

Electronic Supplementary Information

Tunable Regioselective Synthesis of Pyrazolo[3,4-d]pyrimidine Derivatives via Aza-Wittig Cyclization and Dimroth-type rearrangement

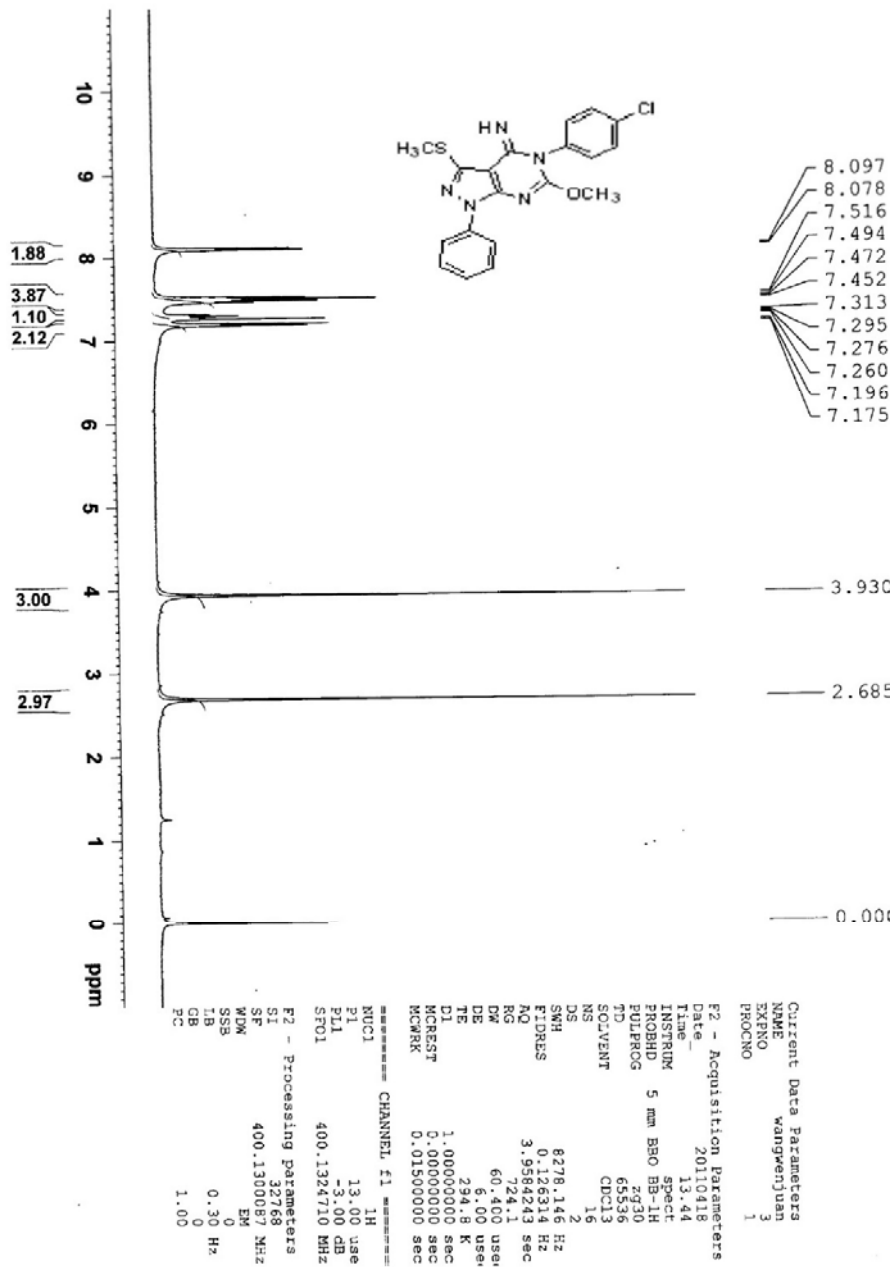
Tao Wang,^{*ab} Jun Xiong,^a Wenjuan Wang,^a Rou Li,^a Xiaoli Tang,^a Fei Xiong^{*ab}

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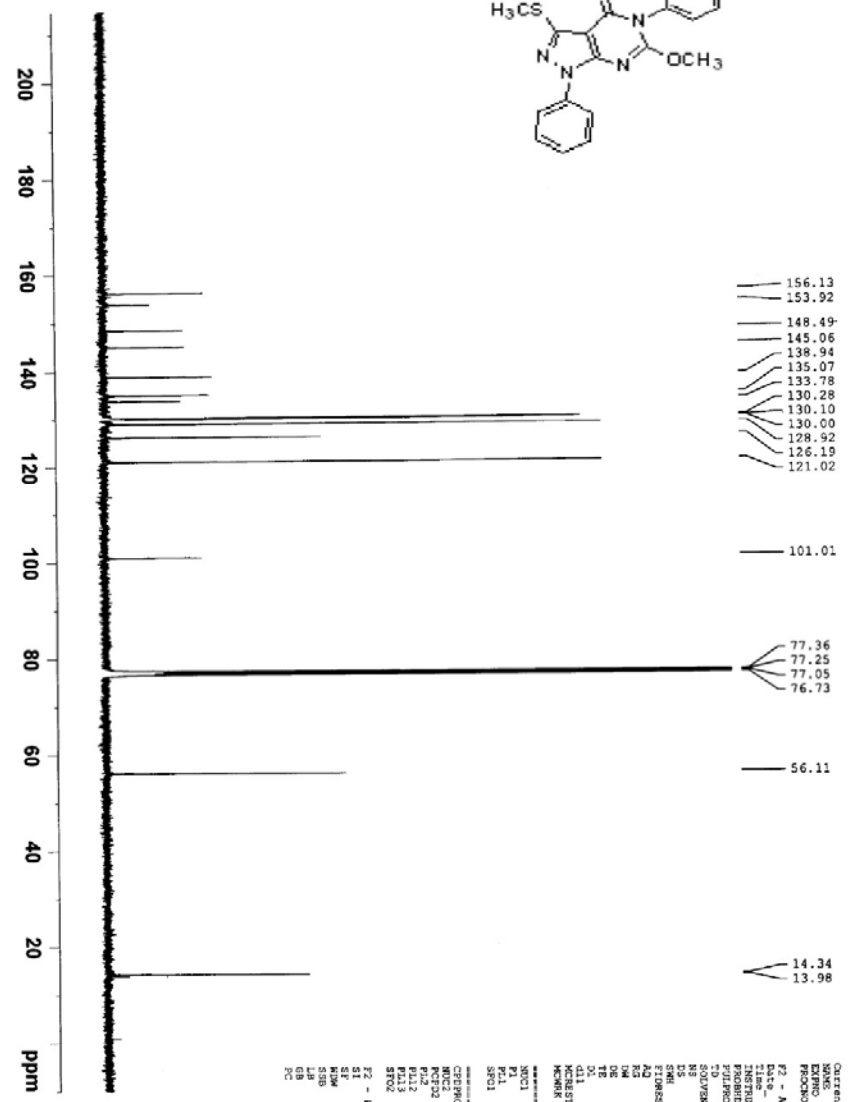
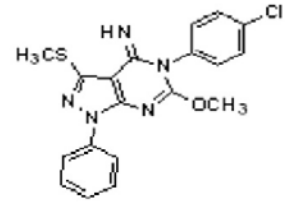
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1: ¹H NMR, ¹³C NMR and IR Spectra of Compounds 3

Compound 3a

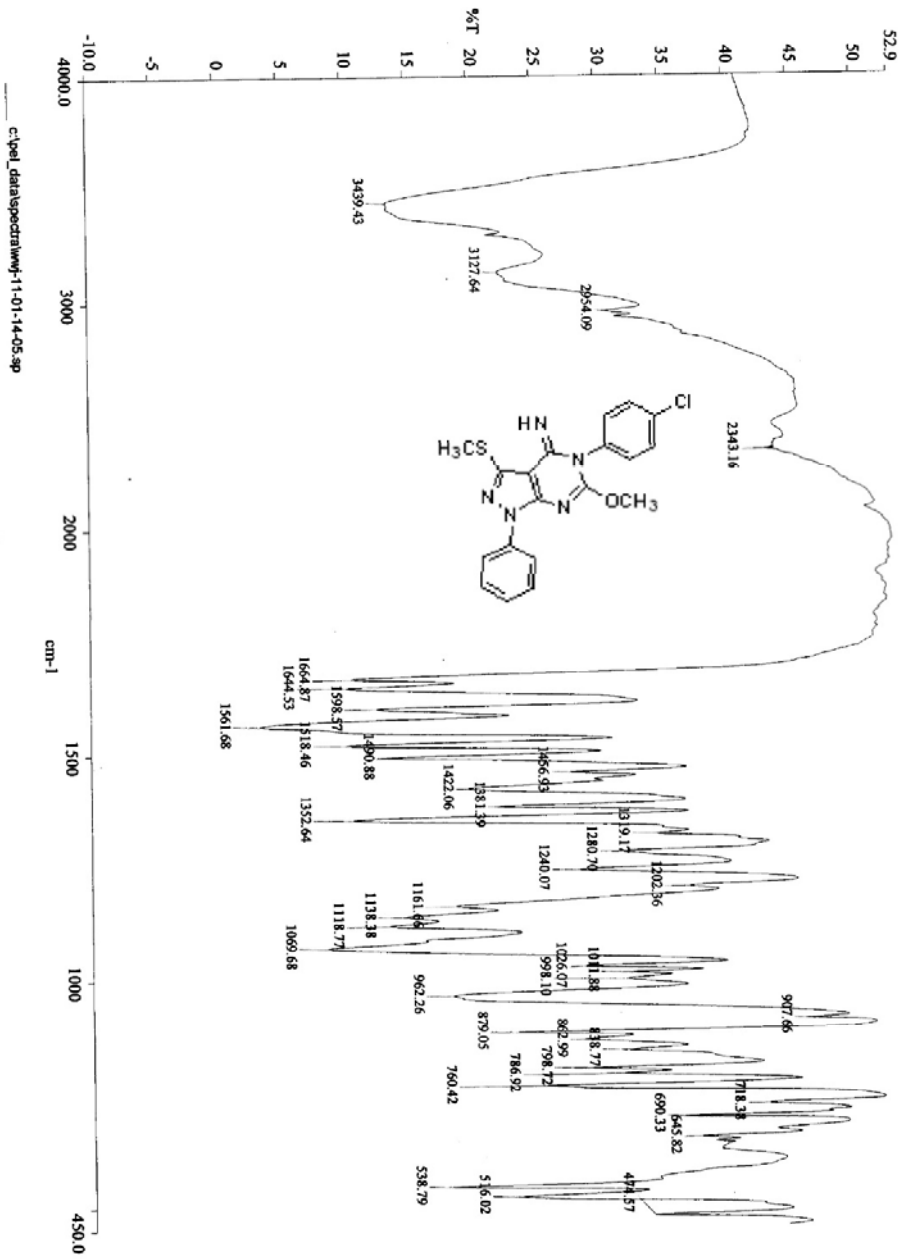


WVJ 4

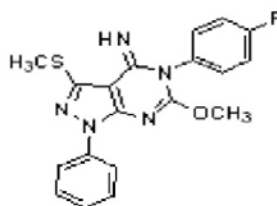


- 156.13
- 153.92
- 148.49
- 145.06
- 138.94
- 135.07
- 133.78
- 130.82
- 130.10
- 130.00
- 128.92
- 126.19
- 121.02
- 101.01
- 77.36
- 77.25
- 77.05
- 76.73
- 56.11
- 14.34
- 13.98

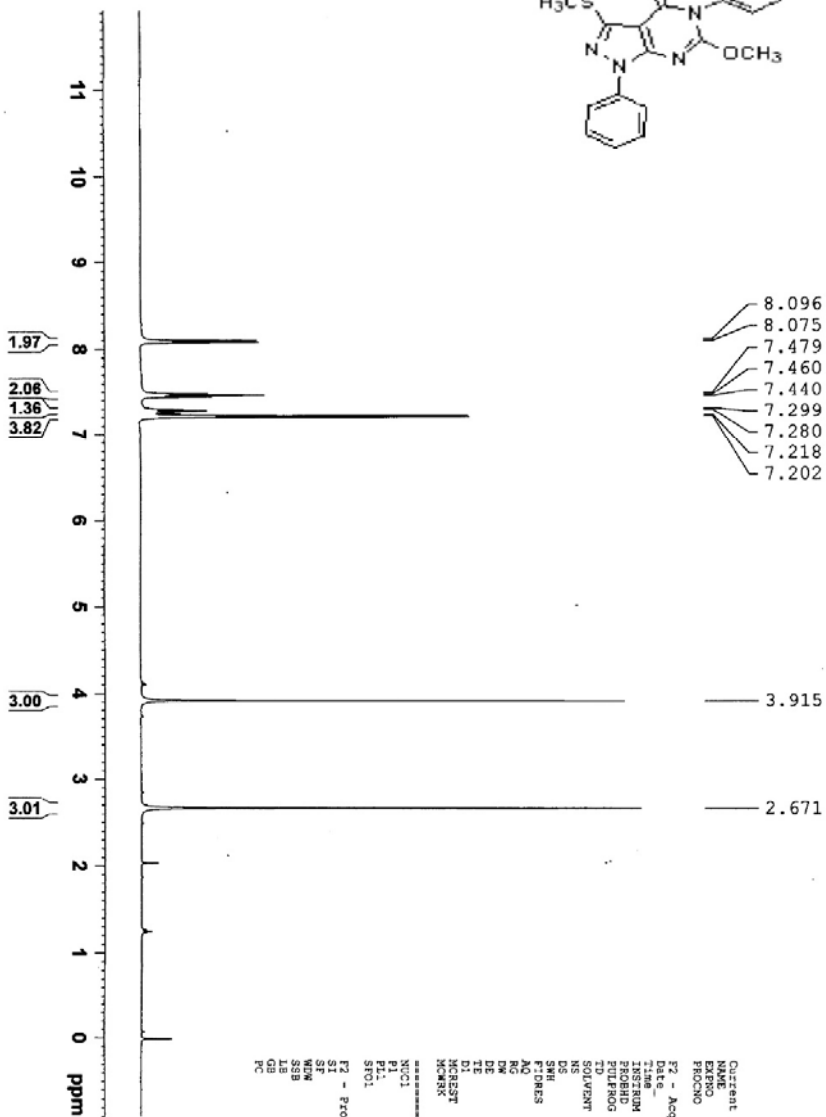
Current Data Parameters
 Name: WVJ 4
 ExpNo: 1
 ProcNo: 1
 F2 - Acquisition Parameters
 Date_: 20191124
 Time: 16:02
 File: WVJ4
 F2P001: 5 mm BBO BB-1H
 F2P002: 299130
 F2P003: 125.761 MHz
 F2P004: CMC13
 F2P005: CMC13
 SFO01: 5144
 NS: 6144
 DS: 4
 SS: 23960.014 Hz
 SFO: 5144
 AQ: 0.346918 sec
 AQ2: 1.364979 sec
 DE: 1.00 usec
 DE2: 20.050 usec
 DE3: 1.00 usec
 DE4: 1.00 usec
 DE5: 2.00000000 sec
 DE6: 0.03000000 sec
 DE7: 0.00000000 sec
 DE8: 0.00000000 sec
 DE9: 0.10000000 sec
 DE10: 0.00000000 sec
 CHANNEL F1 *****
 P1: 1.00 usec
 P2: 8.50 usec
 P3: -2.00 dB
 P4: 100.0228289 MHz
 SFO1: *****
 CHANNEL F2 *****
 P1: 1.00 usec
 P2: 80.00 usec
 P3: -2.00 dB
 P4: 100.6276711 MHz
 SFO2: *****
 F2 - Processing parameters
 SI: 32768
 SF: 100.627680 MHz
 DF: 0
 SR: 0
 L8: 1.00 Hz
 L9: 0
 SC: 1.40



Compound 3b



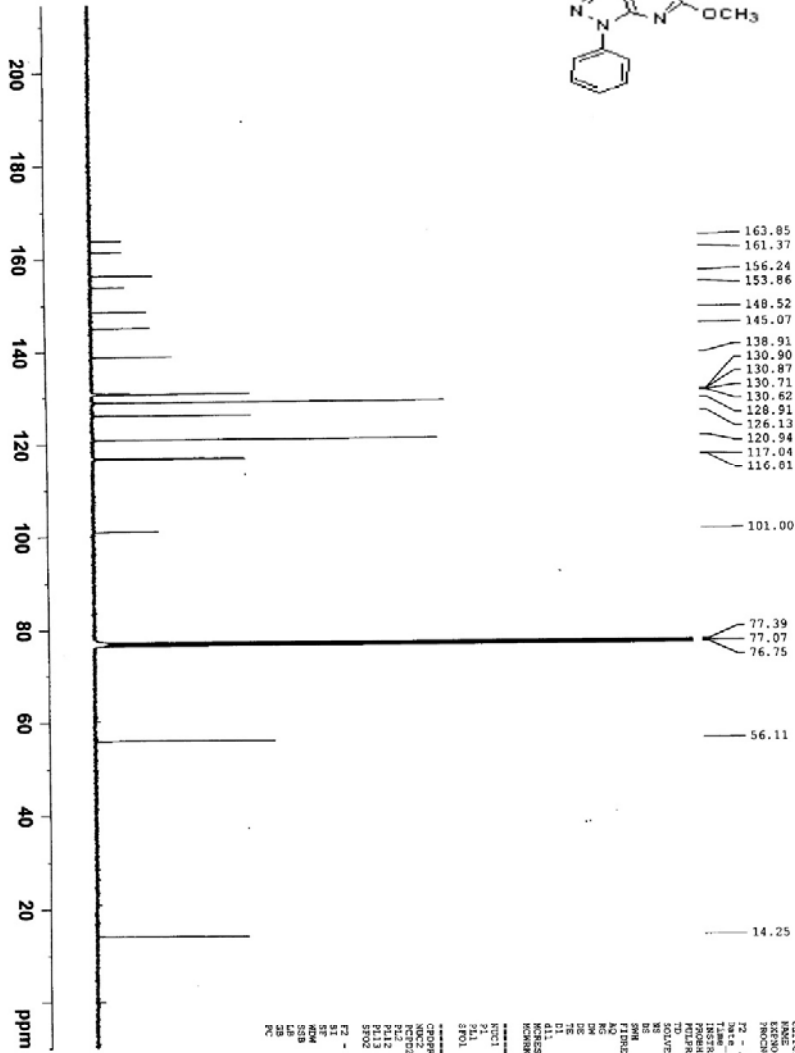
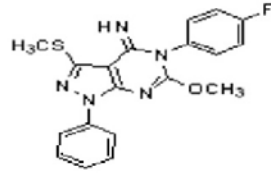
mwj2011030401



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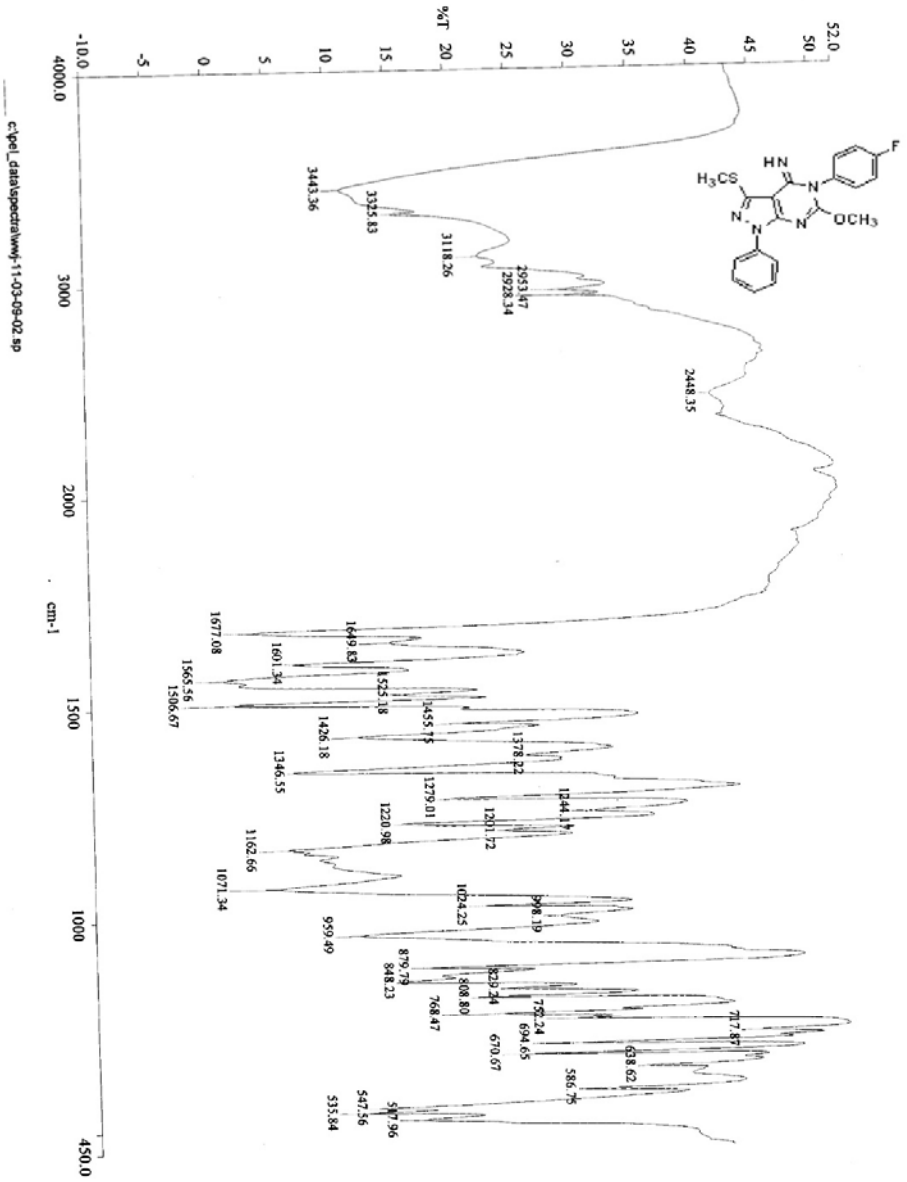
Current Data Parameters
NAME          wangwj
EXPNO         1
PROCNO       1
F2 - Acquisition Parameters
Date_         20110304
Time          12.12
INSTRUM      av400
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
SOLVENT      CDCl3
NS           32
DS           2
SFO1         8278.146 Hz
AQ           0.1714688 sec
RG           31.9584243 sec
RG           574.7
AQ           60.400 usec
TE           290.2 K
DELTA        1.00000000 sec
INTEGRATE    0.01500000 sec
SFO1         400.1324710 MHz
===== CHANNEL f1 =====
NUC1          13
P1            8.18 usec
PL1          -4.00 dB
SFO1         400.1324710 MHz
F2 - Processing parameters
SI           400.130133 MHz
SF           400.130133 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

WUJ3-7-2

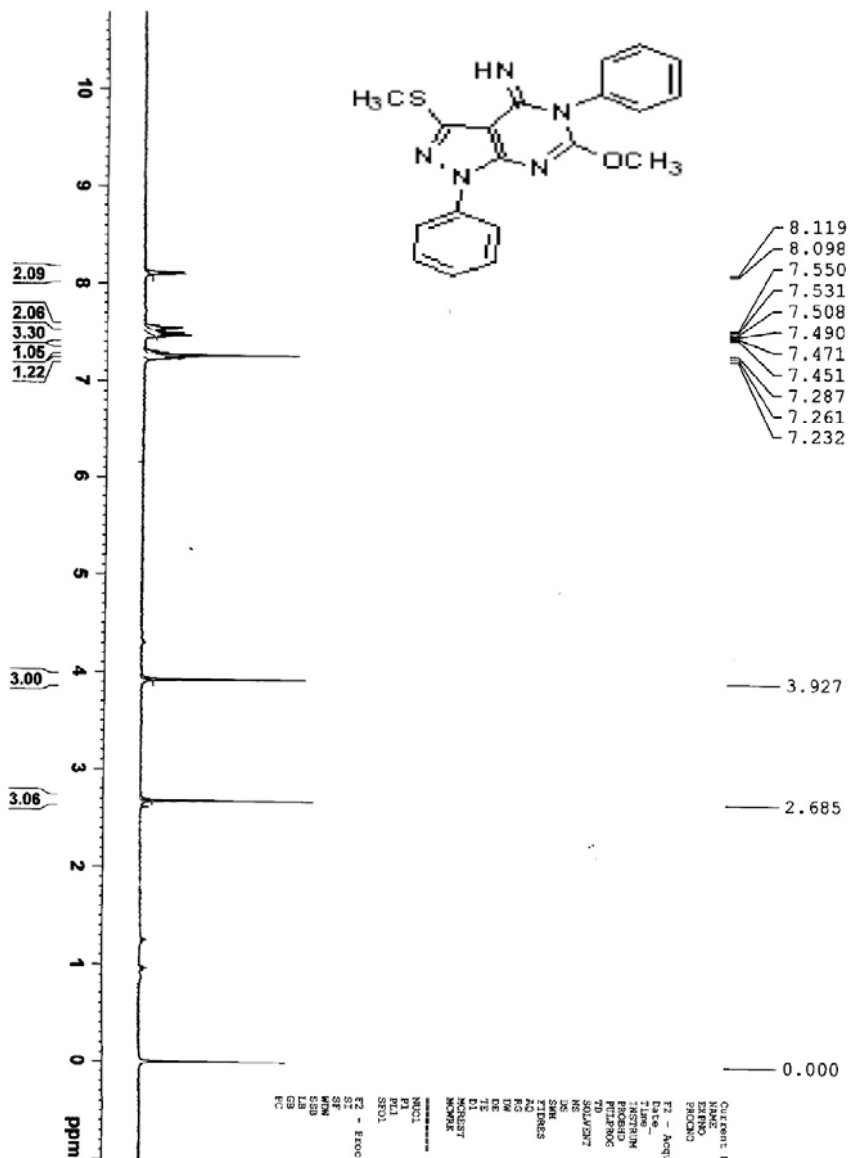
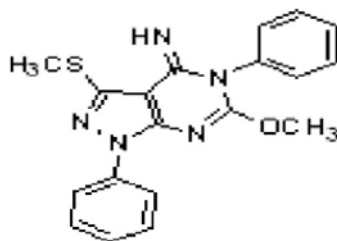


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Current Data Parameters
NAME: WUJ3-7-2
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_ Time: 201109
Time: 12:10
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
SOLVENT: CDCl3
NS: 2568
DS: 4
SWH: 21980.814 Hz
FIDRES: 0.248294 Hz
AQ: 1.18502 sec
RG: 1850.4
AQ: 20.680 usec
DE: 24.70 K
TE: 294.7 K
D1: 2.0000000 sec
DELTA: 0.0000000 sec
DECAY: 0.0000000 sec
RGSS2: 0.0150000 sec
===== CHANNEL f1 =====
NUC1: 13C
P1: 1.50 usec
PL1: -2.00 dB
SFO1: 100.6228228 MHz
===== CHANNEL f2 =====
CPROG2: waltz16
NUC2: 13C
P2: 80.00 usec
PL2: -3.00 dB
PL12: 19.00 dB
PL13: 19.00 dB
SFO2: 400.1166095 MHz
F2 - Processing parameters
SI: 32768
SF: 100.6227712 MHz
WDW: EM
SSB: 0
LB: 1.00 Hz
GB: 0
PC: 1.40
  
```

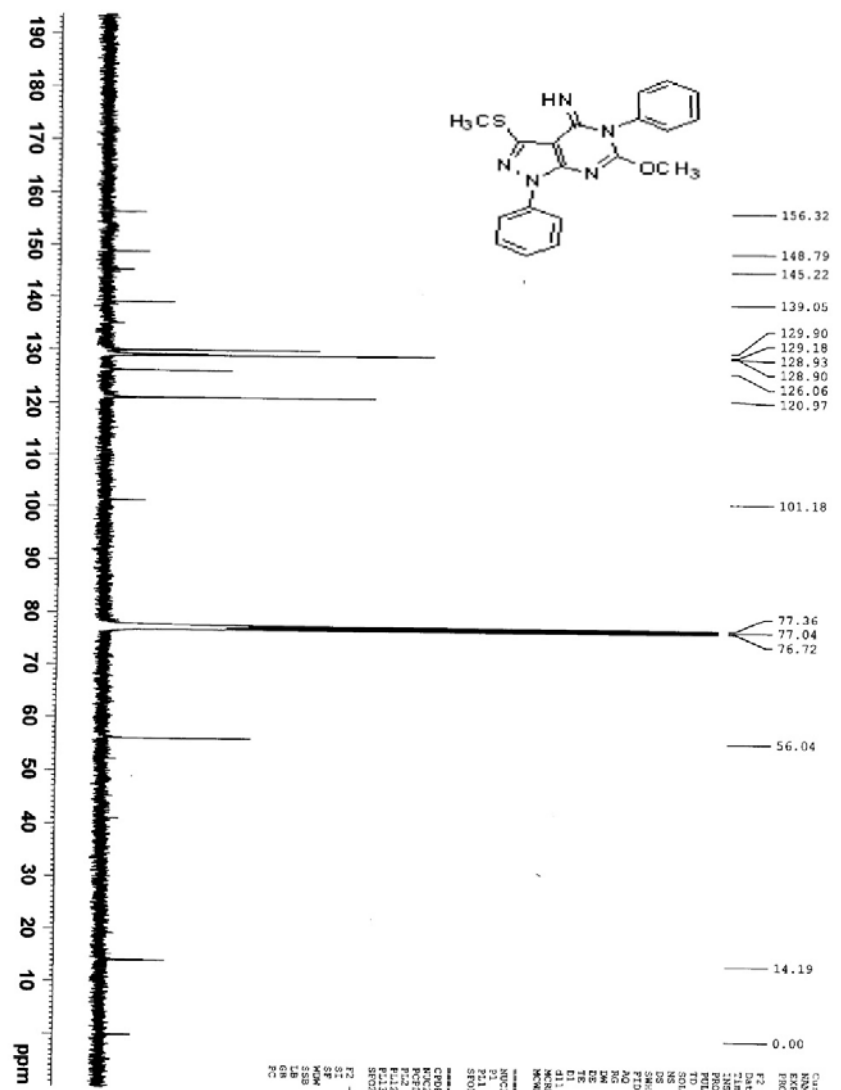
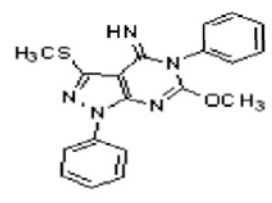


Compound 3c

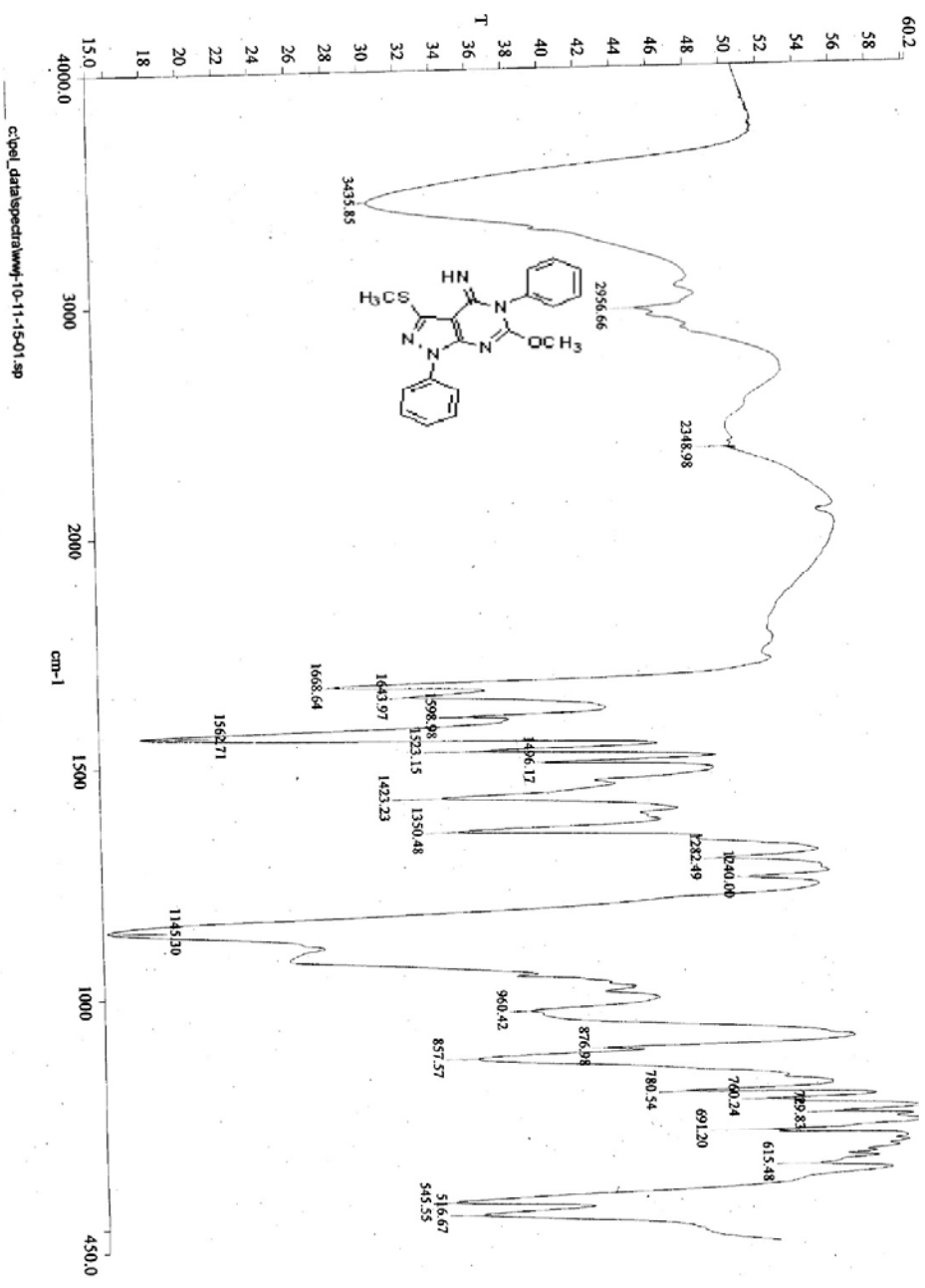


Output Data Parameters
 NAME: compound3
 EXPNO: 24
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20101110
 Time: 14:03
 INSTRUM: spect
 PROBRD: 5 mm BBO BB-1H
 PULPROG: zgpg30
 FIDRES: 0.1630
 SOLVENT: DMSO
 NS: 16
 DS: 4
 SWH: 8378.142 Hz
 SFO: 400.1464010 MHz
 F1: 0.126314 Hz
 F2: 3.9584243 sec
 AQ: 4.421 sec
 DE: 60.460 usec
 TE: 300.2 K
 DE: 61.09 usec
 DI: 205.5 KHz
 D1: 1.3000000 sec
 MCHRG1: 0.0000000 sec
 MCHRG2: 0.0150000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 8.76 usec
 PL1: 0.00 dB
 SFO1: 400.1464010 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 400.1464010 MHz
 WHW: 64
 WDS: 0.36 Hz
 LB: 0
 GB: 1.00

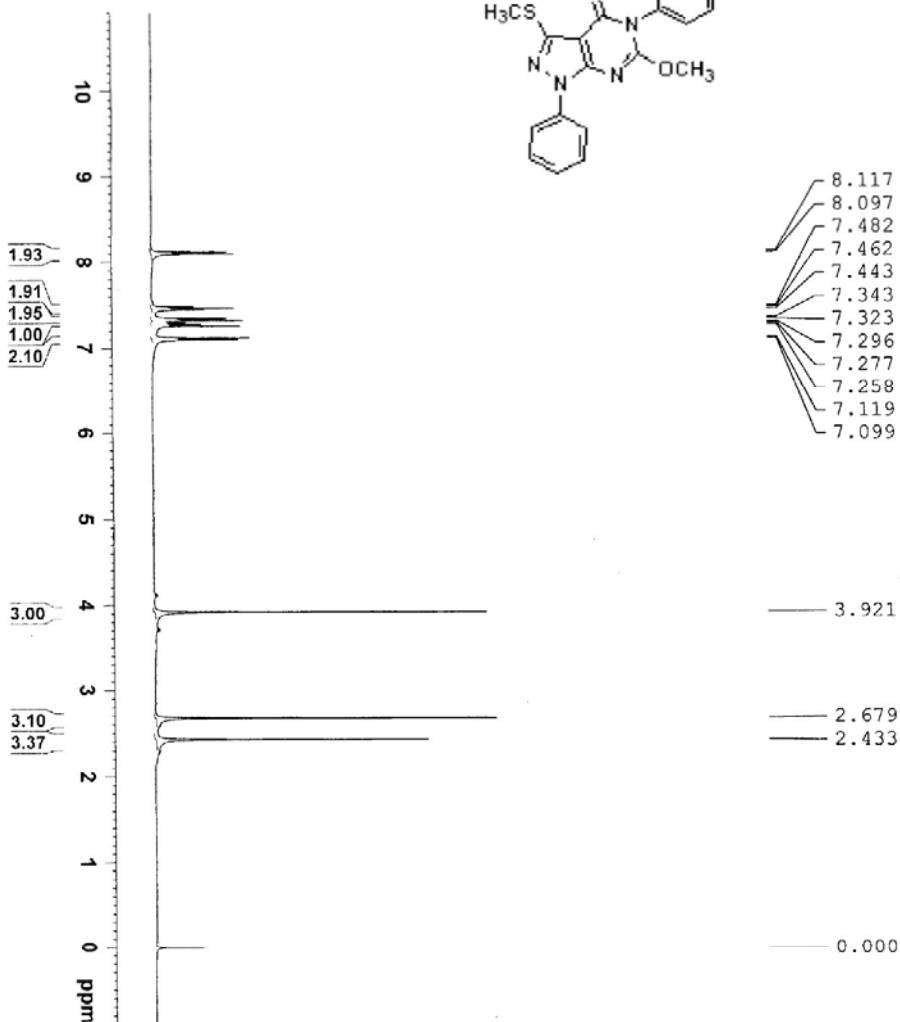
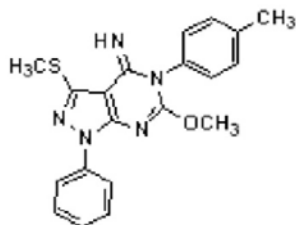
WVJ1



Current Data Parameters
 Name: WVJ1
 ExpNo: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_ : 20101221
 Time: 4:46
 INSTRUM: spect
 PROBNM: 5 mm BBO BB-1H
 PULPROG: zgpg30
 F2: 101.625000 MHz
 F1: 400.116000 MHz
 SOLVENT: CDCl3
 NS: 2165
 DS: 4
 SWH: 23360.814 Hz
 FIDRES: 0.265228 Hz
 AQ: 1.1664735 sec
 RG: 327.500
 DQ: 26.890 usec
 DE: 6.90 usec
 TE: 300.2 K
 D1: 2.0000000 sec
 d11: 0.4300000 sec
 DELT: 0.0150000 sec
 KW: 0.0150000 sec
 ===== CHANNEL f2 =====
 NUC1: 13C
 P1: 8.50 usec
 PL1: -2.00 dB
 SFO1: 100.625000 MHz
 ===== CHANNEL f1 =====
 NUC2: 1H
 P2: 12.00 usec
 PL2: 19.00 dB
 SFO2: 400.116000 MHz
 ===== PROCESSING PARAMETERS =====
 SI: 32768 SPS
 SF: 100.625000 MHz
 MM: 65536
 SSB: 0
 GB: 0
 PC: 1.00 Hz
 LB: 0
 GB: 0
 PC: 1.00 Hz



Compound 3d



7-18-5

- 8.117
- 8.097
- 7.482
- 7.462
- 7.443
- 7.343
- 7.323
- 7.296
- 7.277
- 7.258
- 7.119
- 7.099
- 3.921
- 2.679
- 2.433
- 0.000

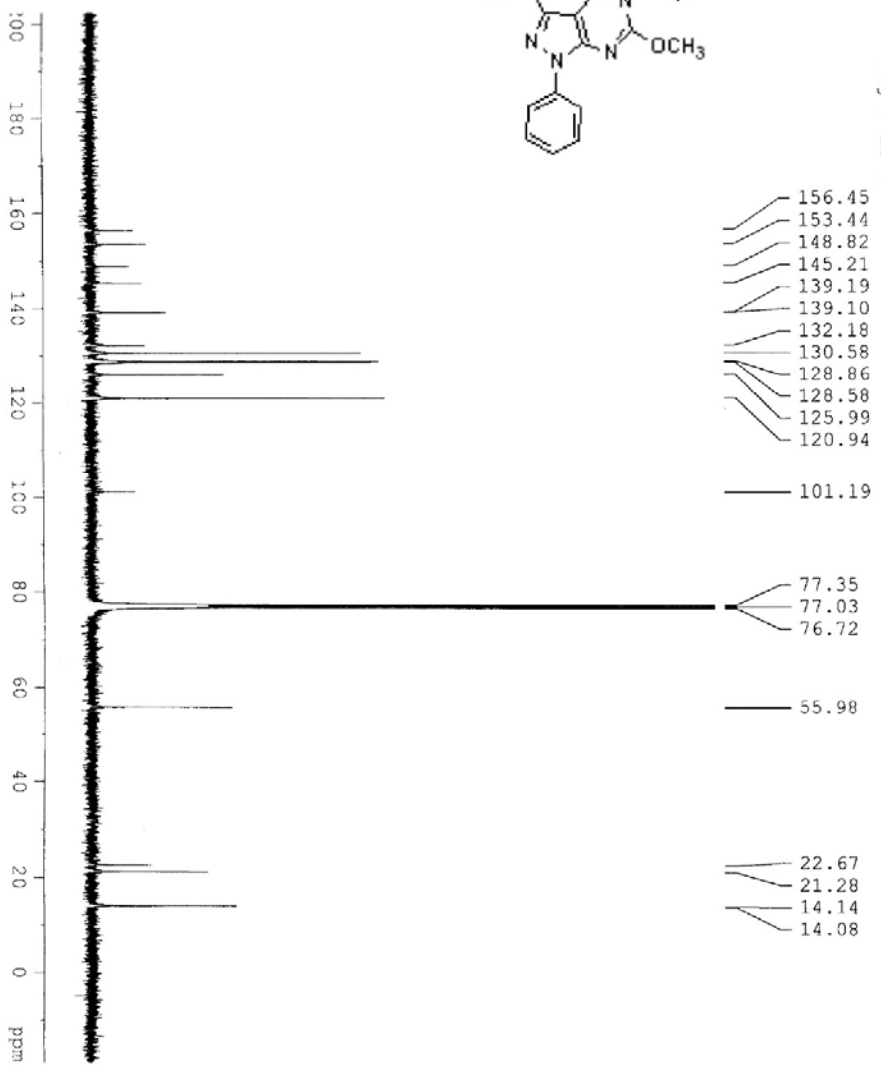
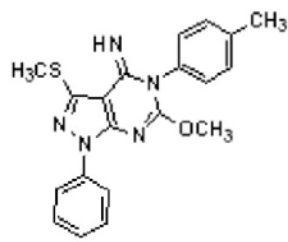
Current Data Parameters
 NAME wangwenjuan
 EXPNO 52
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110718
 Time 14.49
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 362
 DE 60.400 usec
 TE 299.0 K
 D1 1.00000000 sec
 MCREST 0.01500000 sec
 MCPRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

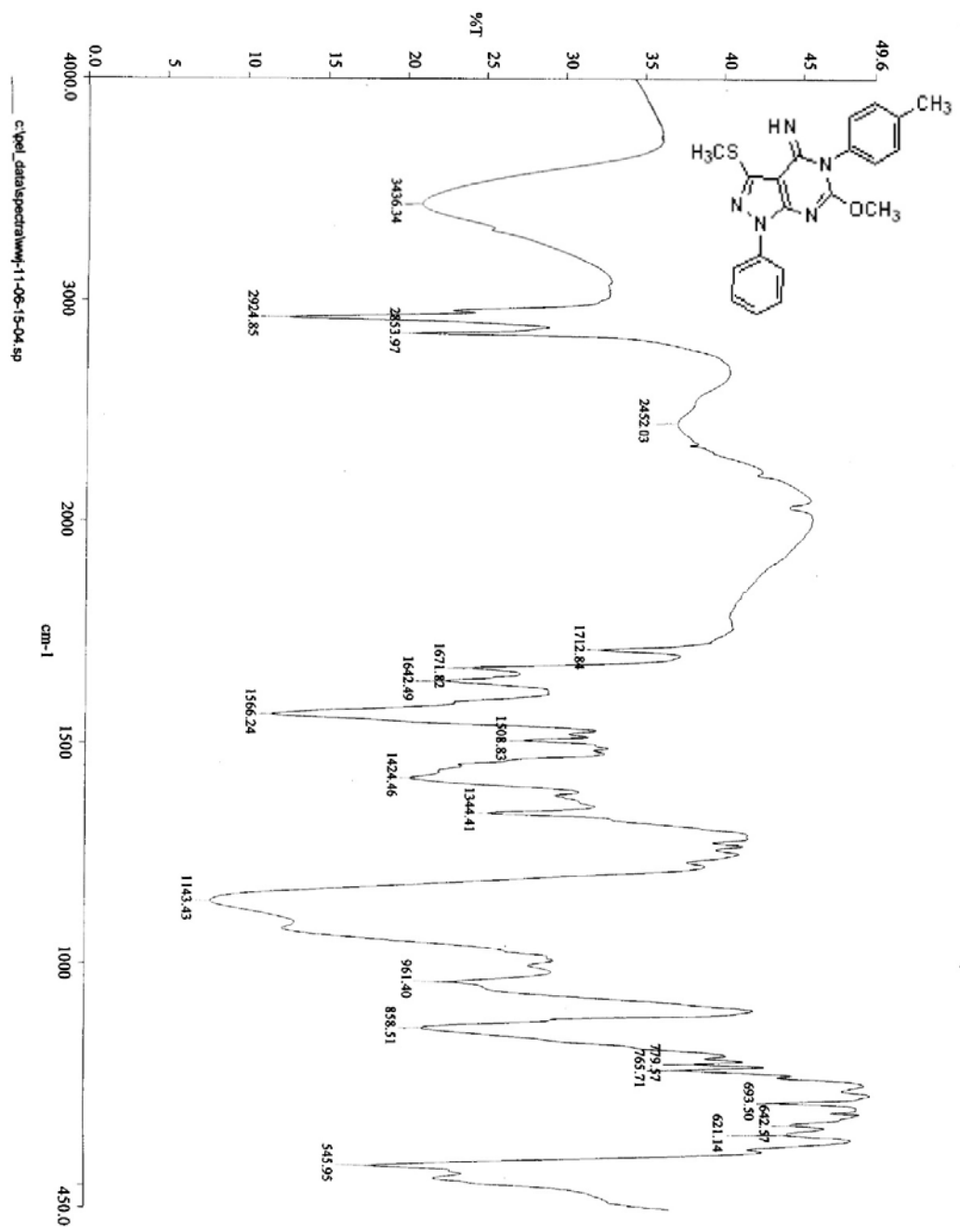
F2 - Processing parameters
 SI 32768
 SF 400.1300039 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

WVJ-7-22-4

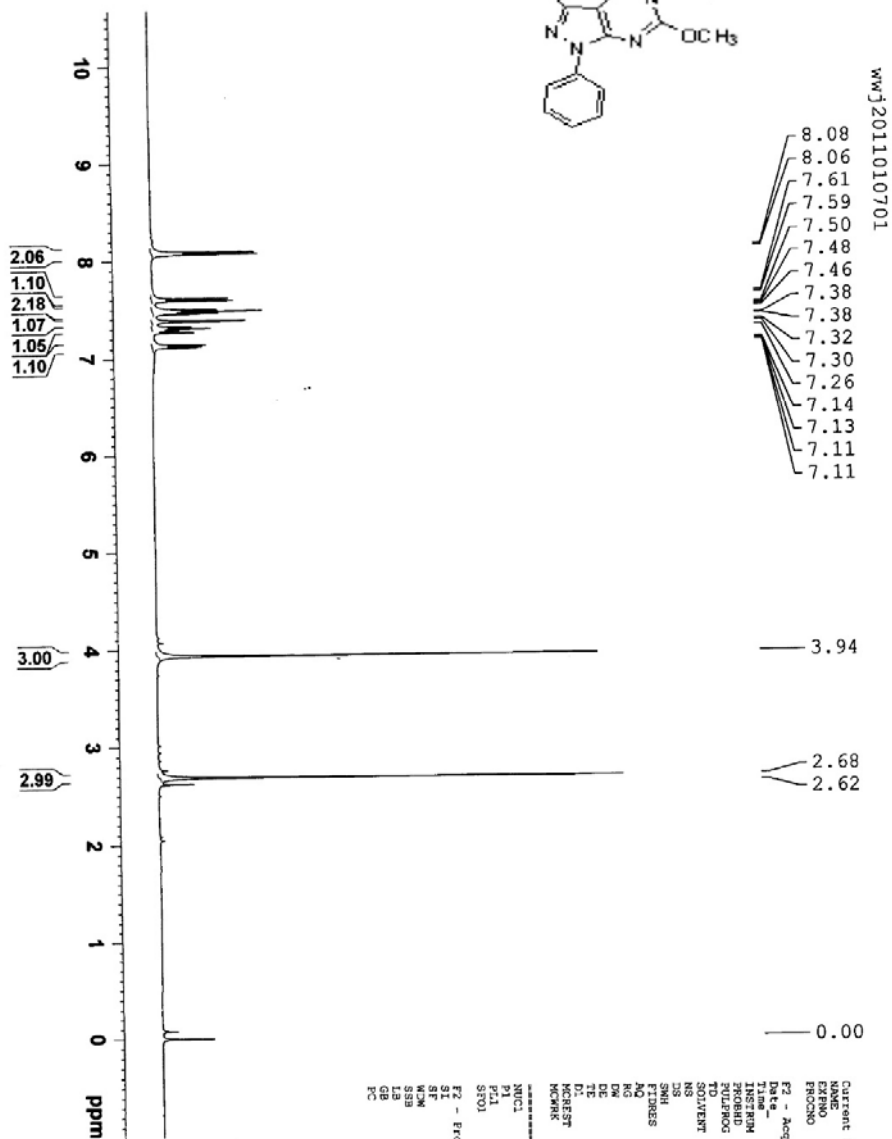
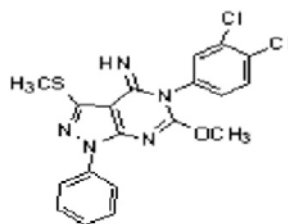


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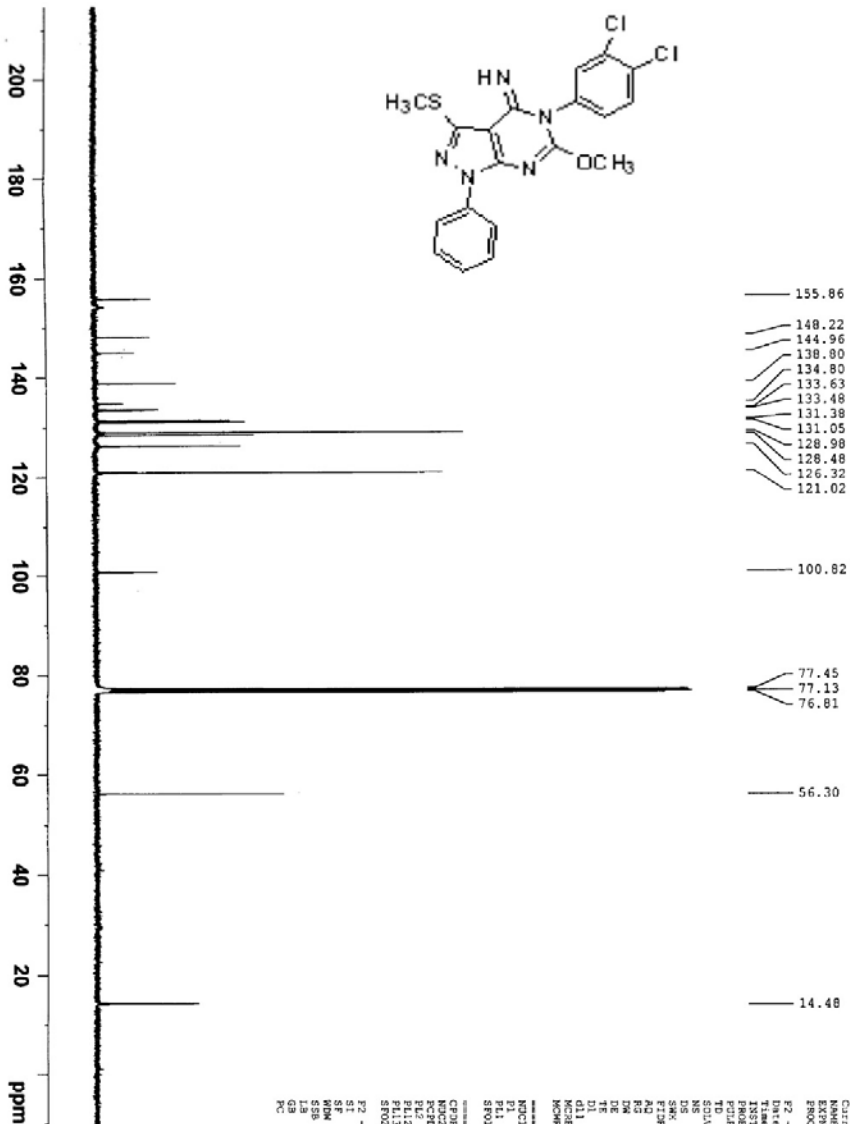
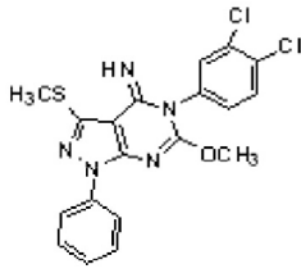
Current Data Parameters
NAME: WVJ-7-22-4
EXPNO: 62
PROCNO: 1
F2 - Acquisition Parameters
Date_Time: 2010728
Time: 15.59
Pulse_Program: zgpg30
PROBHD: 5 mm BBO
PULPROG: zgpg30
TOUPO: 65516
SOLVENT: CDCl3
NS: 2048
DS: 4
SWH: 23990.814 Hz
FIDRES: 0.2362746 Hz
RG: 16384
AQ: 1.3627456 sec
RG: 16384
TM: 20.850 usec
TE: 303.2 K
DE: 0.0000000 sec
AQ1: 0.0000000 sec
DE1: 0.0000000 sec
KCMER: 0.0150000 sec
----- CHANNEL f1: 13C -----
NUC1: 13C
P1: 6.00 usec
PL1: -2.00 dB
SFO1: 100.6250268 MHz
----- CHANNEL f2: 1H -----
NUC2: 1H
P2: 12.00 usec
PL2: -2.00 dB
SFO2: 400.1315005 MHz
----- Processing parameters -----
SI: 32768
SF: 100.6250268 MHz
WDW: EM
SSB: 0
GB: 0
PC: 1.45
  
