

Divergent Synthesis of Benzo[*d*]thiazoles via PIFA-Mediated Cyclization of β -Oxo Thioamides

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^aChangchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun, 130022,

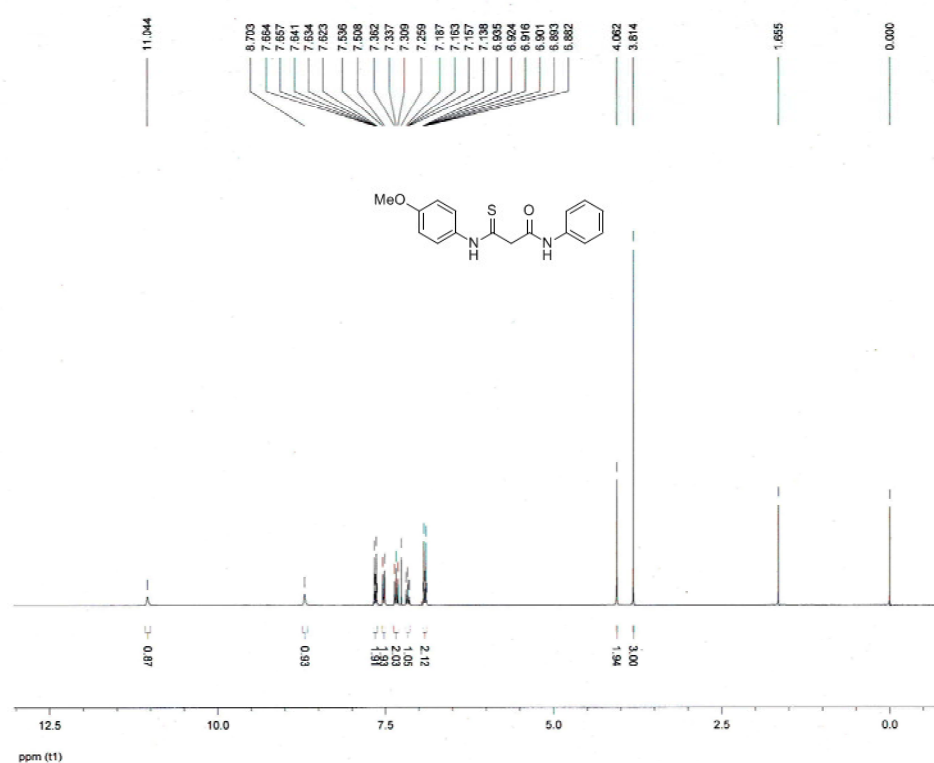
China. ^bDepartment of Chemistry, Northeast Normal University, Changchun, 130024, China.

E-mail: dwdong@ciac.jl.cn

Supplementary Material

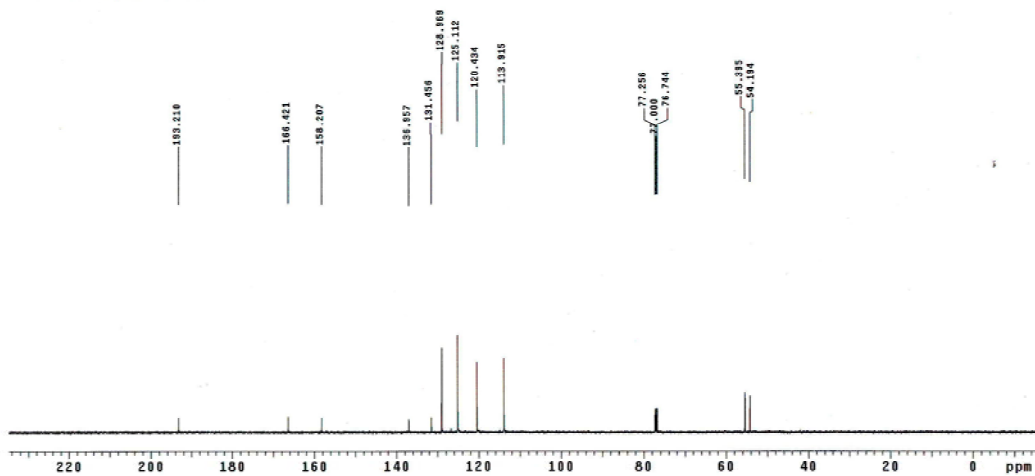
Copies of NMR spectra for compounds 1i-n, 2 and 3

1i

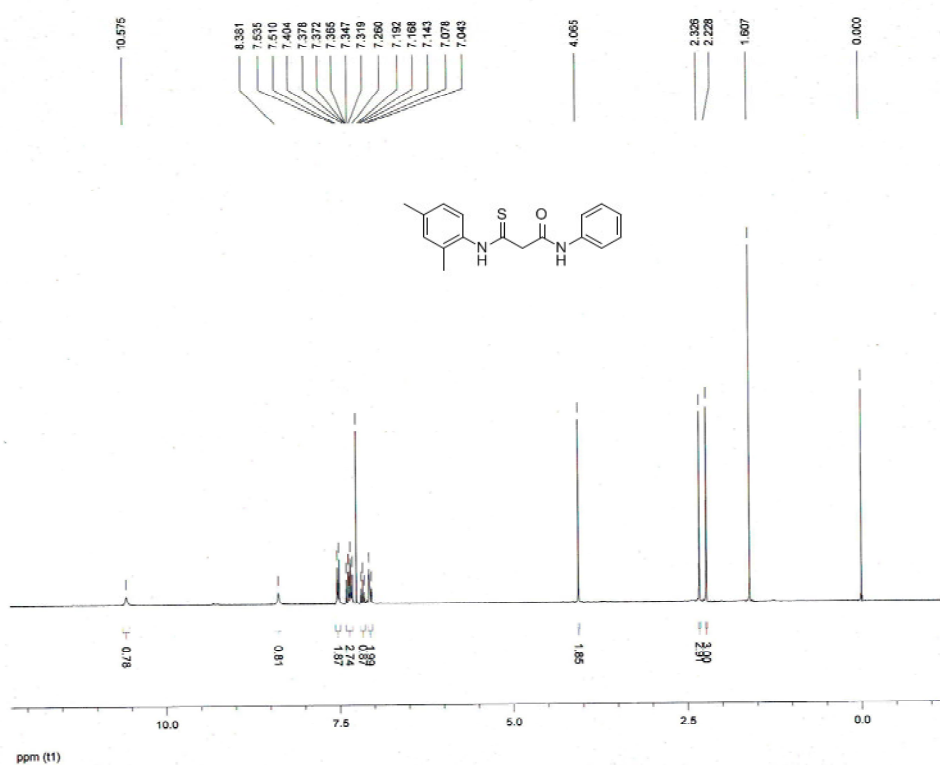


Date: 16 Jul 2009
 Document's Title: Mestres
 Spectrum Title: None
 Frequency (MHz): (f1) 300.130
 Original Points Cou (f1) 16384
 Actual Points Cou (f1) 16384
 Acquisition Time (s) (f1) 2.7329
 Spectral Width (ppm) (f1) 19.975
 Pulse Program: Unknown

