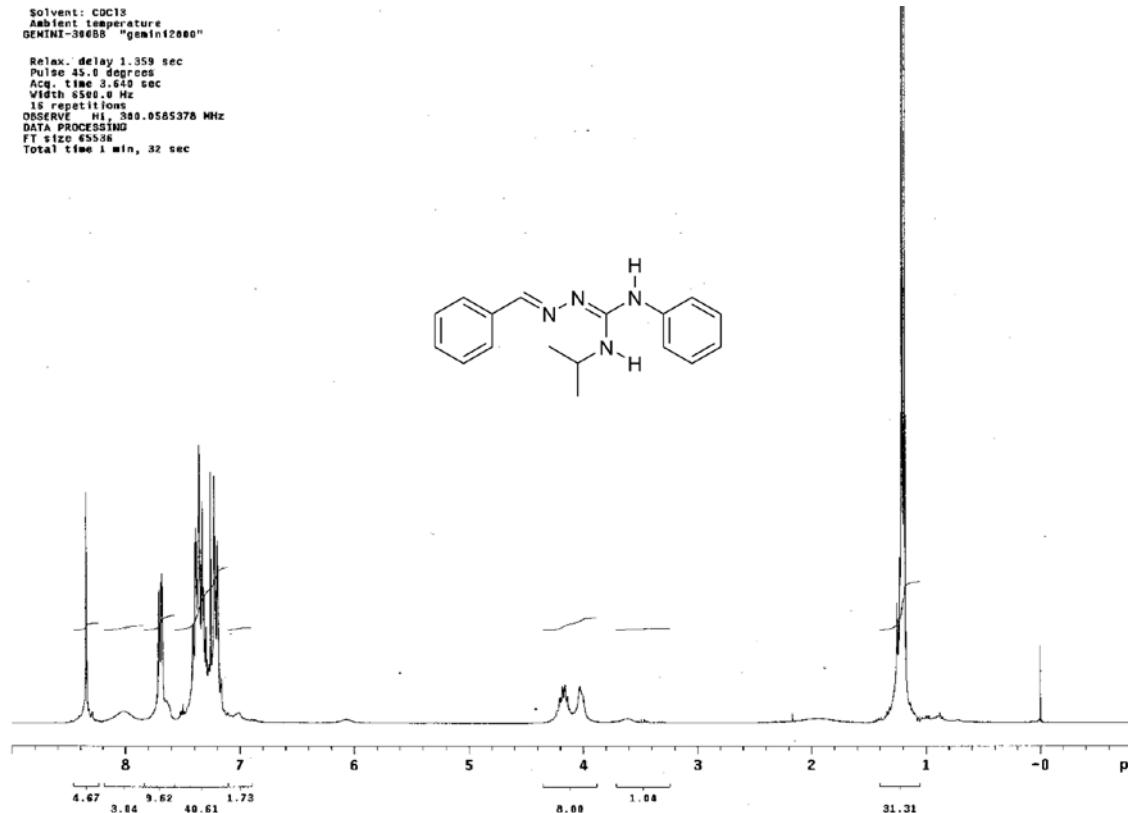
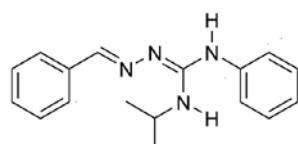


Figure S15. Full ^1H NMR spectrum of compound **2h** (CDCl_3).

```

SAMPLE          DEC. & VT
date Jul 13 2006 dfreq 300.060
solvent   CDCl3 dn   H1
file      exp dpwv  30
        dppf   0
        t1    75.457 dm   vvv
        t2    1.731 dmf  w
        t3    1.731 dmf  8003
        pw    5000
        ip    10664.3 lb   1.00
        p1    10499 wtfile
        is    16 proc   ft
        :pwr  54 fn   not used
        n1    0.7
        d1    0.263 werr
        :of   0 wexp
        st    4999 wbs
        rt    1184 wnt
        :clock s
        gain  not used
        jain  not used
        flags  n
        in    n
        lp    y

DISPLAY
sp   -1416.9
wp   15915.4
v1   51
ic   8
vc   250
zmq  53.06
ls   53.00
rt   770.5
:tp   5699.6
th   29
ins  100.000
nm  no ph