```



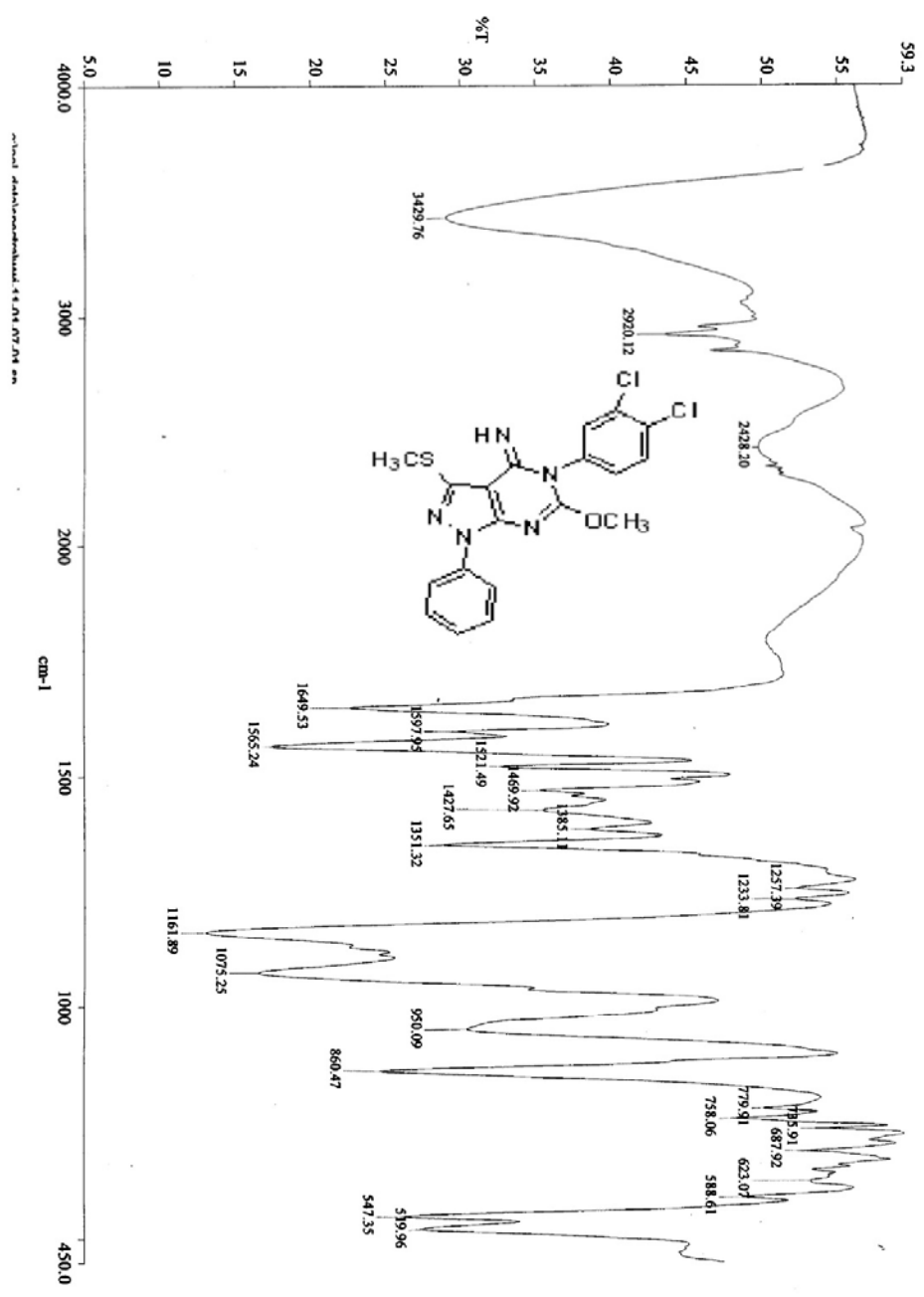
Compound 3c



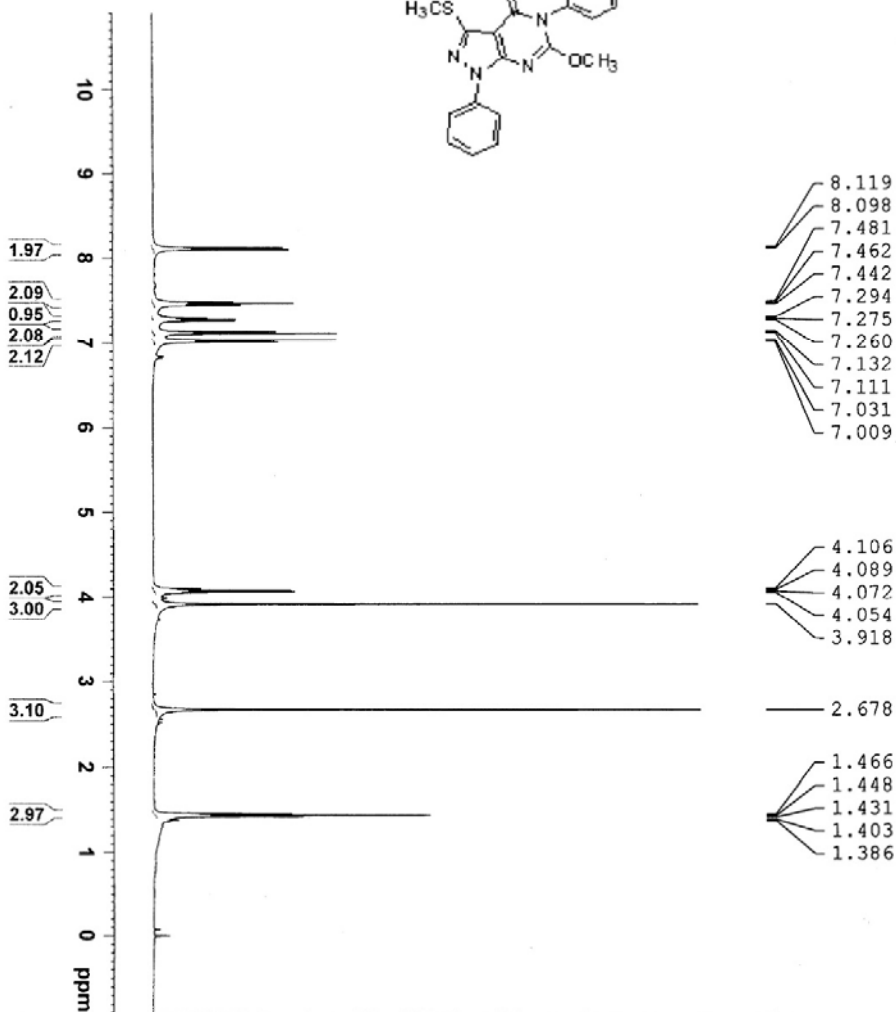
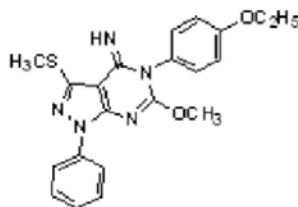
WJ201101100402



Current Data Parameters
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110111
 Time 11:41
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TOUENR 65535
 SOLVENT CDCl3
 NS 797
 DS 4
 SWH 2386.814 Hz
 FIDRES 0.411 Hz
 AQ 1.3664756 sec
 RG 11589.2
 FM 20.00 usec
 TM 289.2 X
 TE 2.4000000 sec
 D1 0.1
 DELT 0.0000000 sec
 ACQRES 0.0000000 sec
 KWNR 0.0150000 sec
 ===== CHANNEL f1 =====
 NUCL1 13C
 P1 8.450 usec
 PL1 -2.50 usec
 SFO1 100.626398 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 WALTZ16
 NUCL2 1H
 P2 80.00 usec
 PL2 0.00 usec
 PL12 1.00 dB
 PL13 14.00 dB
 SFO2 400.1316005 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.617690 MHz
 WHW 0
 CSF 1.00 Hz
 LB 0
 GB 1.40



Compound 3f



- 8.119
- 8.098
- 7.481
- 7.462
- 7.442
- 7.294
- 7.275
- 7.260
- 7.132
- 7.111
- 7.031
- 7.009

- 4.106
- 4.089
- 4.072
- 4.054
- 3.918

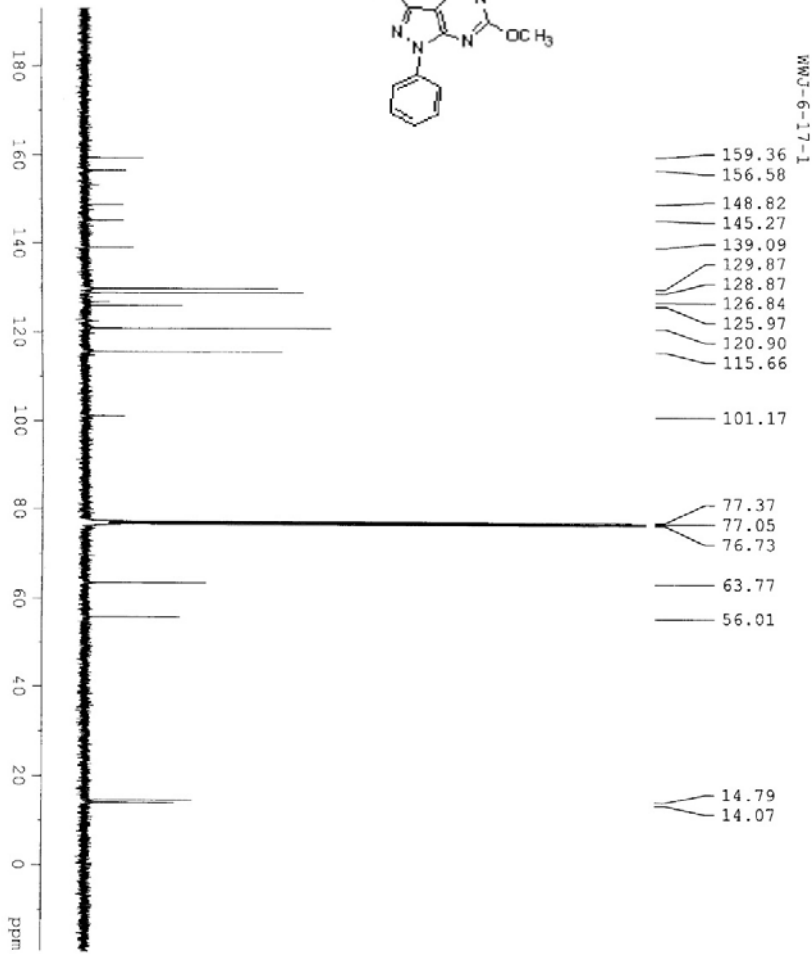
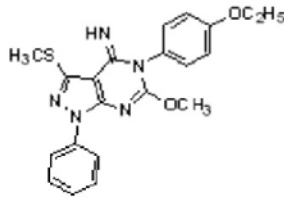
- 2.678
- 1.466
- 1.448
- 1.431
- 1.403
- 1.386

Current Data Parameters
 NAME wangwenjuan
 EXPNO 27
 PROCNO 1

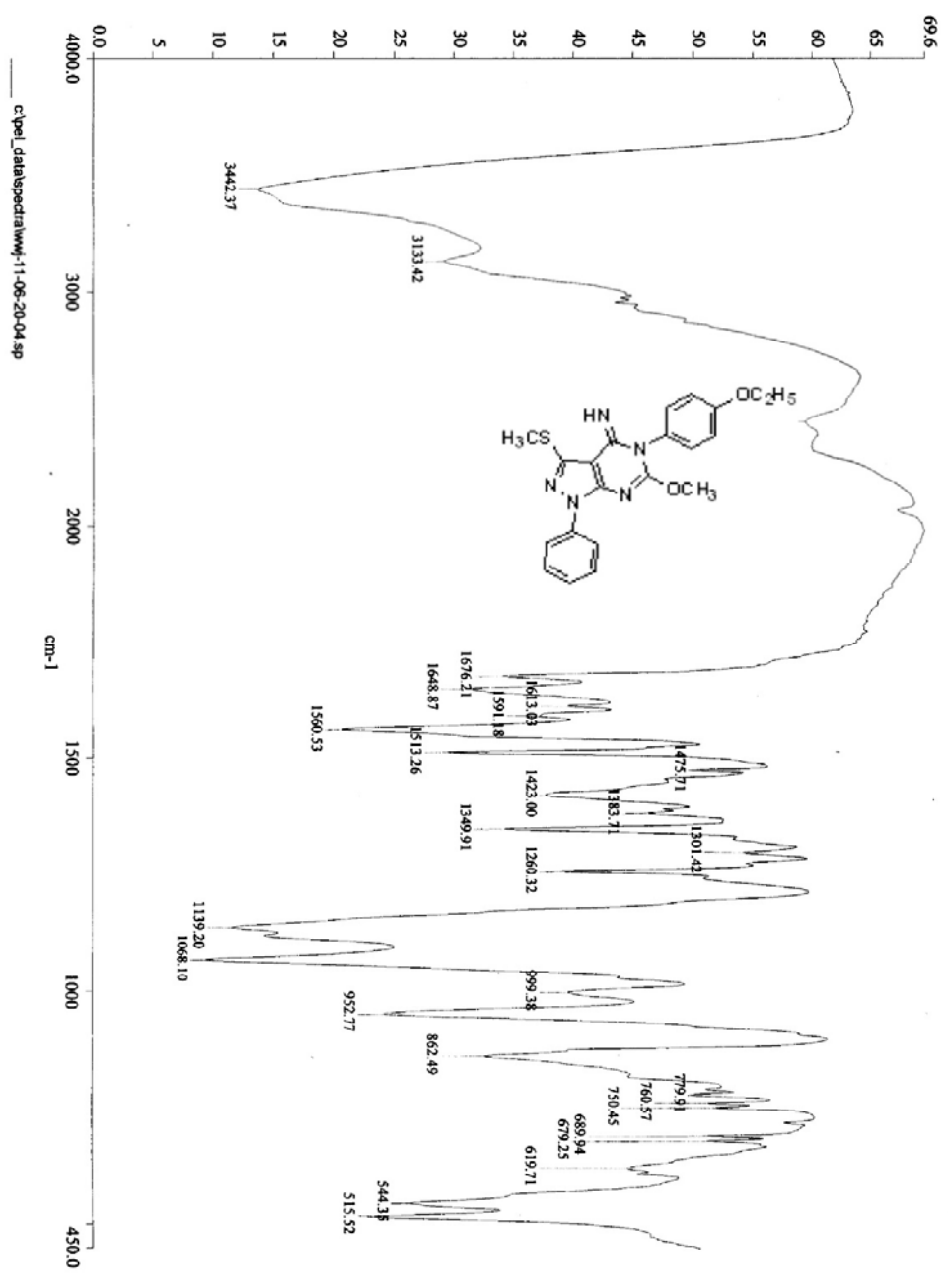
F2 - Acquisition Parameters
 Date_ 20110621
 Time 8.16
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SMH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 362
 DM 60.400 usec
 DE 6.00 usec
 TE 295.1 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

===== CHANNEL f1 =====
 NUCL1 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

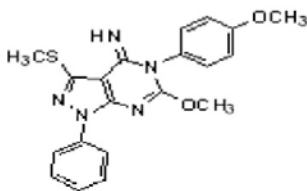
F2 - Processing parameters
 SI 32768
 SF 400.1300092 MHz
 MDW EX
 SSS 0
 LB 0.30 Hz
 GB 0
 PC 1.00



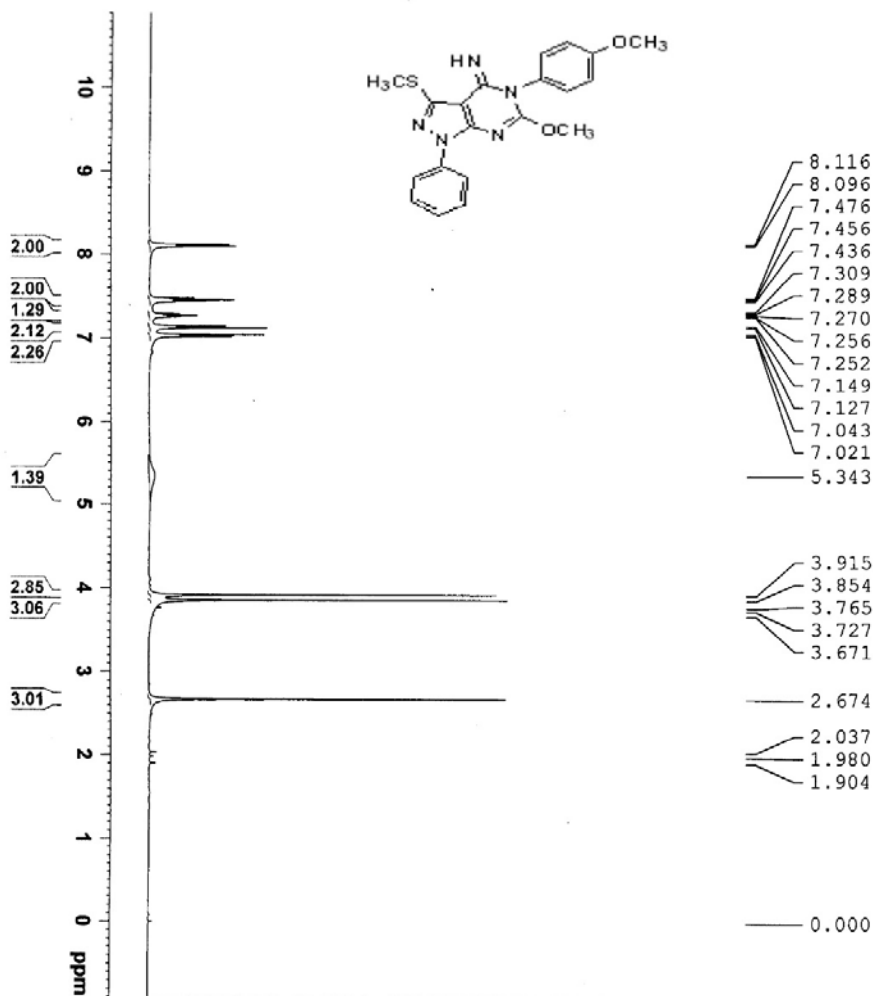
Current Data Parameters
 EXPNO 32
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110624
 Time 11:00:11
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zgpg30
 F2 270.130
 F1 101.623
 SOLVENT CDCl3
 NS 383
 DS 4
 SWH 23980.844 Hz
 FWHM 1.1864758 sec
 AQ 0.085
 SFO 29.6192 sec
 DE 29.6192 sec
 TE 300.2 K
 TS 300.13 K
 d11 0.0200000 sec
 d12 0.0200000 sec
 d13 0.0200000 sec
 d14 0.0200000 sec
 d15 0.0200000 sec
 d16 0.0200000 sec
 d17 0.0200000 sec
 d18 0.0200000 sec
 d19 0.0200000 sec
 d20 0.0200000 sec
 d21 0.0200000 sec
 d22 0.0200000 sec
 d23 0.0200000 sec
 d24 0.0200000 sec
 d25 0.0200000 sec
 d26 0.0200000 sec
 d27 0.0200000 sec
 d28 0.0200000 sec
 d29 0.0200000 sec
 d30 0.0200000 sec
 d31 0.0200000 sec
 d32 0.0200000 sec
 d33 0.0200000 sec
 d34 0.0200000 sec
 d35 0.0200000 sec
 d36 0.0200000 sec
 d37 0.0200000 sec
 d38 0.0200000 sec
 d39 0.0200000 sec
 d40 0.0200000 sec
 d41 0.0200000 sec
 d42 0.0200000 sec
 d43 0.0200000 sec
 d44 0.0200000 sec
 d45 0.0200000 sec
 d46 0.0200000 sec
 d47 0.0200000 sec
 d48 0.0200000 sec
 d49 0.0200000 sec
 d50 0.0200000 sec
 ***** CHANNEL f1 *****
 P1 6.00 usec
 PL1 -2.00 dB
 SFO1 100.622896 MHz
 ***** CHANNEL f2 *****
 P2 18.00 usec
 PL2 18.00 dB
 SFO2 400.1418051 MHz
 F2 - Processing parameters
 SF 100.622896 MHz
 IF 63.151558 MHz
 WB 1.75 Hz
 GB 3
 PC 1.43



Compound 3g



MMJ-6-17-1



- 8.116
- 8.096
- 7.476
- 7.456
- 7.436
- 7.309
- 7.289
- 7.270
- 7.256
- 7.252
- 7.149
- 7.127
- 7.043
- 7.021
- 5.343

- 3.915
- 3.854
- 3.765
- 3.727
- 3.671

- 2.674

- 2.037
- 1.980
- 1.904

- 0.000

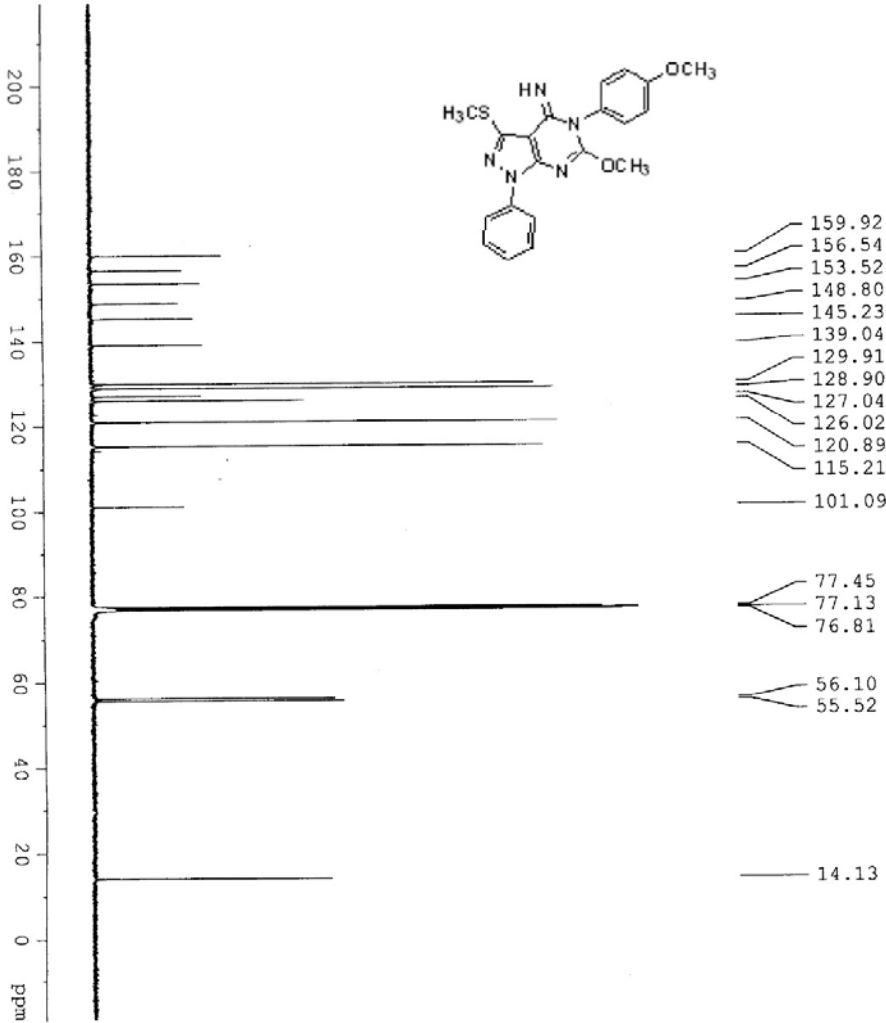
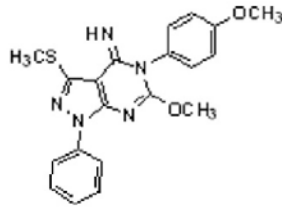
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Current Data Parameters
NAME      wangjuan
EXPNO     22
PROCNO    1

F2 - Acquisition Parameters
Date_     20110617
Time      10.51
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        8278.146 Hz
FIDRES     0.126314 Hz
AQ         3.9584243 sec
RG         161.3
DE         60.400 usec
TE         297.2 K
D1         1.00000000 sec
MCREST     0.00000000 sec
MCMRR      0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         13.00 usec
PL1        -3.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
SI         32768
SF         400.1300111 MHz
WDW        EM
SSB        0
GB         0
PC         1.00
    
```



- 159.92
- 156.54
- 153.52
- 148.80
- 145.23
- 139.04
- 129.91
- 128.90
- 127.04
- 126.02
- 120.89
- 115.21
- 101.09

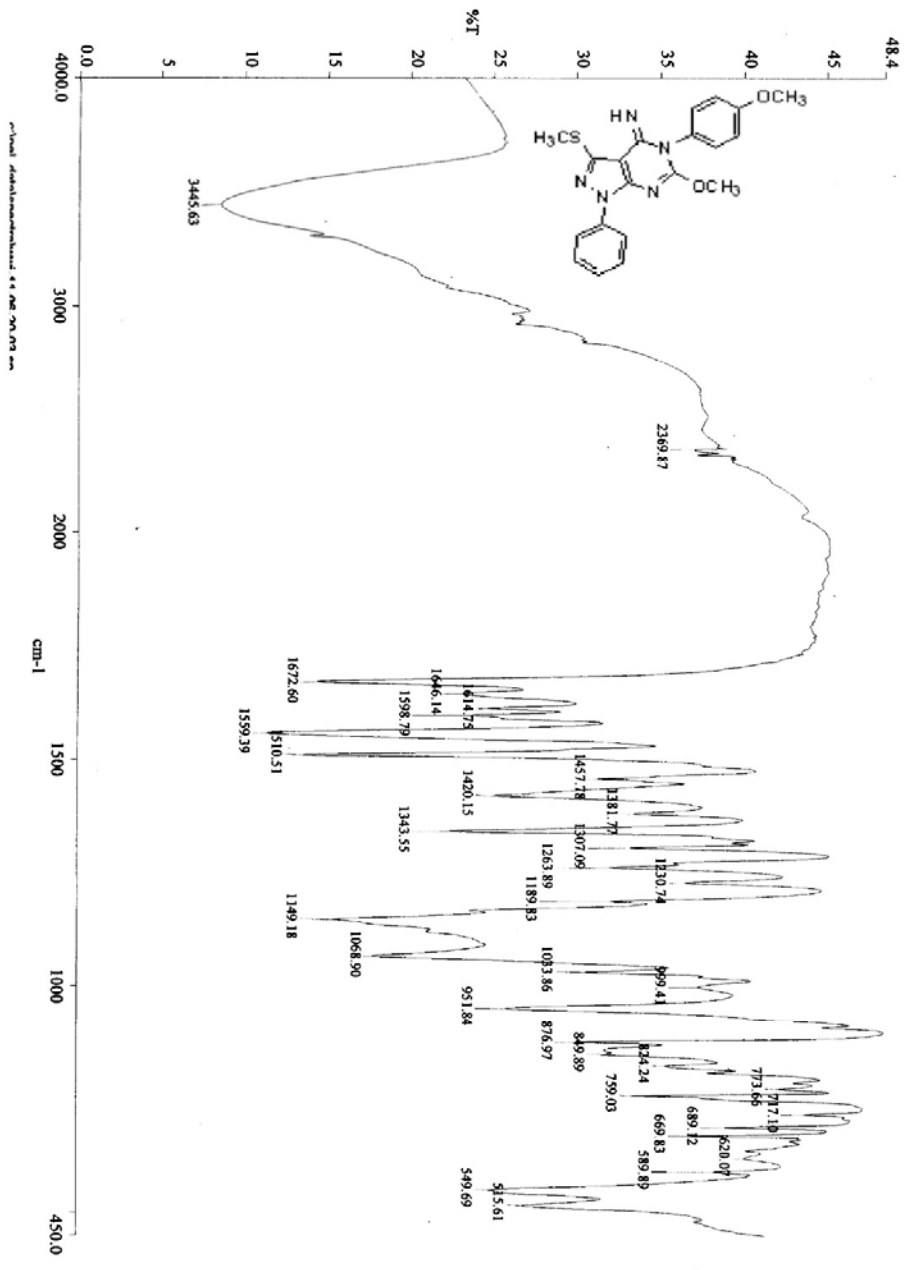
- 77.45
- 77.13
- 76.81

- 56.10
- 55.52

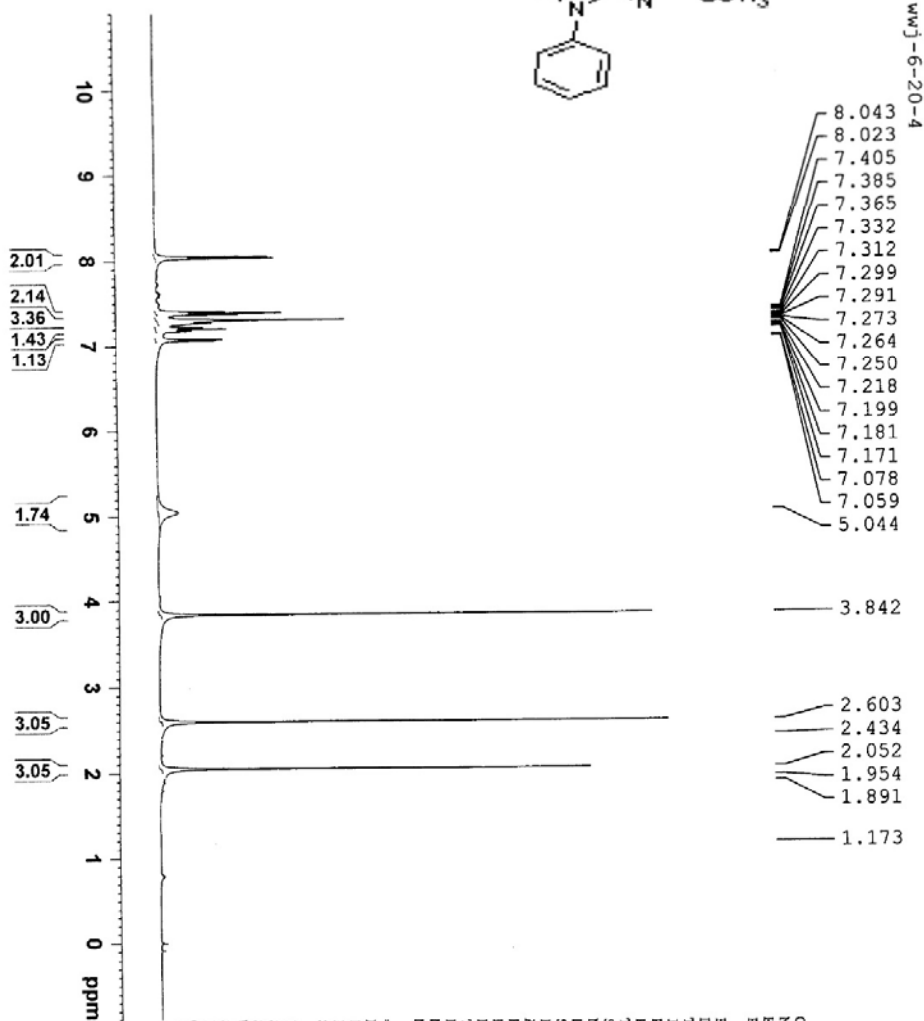
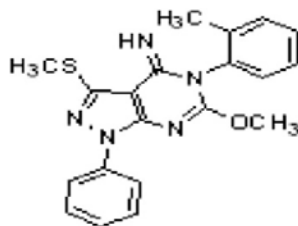
- 14.13