STANDARD CARBON PARAMETERS
 Archive directory: /export/home/11uy/vnmrsvs/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 User: s-14-87
 File: a715
 INOVA-500 "NENU500"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.350 sec
 Width 31421.8 Hz
 84 repetitions
 OBSERVE C13, 125.6754699 MHz
 DECOUPLE H1, 499.8050895 MHz
 Power 40 dB
 CONTINUOUSLY ON
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec

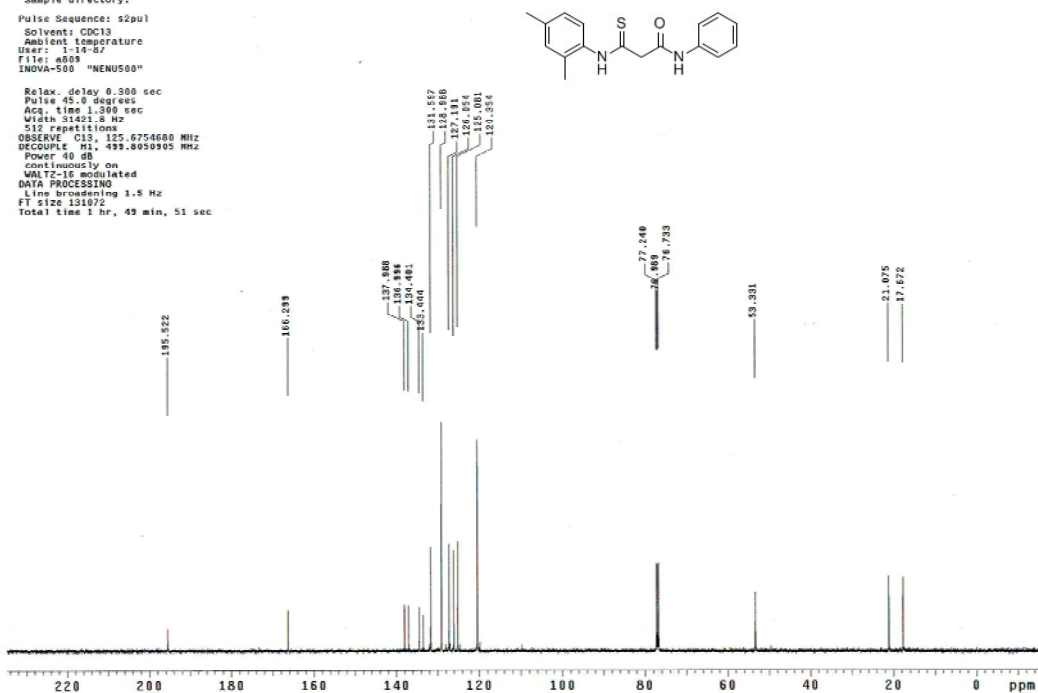


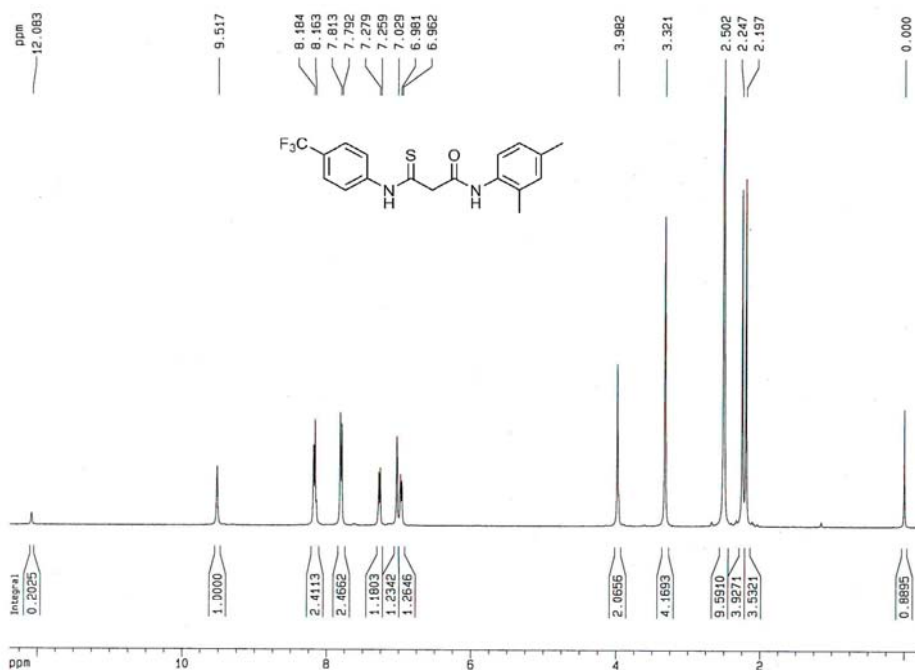
1j



Date: 24 Jul 2009
 Document's Title: Mestre1
 Spectrum Title: None
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 Original Points Cou: (f1) 16384
 Actual Points Coun: (f1) 16384
 Acquisition Time (s): (f1) 2.7329
 Spectral Width (ppm): (f1) 19.975
 Pulse Program: Unknown

STANDARD CARBON PARAMETERS
 Archive directory: /export/home/lluy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 User: 1-18-87
 File: a009
 INOVA-500 "NEU500"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 512 repetitions
 OBSERVE C13, 125.6754680 MHz
 DECOUPLE H1, 499.8090905 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec





HP-10-25-1

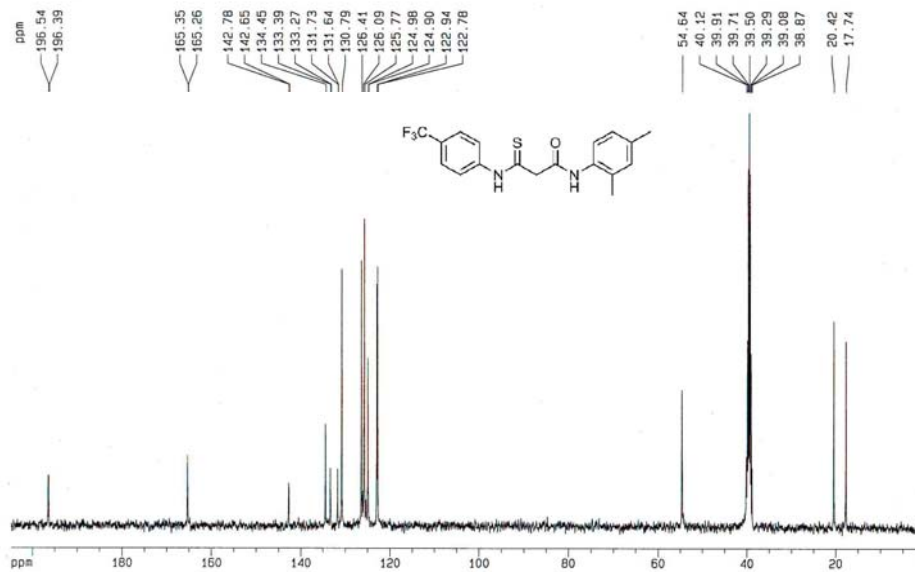
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 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101025
 Time 18.46
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 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 16384
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 5668.934 Hz
 FIDRES 0.346004 Hz
 AQ 1.4451188 sec
 RG 32
 DM 88.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 10.00000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.50 usec
 PL1 -3.00 dB
 SFO1 399.9525185 MHz

F2 - Processing parameters
 SI 85536
 SF 399.9500029 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 10.00

ID NMR plot parameters
 CX 22.00 cm
 CY 15.00 cm
 F1P 12.384 ppm
 F1 4953.08 Hz
 F2P -0.181 ppm
 F2 -72.28 Hz
 PRMCH 0.57113 ppm/c
 HZCH 228.42543 Hz/cm



HP-1026-1

Current Data Parameters
 NAME HPeng
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101026
 Time 18.28
 INSTRUM av400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TO 16384
 SOLVENT DMSO
 NS 478
 DS 0
 SWH 25062.656 Hz
 FIDRES 1.529703 Hz
 AQ 0.3269108 sec
 RG 8192
 DM 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.69999999 sec
 d11 0.03000000 sec

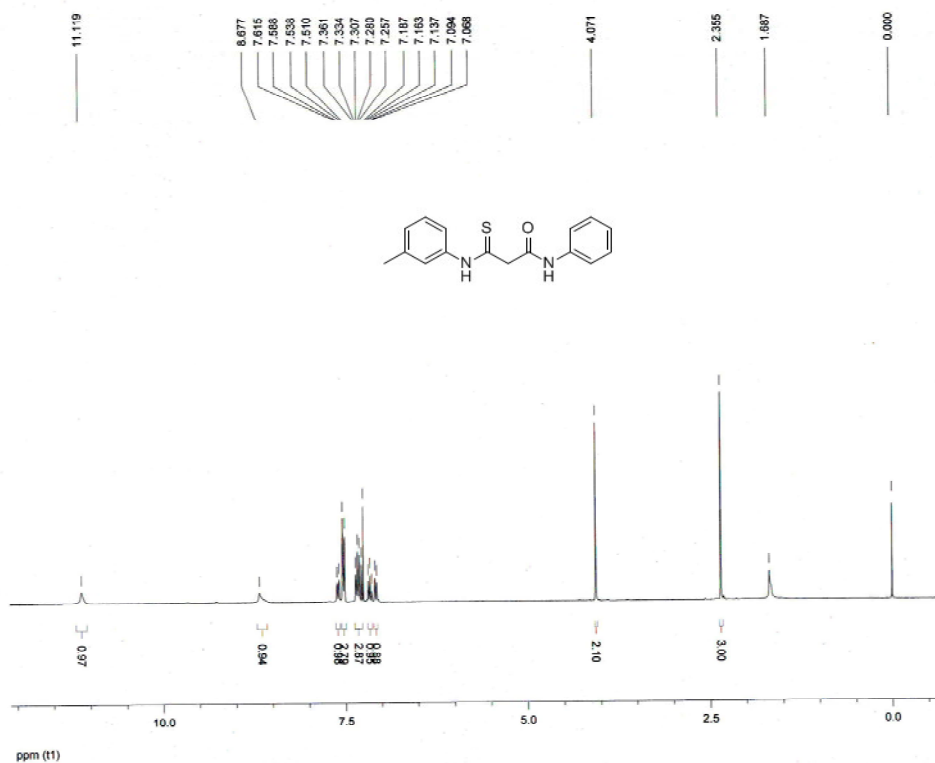
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 NUC1 13C
 P1 2.80 usec
 PL1 -3.00 dB
 SFO1 100.5785294 MHz

***** CHANNEL f2 *****
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 NUC2 1H
 PCDU2 80.00 usec
 PL2 -3.00 dB
 PL12 18.20 dB
 SFO2 399.9515998 MHz