```

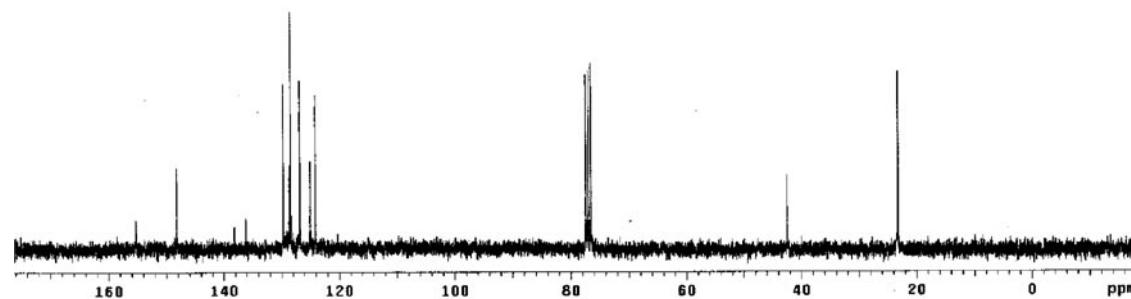
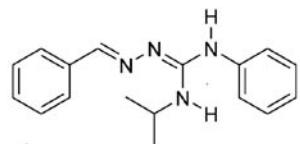


Figure S16. Full ¹³C NMR spectrum of compound **2h** (CDCl₃).

```

SAMPLE          DEC. & VT
date Jun 26 2006 dfreq 300.060
solvent   CDCl3 dn   H1
file      exp dpwv  30
        dppf   0
        t1    8.543 dm   mmn
        t2    1.543 dmf  c
        at    47325 temp  260
        np    6598.0
        pw    5000
        ip    10664.3 lb   25.0
        p1    10499 wtfile
        bs   4 proc   ft
        :pwr  47 fn   not used
        d1    1.358 werr
        tof   0 wexp
        nt   16 wbs
        ct   16 wnt
        :clock s
        gain  not used
        flags  n
        in    n
        dp    y

DISPLAY
sp   116.2
wp   2545.3
v1   434
ic   8
vc   250
zmq  10.18
ls   4140.00
rtf1  1754.2
:tp   0
th   20
ins  1.000
nm  cdc ph

```

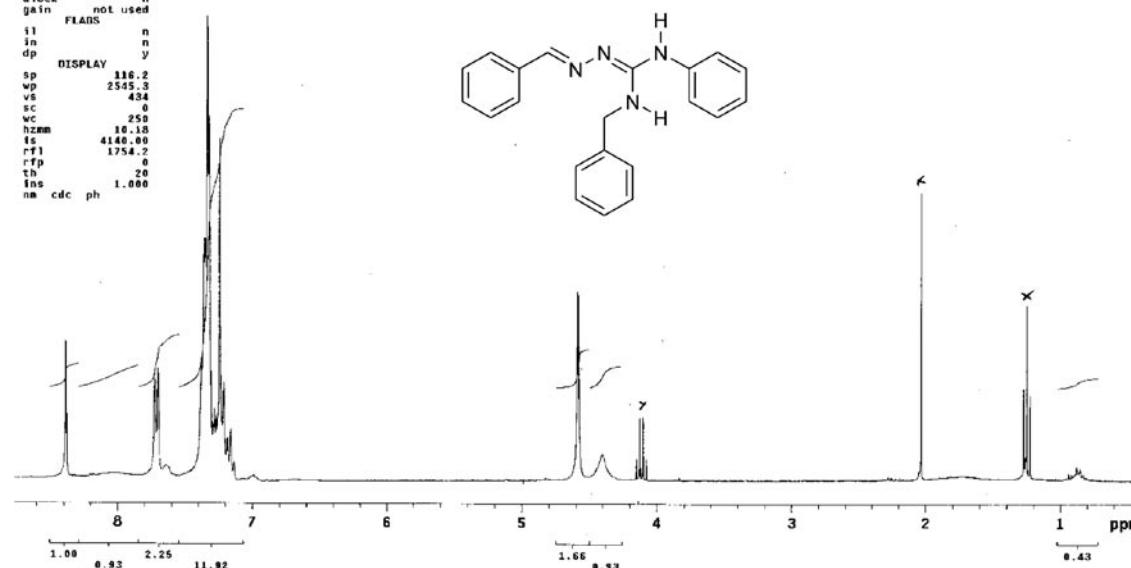
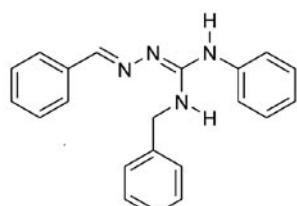