```

Current Data Parameters
NAME      Wmcm6171
EXNO      26
PROCNO    1
----- Acquisition Parameters
Date_     2010620
Time      14.24
INSTRUM   spect
PROBHD    5 mm BBO BbC1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
DE         201
DS         4
SWH        23980.814 Hz
FIDRES    0.3165918 Hz
AQ         1.02213 sec
RG         1021.3
DM         20.850 usec
DE         6.00 usec
TE         300.2 K
D1         2.0000000 sec
d11        0.0300000 sec
MKSRES1   0.0150000 sec
----- CHANNEL f1 -----
NUC1       13C
P1         13C usec
PL1        -2.00 dB
SFO1       100.6278288 MHz
----- CHANNEL f2 -----
NAME      Wmcm6171
PROCNO    1
----- Acquisition Parameters
Date_     2010620
Time      14.24
INSTRUM   spect
PROBHD    5 mm BBO BbC1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
DE         201
DS         4
SWH        23980.814 Hz
FIDRES    0.3165918 Hz
AQ         1.02213 sec
RG         1021.3
DM         20.850 usec
DE         6.00 usec
TE         300.2 K
D1         2.0000000 sec
d11        0.0300000 sec
MKSRES1   0.0150000 sec
----- CHANNEL f2 -----
NUC2       13C
P2         13C usec
PL2        -2.00 dB
SFO2       100.6278288 MHz
----- CHANNEL f3 -----
NAME      Wmcm6171
PROCNO    1
----- Acquisition Parameters
Date_     2010620
Time      14.24
INSTRUM   spect
PROBHD    5 mm BBO BbC1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
DE         201
DS         4
SWH        23980.814 Hz
FIDRES    0.3165918 Hz
AQ         1.02213 sec
RG         1021.3
DM         20.850 usec
DE         6.00 usec
TE         300.2 K
D1         2.0000000 sec
d11        0.0300000 sec
MKSRES1   0.0150000 sec
----- CHANNEL f3 -----
NUC3       13C
P3         13C usec
PL3        -2.00 dB
SFO3       100.6278288 MHz
----- Processing parameters -----
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00
  
```



Compound 3h



wj-6-20-4

Current Data Parameters
NAME wangwenjuan
EXPNO 29
PROCNO 1

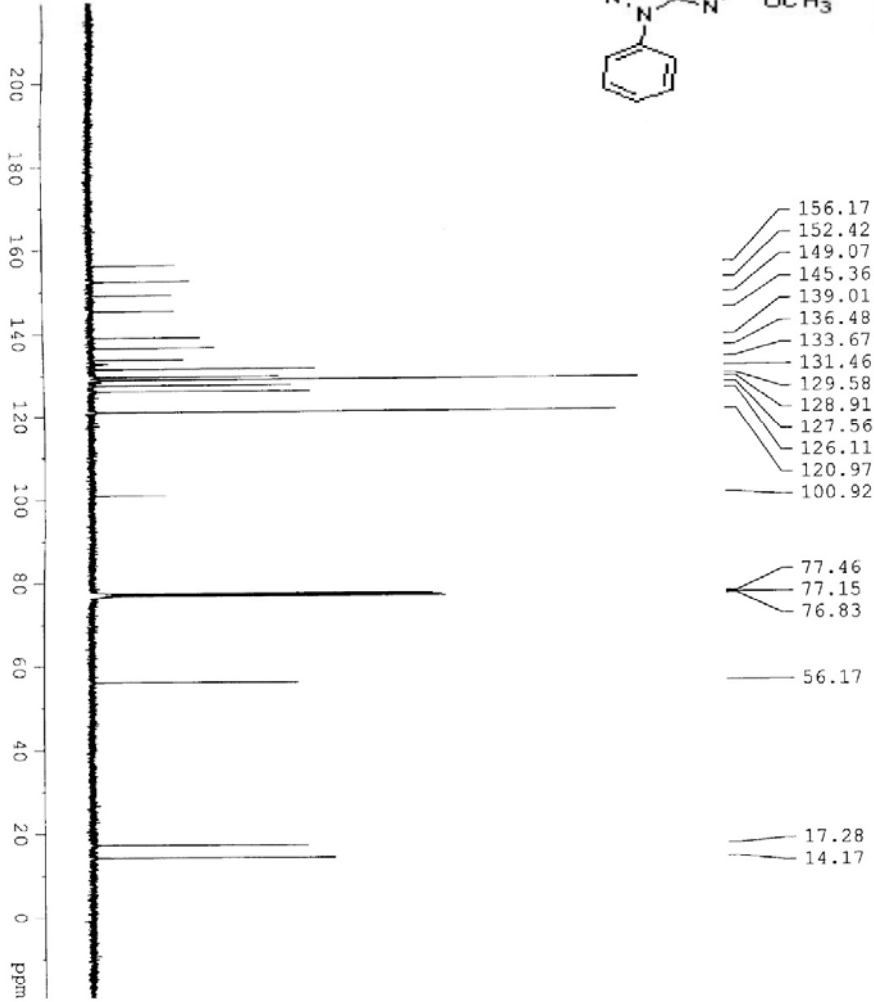
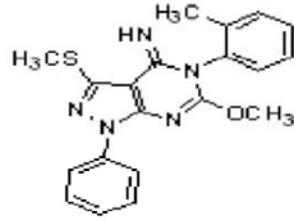
F2 - Acquisition Parameters

Date_ 20110621
Time 8:28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 9278.146 Hz
FIDRES 0.126314 Hz
AQ 3.958443 sec
RG 164.03
DW 60.400 use
DE 295.1 use
TE 1.00000000 sec
DI 0.00000000 sec
RGREST 0.01300000 sec
RGMRK 0.01300000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 13.00 use
PL1 13.00 dB
SFO1 400.1324710 MHz

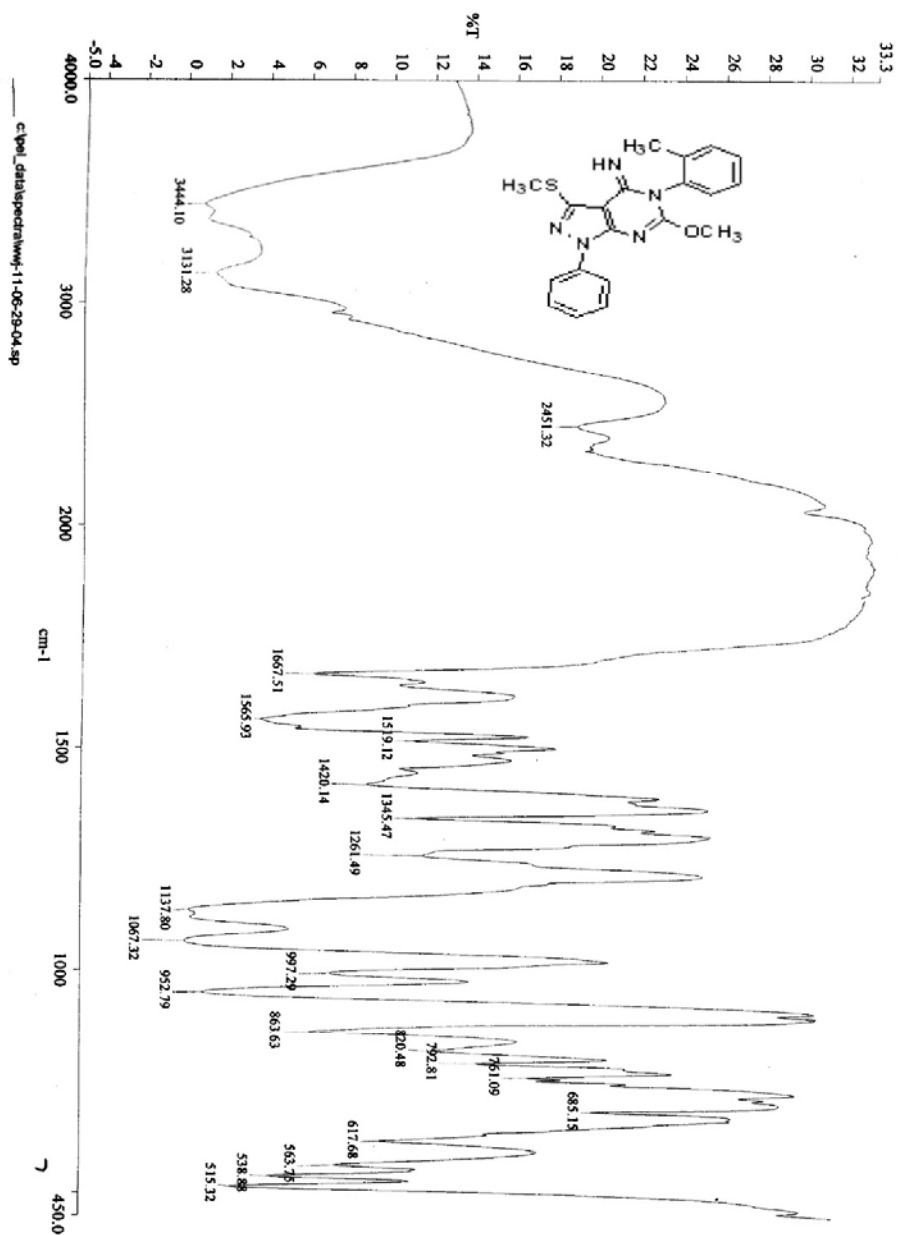
F2 - Processing parameters
SI 327.68 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

WWT-6-22-6

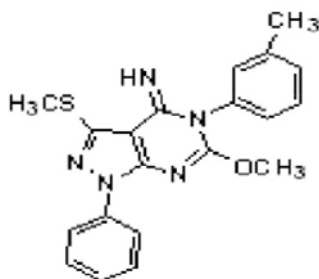


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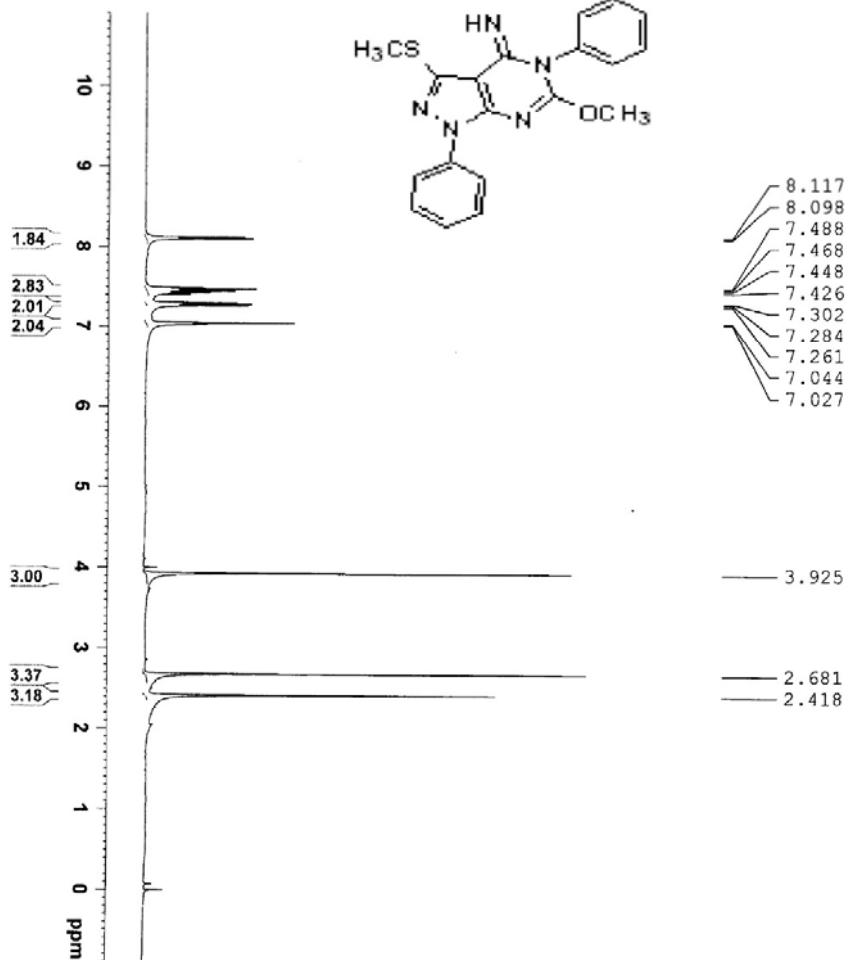
Current Data Parameters
NAME          wwt62206139
EXPNO        39
PROCNO       1
F2 - Acquisition Parameters
Date_         11-57
Time         11:57
INSTRUM      spect
PROBHD       5 mm BBO BP-1H
PULPROG      zgpg30
TD            65536
SFO1         125.761
FIDRES       0.316
AQ           0.1150000
RG           516
DS           4
SWH          23580.814 Hz
FIDRES       0.316
AQ           0.1150000
RG           516
DM           20.850 usec
TE           300.2 K
D1           2.00000000 sec
d11scf      0.05000000 sec
MCMKR      0.01500000 sec
===== CHANNEL f1 =====
NUC1         13
P1           6.00 usec
PL1         -2.00 dB
SFO1         100.628258 MHz
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2         13
P2           80.00 usec
PL2         120.00 dB
PL12        12.00 dB
PL13        12.00 dB
PL14        12.00 dB
SFO2         400.1418000 MHz
F2 - Processing parameters
SI           32768
SF           100.612746 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

Compound 3i



WUJ-6-8-2



Current Data Parameters
NAME wangwenjuan
EXPNO 14
PROCNO 1

F2 - Acquisition Parameters

Date_ 201609
Time_ 9:10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 456.1
DM 60.400 usec
DE 239.2 K
TE 300.2 K
T1 1.0000000 sec
T2 0.0000000 sec
MCREST 0.0100000 sec
MCMER 0.0100000 sec

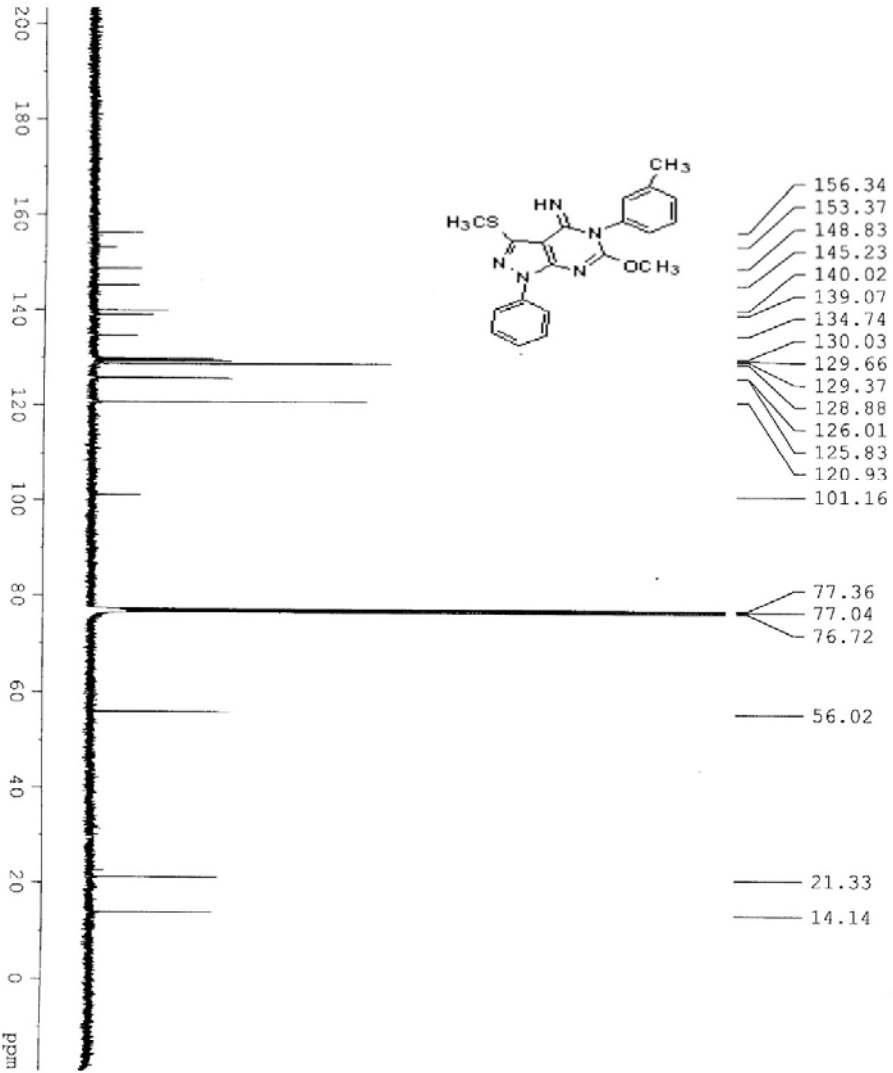
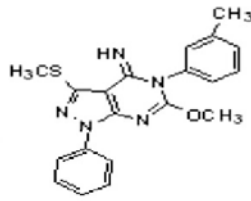
===== CHANNEL f1 =====

NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters

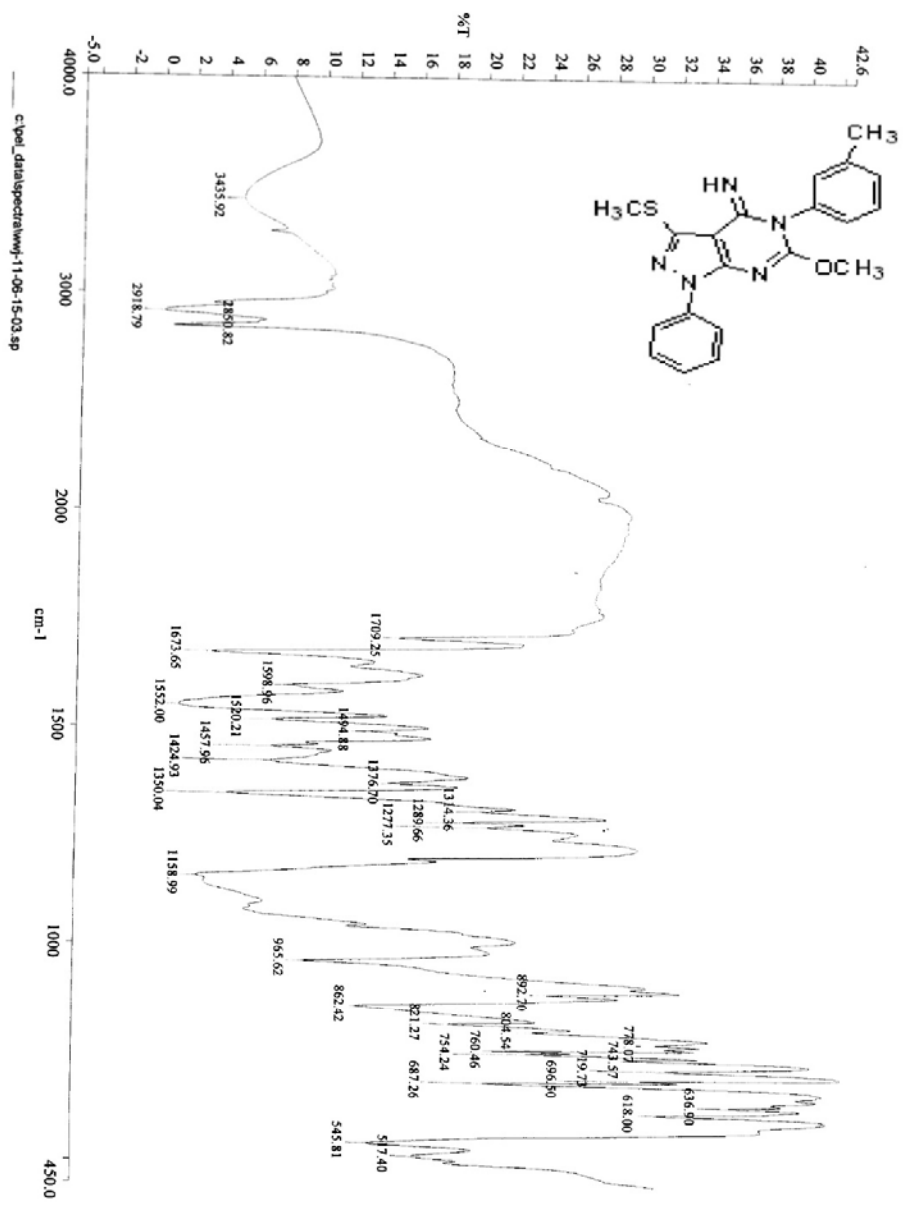
SF 400.130082 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

WJ-6-13-2

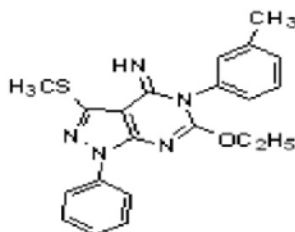


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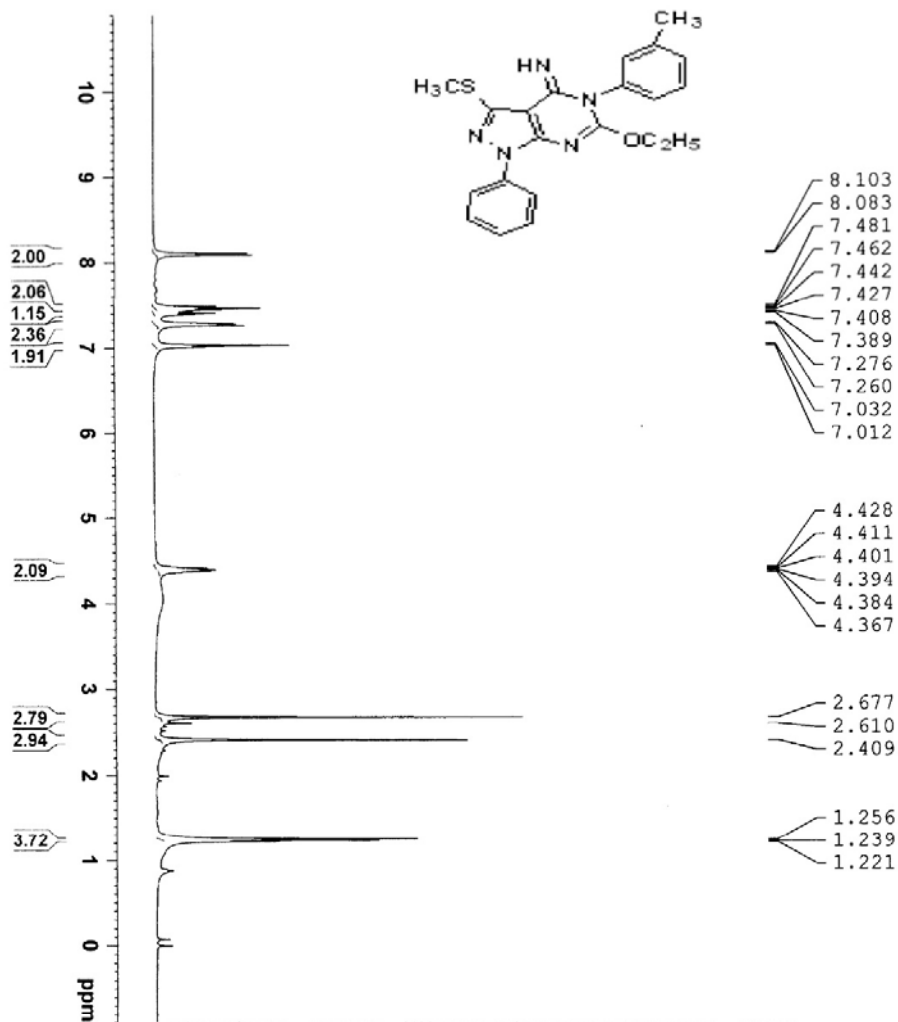
Current Data Parameters
Date_ 20100615
Time_ 15.49
ExpNo 21
ProcNo 1
===== CHANNEL F2 =====
NUC1 13C
P1 5.00 usec
SFO1 100.628298 MHz
===== CHANNEL F1 =====
NUC1 13C
P1 5.00 usec
SFO1 100.628298 MHz
===== CHANNEL F2 =====
CONPFG2 wait16
NUC2 13C
P2 60.00 usec
PERF02 120.00 dB
E2 120.00 dB
F2 12.00 dB
F213 12.00 dB
SFO2 400.1318005 MHz
===== Processing parameters =====
SI 100.6127450 MHz
SF 100.6127450 MHz
K1W EM
SB 1.00 Hz
GB 0
PC 1.40
  
```



Compound 3j



WUJ-6-17-3



- 8.103
- 8.083
- 7.481
- 7.462
- 7.442
- 7.427
- 7.408
- 7.389
- 7.276
- 7.260
- 7.032
- 7.012

- 4.428
- 4.411
- 4.401
- 4.394
- 4.384
- 4.367

- 2.677
- 2.610
- 2.409

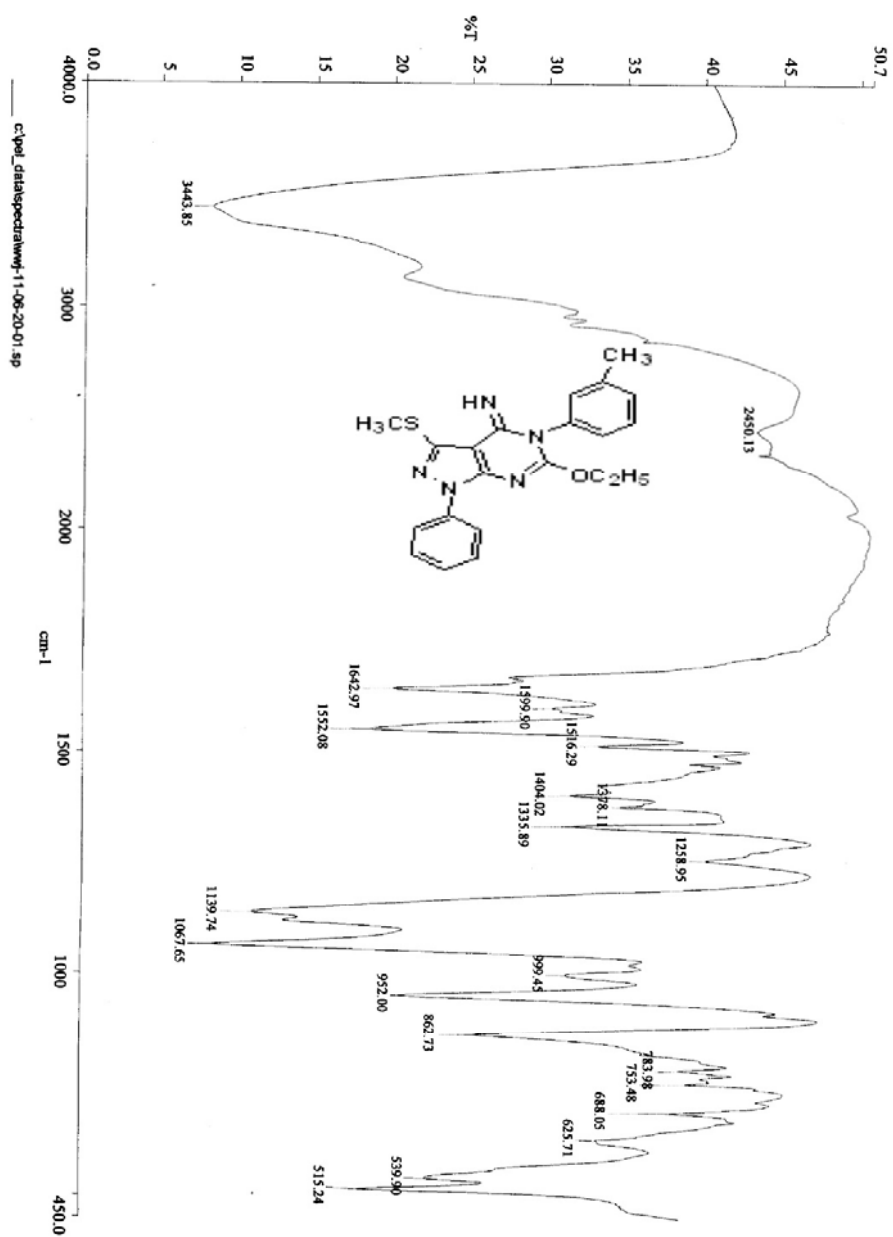
- 1.256
- 1.239
- 1.221

Current Data Parameters
 NAME wangwenjuan
 EXPNO 25
 PROCNO 1

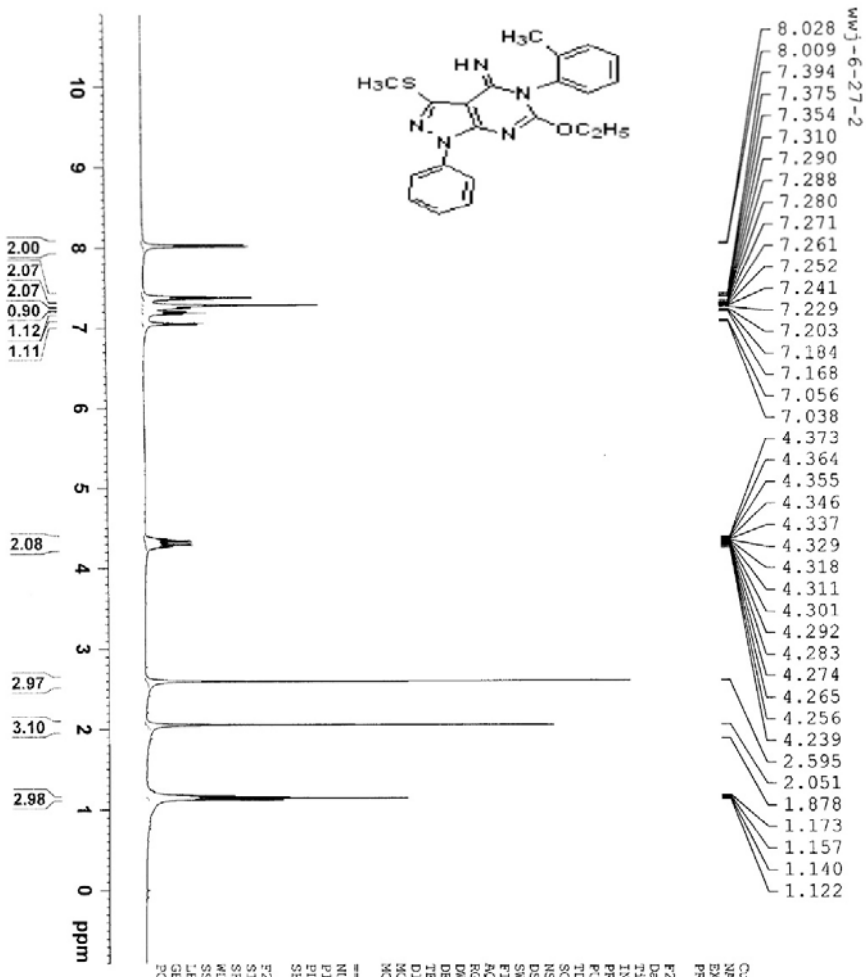
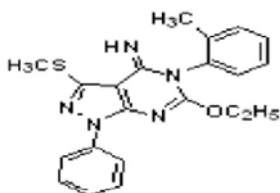
F2 - Acquisition Parameters
 Date_ 20110617
 Time 11.02
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 362
 DW 60.400 usec
 DE 6.00 usec
 TE 297.1 K
 D1 1.00000000 sec
 MCOREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUCL 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300999 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Compound 3k



- 8.028
8.009
7.394
7.375
7.354
7.310
7.290
7.288
7.280
7.271
7.261
7.252
7.241
7.229
7.203
7.184
7.168
7.056
7.038
4.373
4.364
4.355
4.346
4.337
4.329
4.318
4.311
4.301
4.292
4.283
4.274
4.265
4.256
4.239
2.595
2.051
1.878
1.173
1.157
1.140
1.122

2.00
2.07
2.07
0.90
1.12
1.11

2.08

2.97

3.10

2.98

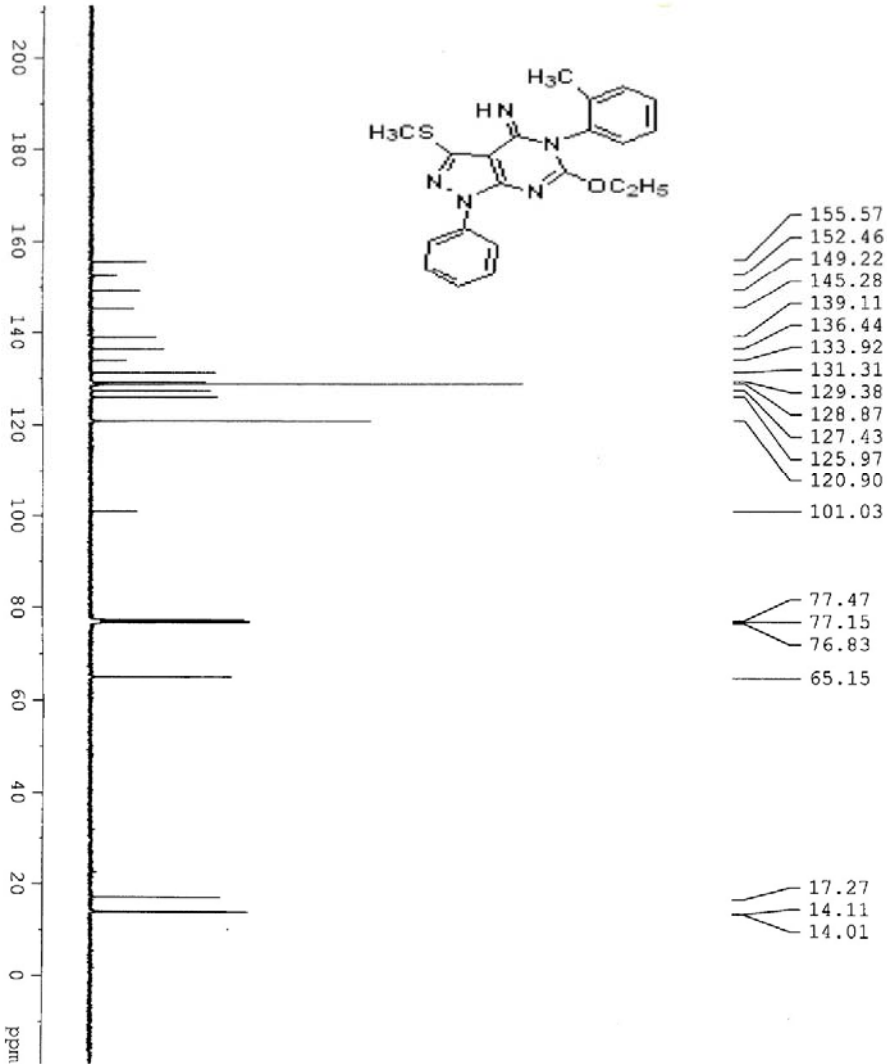
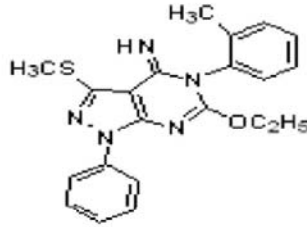
ppm

Current Data Parameters
NAME wangwenjuan
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 201609
Time 15:09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 161.3
DW 60.400 usec
DE 8.400 usec
TE 29.1 K
D1 1.00000000 sec
DELTA 1.00000000 sec
SOLVENT CDCl3
SCANS 0.01500000 sec

CHANNEL f1
NUC1 1H
P1 13.00 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300464 MHz
WDW EX
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



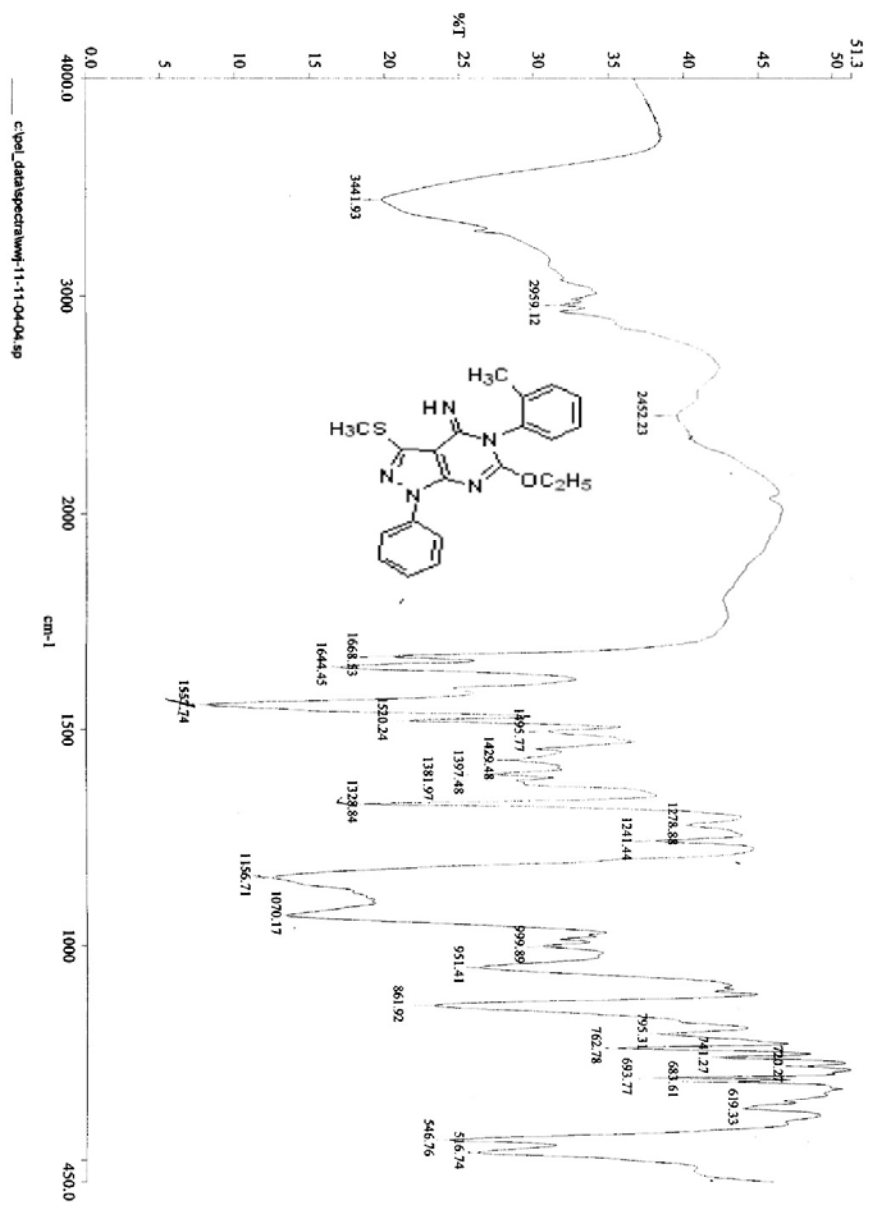
Current Data Parameters
 NAME: Wangpinjuan
 EXPNO: 44
 PROCNO: 1