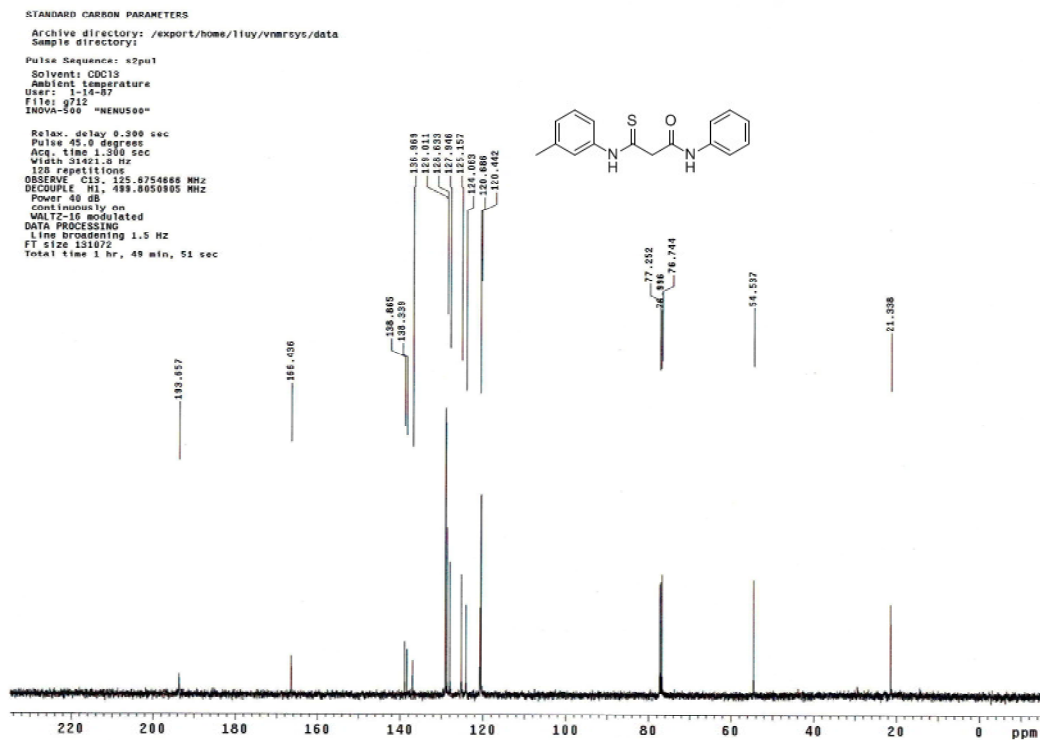
F2 - Processing parameters
 SI 85536
 SF 100.5675982 MHz
 WDW EM
 SSB 0
 LB 4.00 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 22.00 cm
 CY 10.00 cm
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 F1 20596.71 Hz
 F2P -0.464 ppm
 F2 -46.69 Hz
 PRMCH 9.33041 ppm/c
 HZCH 938.33600 Hz/cm

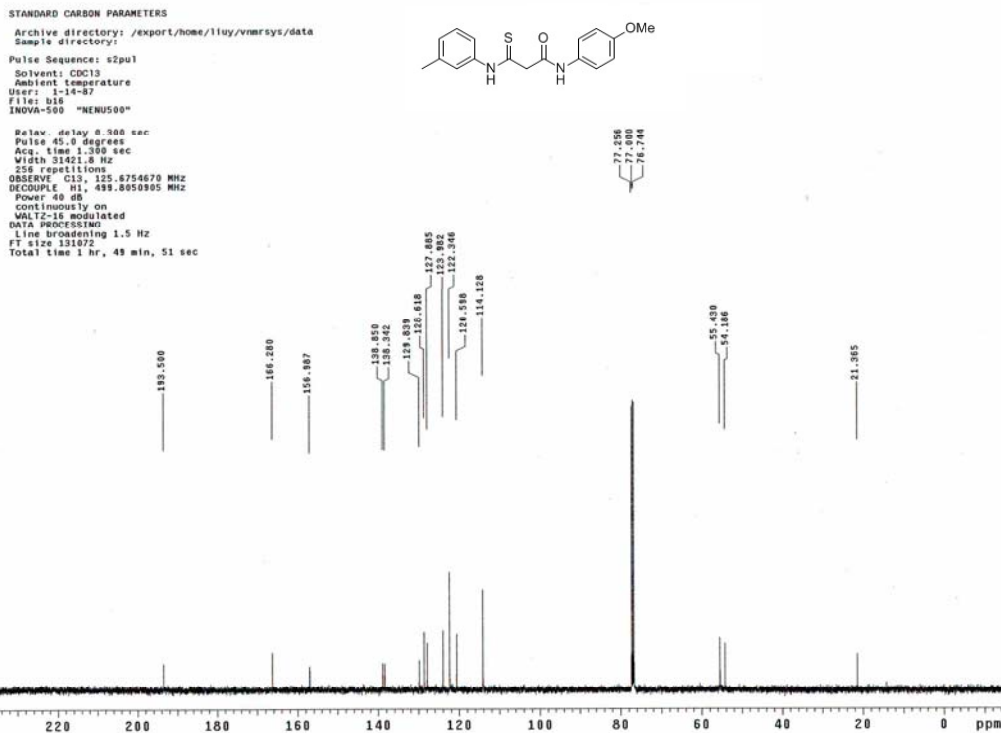
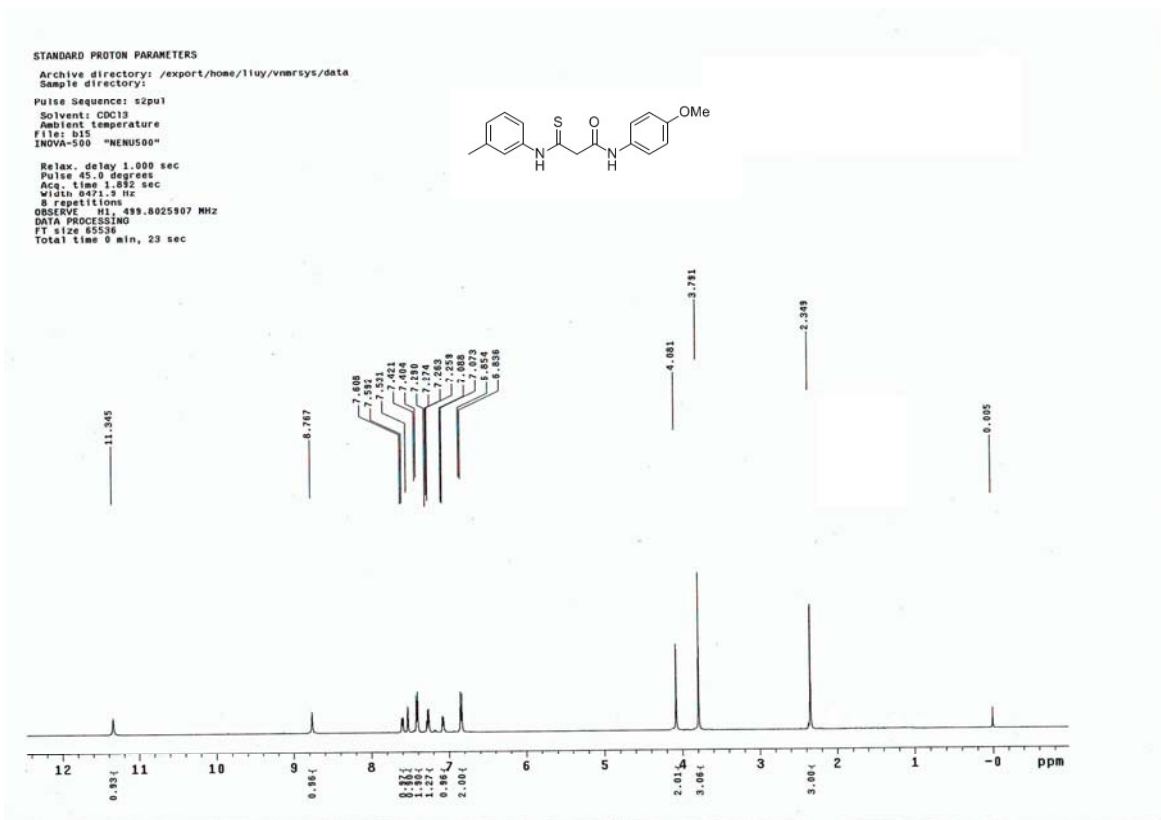
1m