Figure S17. Full ¹H NMR spectrum of compound **2i** (CDCl₃).

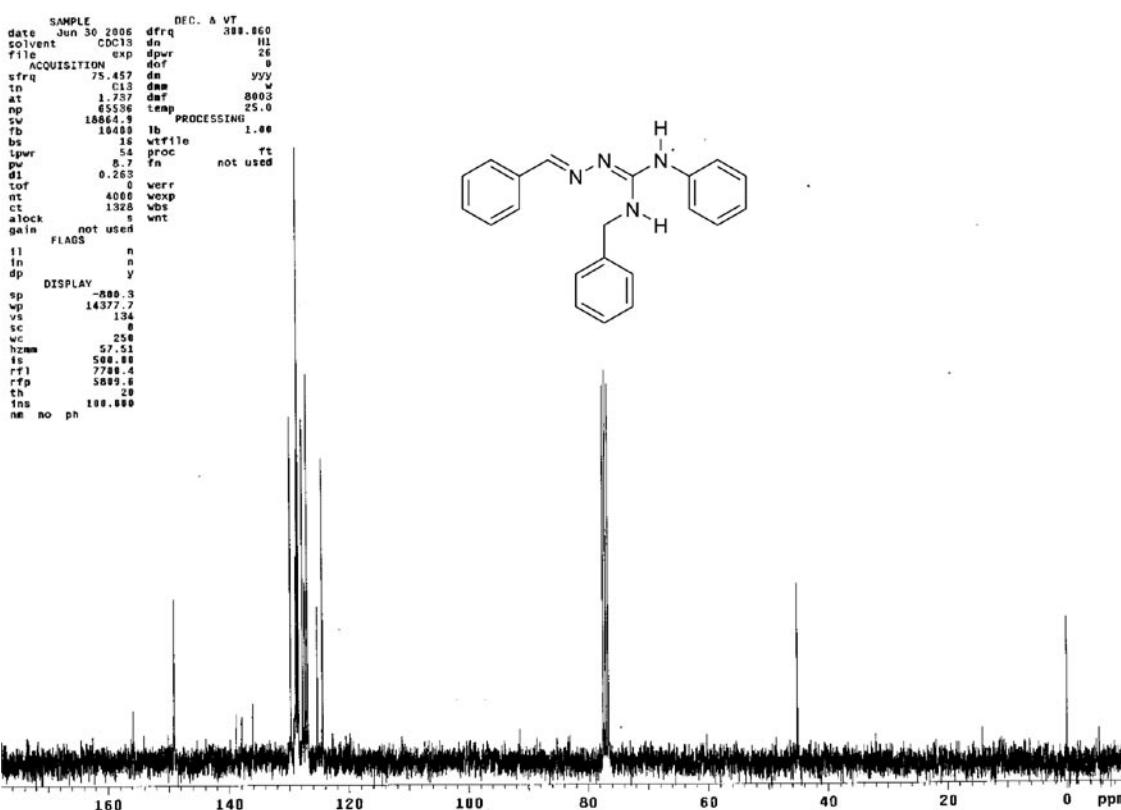


Figure S18. Full ¹³C NMR spectrum of compound 2i (CDCl₃).