F2 - Acquisition Parameters
 Date_ 20110630
 Time 8.07
 TMRQM 1.0000000
 PROBNM 5 ml BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SFO 400.1316035
 SOLVENT CDCl3
 NS 512
 DS 4
 SMH 23980.814 Hz
 AQ 0.0000000
 FIDRES 1.366758 Hz
 RG 5792.6
 MK 20.850 usec
 TE 29.00 usec
 TR 2.00 usec
 DE 6.00 usec
 DI 1.0000000 sec
 D11 0.0300000 sec
 DELT 0.0000000 sec
 KW 0.0000000 sec
 KCMW 0.0100000 sec

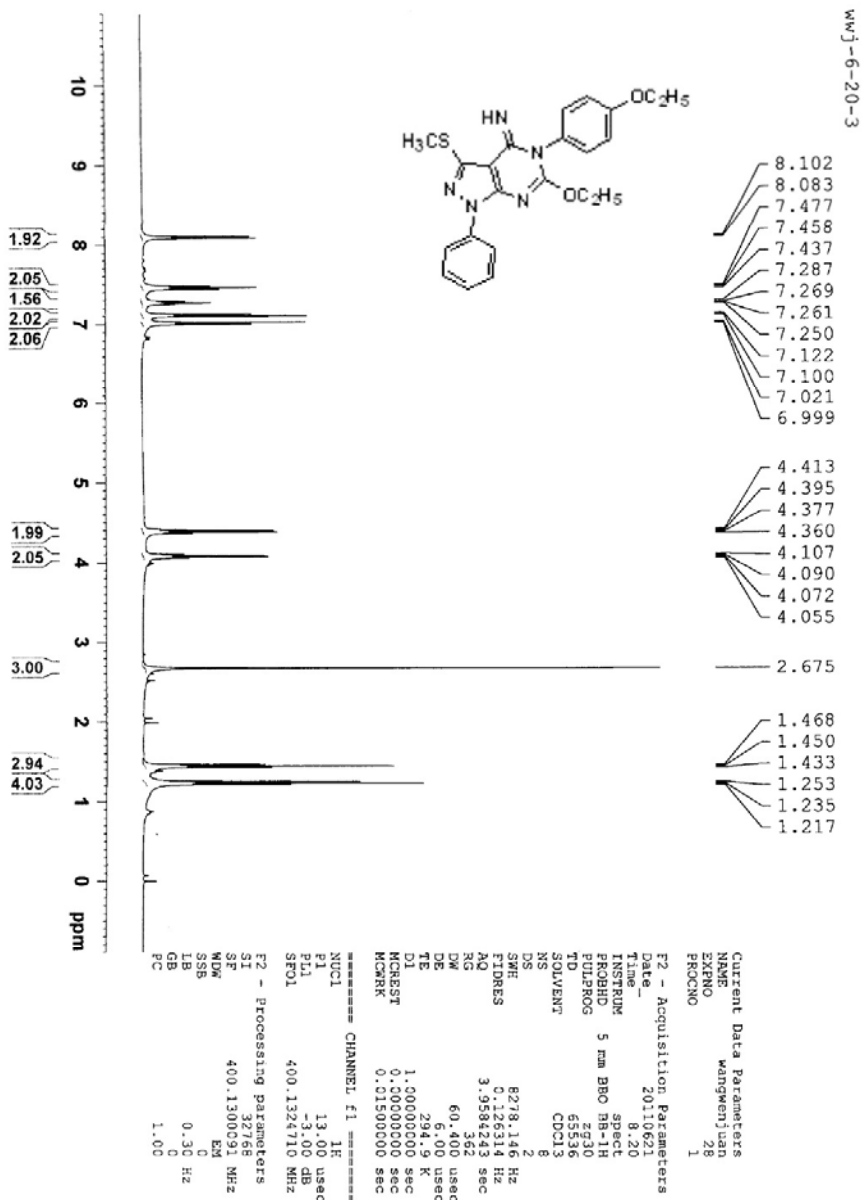
***** CHANNEL f1 *****
 NUC1 13C
 P1 6.00 usec
 PL1 -2.00 dB
 SFO1 100.6282998 MHz

***** CHANNEL f2 *****
 CDEPRG2 waltz16
 RUCF2 1H
 PULP2 80.00 usec
 PLP2 120.00 dB
 PUL12 12.00 dB
 PUL13 12.00 dB
 SFO2 400.1316035 MHz

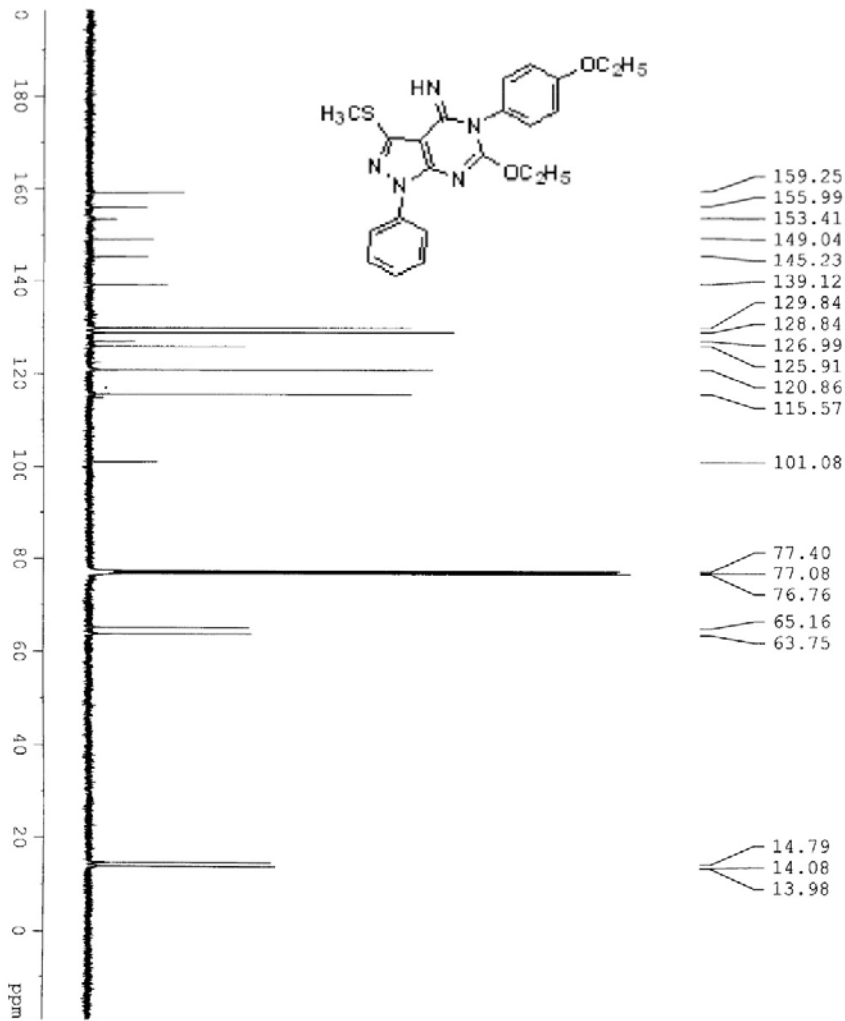
F2 - Processing parameters
 SI 32768
 SF 100.6127890 MHz
 WDW 0
 SSB 0
 LB 1.00 Hz
 GB 0
 EC 1.40



Compound 3l



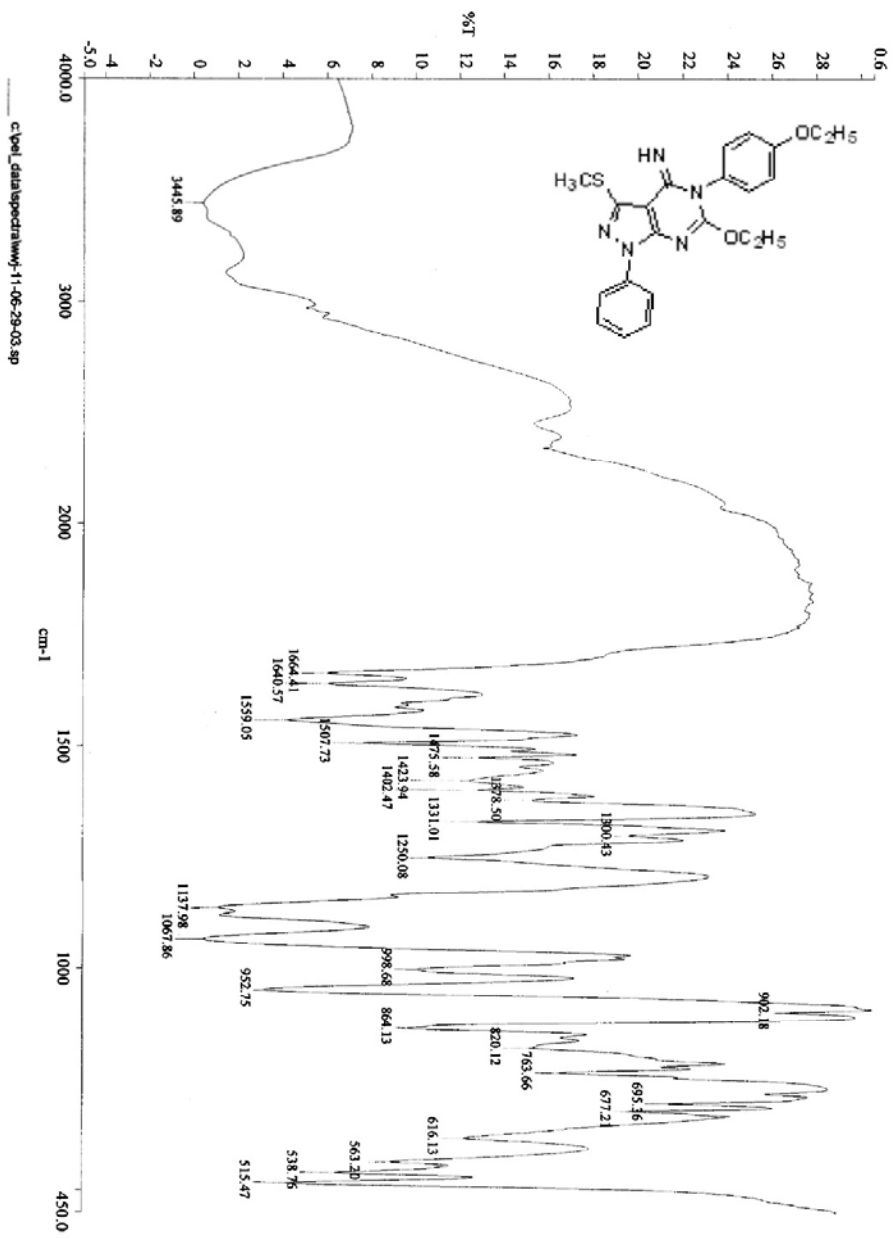
RMJ-6-22-5



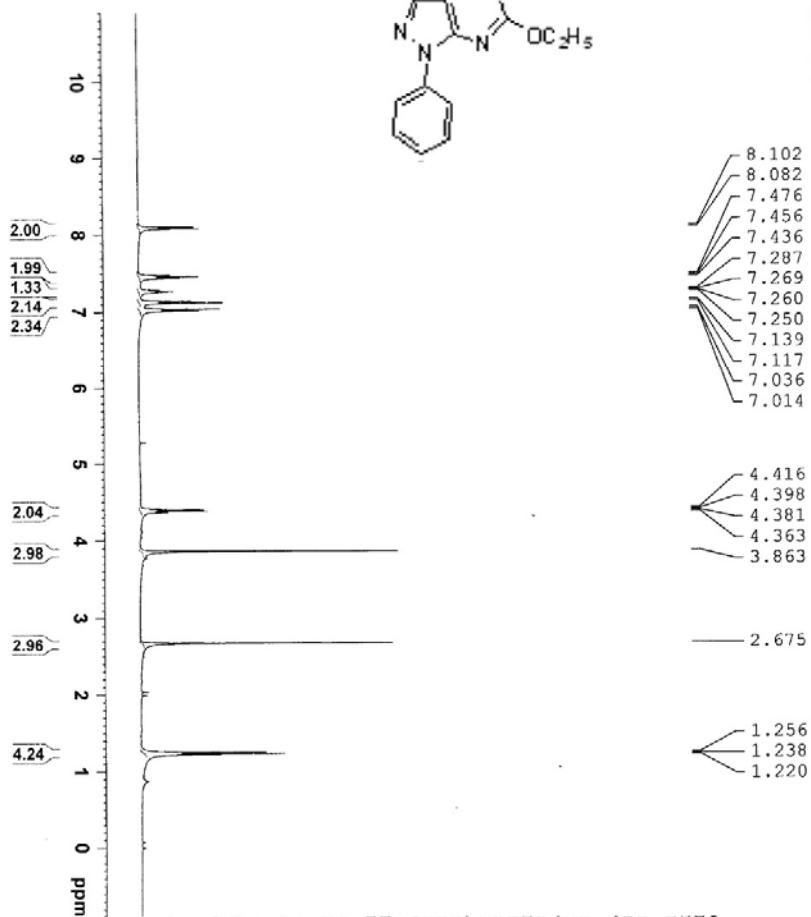
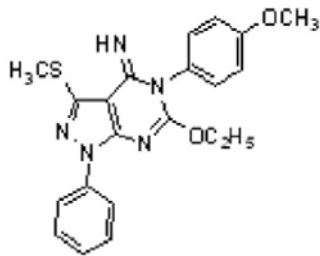
```

Current Data Parameters
NAME      Acquisition3
EXPNO    37
PROCNO   1
F2 - Acquisition Parameters
Date_    20110624
Time     11:12
INSTRUM  spect
PROBHD   5 mm BBO BB-1H
PULPROG  zgpg30
SOLVENT  CDCl3
NS       675
DS       4
SWH      23980.814 Hz
FIDRES   0.365918 Hz
AQ       1.3664726 sec
RG        682
DE       20.852 uSVC
TE       300.2 K
T1       3.09000000 sec
d11      0.03000000 sec
NCREST   0.03000000 sec
SFO1     100.6228296 MHz
===== CHANNEL f1 =====
NUC1      13C
P1       12C
PL1      6.00 uSVC
SFO2     100.6228296 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      13C
P2       80.00 uSVC
PL2      120.00 dB
PL12     12.00 dB
SFO3     400.1314500 MHz
F2 - Processing parameters
SF       100.6127690 MHz
RG        682
DE       20.852 uSVC
TE       300.2 K
T1       3.09000000 sec
d11      0.03000000 sec
NCREST   0.03000000 sec
SFO1     100.6228296 MHz
SFO2     400.1314500 MHz
===== CHANNEL f1 =====
NUC1      13C
P1       12C
PL1      6.00 uSVC
SFO2     100.6228296 MHz
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      13C
P2       80.00 uSVC
PL2      120.00 dB
PL12     12.00 dB
SFO3     400.1314500 MHz
===== CHANNEL f3 =====
SF       100.6127690 MHz
RG        682
DE       20.852 uSVC
TE       300.2 K
T1       3.09000000 sec
d11      0.03000000 sec
NCREST   0.03000000 sec
SFO1     100.6228296 MHz
SFO2     400.1314500 MHz

```



Compound 3m

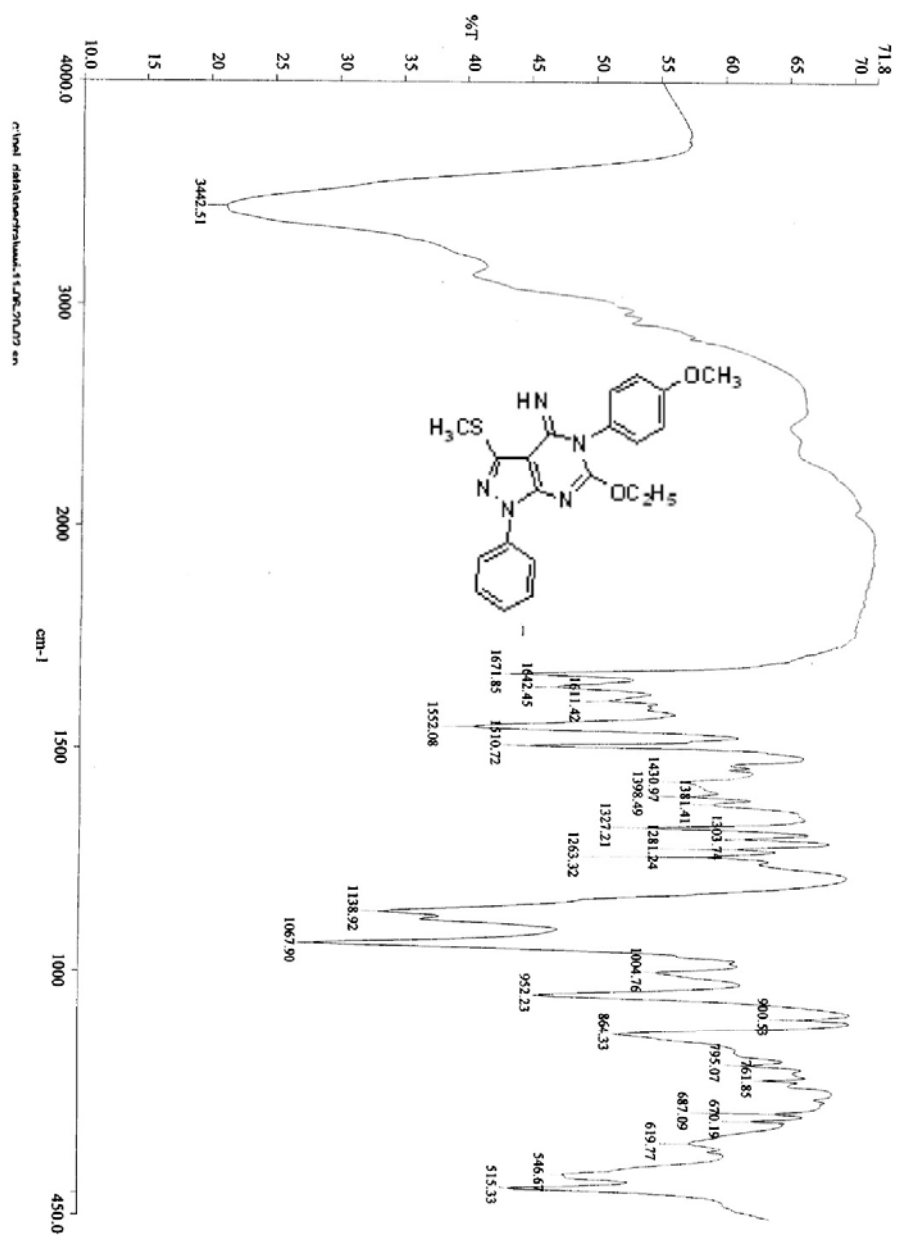


MMJ-6-17-2

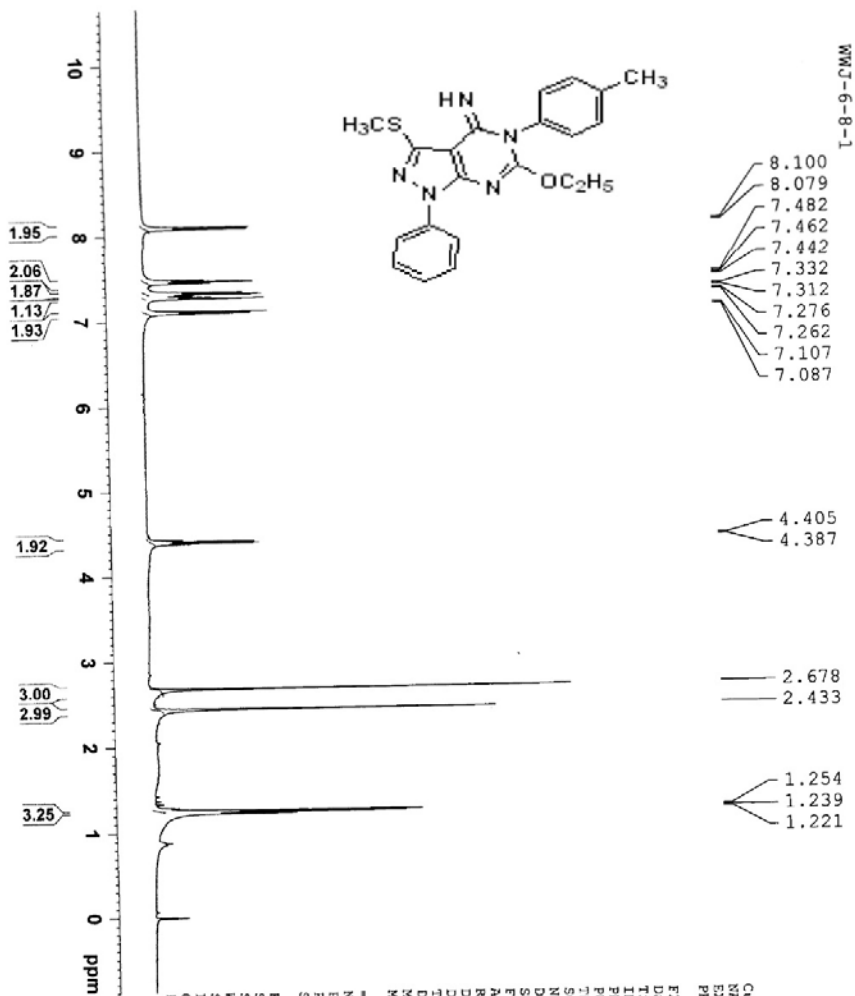
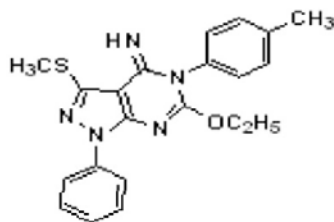
```

Current Data Parameters
NAME          wangenj23
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20110617
Time          10:59
INSTRUM      spect
PROBHD       5 mm BBO BB-1H
PULPROG      zgpg30
TD           65536
SFO1         400.13
D1           0.05000000
DE           6.400
AQ           0.03200000
RG           228.1
WDW          EM
SSB          0
GB           0
PC           1.00
===== CHANNEL f1 =====
NUC1          1H
P1            13.00 usec
PL1          -3.00 dB
SFO1         400.1324710 MHz
F2 - Processing parameters
SI           32768
SF           400.1300091 MHz
WDW          EM
SSB          0
GB           0
PC           1.00
  
```

Compound 3n



8.100
8.079
7.482
7.462
7.442
7.332
7.312
7.276
7.262
7.107
7.087

4.405
4.387

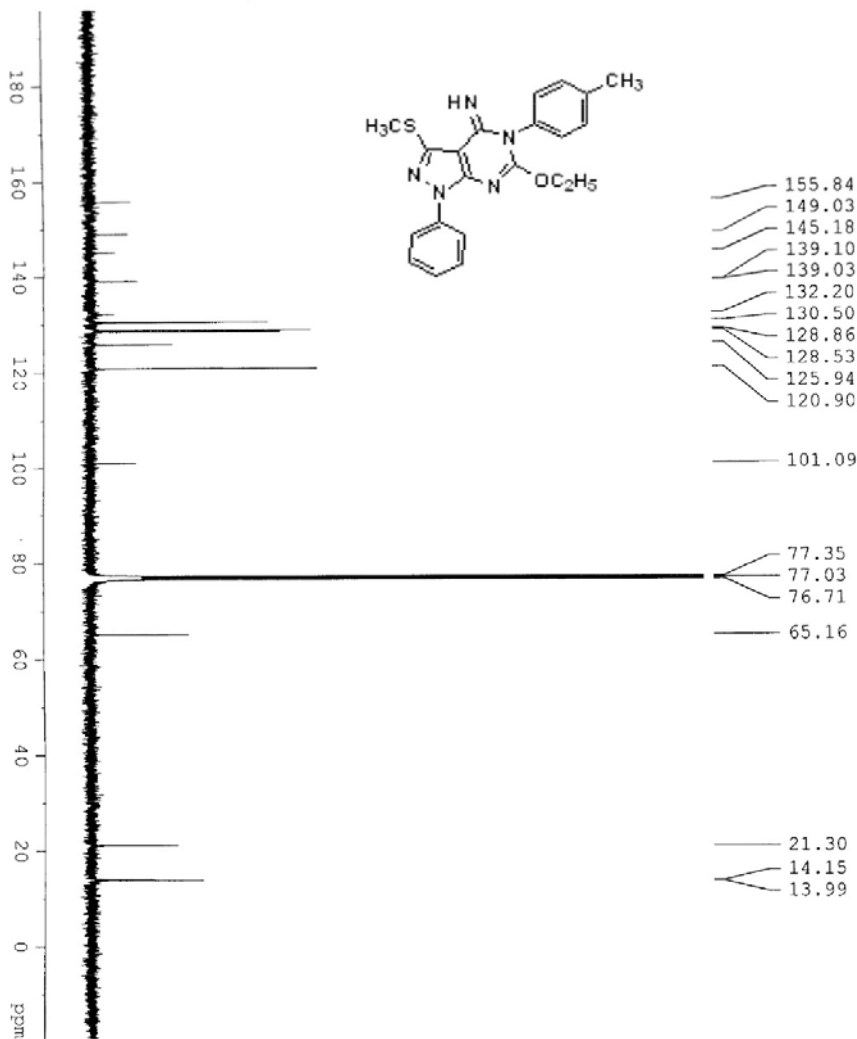
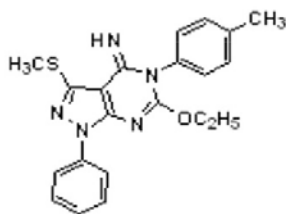
2.678
2.433

1.254
1.239
1.221

WMJ-6-8-1

Current Data Parameters
 NAME wangwenjun
 EXPNO 13
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110609
 Time_ 9.05
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 8279.146 Hz
 FIDRES 0.126214 Hz
 AQ 3.958429 sec
 RG 60.401
 DW 6.00 usec
 DE 295.2 K
 TE 1.0000000 sec
 DI 0.0000000 sec
 MCREST 0.0150000 sec
 MCWRR
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1329710 MHz
 F2 - Processing parameters
 SI 400.1300100 MHz
 SF 400.1300100 MHz
 EQ 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

WMJ-6-13-1



- 155.84
- 149.03
- 145.18
- 139.10
- 139.03
- 132.20
- 130.50
- 128.86
- 128.53
- 125.94
- 120.90
- 101.09
- 77.35
- 77.03
- 76.71
- 65.16
- 21.30
- 14.15
- 13.99

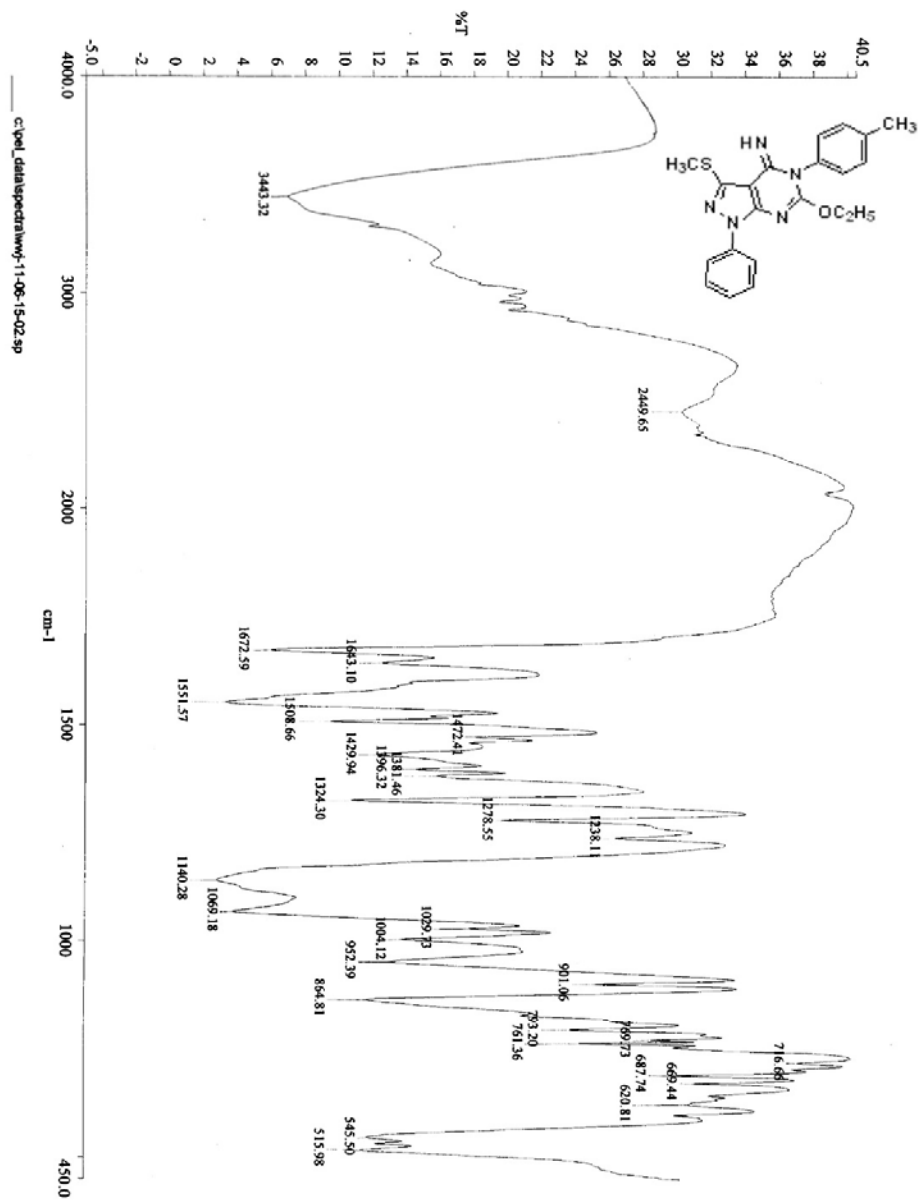
```

Current Data Parameters
Name: WMJ-6-13-1
Date_ Time: 20100615 15.13
INSTRUM: spect
PROBHD: 5 mm BBO Spect
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NUC1: 13C
NUC2: 13C
ORIG: F1
FIDRES: 2390.814 Hz
AQ: 0.064746 sec
RG: 8132
SM: 20.840 usec
DE: 2.00000000 sec
TE: 296.3 K
D1: 2.00000000 sec
d11: 0.05000000 sec
DELTA: 0.05000000 sec
KORRECT: 0.05000000 sec

===== CHANNEL F1 =====
NUC1: 13C
P1: 6.00 usec
PL1: -2.00 dB
SFO1: 100.628268 MHz

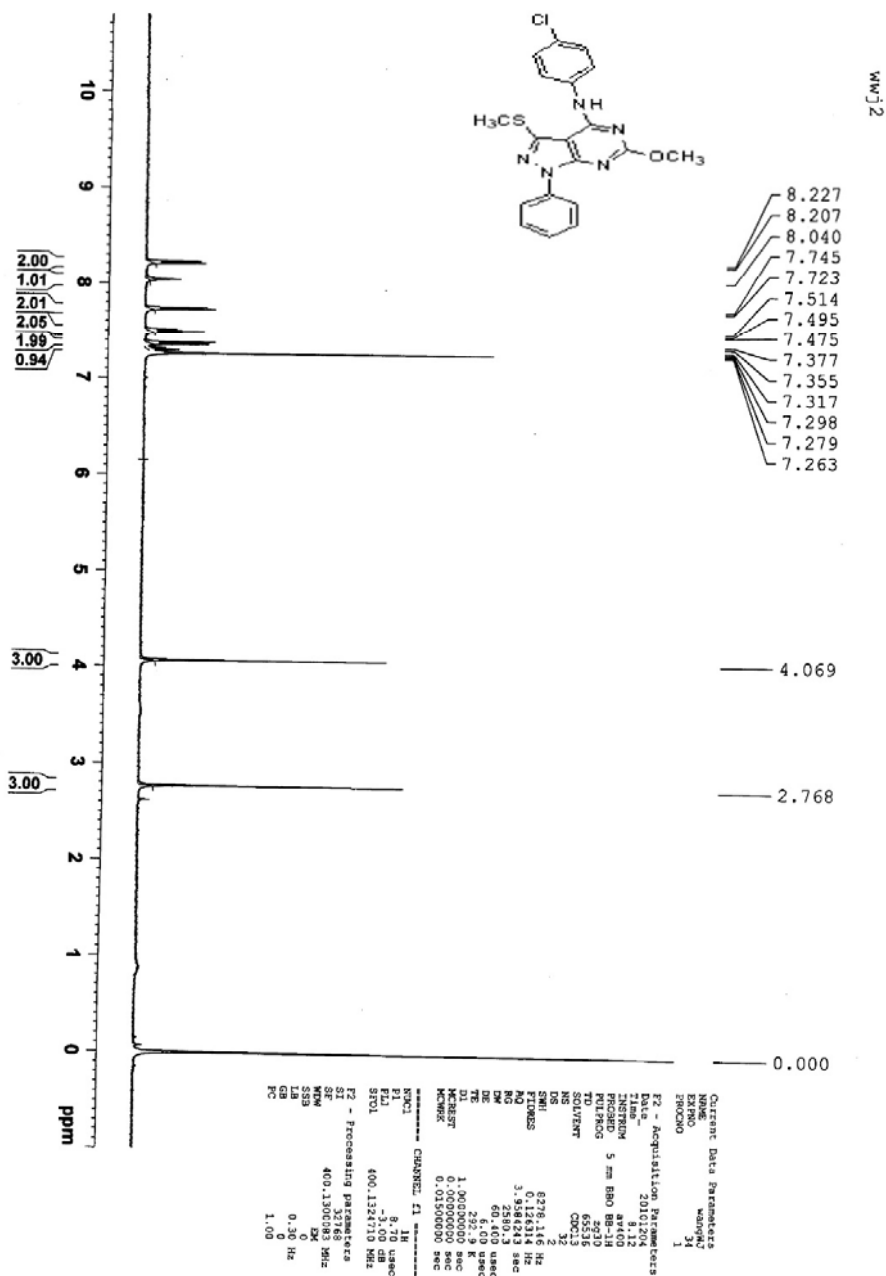
===== CHANNEL F2 =====
NAME: waltz16
NUC1: 13C
NUC2: 13C
PULSE2: 80.00 usec
PCPD2: 120.00 dB
PL2: 120.00 dB
PL12: 120.00 dB
PL13: 120.00 dB
SFO2: 400.131605 MHz

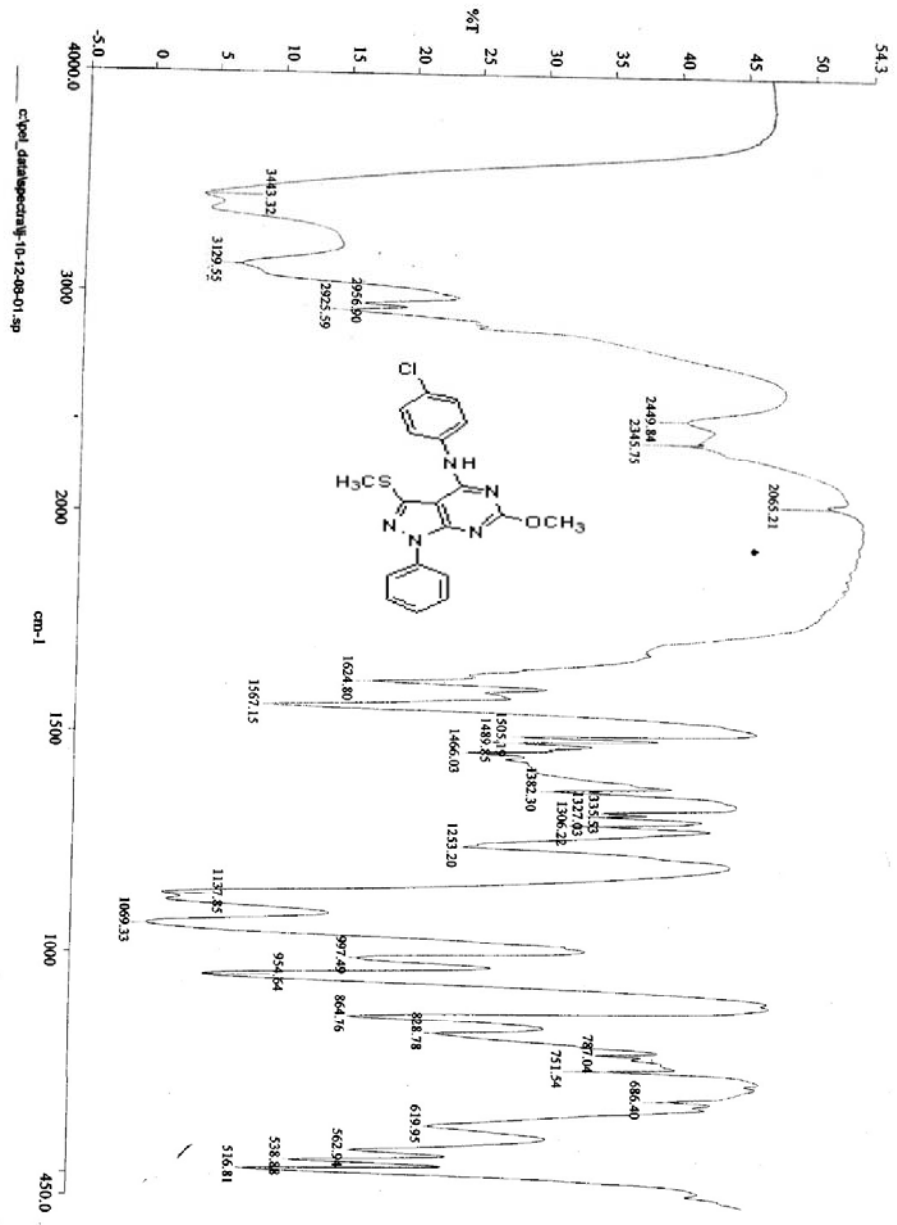
F1 - Processing parameters
SI: 32768
SF: 100.627690 MHz
KHZ: 5M
L2: 1.00 Hz
GB: 0
PC: 1.10
  
```



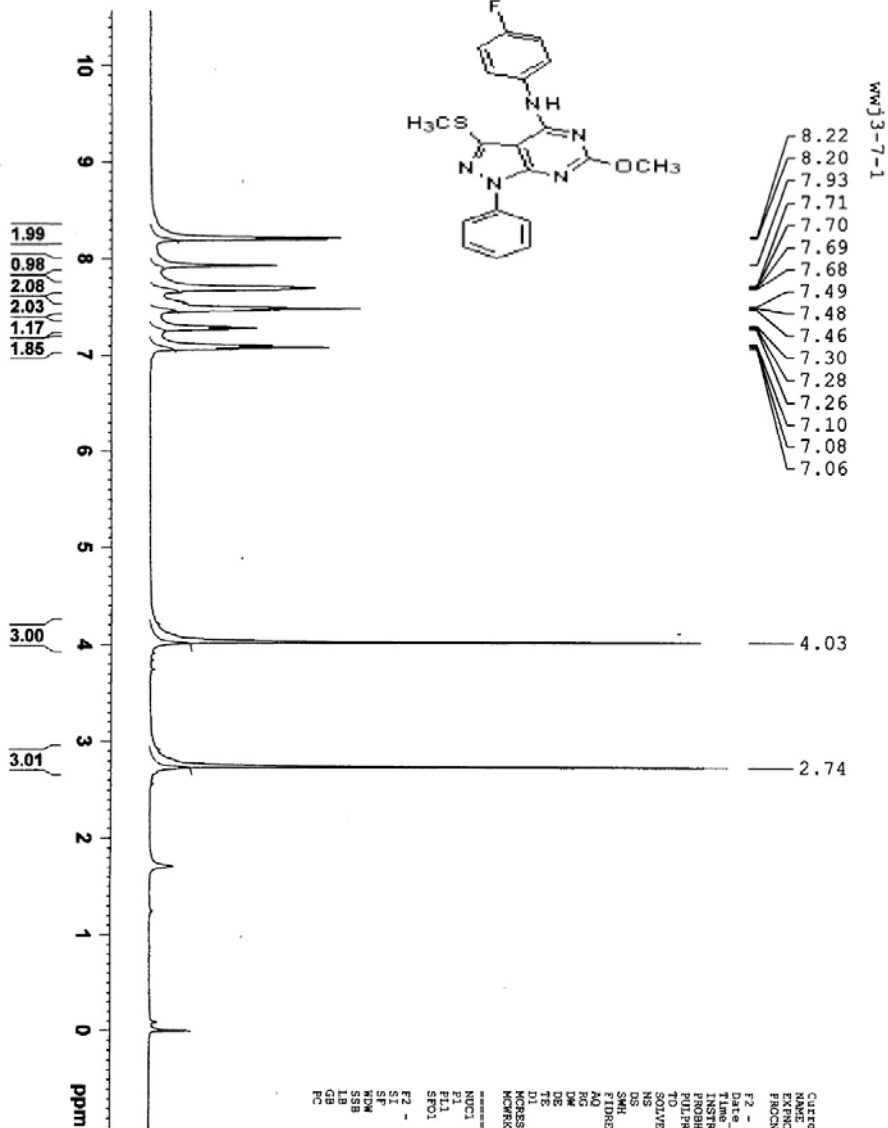
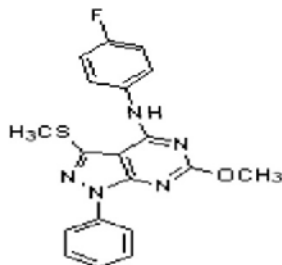
2. ¹H NMR, ¹³C NMR and IR Spectra of Compounds 4