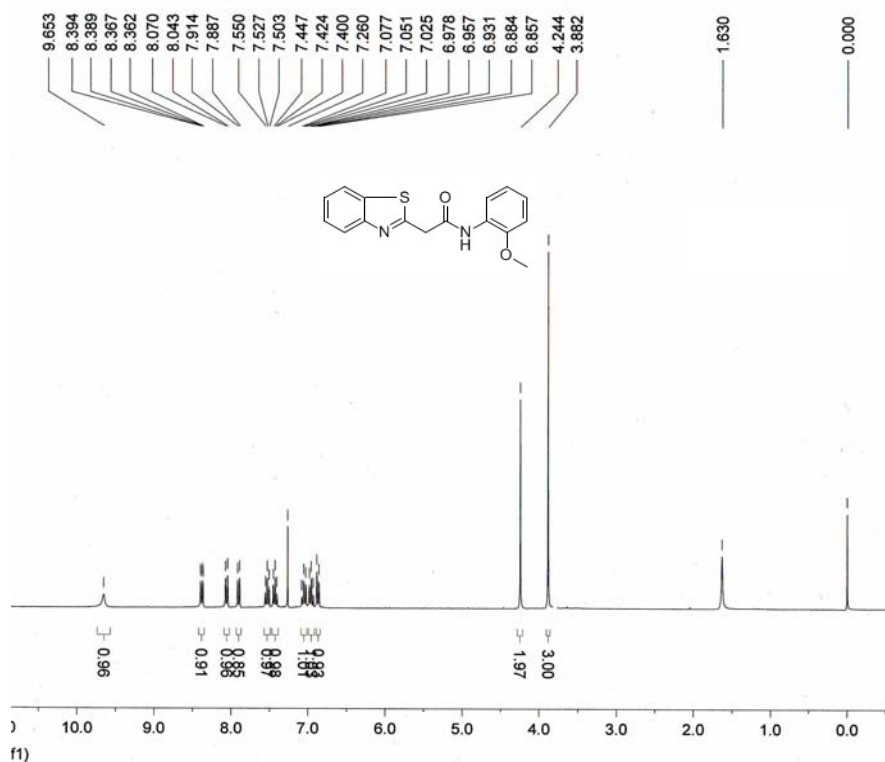
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Original Points Cou: (f1) 16384
Actual Points Coun: (f1) 16384
Acquisition Time (s): (f1) 2.7329
Spectral Width (ppm): (f1) 19.975
Pulse Program: Unknown