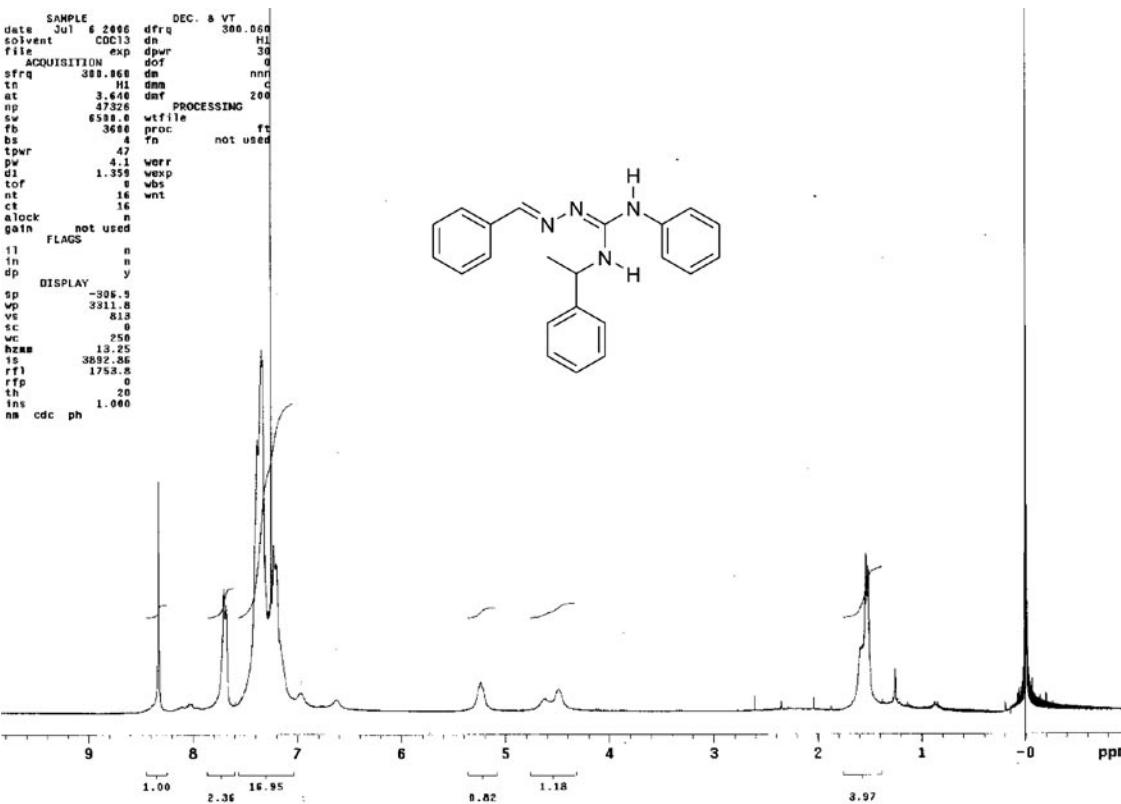
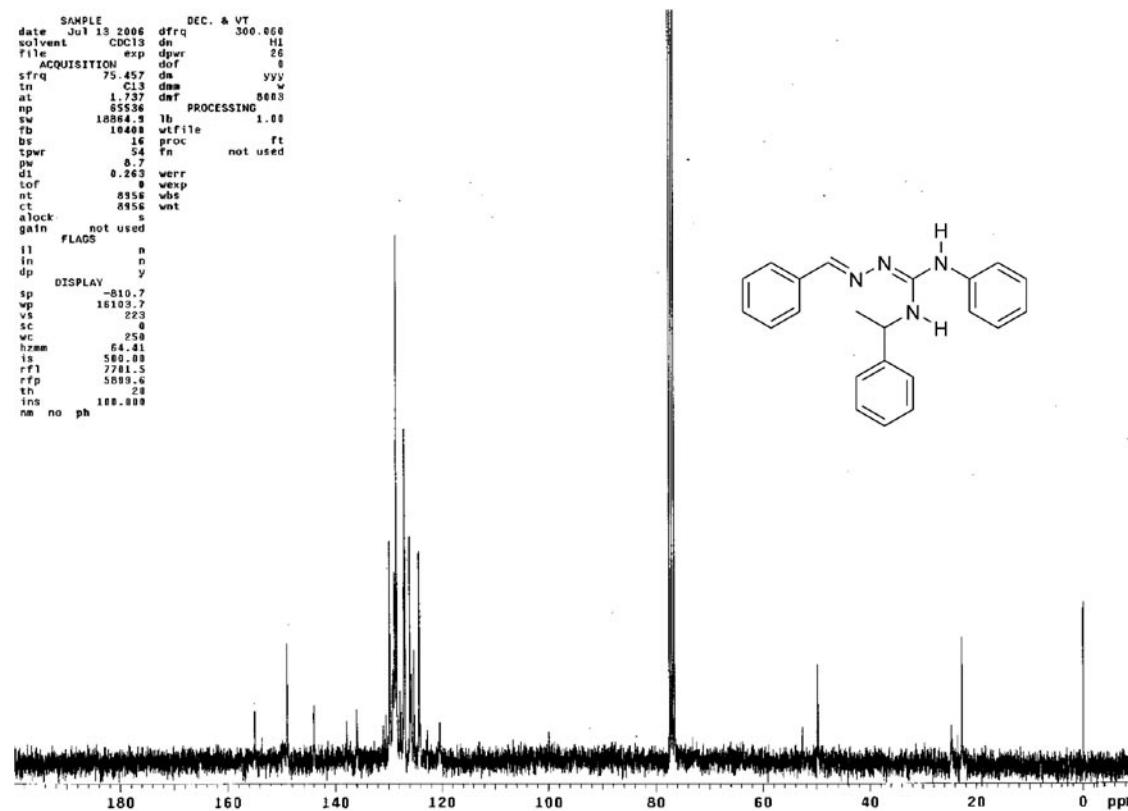