Compound 4a





Compound 4b

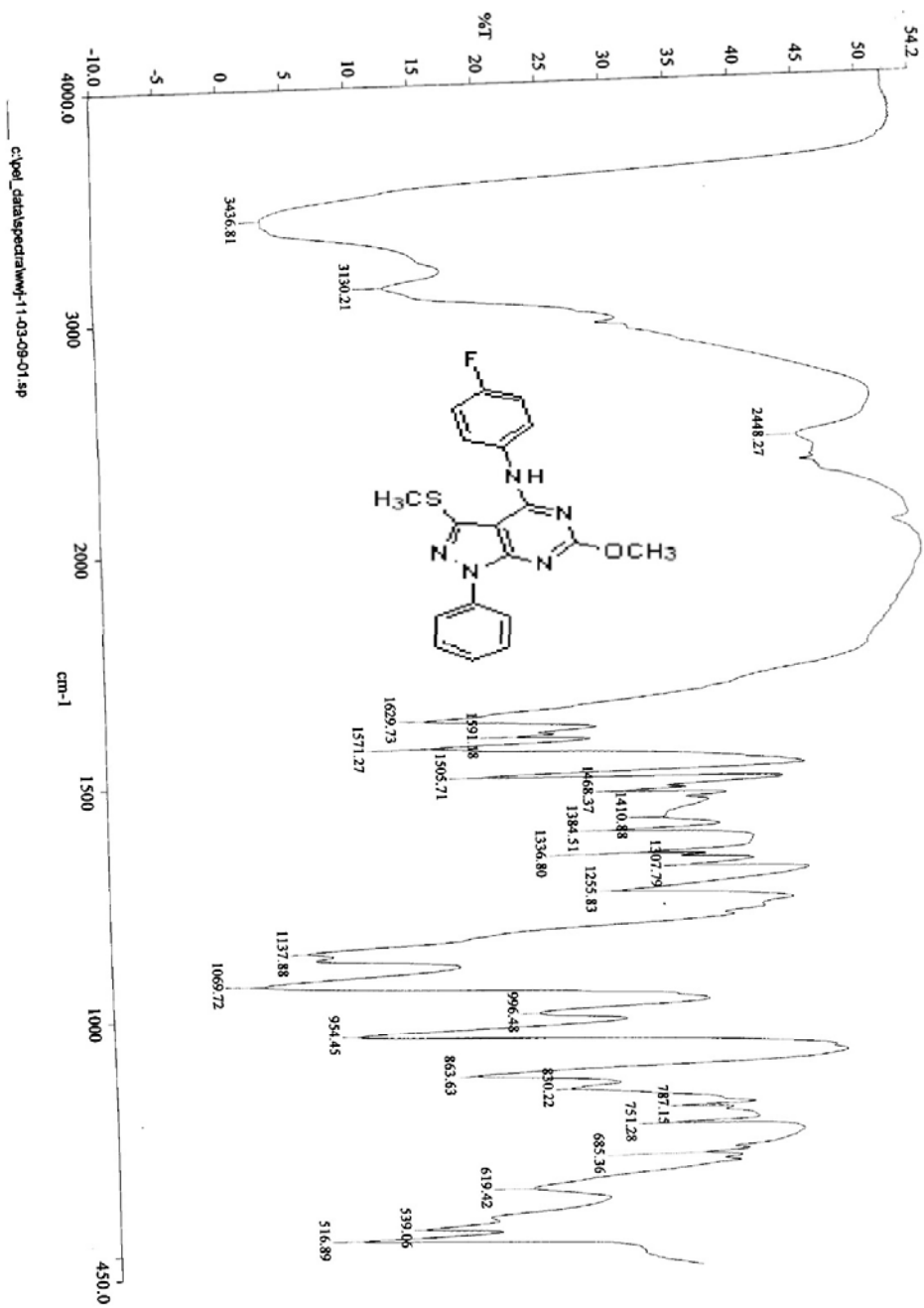


WJ3-7-1

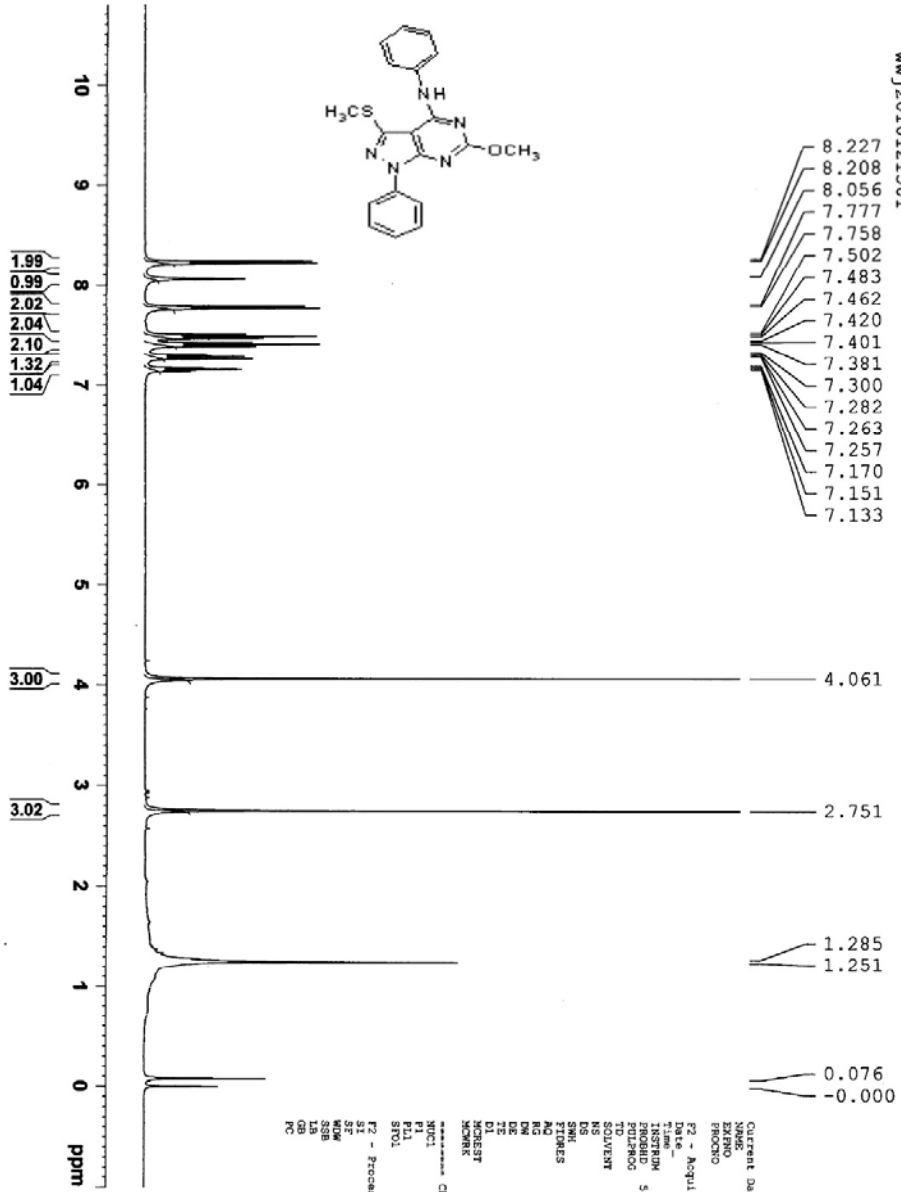
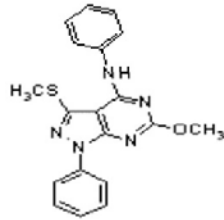
Current Data Parameters
 NAME: wanyu
 EXPNO: 58
 PROCNO: 1

F2 - Acquisition Parameters
 Date_ 20110311
 Time 7:54
 INSTRUM: spect
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 2
 DS: 4
 SWH: 8278.146 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.9584243 sec
 RG: 412
 RW: 60.412 usec
 DE: 6.00 usec
 TE: 291.5 K
 DI: 1.00000000 sec
 DCREST: 0.00000000 sec
 MCPRG1: 0.01300000 sec
 ***** CHANNEL f1 *****
 NUCL1: 1H
 P1: 9.10 usec
 PL1: -3.00 dB
 SFO1: 400.1324710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300100 MHz
 KW: 64
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00



Compound 4c



Wwj2010121301

8.227
8.208
8.056
7.777
7.758
7.502
7.483
7.462
7.420
7.401
7.381
7.300
7.282
7.263
7.257
7.170
7.151
7.133

4.061

2.751

1.285

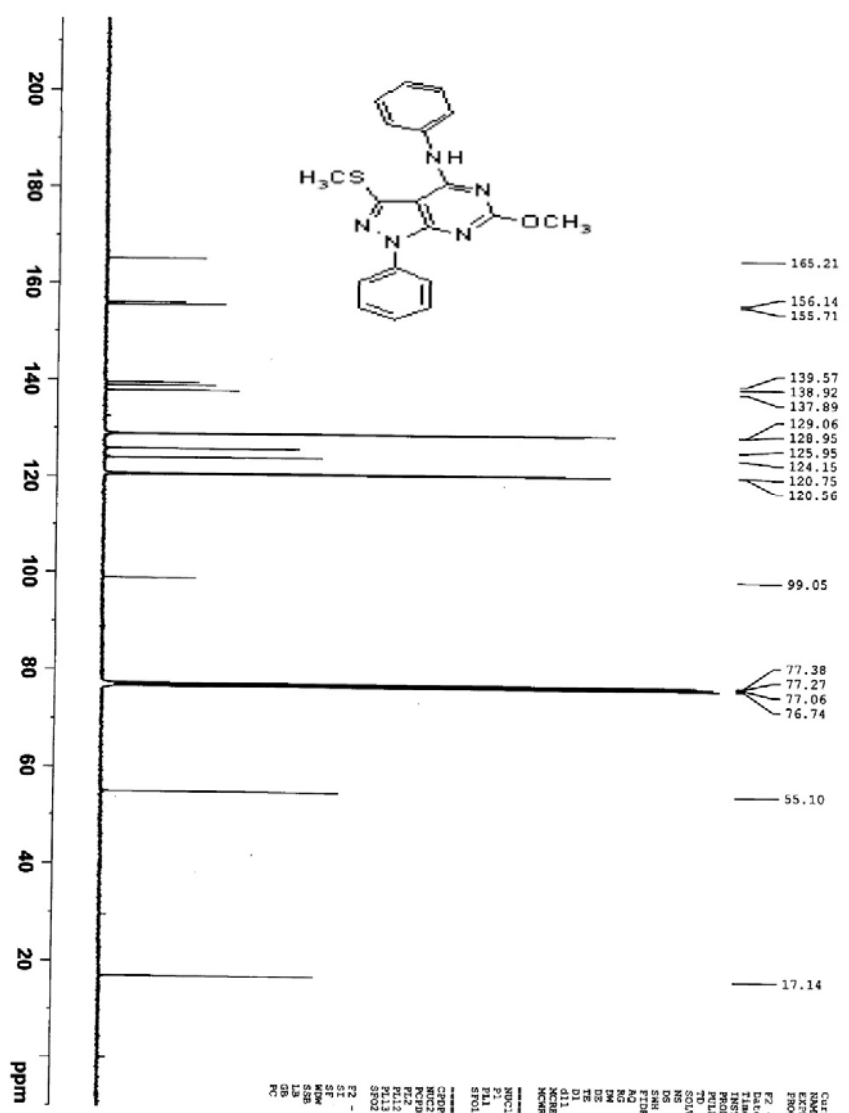
1.251

0.076

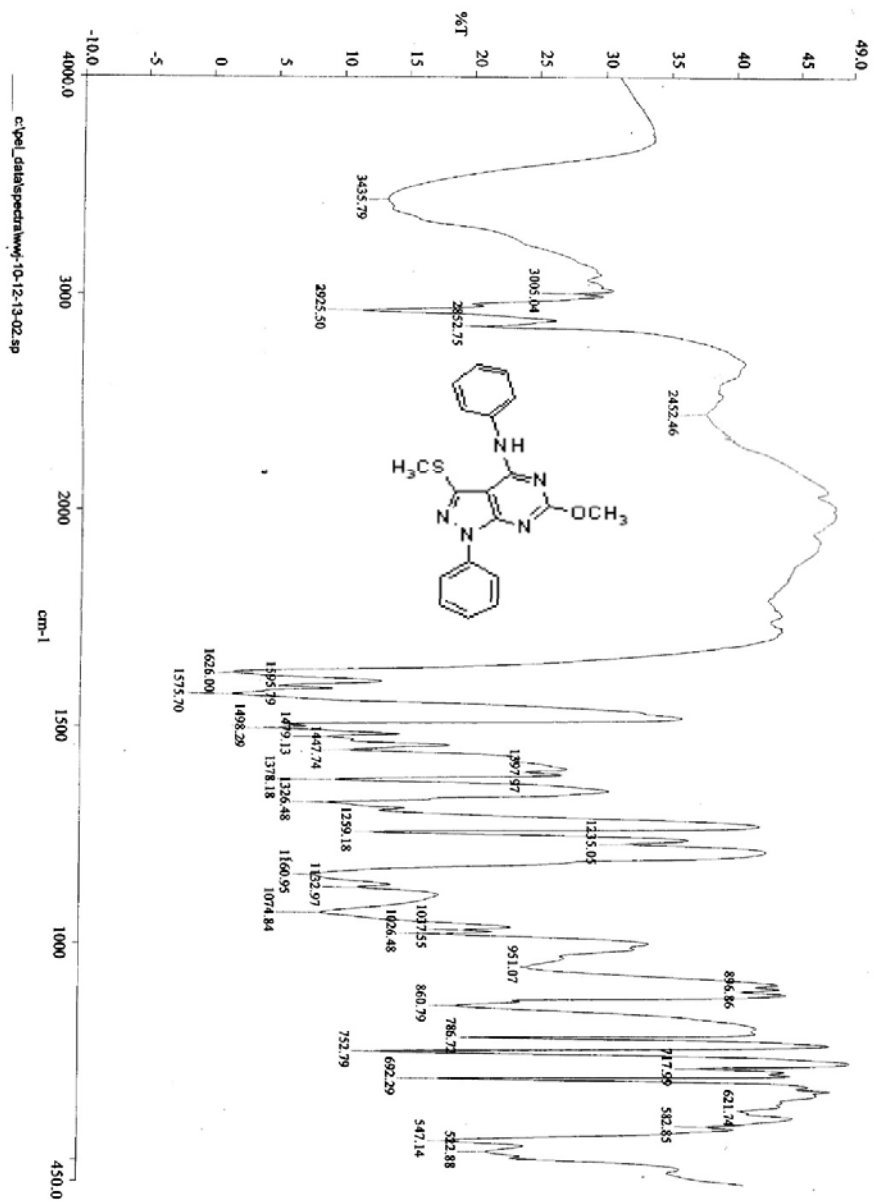
-0.000

Current Data Parameters
Date_ 20101213
Time_ 14:50
INSTRUM 5 mm BBO BB31
PROBHD 513
TD 6536
SOLVENT CDCl3
NS 32
DS 8
SWH 8778.145 Hz
FIDRES 0.126314 Hz
AQ 1.398423 sec
RG 655
DM 50.400 usec
DE 5.00 usec
DI 1.0000000 sec
DC 0.0000000 sec
MCNMR 0.01500000 sec
----- CHANNEL f1 -----
NUC1 13C
P1 1R
PI 9.70 usec
PL 0.00 dB
SFO1 400.1326710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300111 MHz
WDW EM
SSB 0
GB 0
PC 1.00

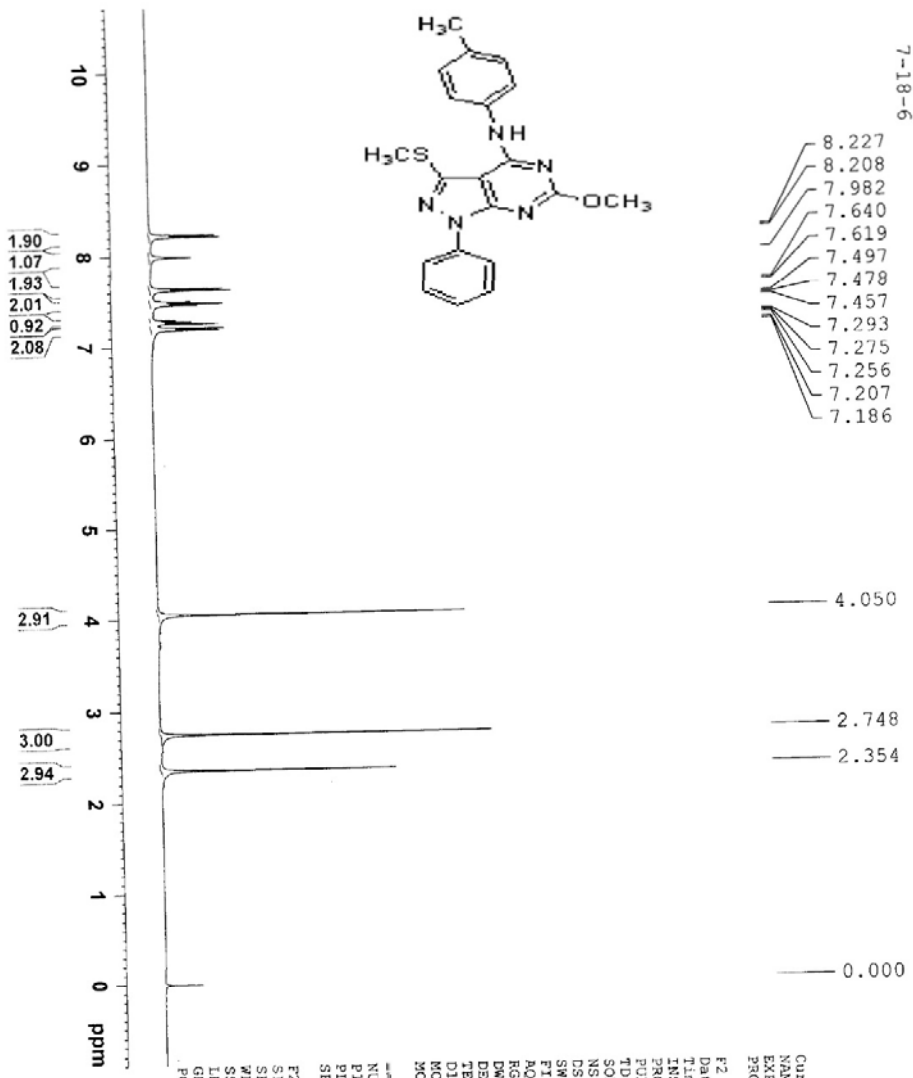
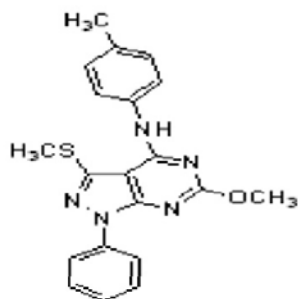
mwj



Current Data Parameters
 NAME: 20101219
 EXNO: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20101219
 Time: 11:17
 INSTRUM: spect
 PROBRD: 5 mm BBO BB-1H
 PULPROG: zgpg30
 FIDRES: 0.0001000
 SOLVENT: CDCl3
 NS: 2048
 DS: 4
 SWH: 23980.314 Hz
 FIDRES: 0.365918 Hz
 AQ: 1.3644176 sec
 RG: 327.500
 DW: 20.450 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 2.00000000 sec
 d11: 0.03000000 sec
 ACQRES: 0.00000000 sec
 NSCAN: 0.01900000 sec
 ===== CHANNEL F1 =====
 P1: 12.00 usec
 PL1: -2.00 dB
 SFO1: 100.6282589 MHz
 ===== CHANNEL F2 =====
 CPDPRG2: waltz16
 VPP2: 1.00 usec
 PCPD2: 80.00 usec
 FZ2: -3.00 dB
 PL2: 14.00 dB
 PL12: 14.00 dB
 SFO2: 400.1316905 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 100.617762 MHz
 DS: 4
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.00



Compound 4d



7-18-6

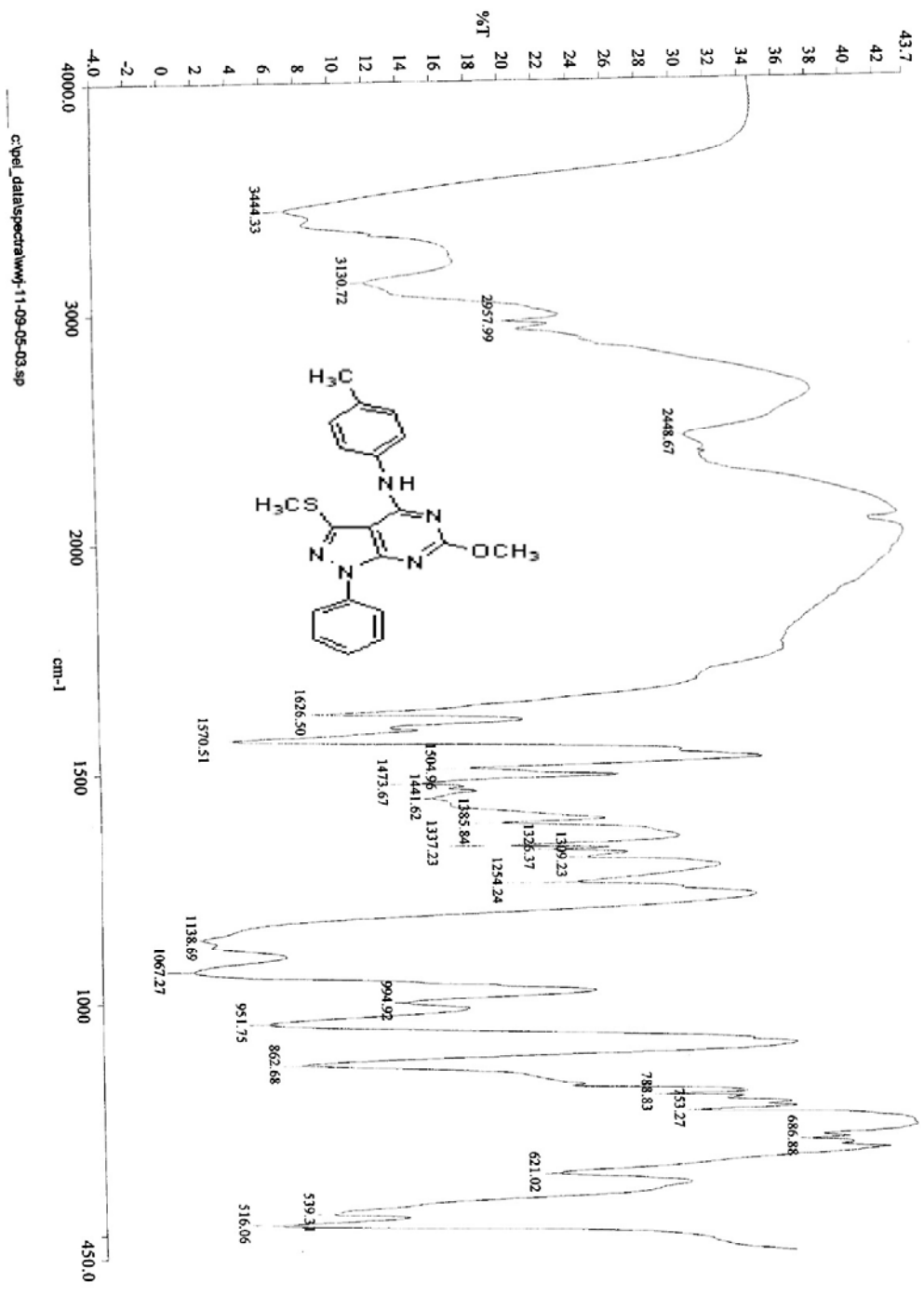
Current Data Parameters
 NAME wangwenjuan
 EXPNO 53
 PROCNO 1

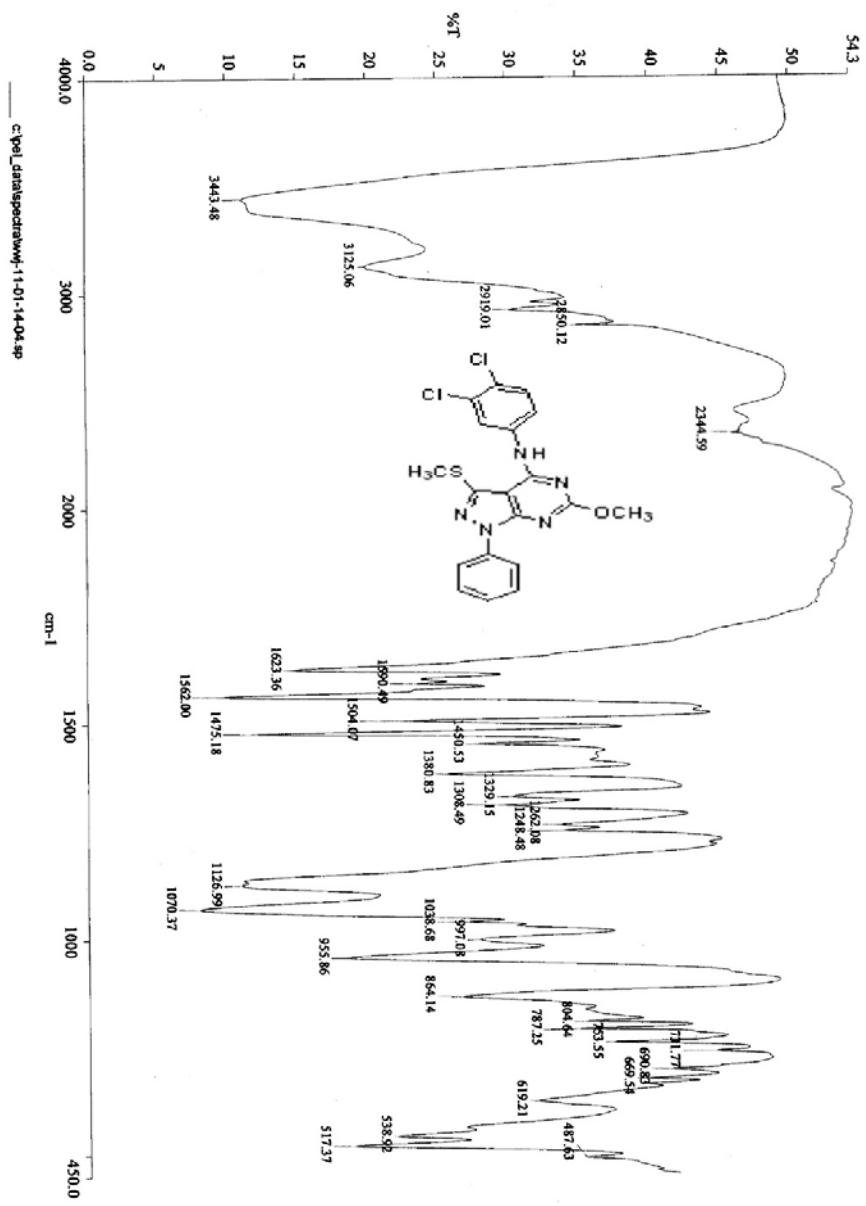
F2 - Acquisition Parameters

Date_ 20110718
 Time 14.53
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 362
 DE 60.400 usec
 DM 6.00 usec
 TE 299.0 K
 DI 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

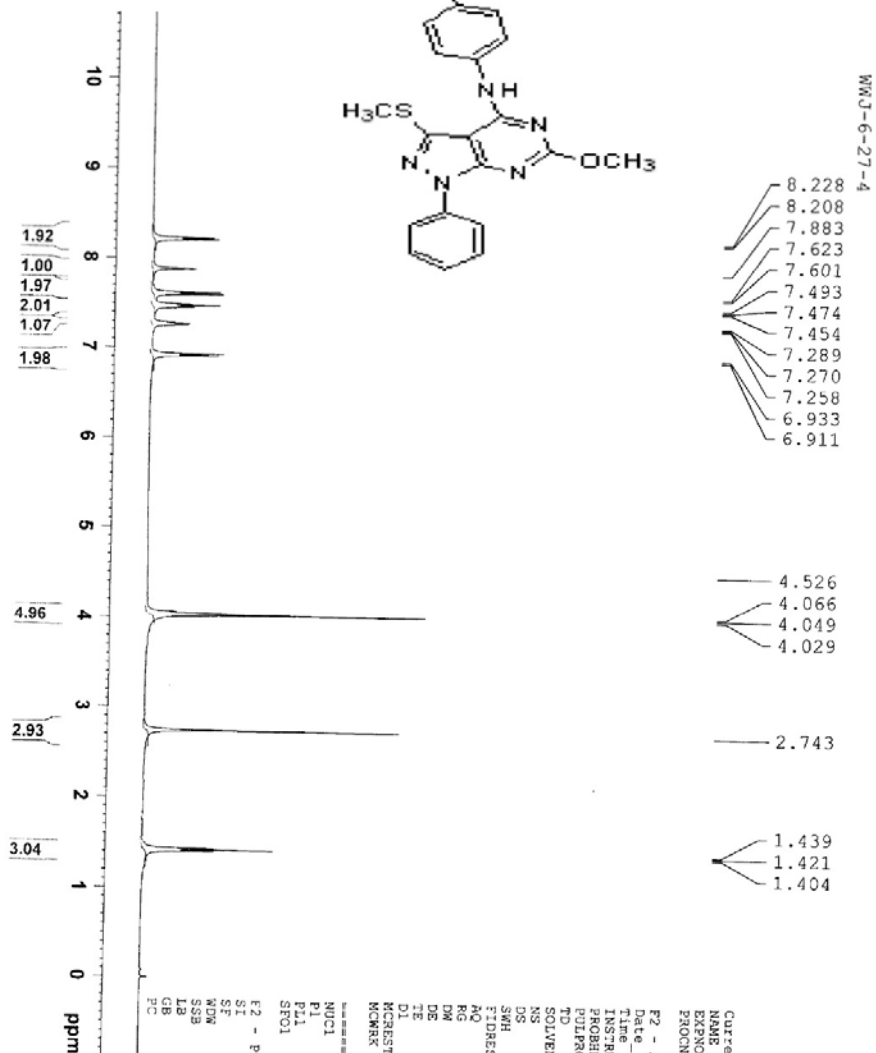
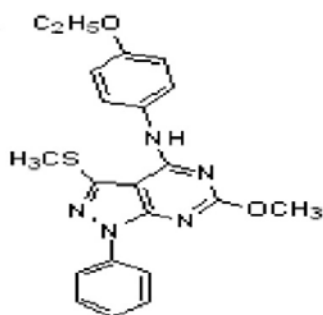
===== CHANNEL f1 =====
 NUCL 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300105 MHz
 WDM FM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Compound 4f



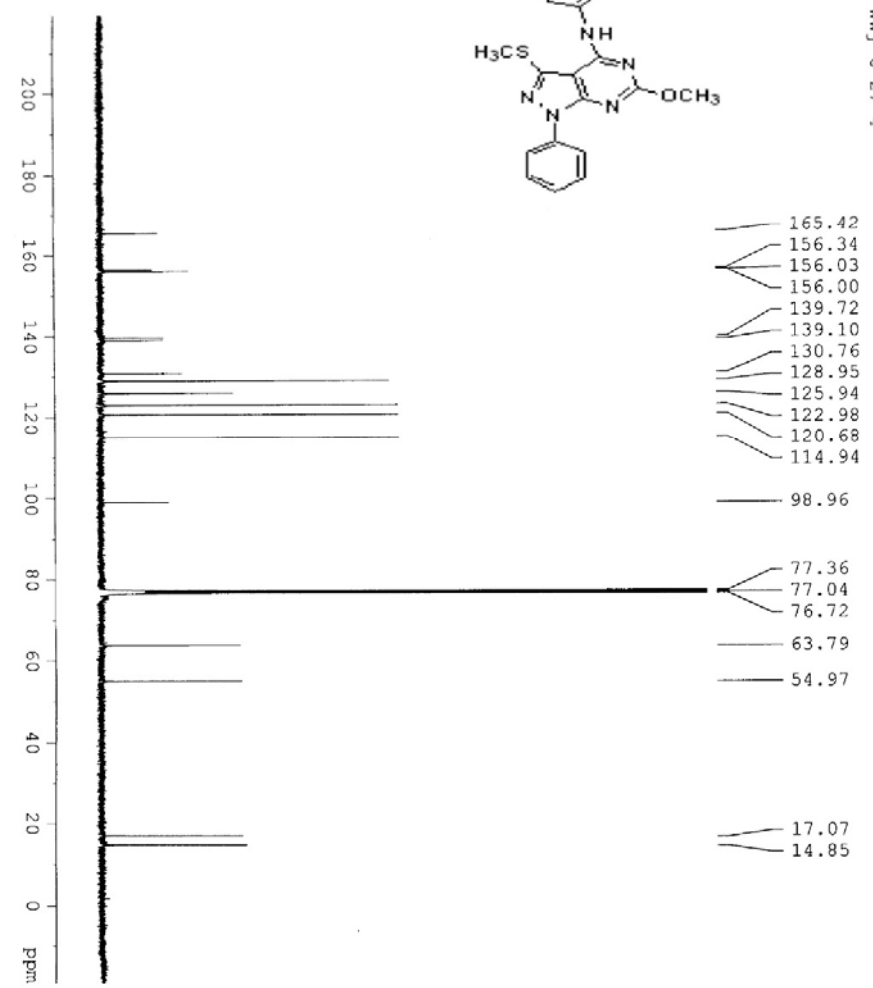
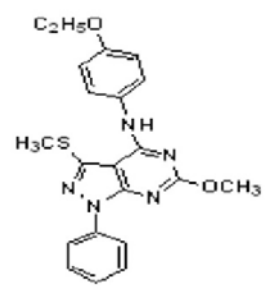
Current Data Parameters
 NAME wangwenjuan
 EXPNO 42
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110628
 Time 15.22
 PROGRAM spect
 PROBRW 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SFO1 400.1324710 MHz
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 8279.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 362
 DE 60.400 usec
 TE 295.1 K
 ACQST 1.00000000 sec
 PCASST 0.00000000 sec
 MCHST 0.01500000 sec

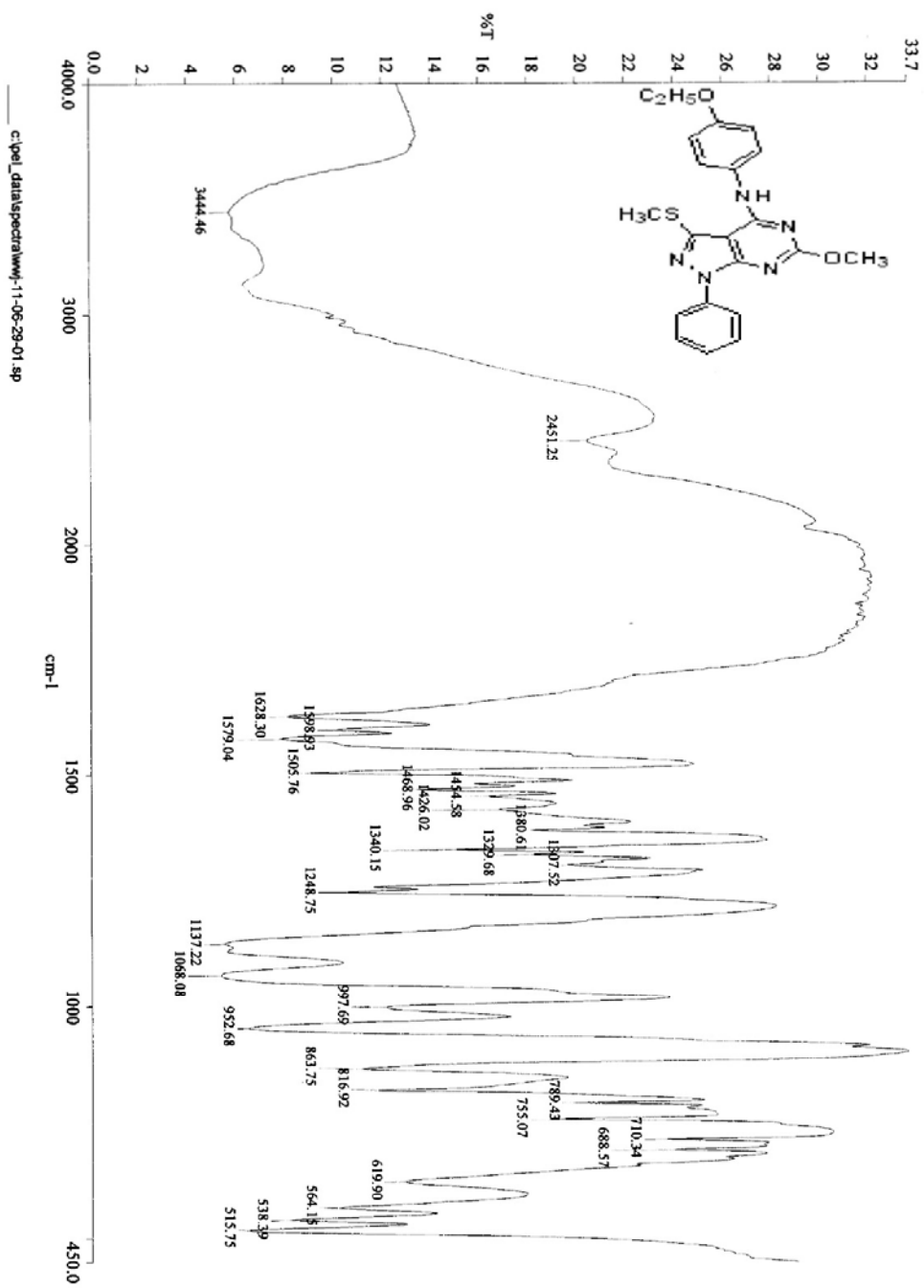
===== CHANNEL f1 =====
 NUCL1 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130096 MHz
 KCM EM
 SSB C
 DB 0
 PC 1.00

WJ-6-27-4

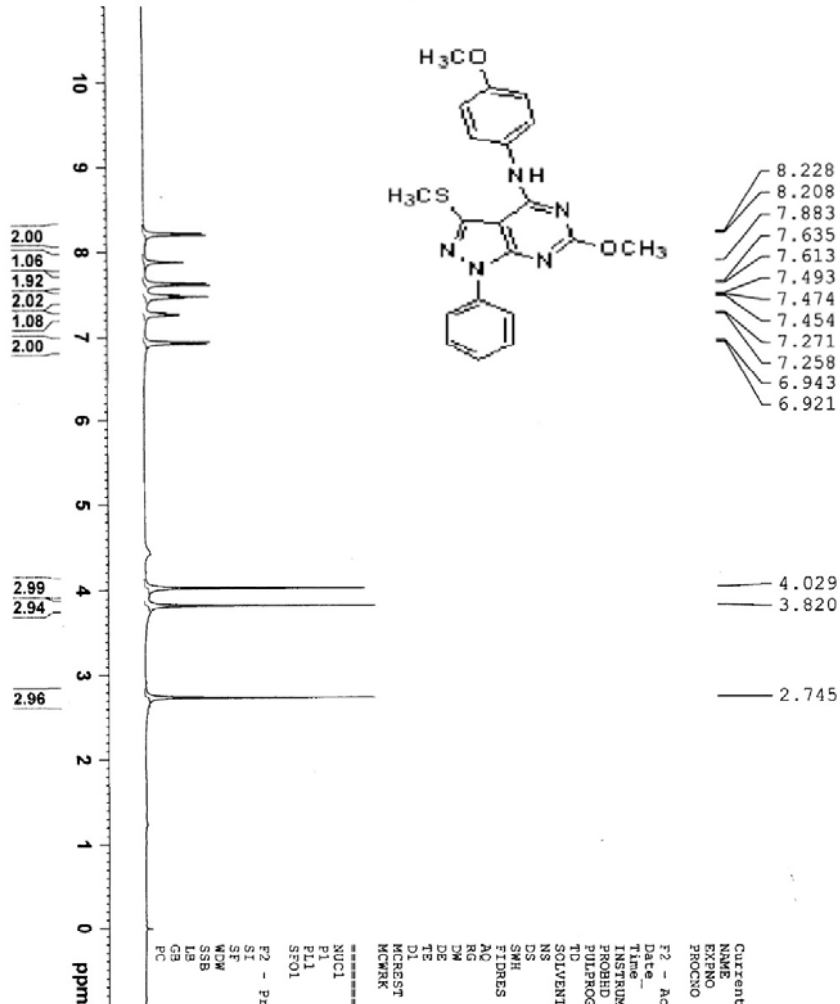
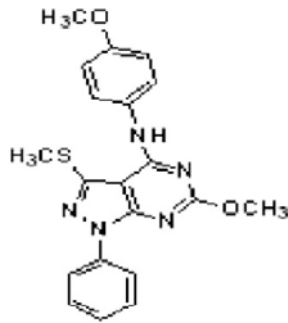


Current Data Parameters
 NAME: samengujian
 SAMPLE: 43
 PROBNM: 43
 P2 - Acquisition Parameters
 Date_: 2012-07-27
 Time: 20.33
 INSTRUM: spect
 PROBHD: 5 mm BBO BB-1H
 PULPROG: zgpg30
 TD: 65536
 SFO: 400.131603
 SOLVENT: CDCl3
 NS: 228
 DS: 4
 SWH: 23980.814 Hz
 FIDRES: 0.365918 Hz
 AQ: 1.208425 sec
 RG: 327.5
 SW: 20.850 usec
 SF: 30.0 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 2.00000000 sec
 d11: 0.03000000 sec
 d12: 0.03000000 sec
 d13: 0.03000000 sec
 ACQMSK: 0.01500000 sec
 N1: 1.00000000 sec
 N2: 1.00000000 sec
 N3: 1.00000000 sec
 ===== CHANNEL f1 =====
 NU1: 1
 F1: 6.30 usec
 FL1: -2.00 dB
 SFO1: 100.6258298 MHz
 ===== CHANNEL f2 =====
 C1PRPG2: waltz16
 NU2: 2
 F2: 6.30 usec
 FL2: 120.00 dB
 FL3: 12.00 dB
 FL4: 12.00 dB
 SFO2: 400.131603 MHz
 P1 - Processing parameters
 SI: 32768
 SF: 100.6171890 MHz
 KM: 32
 LB: 1.00 Hz
 GB: 0
 PC: 1.40