1n



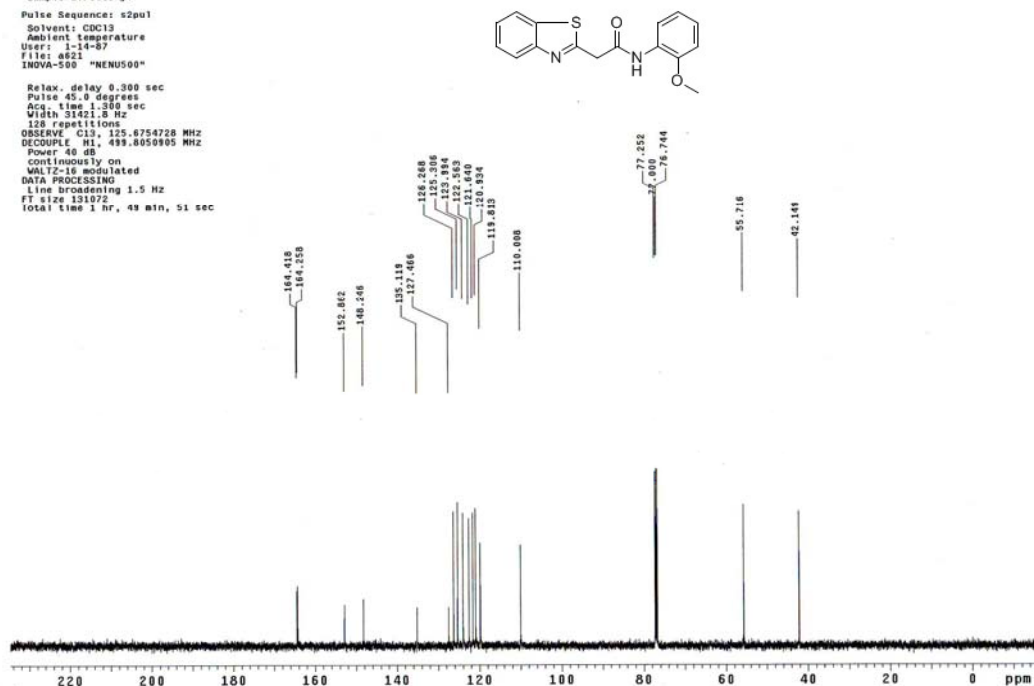
2a



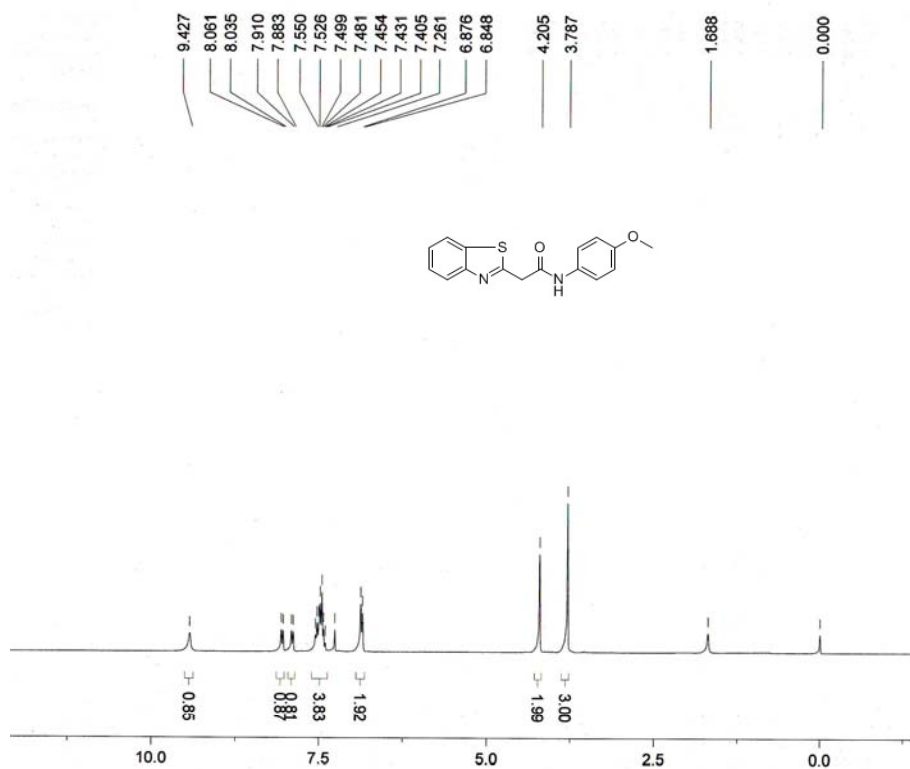
Date: 12 Nov 2009
 Document's Title: 1
 Spectrum Title: None
 Frequency (MHz): (f1) 300.132
 Original Points Count: (f1) 16384
 Actual Points Count: (f1) 32768
 Acquisition Time (sec): (f1) 2.7329
 Spectral Width (ppm): (f1) 19.975
 Pulse Program: ZG
 Temperature: 673.16
 Number of Scans: 5
 Acq. Date: Fri Jun 05 04:43:12 PM

STANDARD CARBON PARAMETERS

Archive directory: /export/home/11uy/vnmrSYS/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 User: i-14-87
 File: 0823
 INOVA-500 "NENU500"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.390 sec
 Width 31421.8 Hz
 128 repetitions
 OBSERVE C13, 125.6754728 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power 49 dB
 continuously on
 MWTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec

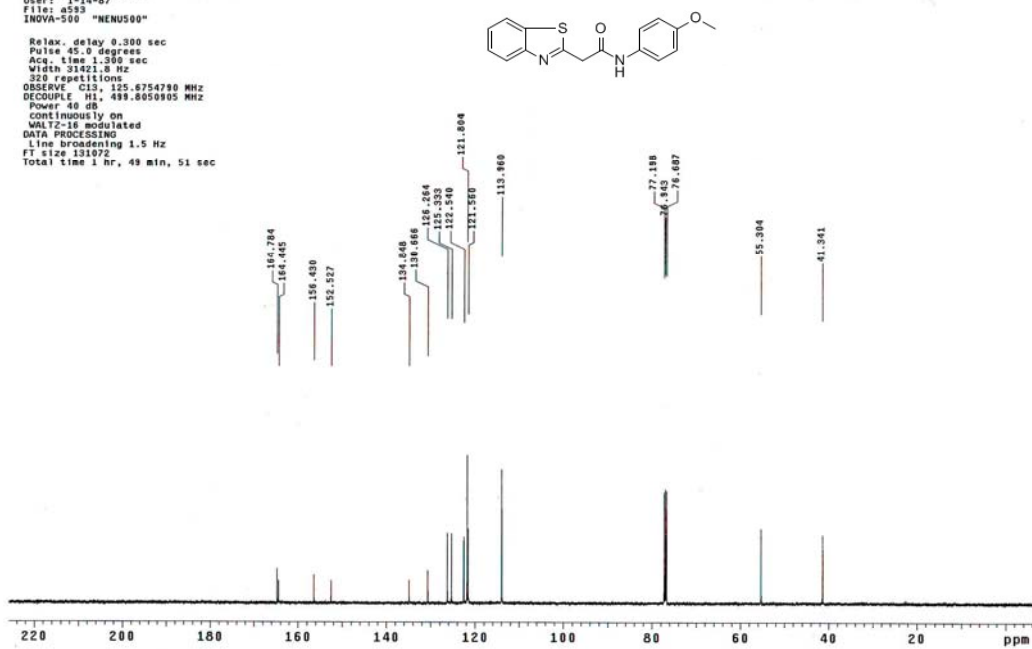


2b

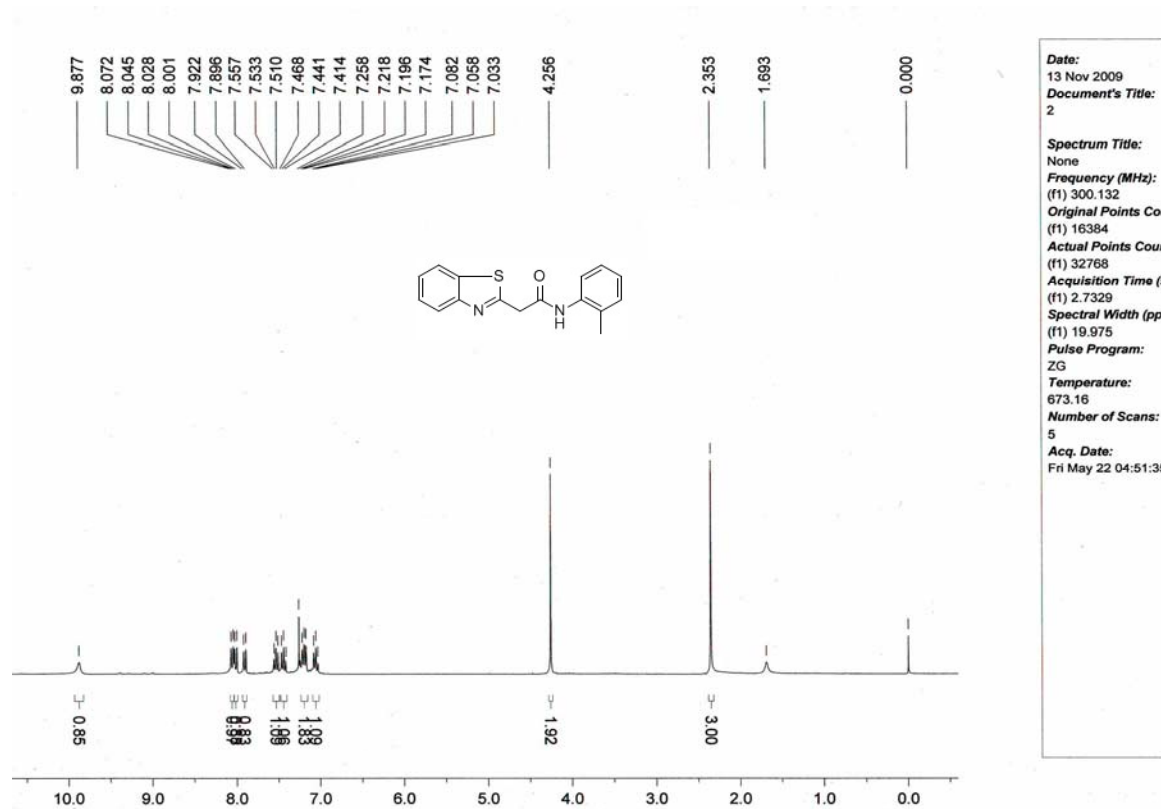


Date: 10 Jun 2009
 Document's Title: Mestrel
 Spectrum Title: None
 Frequency (MHz): (f1) 300.130
 Original Points Count: (f1) 16384
 Actual Points Count: (f1) 16384
 Acquisition Time (sec): (f1) 2.7329
 Spectral Width (ppm): (f1) 19.975
 Pulse Program: Unknown

STANDARD CARBON PARAMETERS
 Archive directory: /export/home/11uy/vmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient Temperature
 User: 1-14-87
 File: 4553
 INOVA-500 "NENUS90"
 Relax. delay 0.300 sec
 Pulse 45.0 degree
 Acq. time 1.300 sec
 Width 31421.0 Hz
 320 repetitions
 OBSERVE C13, 125.6754780 MHz
 DECOUPLE H1, 499.8650805 MHz
 Power 40 db
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131872
 Total time 1 hr, 49 min, 51 sec

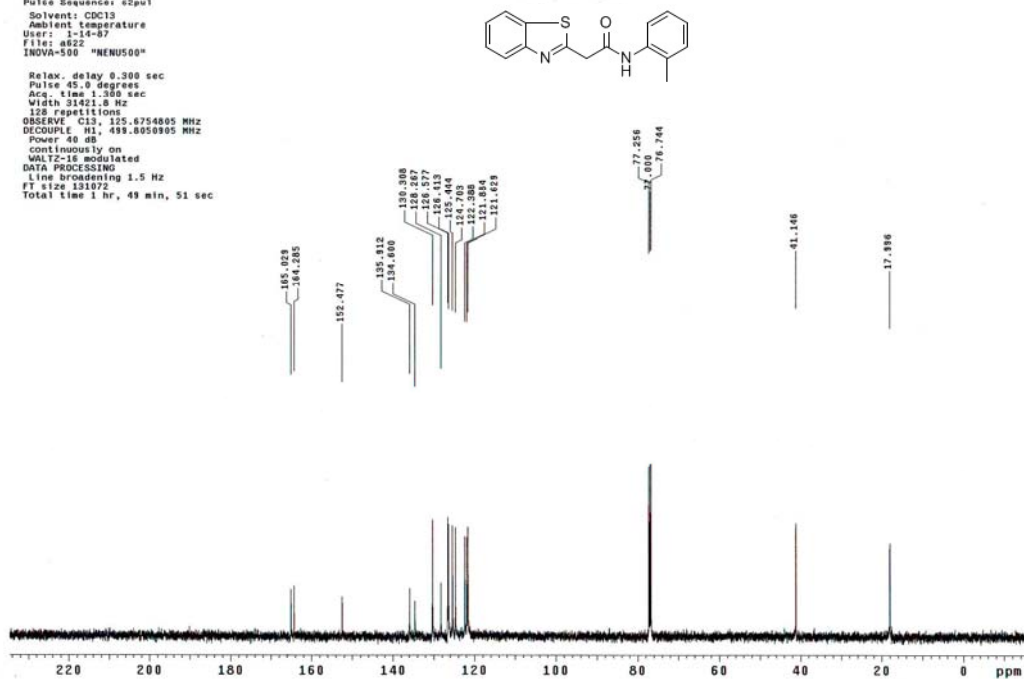


2c

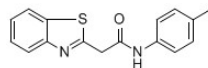
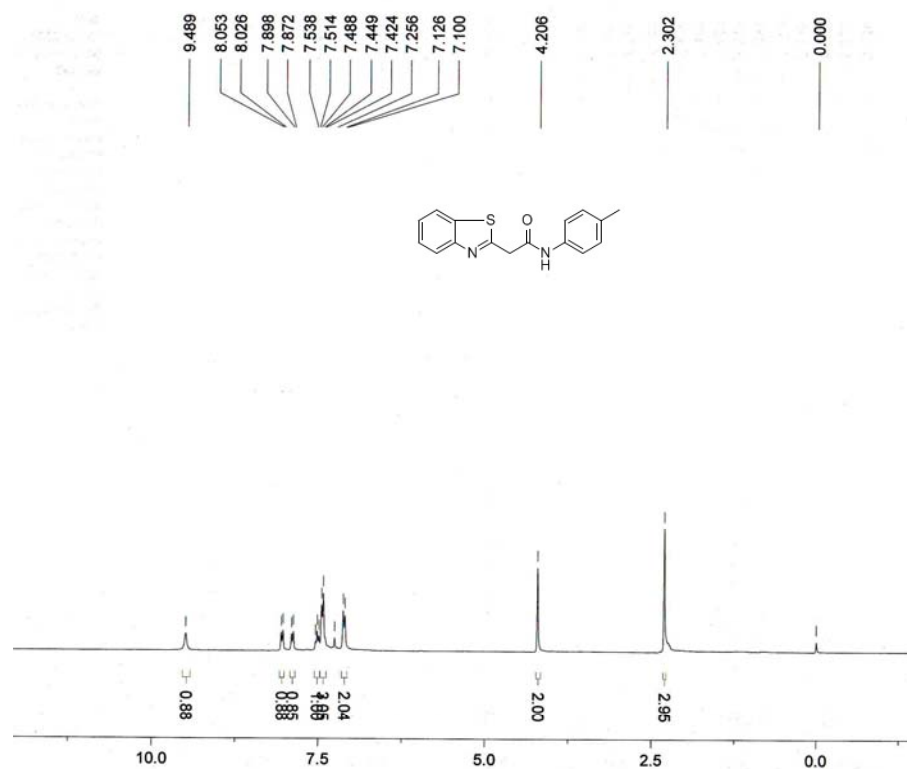