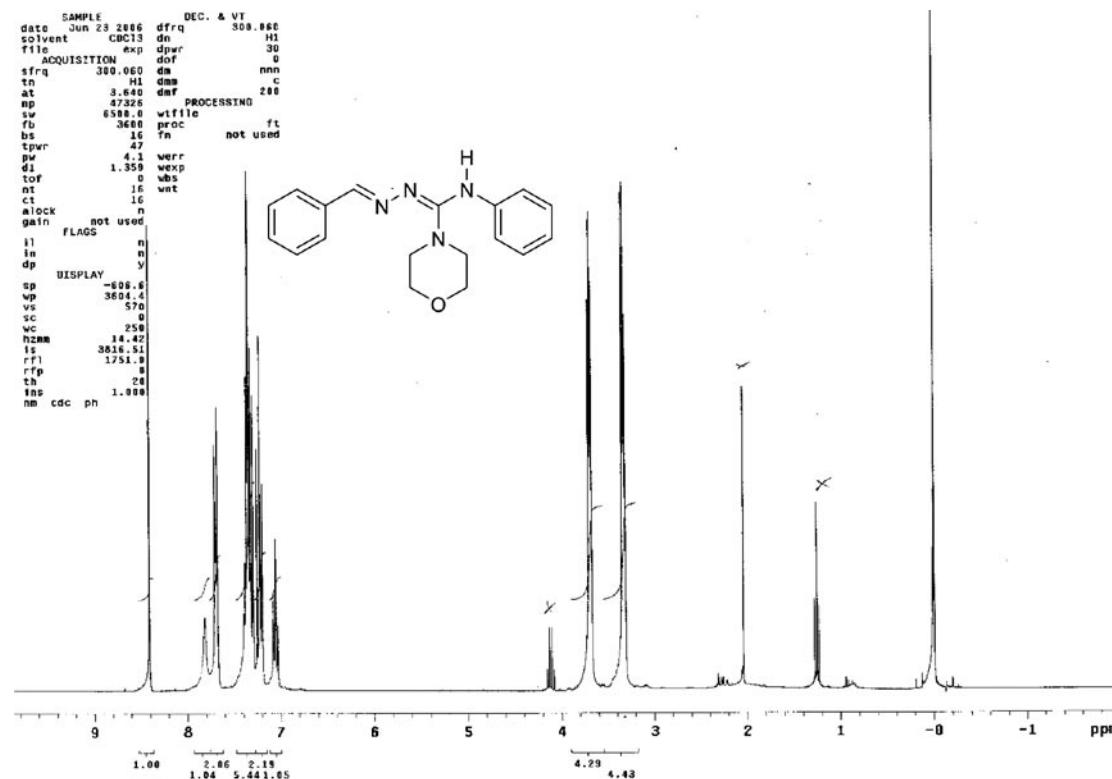