Compound 4g

WUJ-6-27-5



Current Data Parameters
 NAME wangwenjuan
 EXPNO 43
 PROCNO 1

F2 - Acquisition Parameters

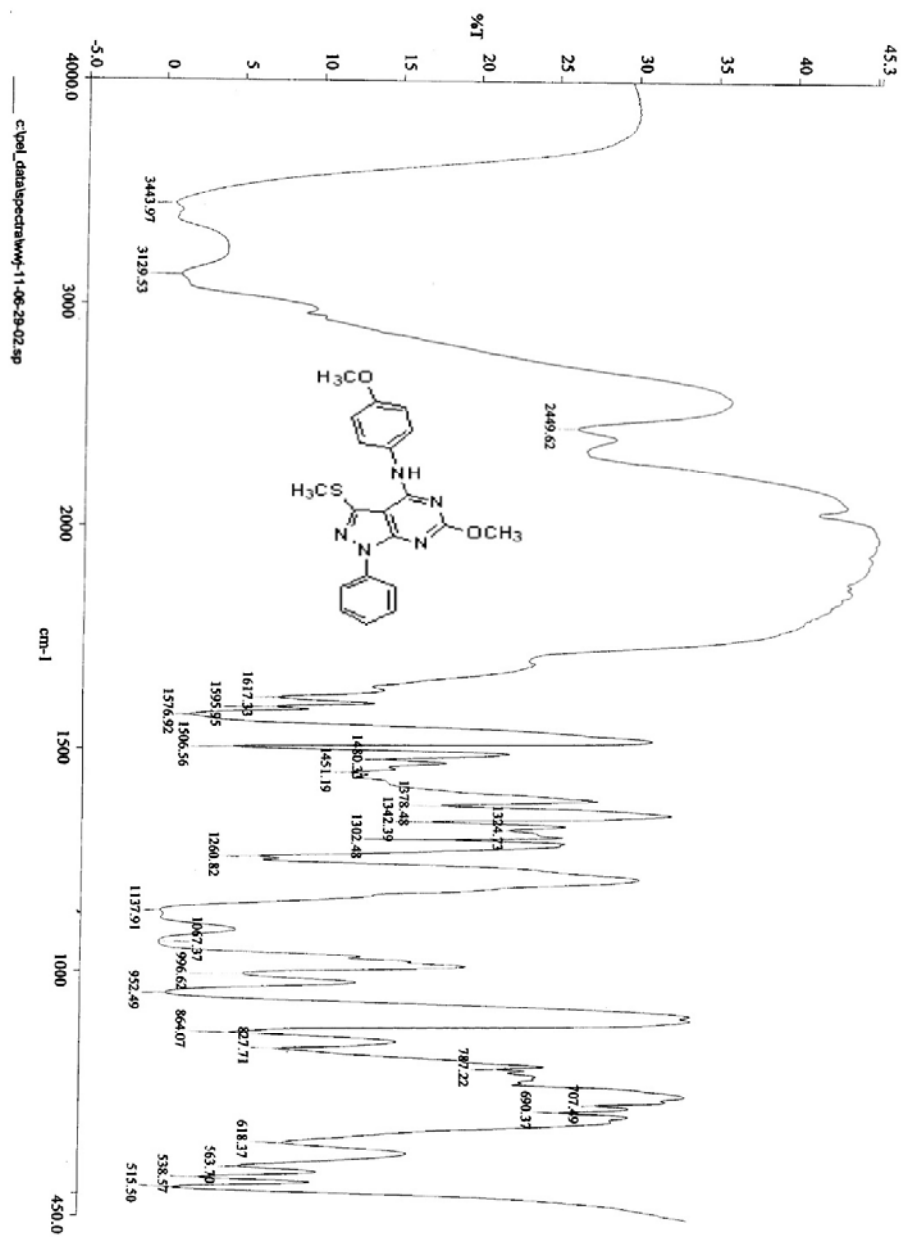
Date 20110628
 Time 15:28
 INSTRUM spect
 PULPROG zgpg30
 FREQH0 5 mm SBO B1-41
 FIDRES 65336
 TD 65336
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 362
 DM 60.400 usec
 DE 6.00 usec
 TE 299.1 K
 DI 1.0000000 sec
 SFO1 400.1324710 MHz
 HCNM 0.0150000 sec

CHANNEL f1

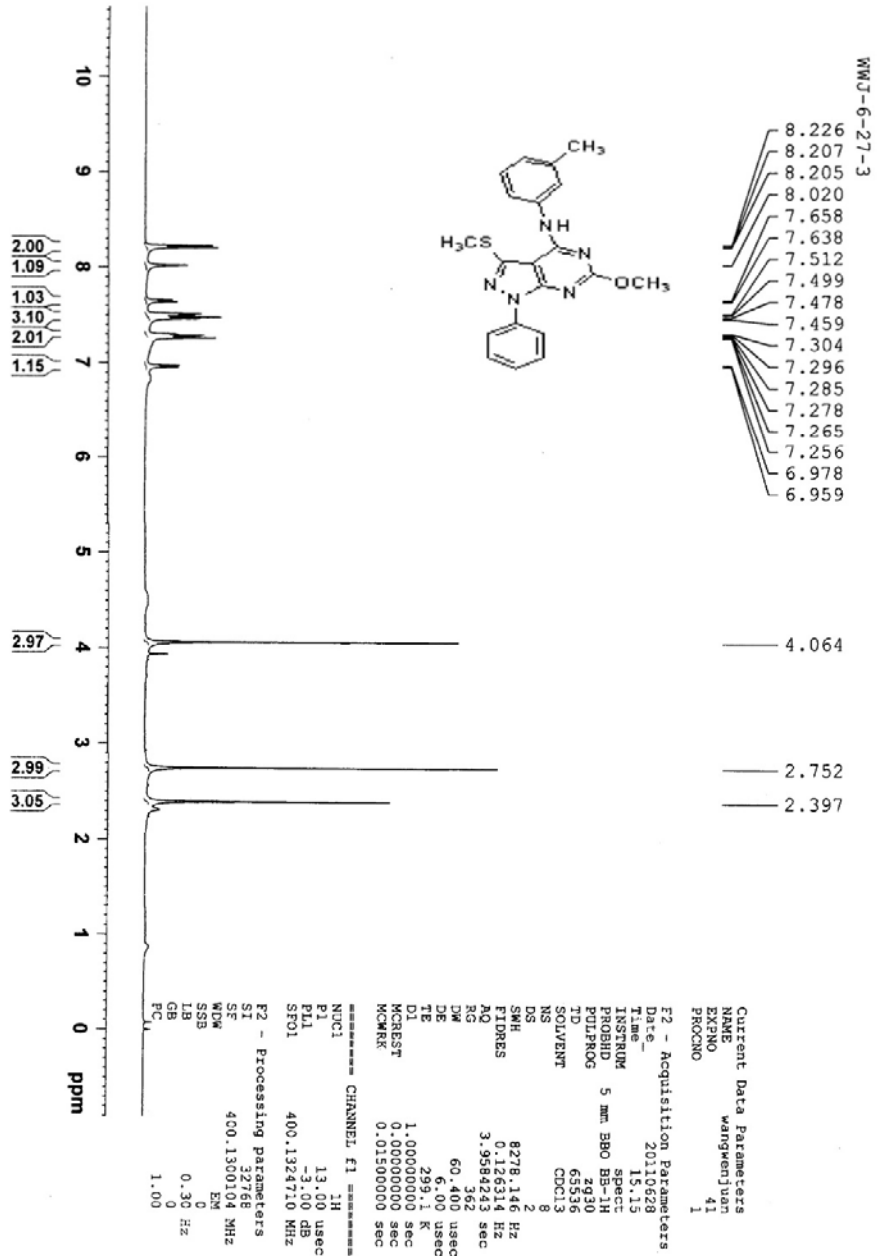
NUC1 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

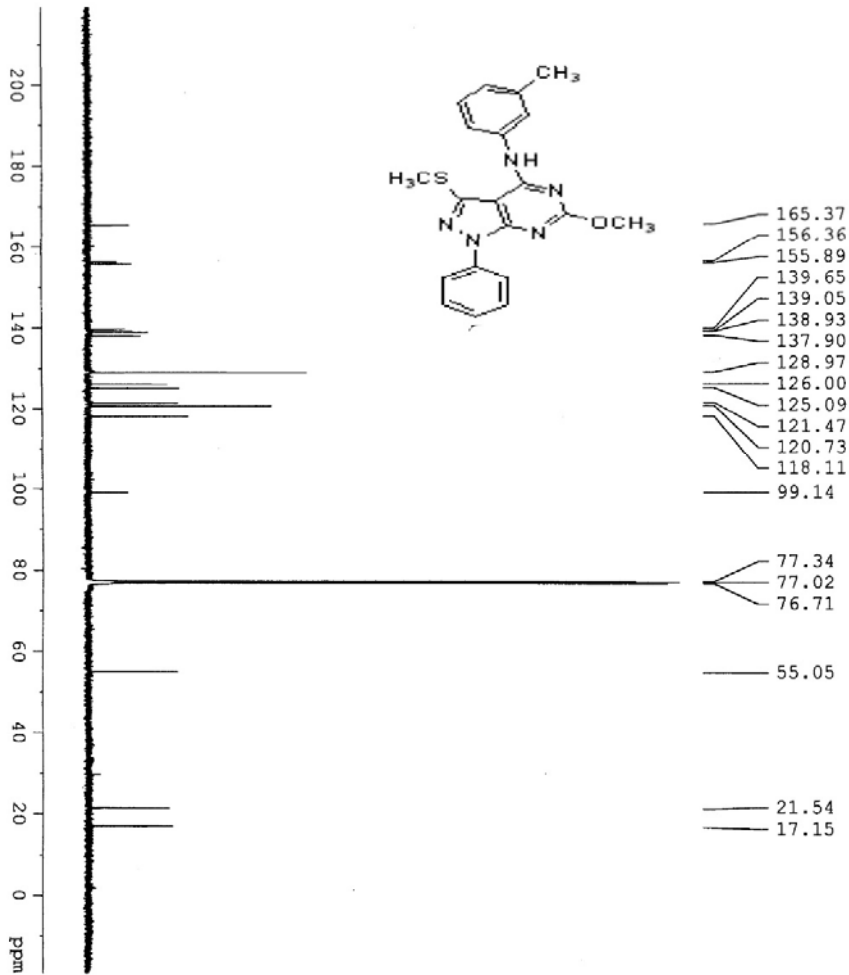
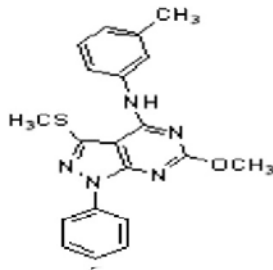
F2 - Processing parameters

SI 32768
 SF 400.130098 MHz
 WDW RM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



Compound 4h





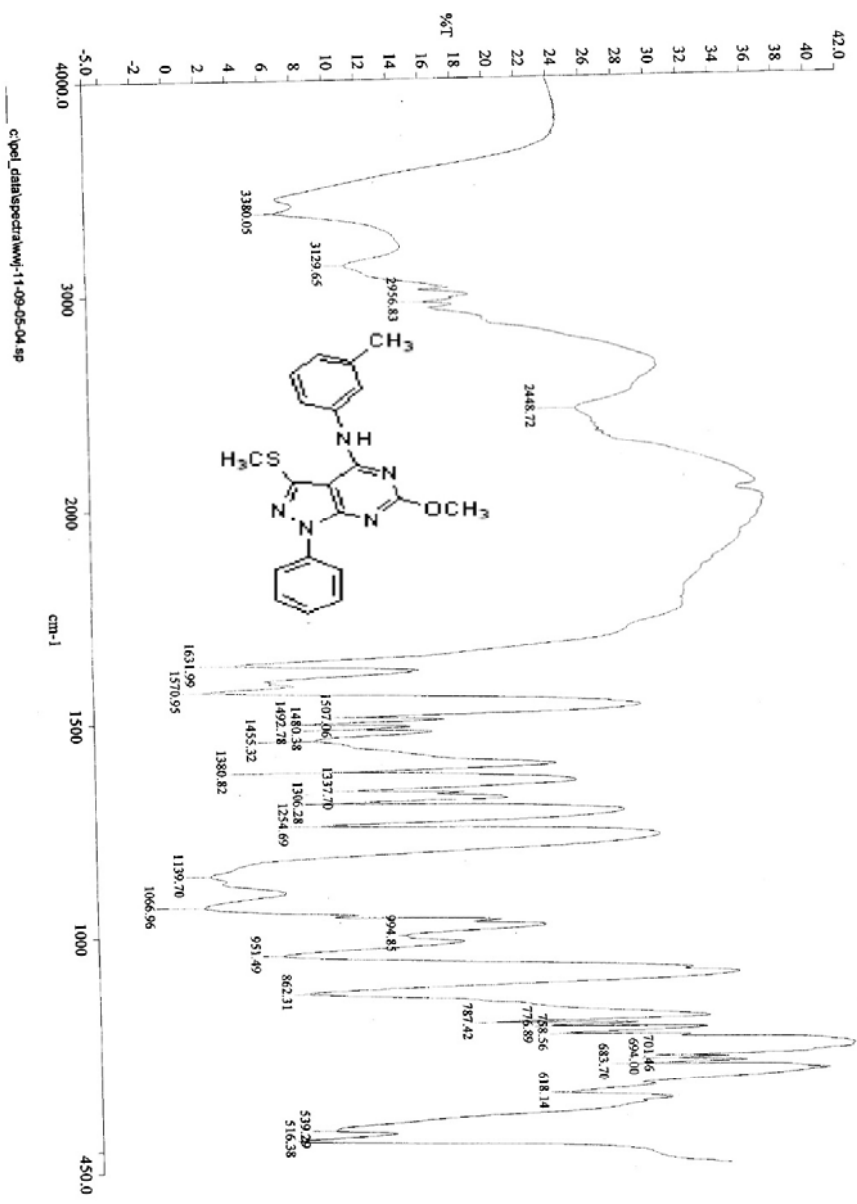
- 165.37
- 156.36
- 155.89
- 139.65
- 139.05
- 138.93
- 137.90
- 128.97
- 126.00
- 125.09
- 121.47
- 120.73
- 118.11
- 99.14
- 77.34
- 77.02
- 76.71
- 55.05
- 21.54
- 17.15

Current Data Parameters
 EXPNO 4
 F2 - Acquisition Parameters
 Date_ 20110701
 Time 23.06
 INSTRUM 5 mm BBO Spect
 PULPROG zgpg30
 TD 65536
 SFO2 400.1316005 MHz
 SOLVENT CDCl3
 NS 1024
 DS 4
 SM 33981.814 Hz
 AQ 1.566715 sec
 RG 120642.5
 DM 29.650 usec
 DE 1.00000000
 TE 301.3 K sec
 D1 2.00000000 sec
 D11 0.20000000 sec
 MCHEST 0.01500000 sec
 MCHMR 0.01500000 sec

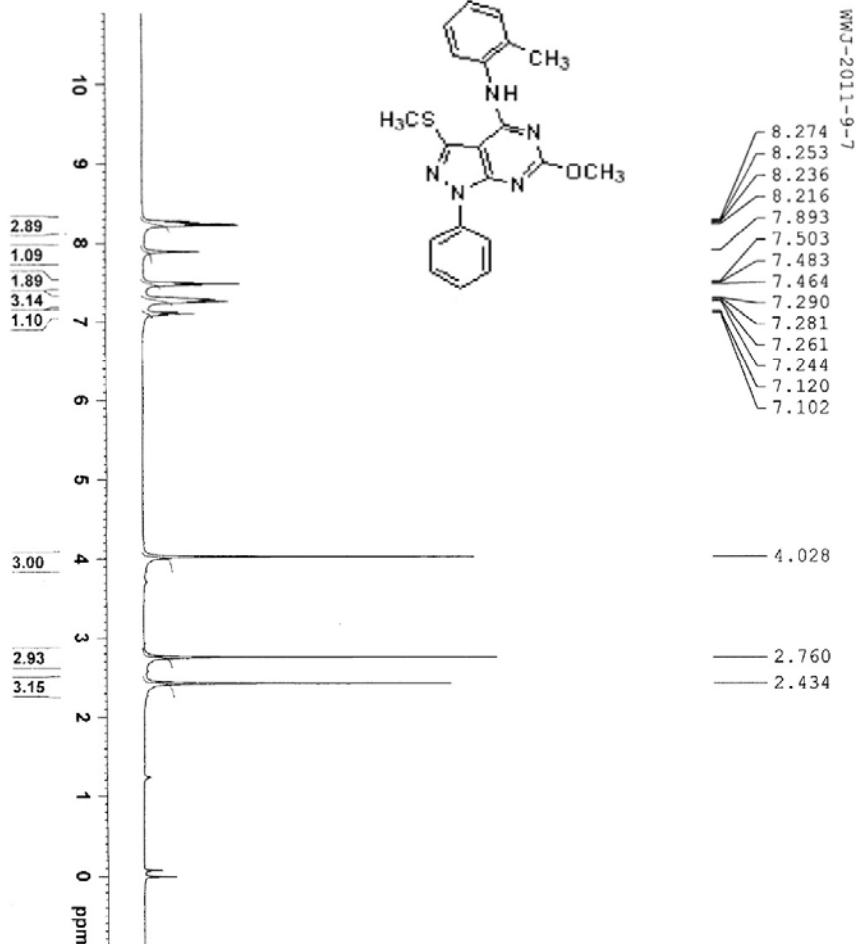
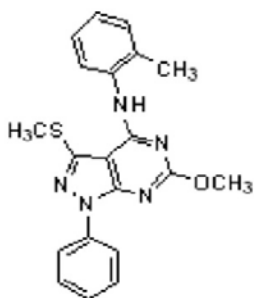
----- CHANNEL f1 -----
 NU01 13C
 P1 6.00 usec
 PL 0.00 dB
 SFO1 100.626250 MHz

----- CHANNEL f2 -----
 nu02 1H
 PCP02 180.00 usec
 P12 120.00 dB
 P13 12.00 dB
 P14 12.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6121650 MHz
 N 65536
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



Compound 4i



MMJ-2011-9-7

- 8.274
- 8.253
- 8.236
- 8.216
- 7.893
- 7.503
- 7.483
- 7.464
- 7.290
- 7.281
- 7.261
- 7.244
- 7.120
- 7.102

4.028

2.760

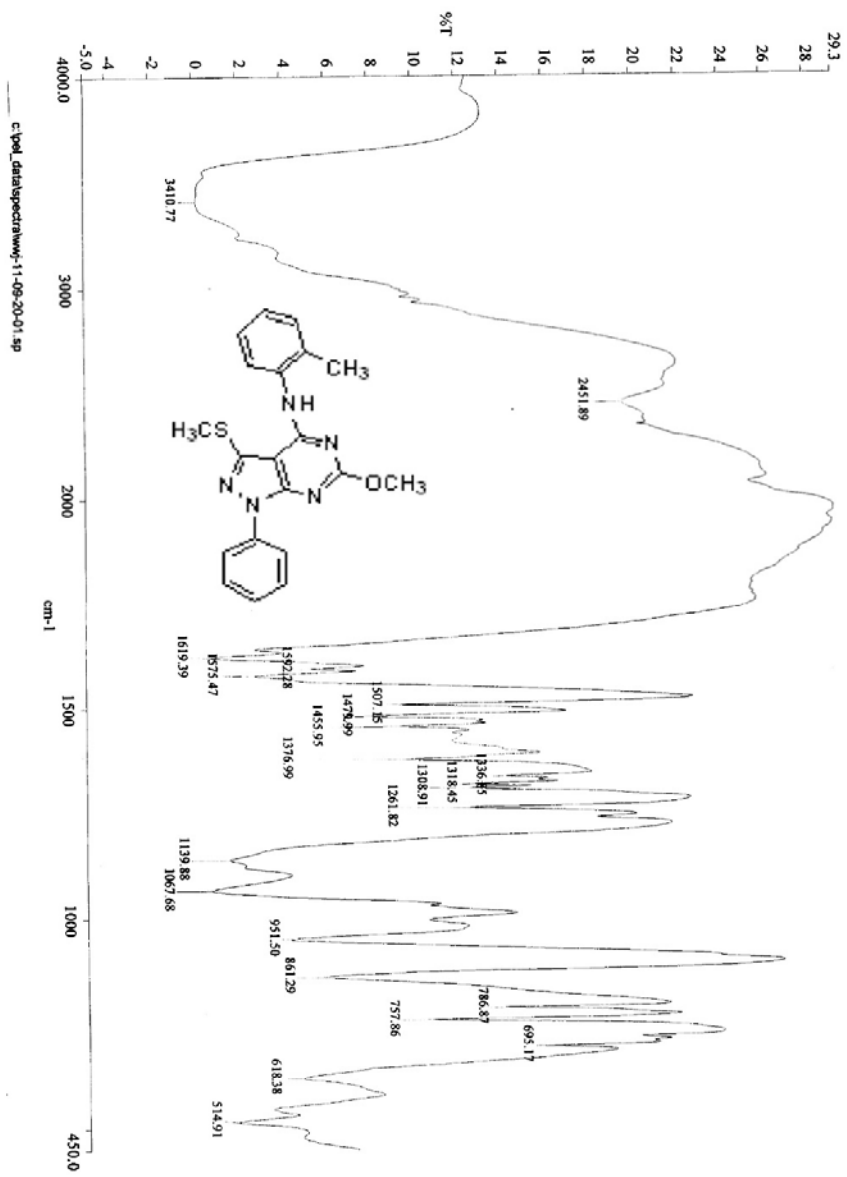
2.434

Current Data Parameters
 NAME wangpenjun
 EXPNO 3
 PROCNO 1

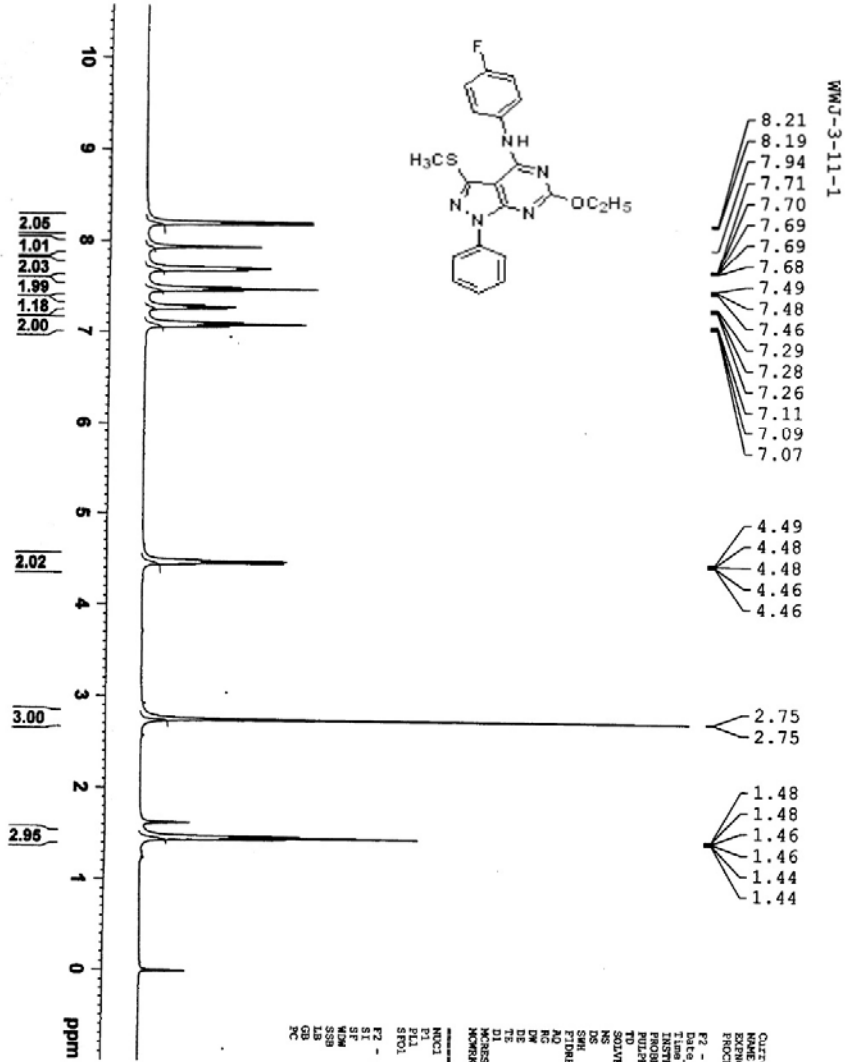
F2 - Acquisition Parameters
 Date_ 20110907
 Time 15.06
 INSTRUM spect
 PROBD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.12634 Hz
 AQ 3.9586243 sec
 RG 35.9
 DW 60.400 usec
 DE 6.00 usec
 TE 297.1 K
 D1 1.00000000 sec
 MCRES1 0.00000000 sec
 KCMR1 0.01500000 sec

***** CHANNEL f1 *****
 NUCL 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300115 MHz
 WDM 2
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

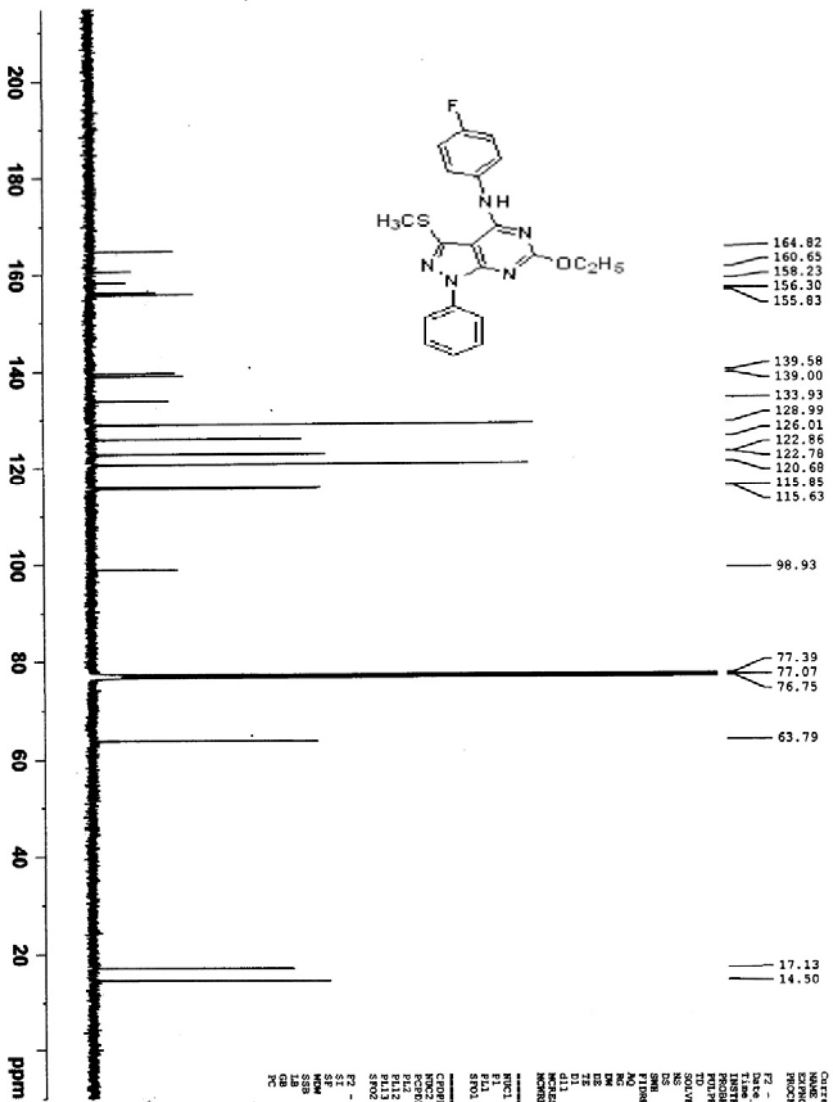
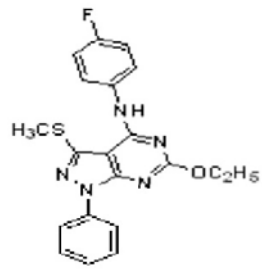


Compound 4j



Current Data Parameters
 Name: WWD-3-11-1
 ExpNO: 1
 F2 - Acquisition Parameters
 Date_ 20110314
 Time: 14.36
 INSTRUM: spect
 PULPROG: zgpg30
 TO: 65536
 SOLVENT: CDCl3
 DS: 16
 SWH: 8278.146 Hz
 FIDRES: 0.126314 Hz
 AQ: 3.994243 sec
 RG: 60.400 usec
 DE: 6.00 usec
 TE: 292.2 K
 D1: 1.00000000 sec
 MANSST: 0.00000000 sec
 AQC: 0.01500000 sec
 CHANNEL: f1
 NUC1: 1H
 P1: 8.00 usec
 F1: 3.00 dB
 SFO1: 400.126410 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 400.130050 MHz
 WIDW: 0
 SSB: 0.30 Hz
 GB: 0
 PC: 1.40

wvj20110316



164.82
160.65
158.23
156.30
155.83
139.58
139.00
133.93
128.99
126.01
122.86
122.78
120.68
115.85
115.63
98.93
77.39
77.07
76.75
63.79
17.13
14.50

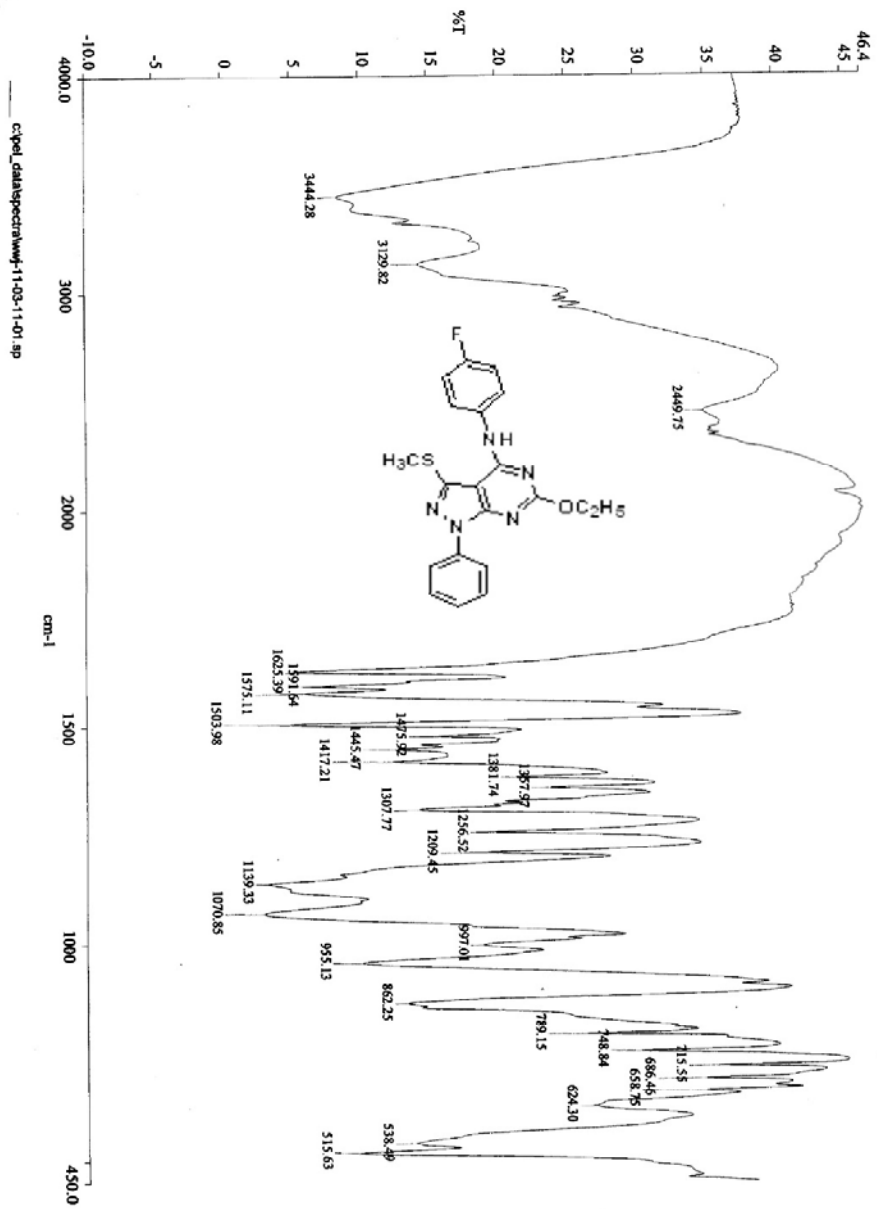
```

Current Data Parameters
NAME:
EXPNO: 1
PROCNO: 1
F2 - Acquisition Parameters
Date_   : 20110316
Time    : 11:37
INSTRUM : 5 mm BBO Av400
PROBHD  : 5mmBBO
PULPROG : zgpg30
TD       : 65536
SOLVENT : CDCl3
NS       : 1024
DS       : 4
SWH      : 23990.814 Hz
AQ       : 0.0042444 sec
RG       : 13004
FIDRES   : 1.3664756 sec
AQ       : 20.850 usec
RG       : 298.1 K
SI       : 2.0000000 sec
D1       : 0.0000000 sec
DELTA    : 0.0000000 sec
MORPH    : 0.0150000 sec

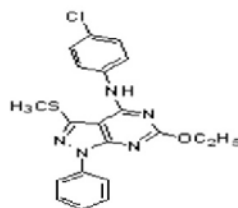
===== CHANNEL f1 =====
NUC1     : 13C
P1       : 8.10 usec
PL1      : -2.00 dB
SFO1     : 100.6282698 MHz

===== CHANNEL f2 =====
CPDPRG2  : waltz16
NUC2     : 1H
PCPD2    : 90.00 usec
PCPD2    : 90.00 usec
PL12     : 10.27 dB
PL12     : 10.27 dB
PL13     : 14.00 dB
SFO2     : 400.1516902 MHz

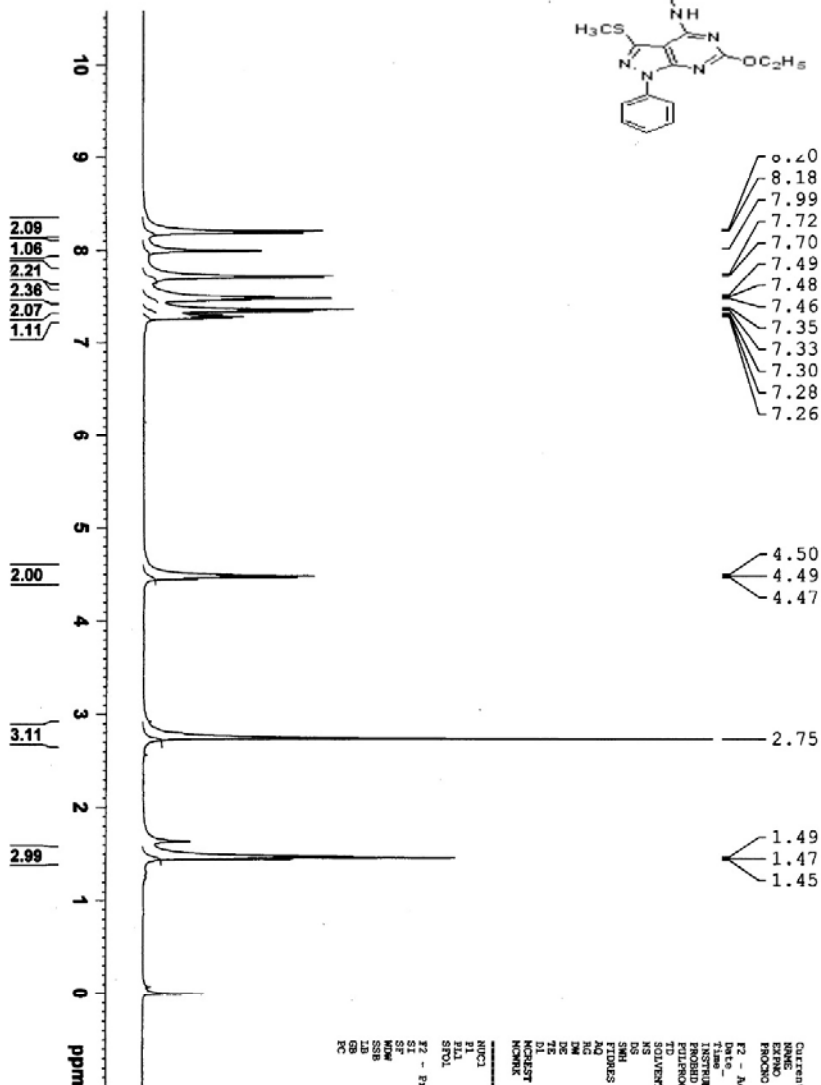
F2 - Processing parameters
SI       : 32768
SF       : 100.6127850 MHz
WDW      : EM
SSB      : 0
GB       : 0
PC       : 1.40
  
```

Compound 4k



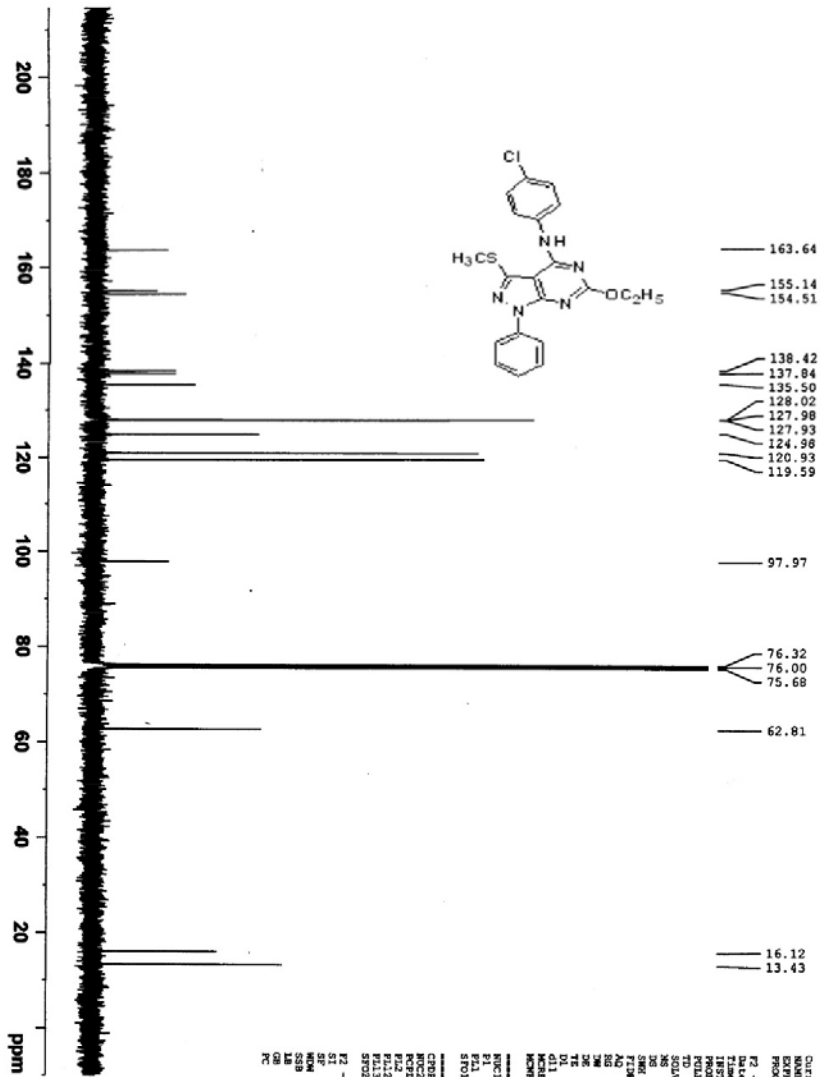
MWJ2011011001



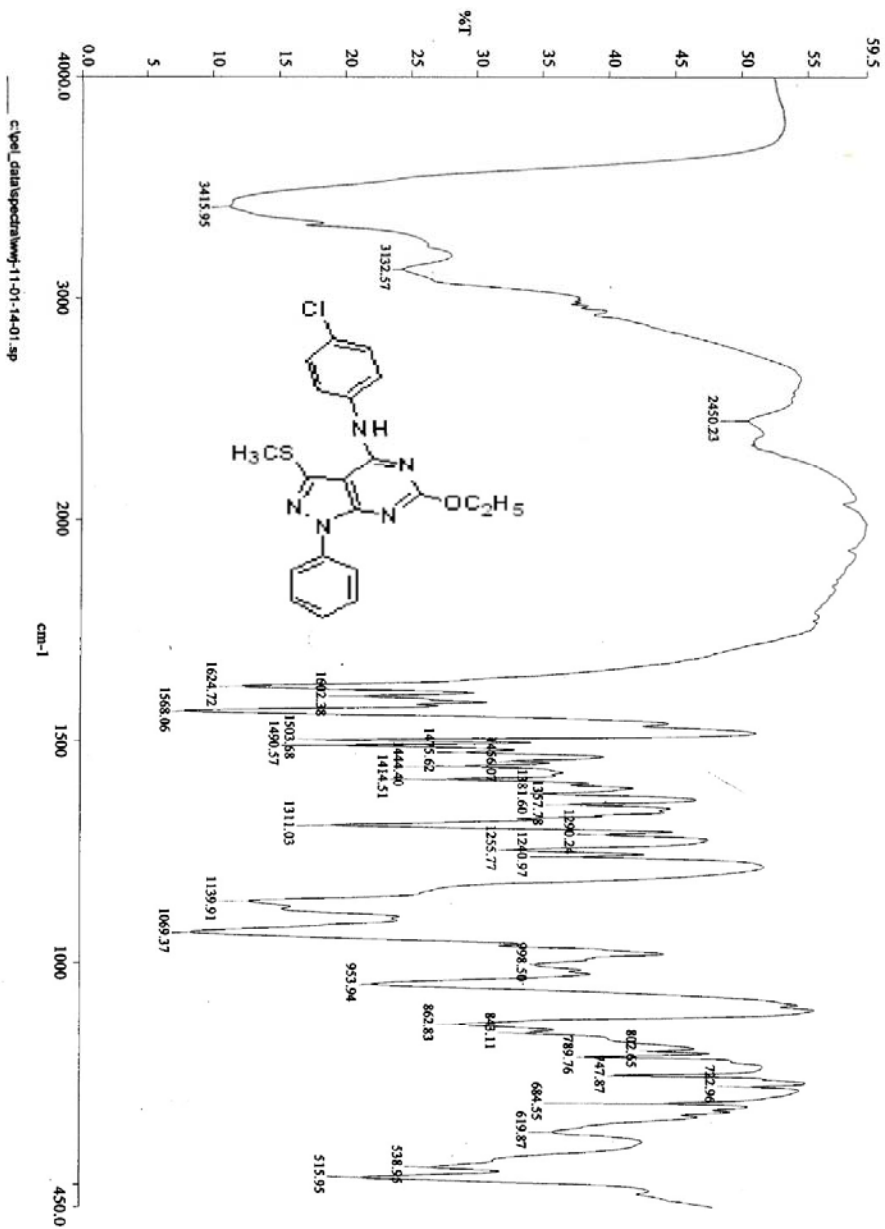
```

Current Data Parameters
Date_ 20110111
Time_ 10.07
INSTRUM 5 mm BBO
PROBHD 5
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2
DS 2
SWH 8278.146 Hz
FIDRES 0.142314 Hz
AQ 3.794511 sec
RG 645.1
DM 60.400 usec
DE 6.000 usec
TE 29.00 usec
SI 1.00000000 sec
SFO1 400.1300000 MHz
KORRES 0.02000000 sec
----- CHANNEL f1 -----
NUC1 1H
P1 18.00 usec
PL1 -3.00 dB
SFO1 400.132715 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
GB 0
PC 1.00
  
```

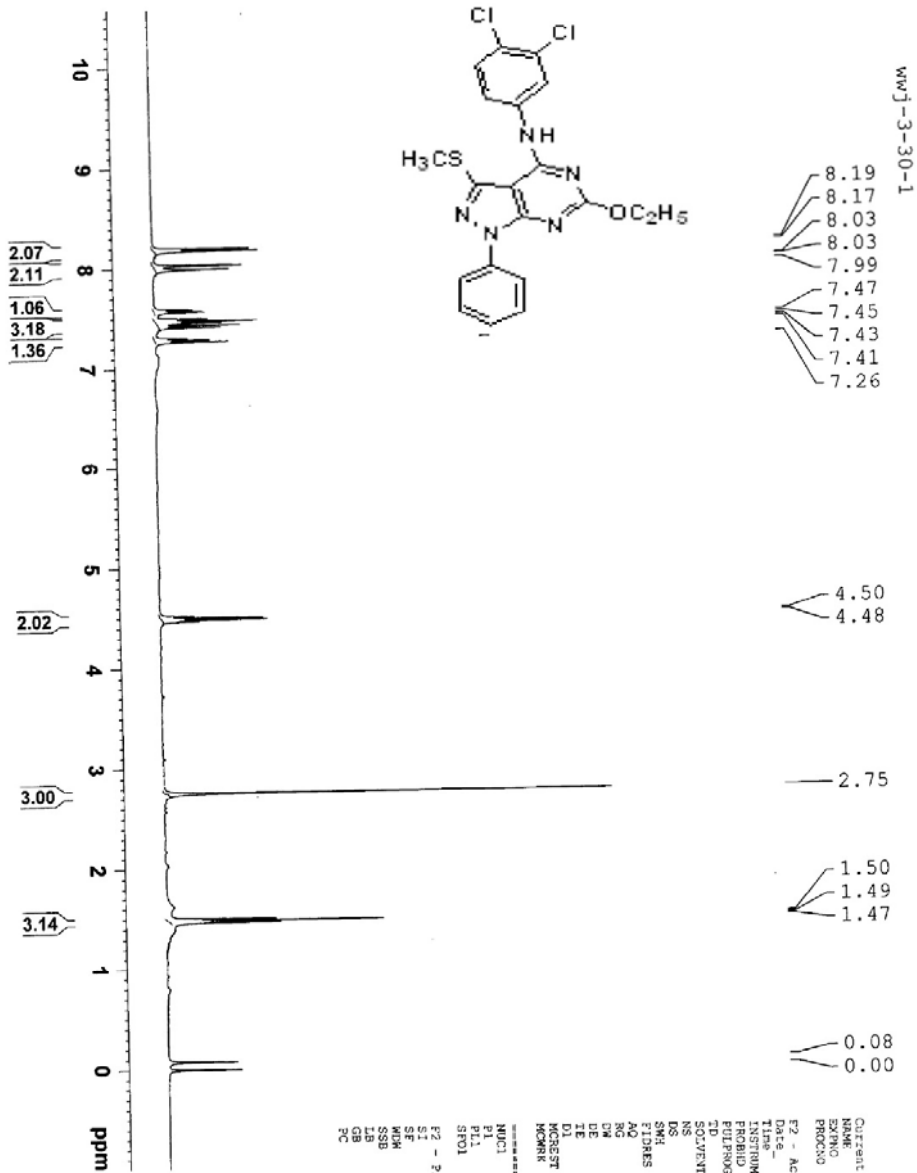
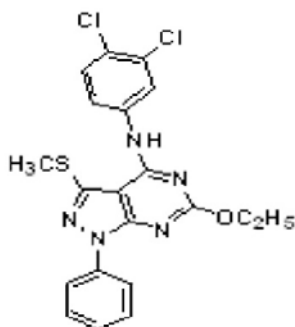
wwj2011030202



Current Data Parameters
 Name: 20110302
 RecNo: 1
 ExpNo: 1
 F1 - Acquisition Parameters
 Date_Time: 20110304 22:09
 File: 20110304_11
 Instrument: 5 MM BBO AV400
 Processor: zgpg30
 F2 - Processing parameters
 SI: 32768
 SF: 100.628784 MHz
 AQ: 4.000000 sec
 EQ: 1.000000 sec
 FIDRES: 0.000000 Hz
 AQRES: 0.0250000 sec
 CHANNEL: f1
 P1: 13C 13C usec
 P2: 91C 91C usec
 P3: 100.628784 MHz
 SFO1: 100.628784 MHz
 CHANNEL: f2
 MVT: 16
 CPDPRG2: waltz16
 PCPD2: 80.00 usec
 P12: -3.00 dB
 P13: 10.00 dB
 P14: 10.00 dB
 SFO2: 400.1316005 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 100.628784 MHz
 AQ: 4.000000 sec
 EQ: 1.000000 sec
 FIDRES: 0.000000 Hz
 AQRES: 0.0250000 sec



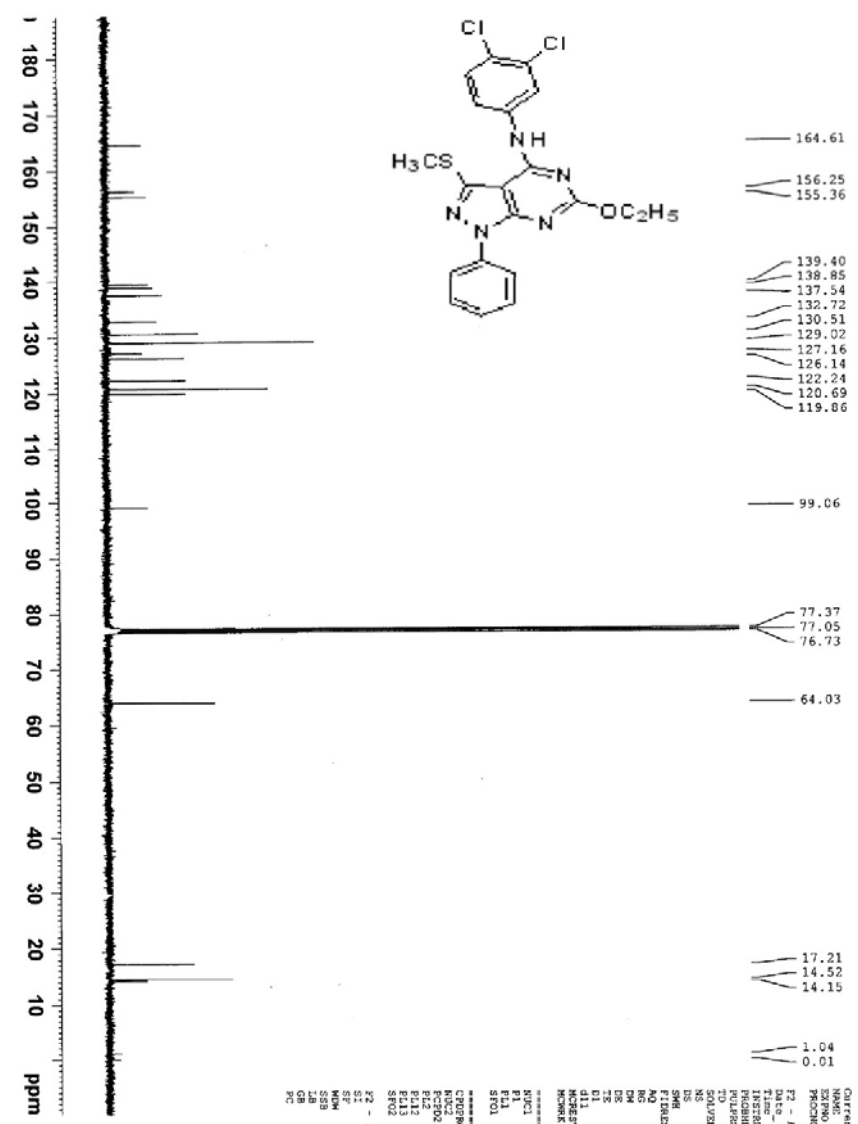
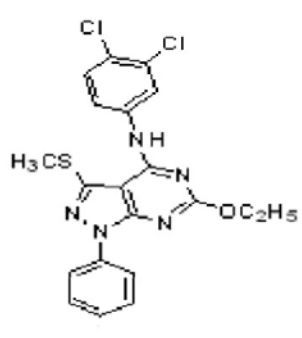
Compound 4l



MWJ-3-30-1

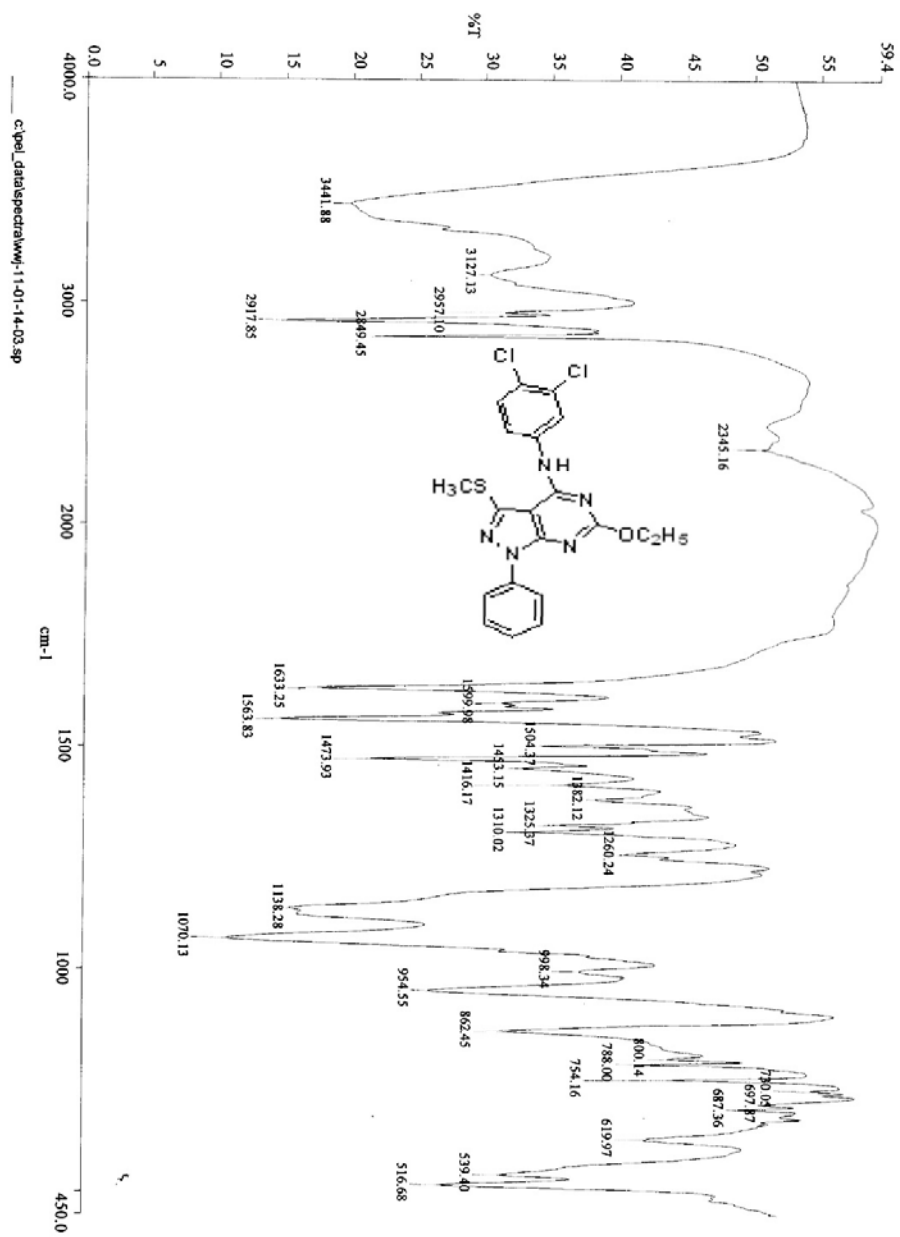
Current Data Parameters
 Name: MWJ-3-30-1
 ExpNo: 1
 ProcNo: 1
 F2 - Acquisition Parameters
 Date_: 20110311
 Time: 16:12
 Instrument: AV400
 PROBHD: 5 mm BBO BB-1H
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 16
 DS: 4
 SWH: 6378.146 Hz
 FIDRES: 0.156314 Hz
 AQ: 3.9584243 sec
 RG: 574.7
 GW: 60.400 usec
 DE: 291.9 usec
 TE: 300.2 K
 DI: 1.00000000 sec
 MCREST: 0.00000000 sec
 MCWNR: 0.01500000 sec
 ===== CHANNEL f1 =====
 NUCL1: 1H
 P1: 8.00 usec
 PL1: -3.00 dB
 SFO1: 400.1324710 MHz
 F2 - Processing parameters
 SF: 327.68 MHz
 WDM: 400.1320098 MHz
 SSB: EM
 LB: 0 Hz
 GB: 0 Hz
 CB: 1.00

WJ-4-1

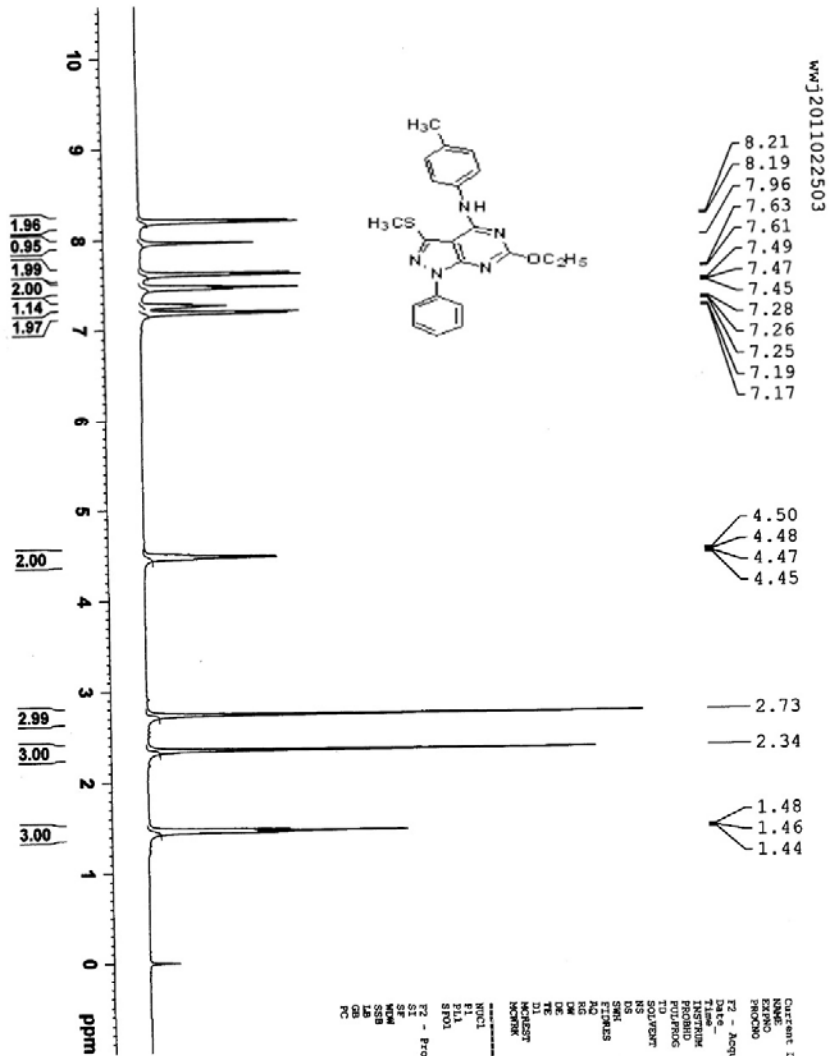


Current Data Parameters

NAME	WJ-4-1
EXPNO	1
PROCNO	1
F2 - Acquisition Parameters	
Date_	20100805
Time	14:43
INSTRUM	g4000
PROBHD	5 mm BBO
PULPROG	zgpg30
TD	65536
SF	100.626120
SOLVENT	CDCl3
NS	512
DS	4
SWH	23980.814 Hz
FIDRES	0.165918 Hz
AQ	1.325918 sec
RG	13004
DM	20.850 usec
DE	291.2 K usec
TE	293.2 K
D1	2.00000000 sec
d11	0.01000000 sec
DELTA	0.01000000 sec
MONKX	0.01500000 sec
===== CHANNEL f1 =====	
NUC1	13C
PT	8.70 usec
PL1	2.00 dB
ST1	100.626120 MHz
===== CHANNEL f2 =====	
NUC2	1H
PT2	90.00 usec
PL2	0.00 dB
PL12	19.00 dB
PL13	14.00 dB
PL14	14.00 dB
PL15	14.00 dB
PL16	14.00 dB
PL17	14.00 dB
PL18	14.00 dB
PL19	14.00 dB
PL20	14.00 dB
===== Processing parameters =====	
SI	32768
SF	100.626120 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



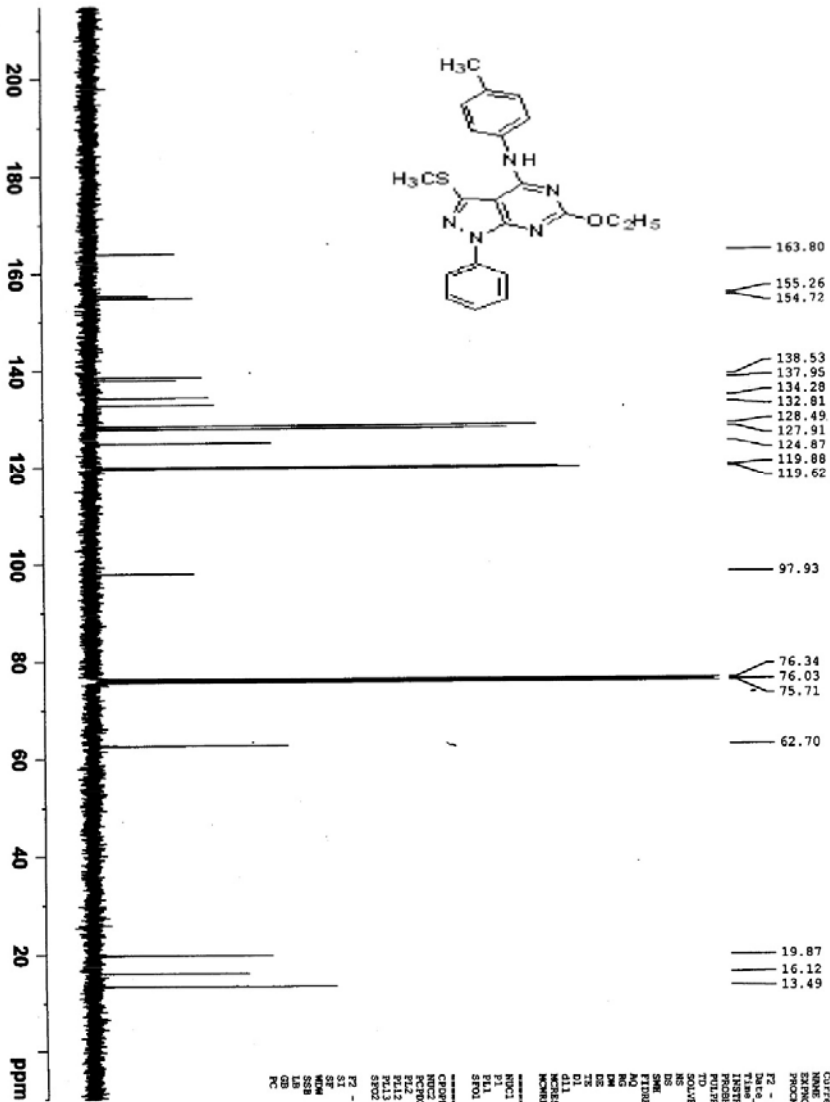
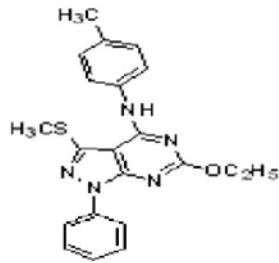
Compound 4m



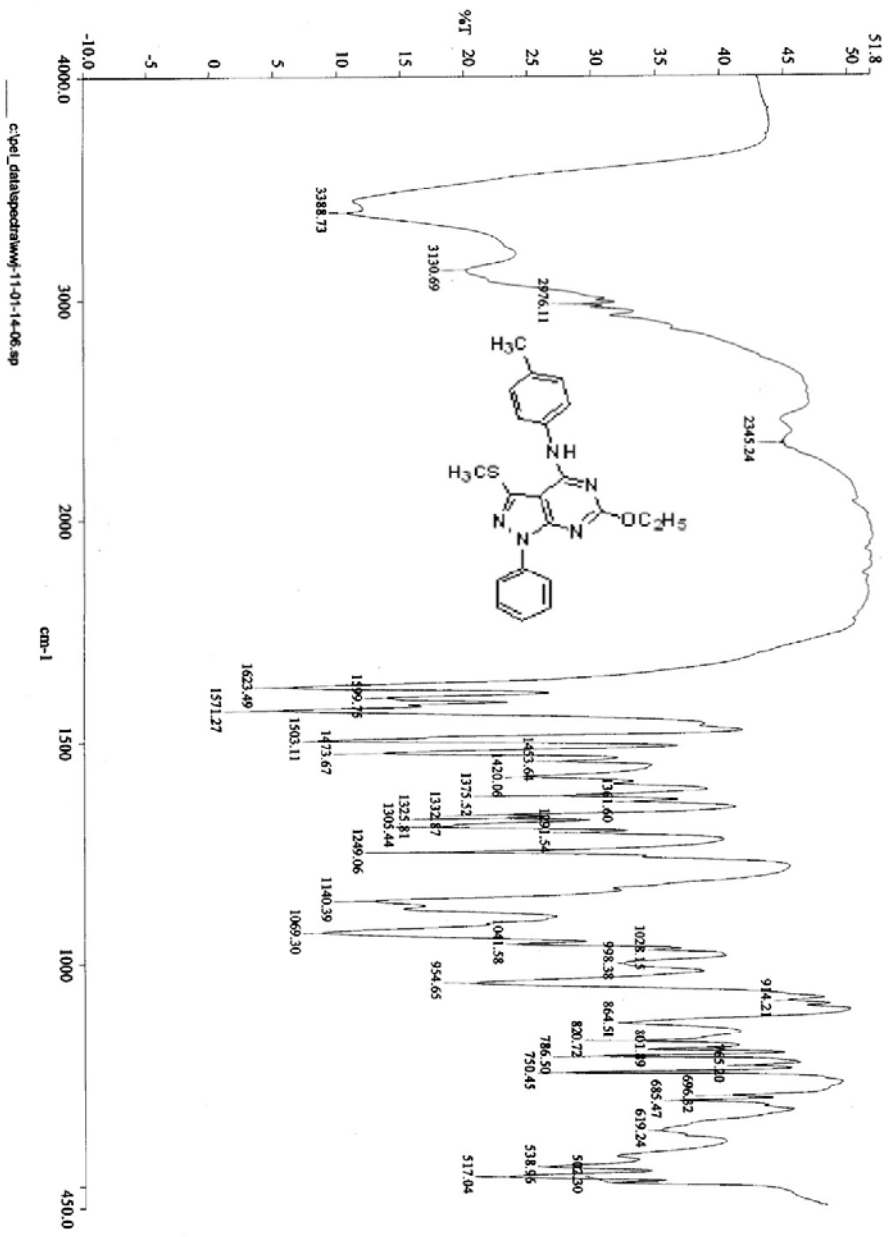
WJ2011022503

Current Data Parameters
 Name: WJ2011022503
 ExpNo: 1
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20110901
 Time: 14:00
 INSTRUM: spect
 PROBNM: 5 mm BBO BB-1H
 PULPROG: zgpg30
 TD: 65536
 TO: 0.00000000
 T1: 0.00000000
 T2: 0.00000000
 T3: 0.00000000
 T4: 0.00000000
 T5: 0.00000000
 T6: 0.00000000
 T7: 0.00000000
 T8: 0.00000000
 T9: 0.00000000
 T10: 0.00000000
 T11: 0.00000000
 T12: 0.00000000
 T13: 0.00000000
 T14: 0.00000000
 T15: 0.00000000
 T16: 0.00000000
 T17: 0.00000000
 T18: 0.00000000
 T19: 0.00000000
 T20: 0.00000000
 T21: 0.00000000
 T22: 0.00000000
 T23: 0.00000000
 T24: 0.00000000
 T25: 0.00000000
 T26: 0.00000000
 T27: 0.00000000
 T28: 0.00000000
 T29: 0.00000000
 T30: 0.00000000
 T31: 0.00000000
 T32: 0.00000000
 DS: 8278.146 Hz
 SFO: 400.1327110 MHz
 FIDRES: 0.126334 Hz
 AQ: 3.9586243 sec
 RG: 655.35
 DE: 60.100 usec
 TE: 283.2 K
 T1RHO: 1.00000000 sec
 T2RHO: 0.00000000 sec
 T3RHO: 0.00000000 sec
 T4RHO: 0.00000000 sec
 T5RHO: 0.00000000 sec
 T6RHO: 0.00000000 sec
 T7RHO: 0.00000000 sec
 T8RHO: 0.00000000 sec
 T9RHO: 0.00000000 sec
 T10RHO: 0.00000000 sec
 T11RHO: 0.00000000 sec
 T12RHO: 0.00000000 sec
 T13RHO: 0.00000000 sec
 T14RHO: 0.00000000 sec
 T15RHO: 0.00000000 sec
 T16RHO: 0.00000000 sec
 T17RHO: 0.00000000 sec
 T18RHO: 0.00000000 sec
 T19RHO: 0.00000000 sec
 T20RHO: 0.00000000 sec
 T21RHO: 0.00000000 sec
 T22RHO: 0.00000000 sec
 T23RHO: 0.00000000 sec
 T24RHO: 0.00000000 sec
 T25RHO: 0.00000000 sec
 T26RHO: 0.00000000 sec
 T27RHO: 0.00000000 sec
 T28RHO: 0.00000000 sec
 T29RHO: 0.00000000 sec
 T30RHO: 0.00000000 sec
 T31RHO: 0.00000000 sec
 T32RHO: 0.00000000 sec
 CHANNEL F1
 NUCL: 1H
 P1: 12.00 usec
 PL1: 0.00 dB
 SFO1: 400.1327110 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 400.1300133 MHz
 WDM: 0
 LB: 0
 GB: 0.30 Hz
 CB: 0
 PC: 1.00

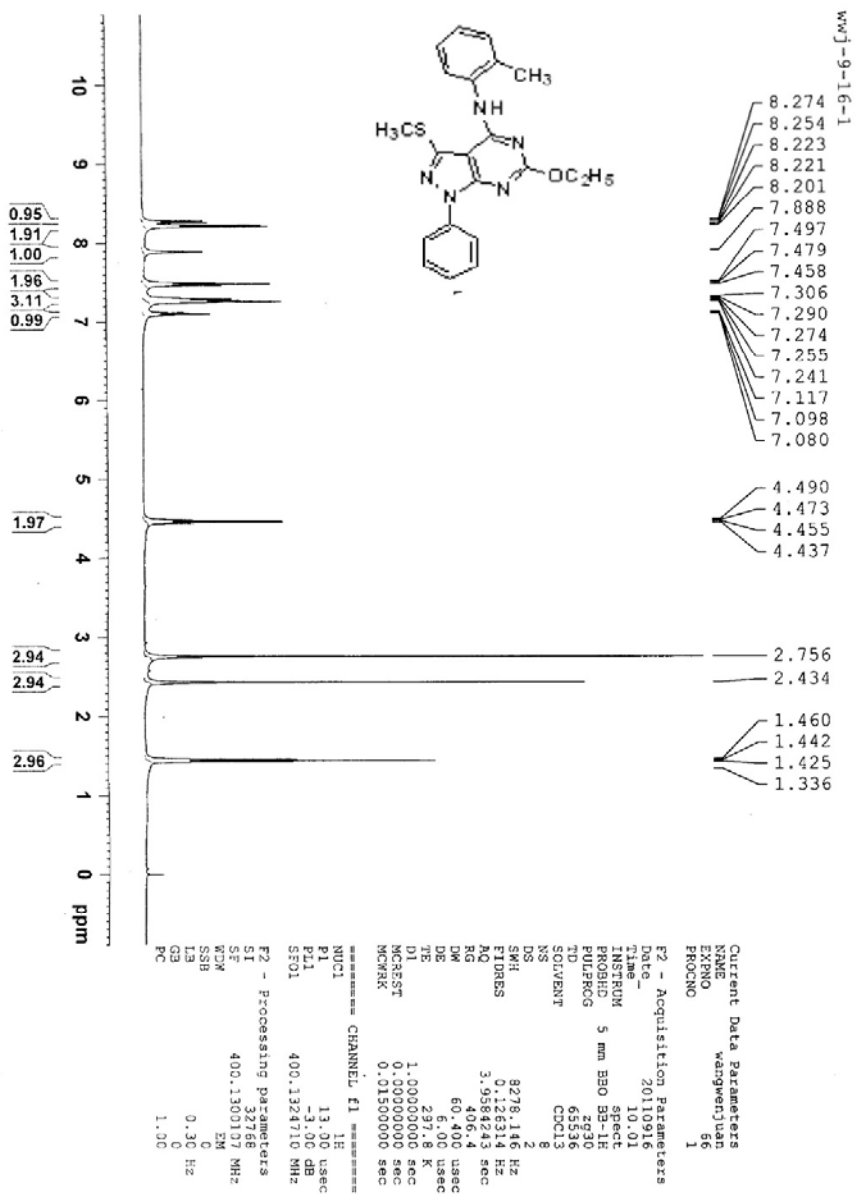
HWJ2011030201



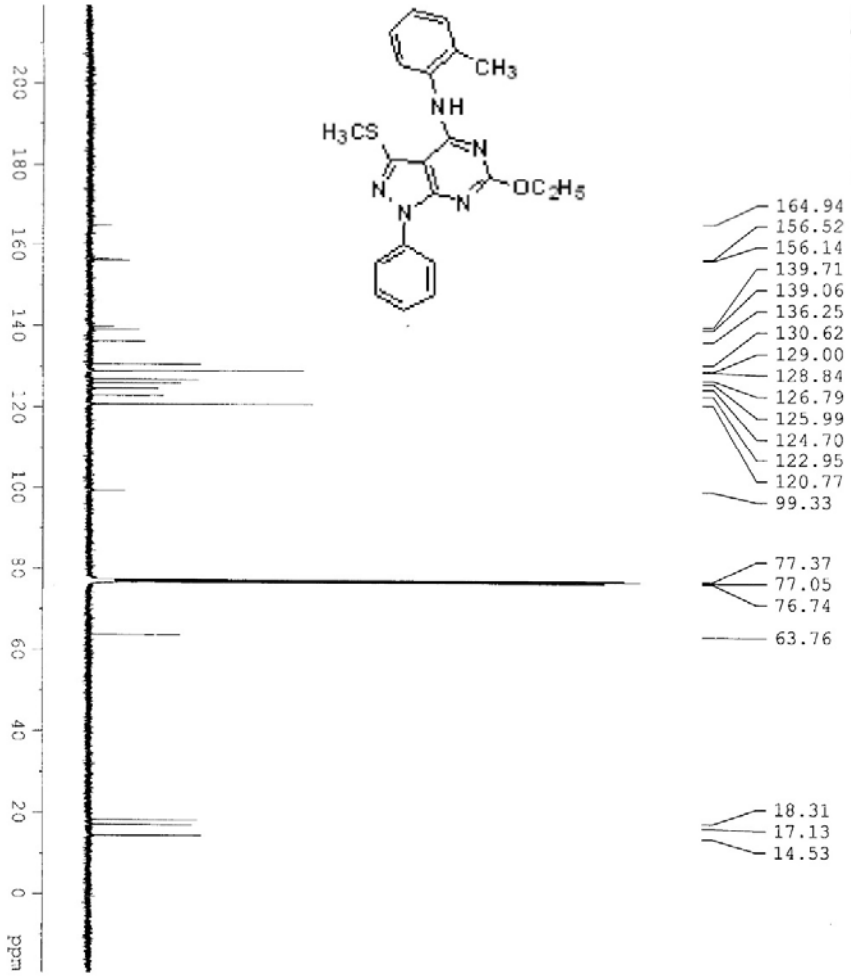
Current Data Parameters
 Date 20110304
 Time 13:57
 INSTRUM 5 MM BBO
 PULPROG zgpg30
 TOU 62516
 TD 63
 SFO 100.628228 MHz
 F2 - Acquisition Parameters
 Date 20110304
 Time 13:57
 INSTRUM 5 MM BBO
 PULPROG zgpg30
 TOU 62516
 TD 63
 SFO 100.628228 MHz
 F2 - Processing parameters
 Date 20110304
 Time 13:57
 INSTRUM 5 MM BBO
 PULPROG zgpg30
 TOU 62516
 TD 63
 SFO 100.628228 MHz
 F2 - Processing parameters
 Date 20110304
 Time 13:57
 INSTRUM 5 MM BBO
 PULPROG zgpg30
 TOU 62516
 TD 63
 SFO 100.628228 MHz



Compound 4n

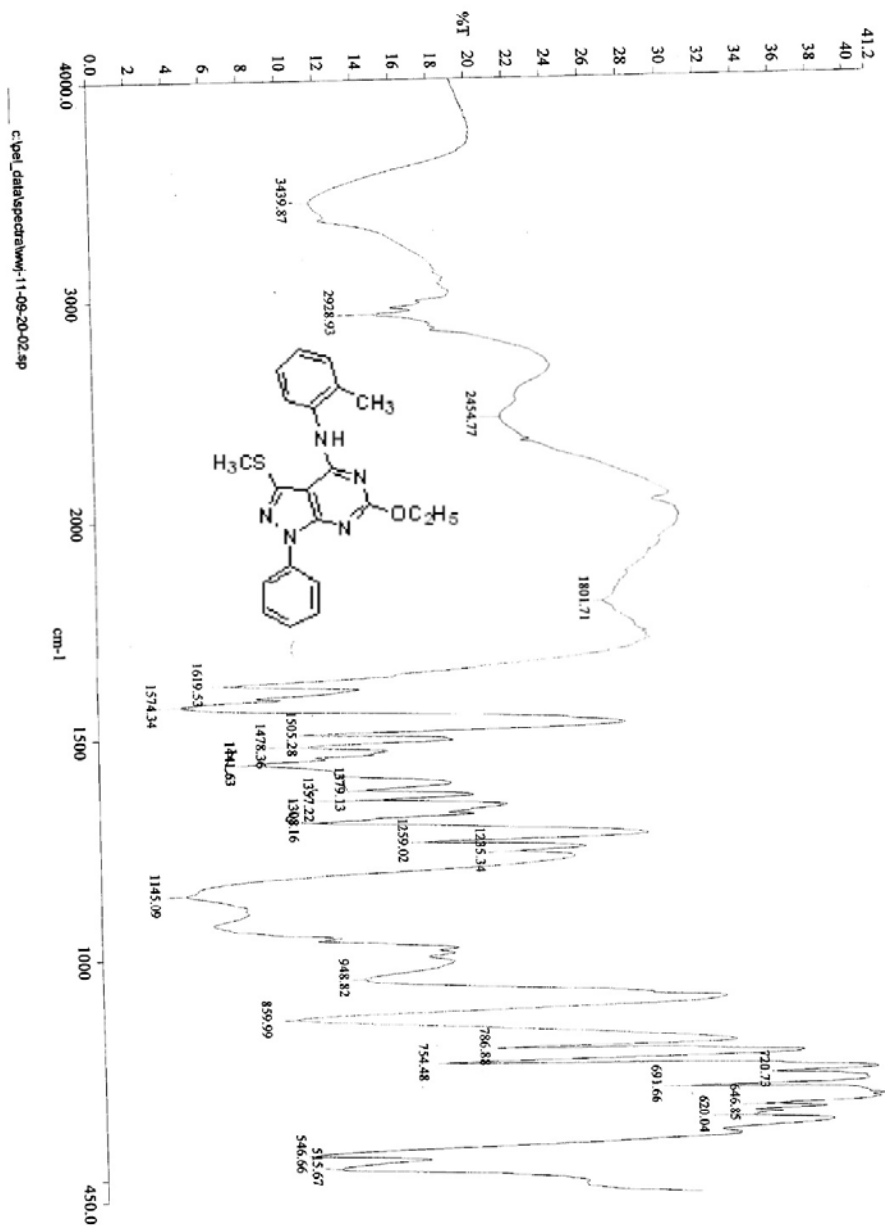


wjf-2011-9-16-1

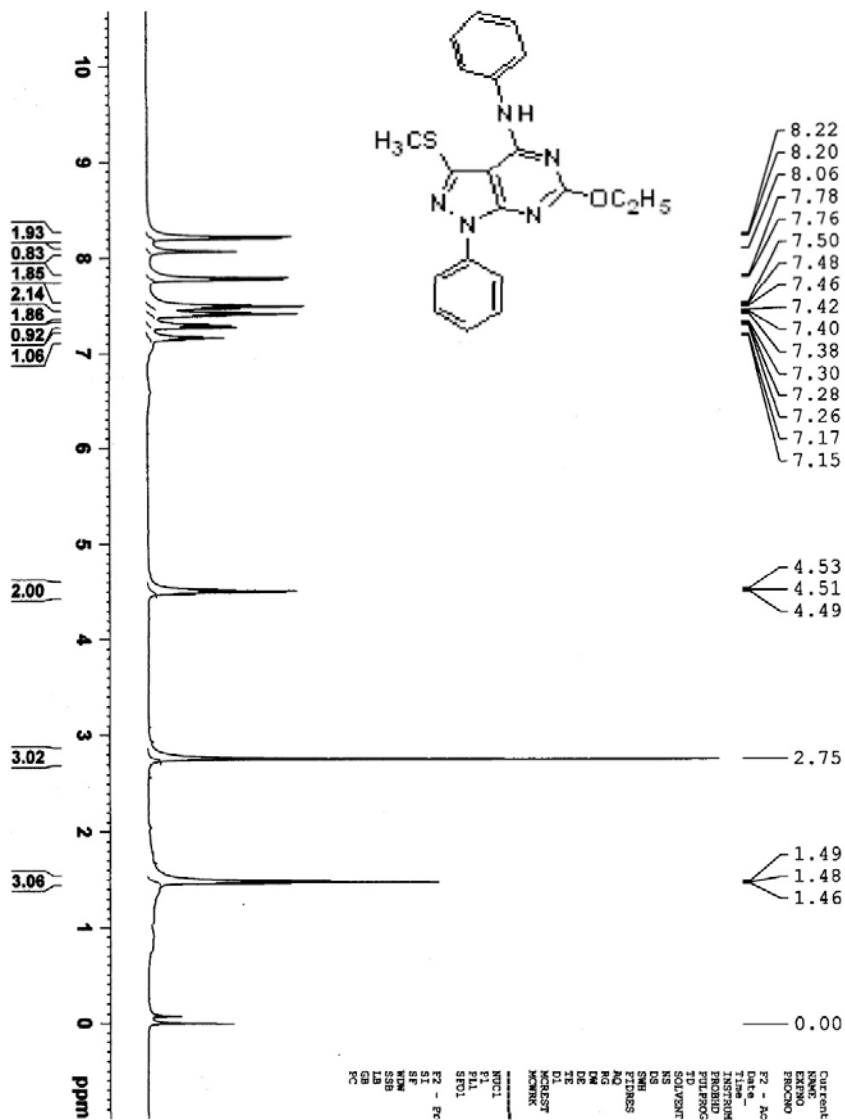


```

Current Data Parameters
NAME      hemipresion
EXPNO    69
PROCNO   1
----- Acquisition Parameters -----
Date_     20110929
Time      17:22:23
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        1024
DS        4
SFO       25860.814 Hz
FIDRES    0.385918 Hz
AQ        1.3166726 sec
RG         655
WDW        EM
SSB        0
GB         0
PC         20.850 usec
TE         300.2 K
NUC1       13
NUC2       13
DE         6.100 usec
d11prog   2.00000000 sec
d11start  0.01000000 sec
d11stop   0.01000000 sec
MKRF      0.01000000 sec
***** CHANNEL f1 *****
PC1       5.00 usec
PL1       -2.00 dB
NUC1      13
SFO1      100.628298 MHz
***** CHANNEL f2 *****
CPDPRG2   waltz16
NUC2      13
PC2       60.00 usec
PL2       120.00 dB
PL12      120.00 dB
PL13      120.00 dB
SFO2      400.131505 MHz
----- Processing parameters -----
SI        32768
SF        100.613690 MHz
RG         655
AQ         1.00 Hz
DE         1.40
PC         1.40
  