Figure S19. Full ¹H NMR spectrum of compound 2j (CDCl₃).

Figure S20. Full ¹³C NMR spectrum of compound 2j (CDCl₃).Figure S21. Full ¹H NMR spectrum of compound 2k (CDCl₃).

```

SAMPLE          DEC. & VT
date   Jun 23 2005 dfrq    300.068
solvent   CDCl3 dn      H1
file     exp      dppr    25
ACQUISITION 75.457 dm      VVY
sfrq      C13 dms      V
at       1.37 dmf      6995
sp       6554.0 PROCESSING
sw      18864.9 lb      1.00
fb      18400 wtffile
hs       16 proc      ft
tpwr      54 Tm      not used
d1      0.248 warr
d1f      0 wexp
nt      2848 wbs
ct      2848 wnt
tlock      3
gain      not used
FLADS
i1      n
in      n
dp      y
DISPLAY
sp      -1495.8
wp      15872.0
v1      142
sc      8
vc      256
hzam      60.23
ts      581.00
rt1      7741.5
rfp      5009.6
th      9
ins      100.000
nm no ph

```

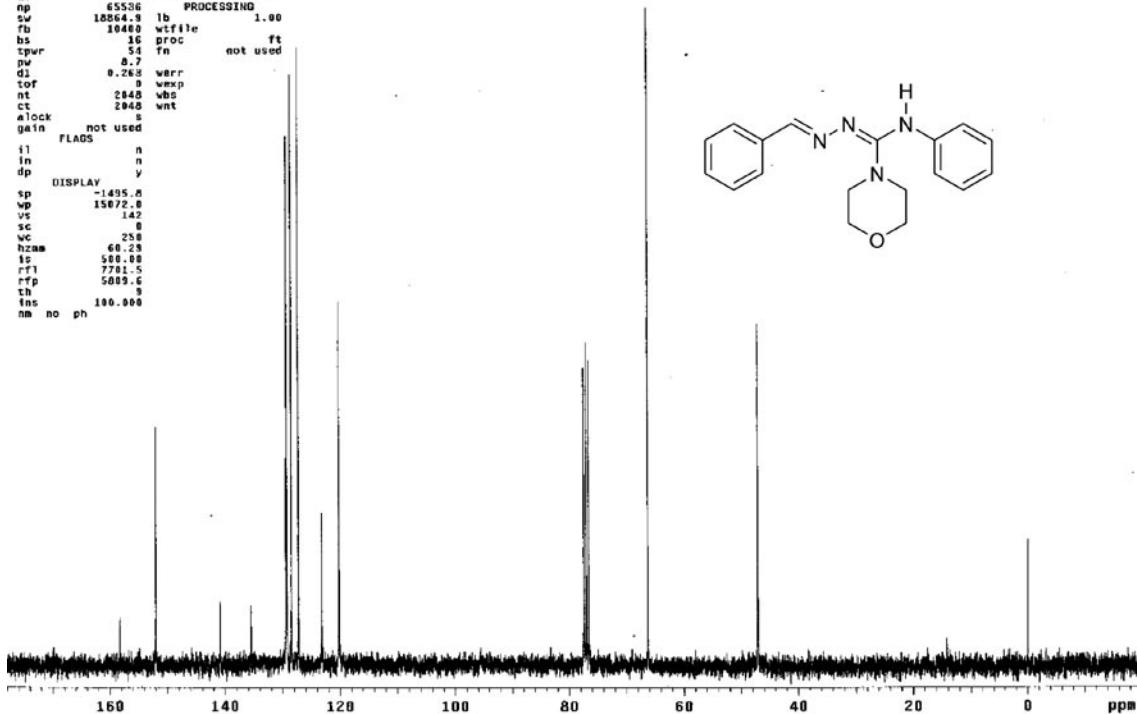


Figure S22. Full ^{13}C NMR spectrum of compound **2k** (CDCl_3).