```



Compound 4o



wwj2011011002

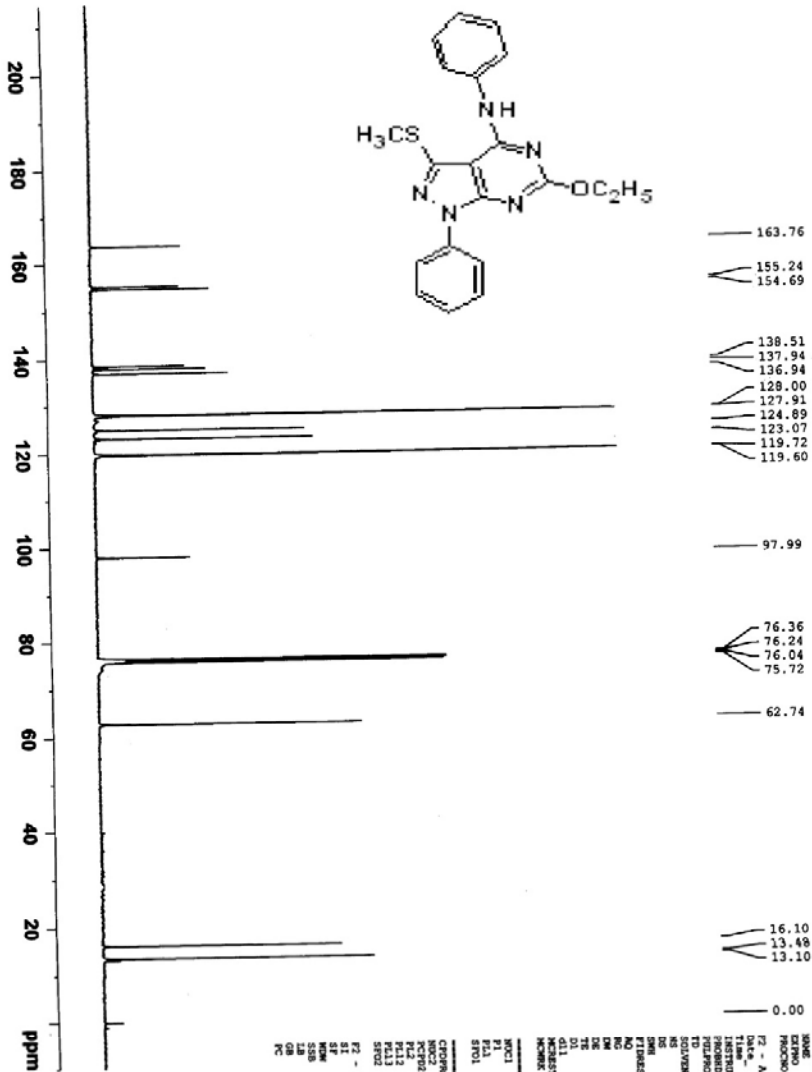
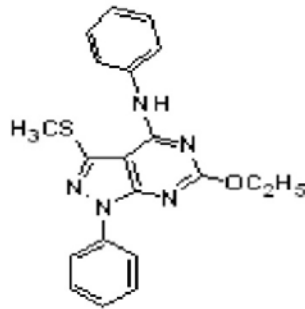
Current Data Parameters
 NAME: 4o
 EXNO: 45
 EPOCH: 1

F2 - Acquisition Parameters
 Date_: 20110111
 Time: 10:20
 INSTR: spect
 ENDOR: 5 mm BBO BB-1H
 PULPROG: zg30
 TD: 65536
 SFO: 400.1324710
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8278.146 Hz
 FIDRES: 0.124934 Hz
 AQ: 3.434944 sec
 RG: 574.7
 DW: 60.400 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 1.00000000 sec
 DELT: 0.00000000 sec
 ACQRES: 0.01500000 sec
 MCHNK: *****

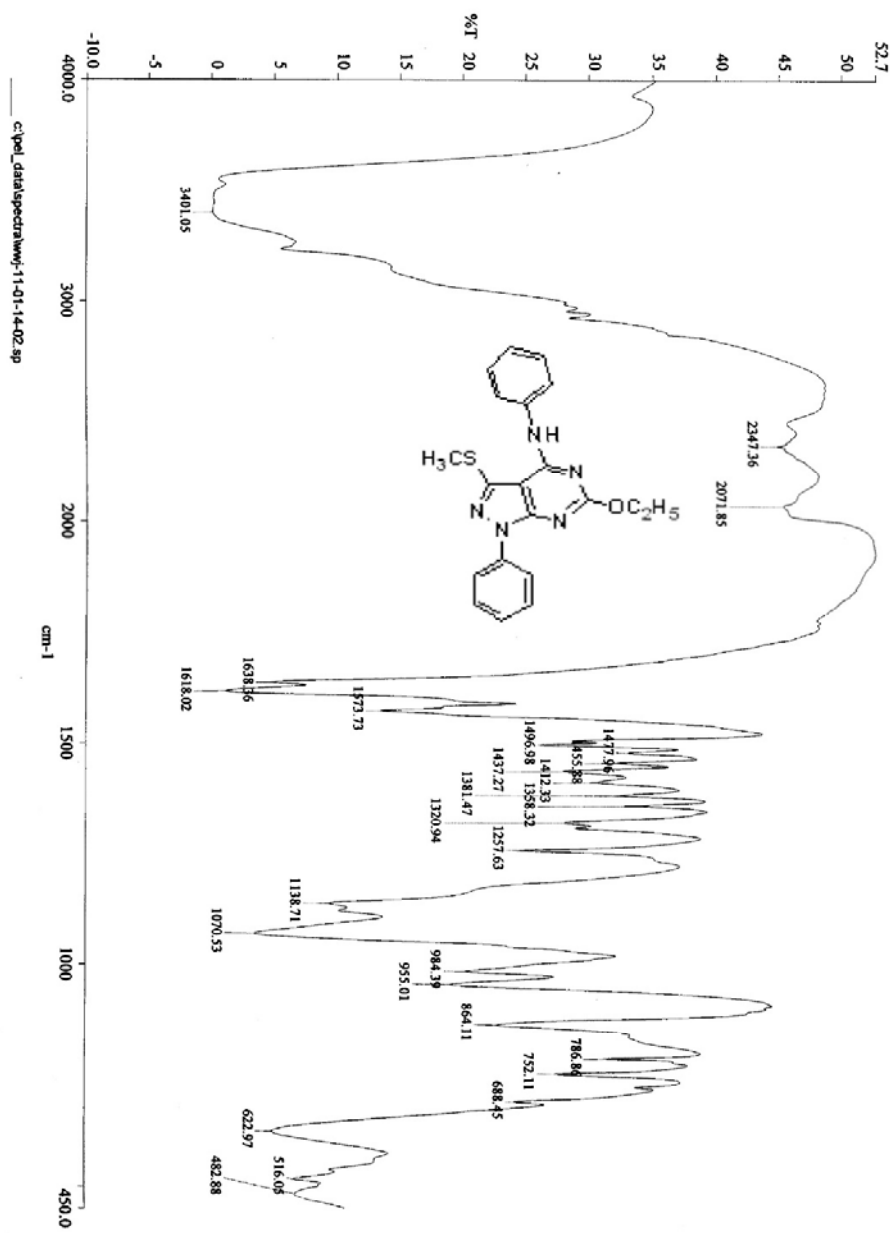
CHANNEL F1 *****
 NUC1: 1H
 P1: 8.00 usec
 PL1: 0.00 dB
 SFO1: 400.1324710 MHz

F2 - Processing parameters
 SI: 32768
 SF: 400.1300187 MHz
 WVM: 0
 SSB: 0
 GB: 0
 PC: 1.00

NWJ2011022501

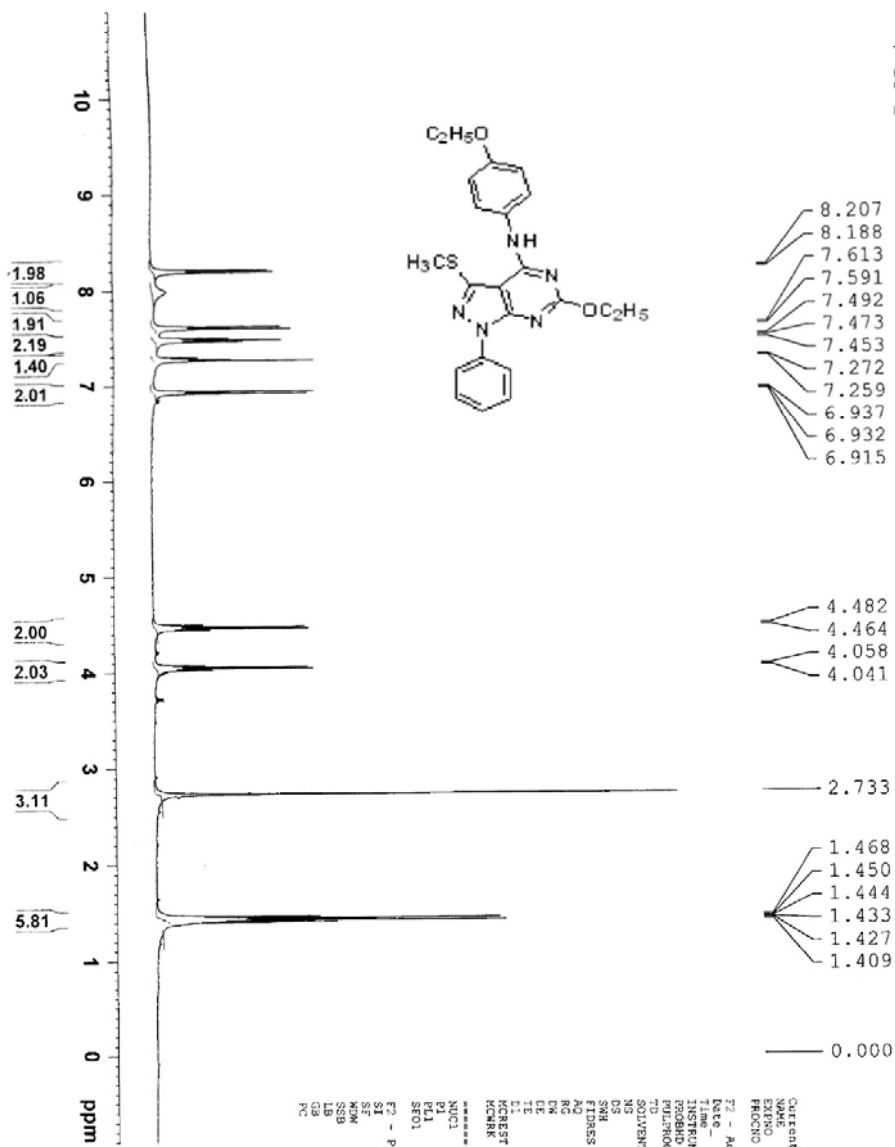


Current Data Parameters
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110904
 Time 14:09
 INSTRUM spect
 PROBRID 5 mm BBO BB-1H
 PULPROG zgpg30
 FIDRES 0.000000
 AQ 0.000000
 SOLVENT CDCl3
 NS 6192
 DS 4
 SWH 23980.614 Hz
 FWHM 0.365918 Hz
 NO 1.1864725 sec
 SFO 120.622858 MHz
 DM 29.850 usec
 DE 2.0000000 sec
 TE 300.2 K
 D1 0.03000000 sec
 d11 0.03000000 sec
 DELT 0.03000000 sec
 ACQPRG2 NAMEZ
 CHANNEL F1 13C
 NU1 8.710 usec
 FI 1.00
 FAL 100.622858 MHz
 SFO1 100.622858 MHz
 CHANNEL F2 1H
 NU2 18 usec
 FI 1.00
 FAL 400.126000 MHz
 SFO2 400.126000 MHz
 F2 - Processing parameters
 SI 100.622858 MHz
 SF 100.622858 MHz
 WDM 84
 SSB 0
 GB 1.00 Hz
 PC 1.00



Compound 4p

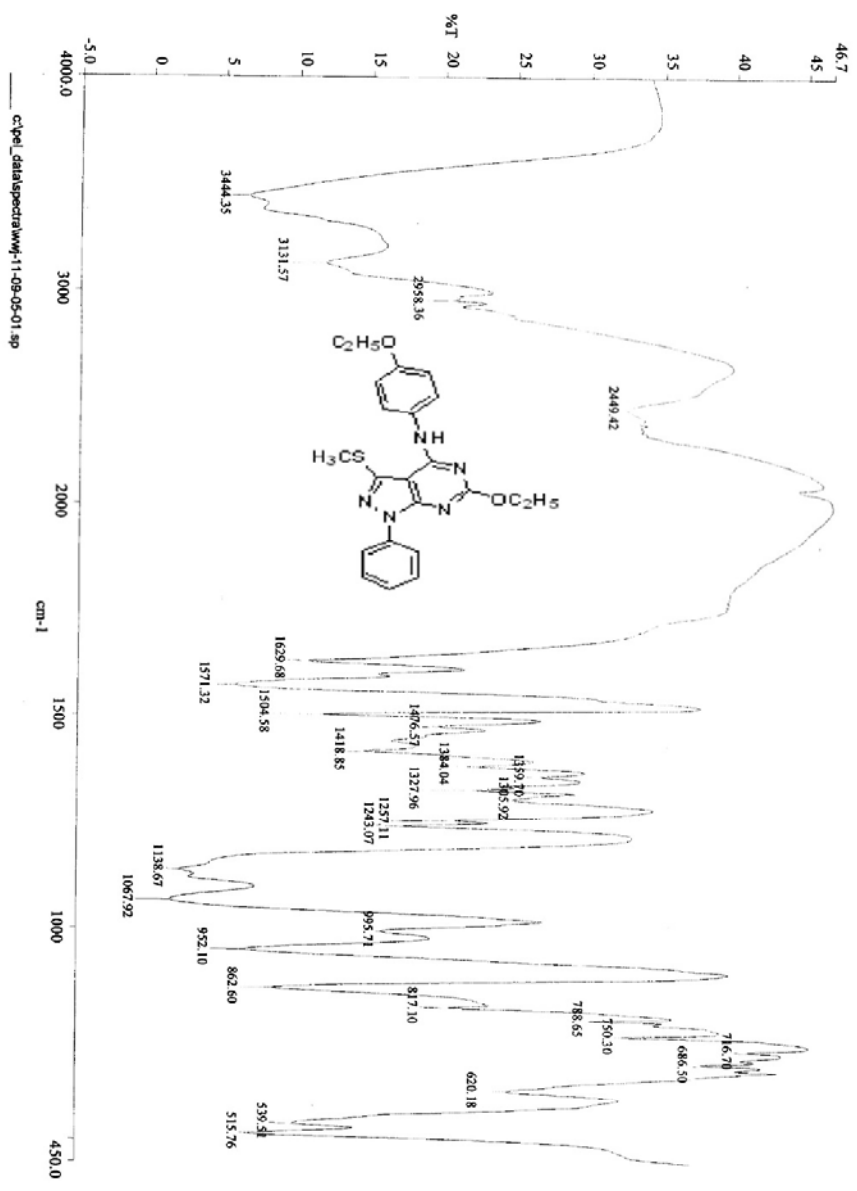
7-18-2



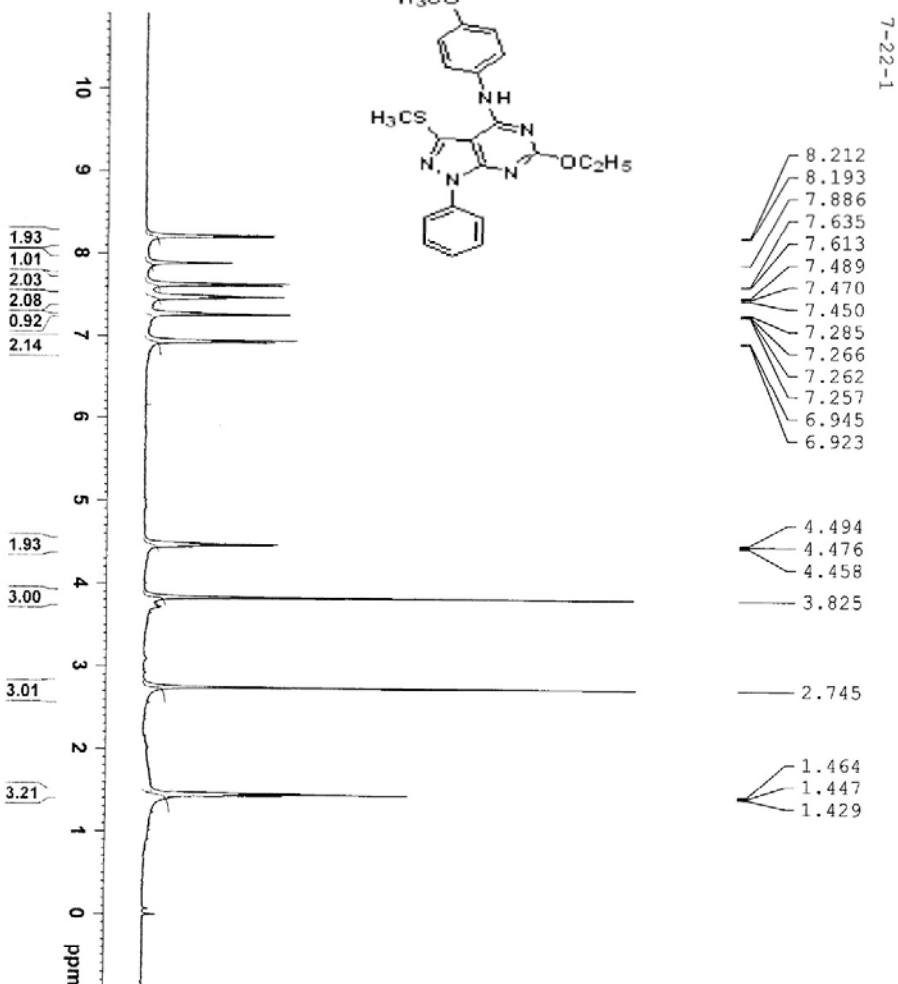
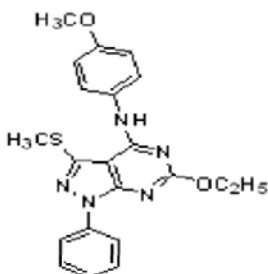
```

Current Data Parameters
NAME: wangyuanjun_49
EXPNO: 1
PROCNO: 1
Date_ 2011.07.18
Time: 14.21.36
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
SOLVENT: CDCl3
NS: 8
DS: 2
SWH: 8279.146 Hz
F2: 400.136099 MHz
FIDRES: 3.1584243 sec
AQ: 0.0000000 sec
RG: 512
AQ: 0.0000000 sec
SFO1: 400.136099 MHz
PC: 1.00
===== CHANNEL f1 =====
NUC1: 1H
P1: 13.00 usec
PL1: -1.00 dB
SFO1: 400.136099 MHz
=====
F2 - Acquisition Parameters
Date_ 2011.07.18
Time: 14.21.36
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
SOLVENT: CDCl3
NS: 8
DS: 2
SWH: 8279.146 Hz
F2: 400.136099 MHz
FIDRES: 3.1584243 sec
AQ: 0.0000000 sec
RG: 512
AQ: 0.0000000 sec
SFO1: 400.136099 MHz
PC: 1.00
=====
F2 - Processing parameters
SI: 32768
SF: 400.136099 MHz
WDW: EM
SSB: 0
LB: 0.30 Hz
GB: 0
PC: 1.00

```

Compound 4q



Current Data Parameters
 NAME wangwenjuan
 EXPNO 54
 PROCNO 1

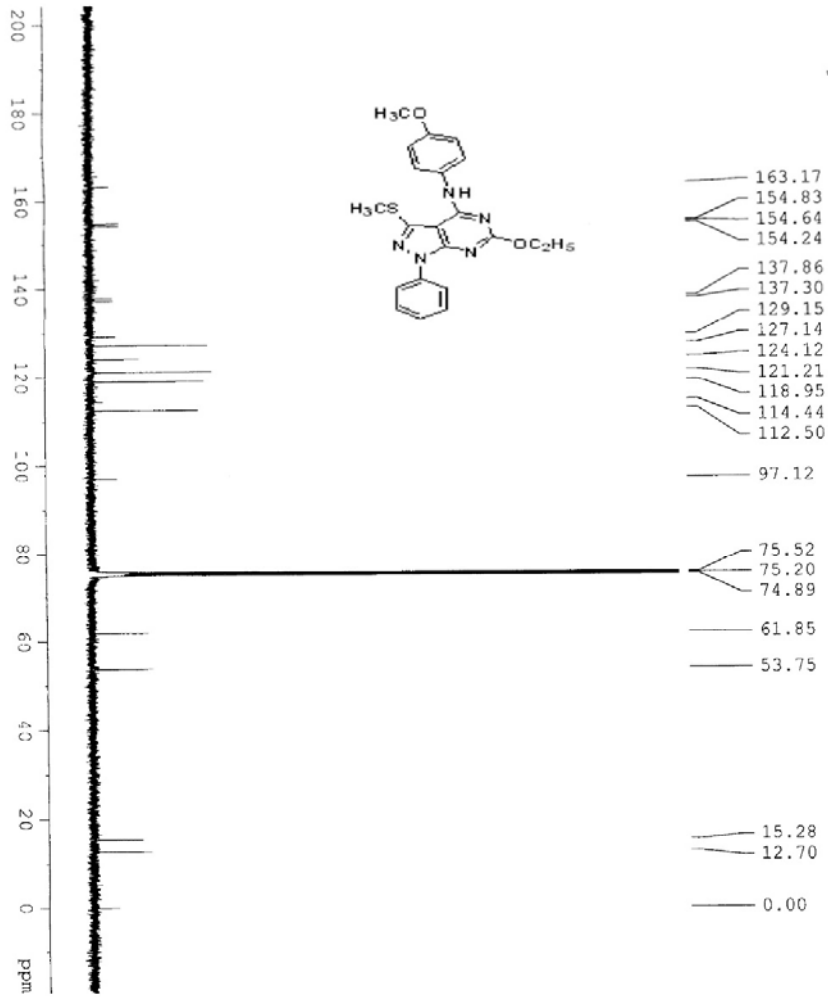
F2 - Acquisition Parameters

Date_ 20110722
 Time 15.53
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 2930
 FIDRES 0.16314 Hz
 AQ 3.9584243 sec
 RG 362
 DE 60.400 usec
 DM 6.00 usec
 TE 300.3 K
 DI 1.00000000 sec
 KRFREQ 0.00000000 sec
 KCMRN 0.01500000 sec

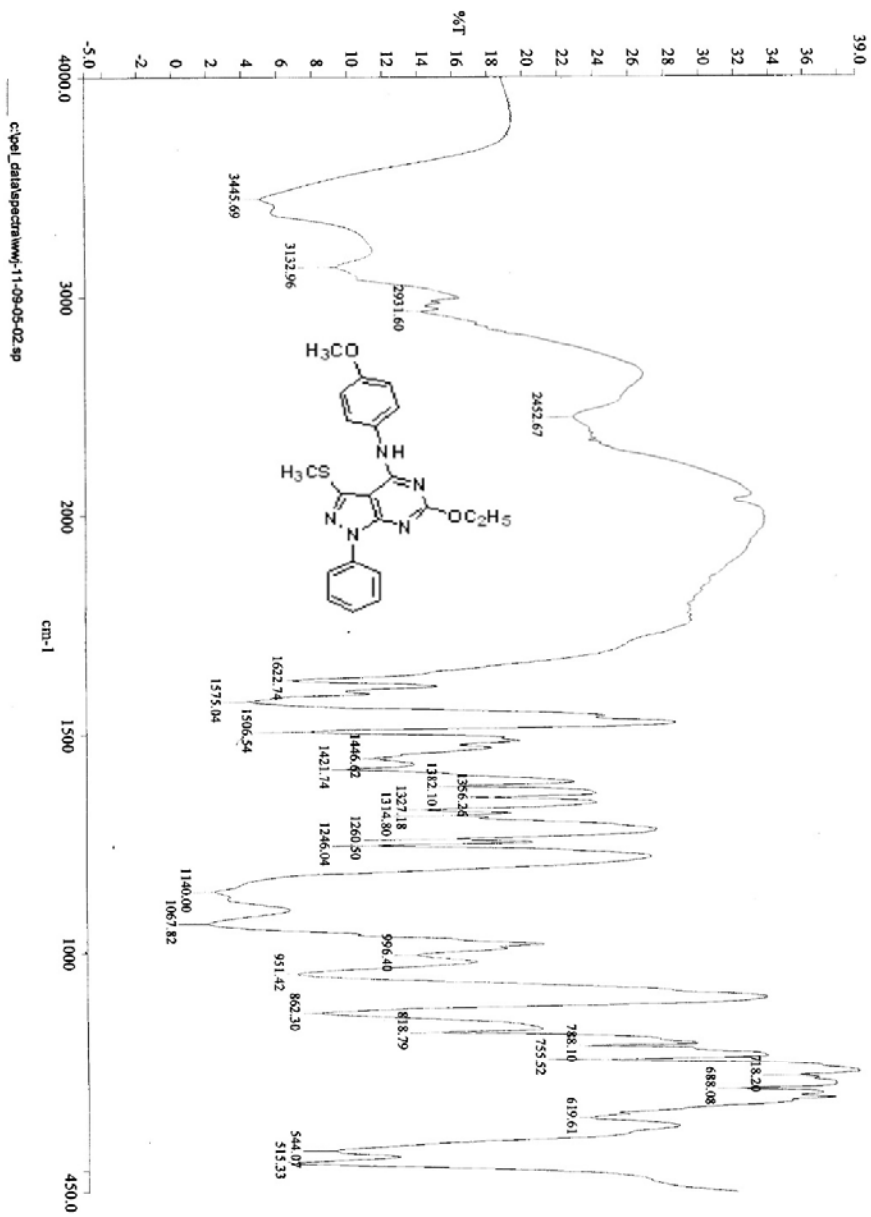
***** CHANNEL f1 *****
 NUC1 1H
 P1 13.00 usec
 PL1 -3.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300105 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

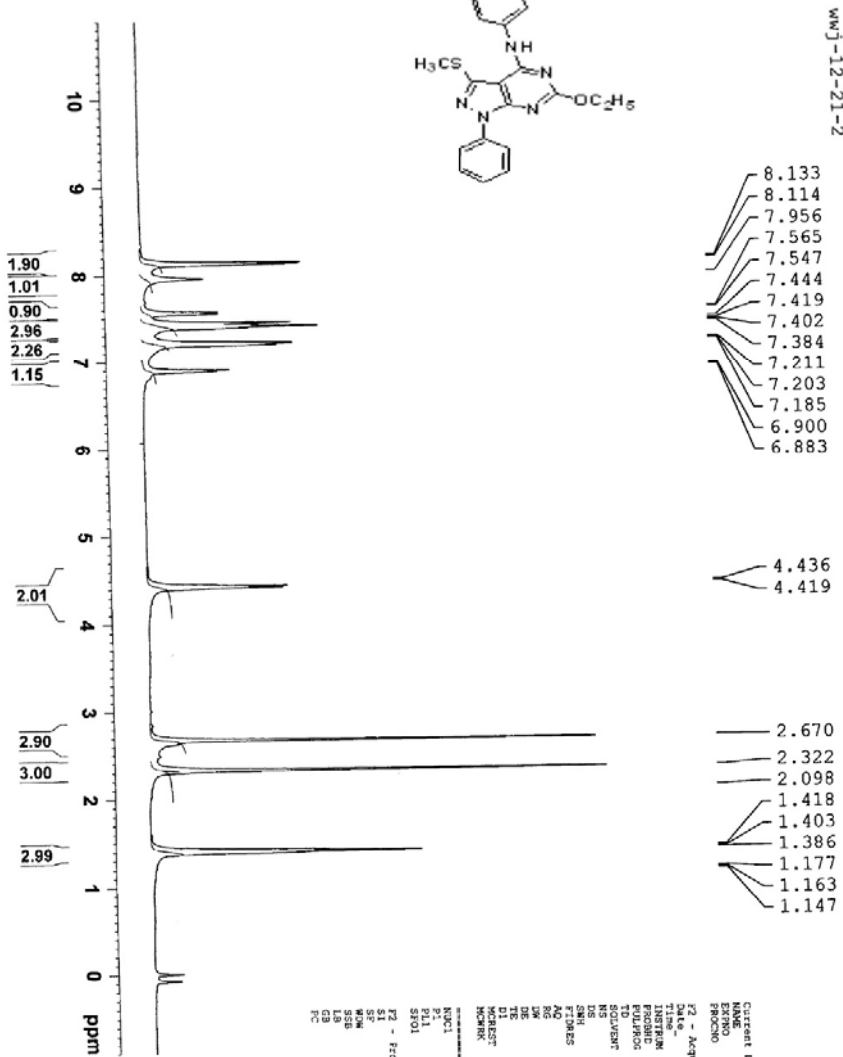
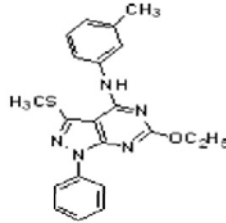
wwj-7-22-1



Current Data Parameters
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20110725
 Time 22:22:00
 INSTRUM spect
 PROBRD 5 mm BBO BB-1H
 P1 12.00
 T1 2.00
 T2 0.50
 SOLVENT CDCl3
 NS 963
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.345918 Hz
 AQ 1.344384 sec
 RG 654
 IN 2048
 FWHM 302.6 Hz
 SFO 400.146000 MHz
 T 302.6 K
 D1 2.20000000 sec
 DELT 0.20000000 sec
 ACQ 0.31500000 sec
 KWAVE 0.31500000 sec
 ===== CHANNEL f1 =====
 NUCL1 13C
 P1 4.00 usec
 PL 0.00 dB
 SFO1 100.628380 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 CHANDEL f2
 NUCL2 1H
 P2 12.00 usec
 PL2 0.00 dB
 SFO2 400.146000 MHz
 F2 - Processing parameters
 SI 32768
 SF 100.628380 MHz
 W 400.146000 MHz
 EQ 0
 SSB 0 Hz
 GB 0
 PC 1.00

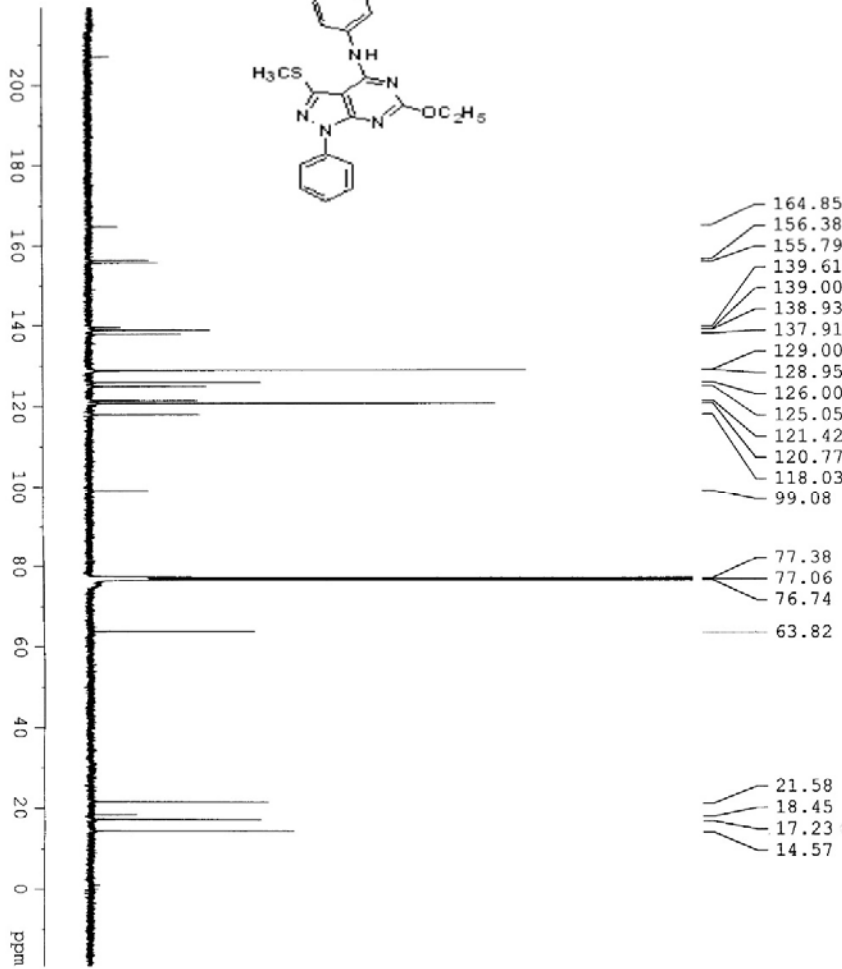
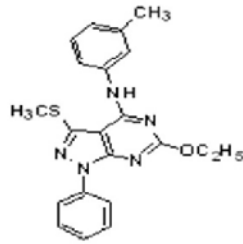


Compound 4r

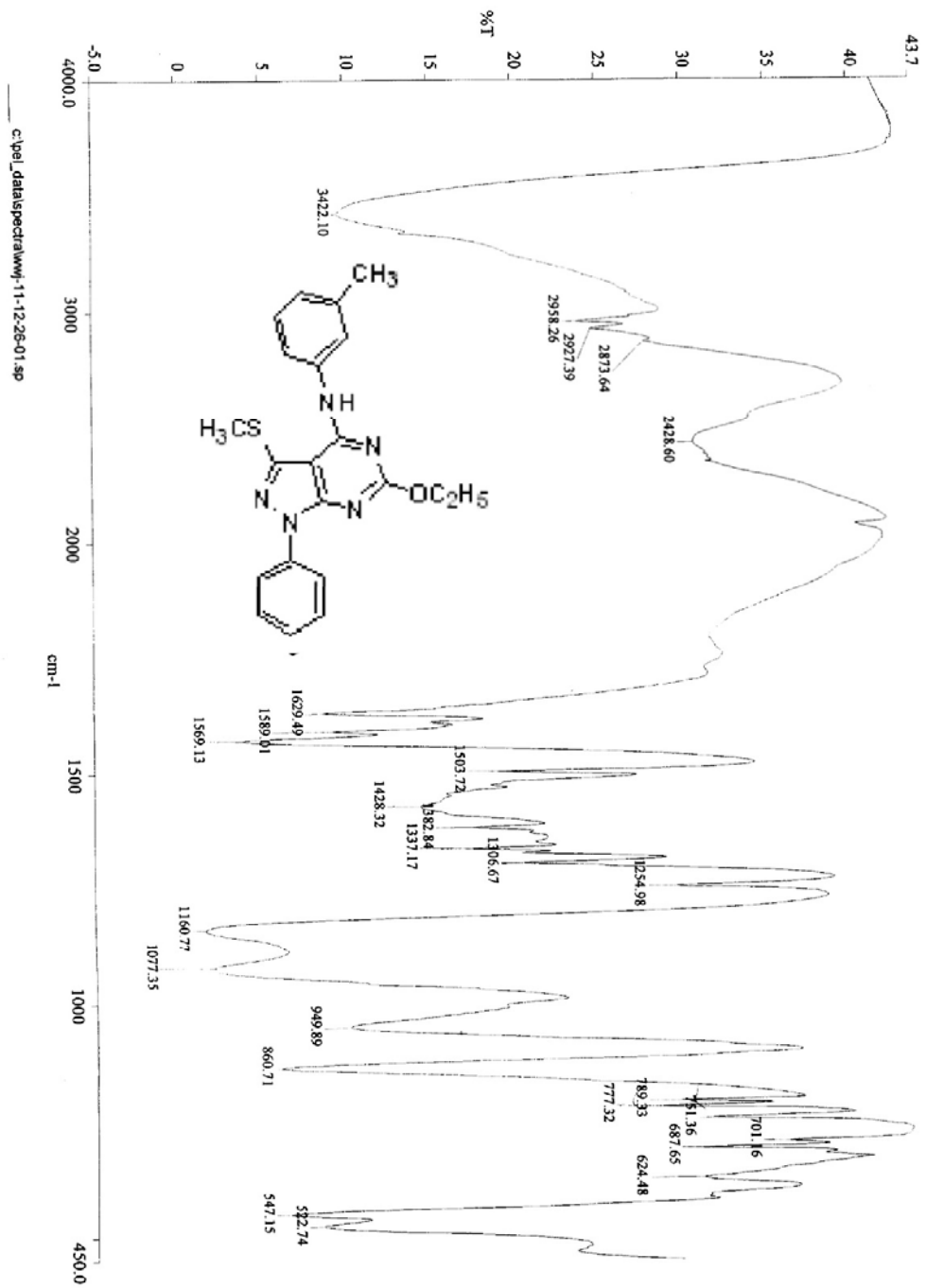


- 8.133
- 8.114
- 7.956
- 7.565
- 7.547
- 7.444
- 7.419
- 7.402
- 7.384
- 7.211
- 7.203
- 7.185
- 6.900
- 6.883
- 4.436
- 4.419
- 2.670
- 2.322
- 2.098
- 1.418
- 1.403
- 1.386
- 1.177
- 1.163
- 1.147

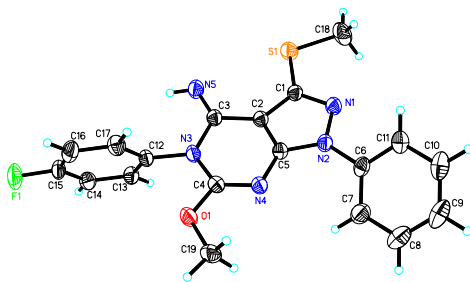
Current Data Parameters
 Name wangsm0111
 ExpNO 111
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 2011221
 Time 9:14
 Operator wangsm
 PROBRG 5 mm QNP 1H
 FREQREF 400.132710 MHz
 PULPROG zgpg30
 TD 65536
 SFO 400.132710 MHz
 CQ213
 SI 32768
 SF 400.132710 MHz
 DS 16
 DE 1.5
 IE 8218.146 Hz
 BE 1.0000000
 FIDRES 0.124314 Hz
 AQ 3.3944724 sec
 DE 60.400 usec
 SE 2.00
 TE 300.2 K
 DE 6.00 usec
 HE 1.0000000 sec
 DI 0.0000000 sec
 MEHEST 0.0100000 sec
 MCHMR
 ===== CHANNEL f1 =====
 NUC1 13C
 P1 13.00 usec
 PL1 -1.00 dB
 F1 100.132710 MHz
 SFO1 400.132710 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.132710 MHz
 DS 16
 SE 2.00
 SF 400.132710 MHz
 DE 6.00 usec
 HE 1.0000000 sec
 DI 0.0000000 sec
 MEHEST 0.0100000 sec



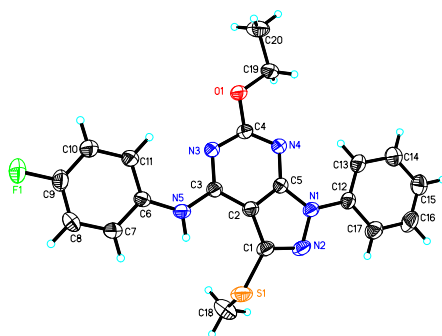
Current Data Parameters
 NAME: maripamjuan
 EXPNO: 113
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_ Time: 20111226 12:52
 INSTRUM: spect
 PROBRD: 5 mm BBO BB-1H
 PULPROG: zgpg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 5120
 DS: 4
 SWH: 23960.814 Hz
 FIDRES: 0.3645918 Hz
 AQ: 1.3644756 sec
 RG: 2048
 DW: 20.850 usec
 DE: 6.00 usec
 TE: 300.2 K
 D1: 2.0000000 sec
 d11: 0.0000000 sec
 d12: 0.0000000 sec
 d13: 0.0000000 sec
 d14: 0.0000000 sec
 MARKS: 0.0000000 sec
 ===== CHANNEL f1 =====
 NU1: 131
 P1: 6.00 usec
 PL1: -2.00 dB
 SFO1: 100.628298 MHz
 ===== CHANNEL f2 =====
 NAME: waltz16
 CPDPRG2: waltz16
 F2: 100.628298 MHz
 P2: 120.00 usec
 PL2: 120.00 dB
 PL12: 12.00 dB
 PL13: 12.00 dB
 PL14: 12.00 dB
 SFO2: 400.131008 MHz
 F2 - Processing parameters
 SI: 32768
 SF: 100.627495 MHz
 DS: 4
 MS: EX
 AS: 0
 L8: 1.00 Hz
 GB: 0
 PC: 1.40



3: Diagram of 3b and 4j



3b



4j