STANDARD CARBON PARAMETERS

Archive directory: /export/home/liuy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDC13
 Ambient Temperature
 User: i-14-87
 File: a622
 INOVA-500 "NENUS00"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.380 sec
 Width 31421.8 Hz
 128 repetitions
 OBSERVE c13, 125.6754805 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec



2d



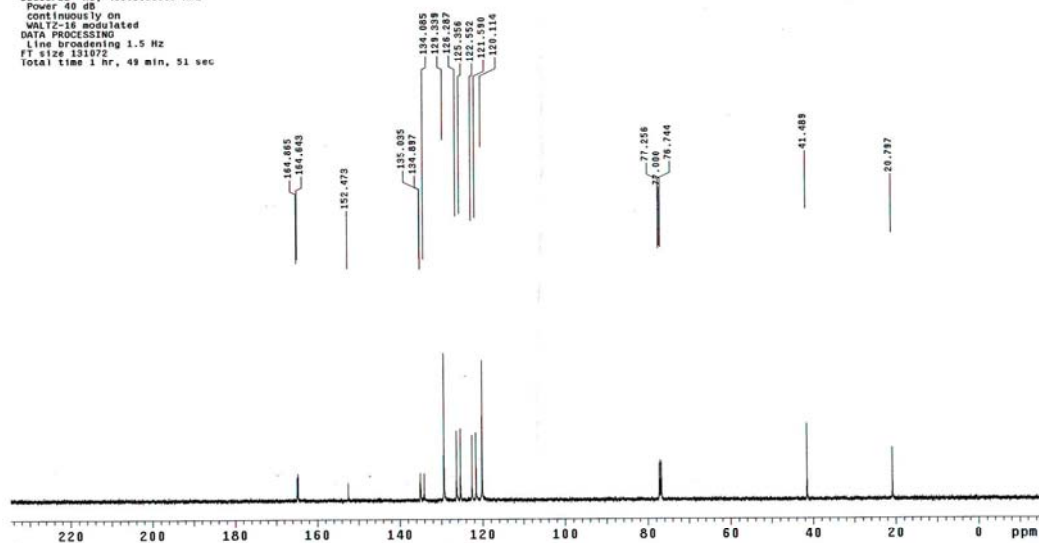
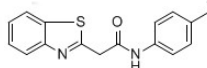
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10 Jun 2009
Document's Title:
Mestre2
Spectrum Title:
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Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 16384
Acquisition Time (sec):
(f1) 2.7329
Spectral Width (ppm):
(f1) 19.975
Pulse Program:
Unknown

STANDARD CARBON PARAMETERS

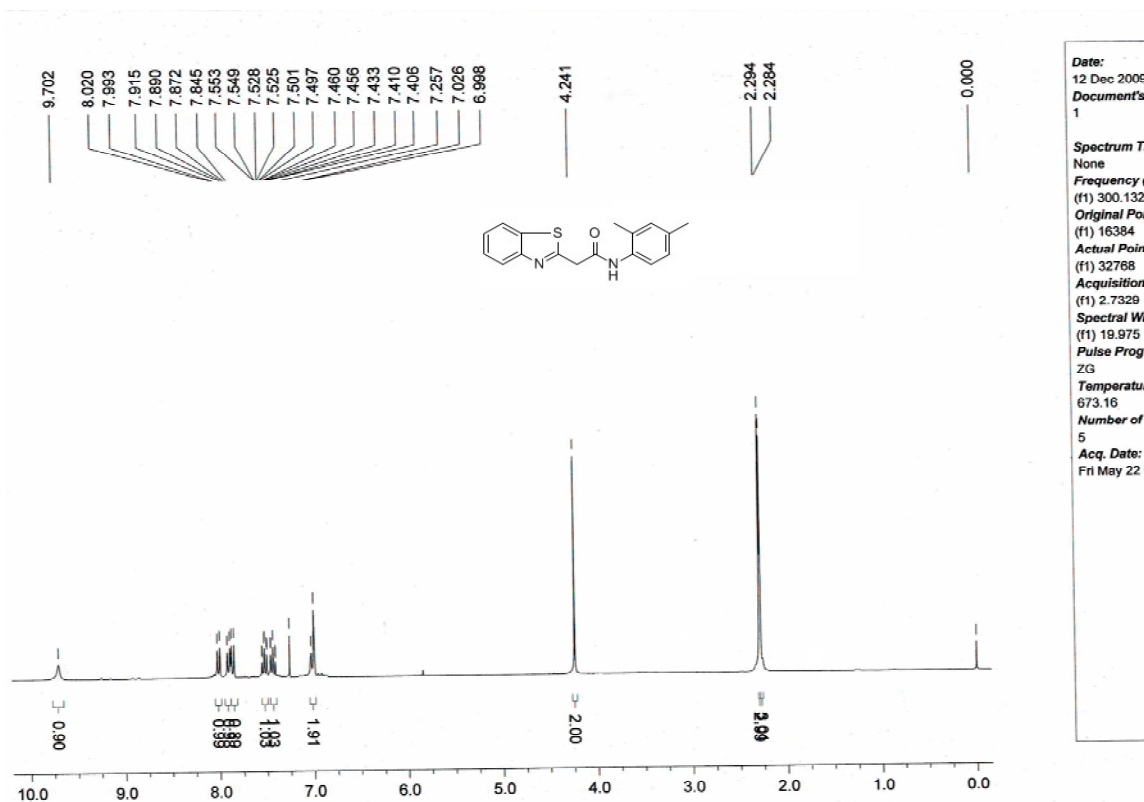
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Sample directory:

Pulse Sequence: s2ou1
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: 8071
INOVA-500 "NENUS00"

Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 Repetitions
OBSERVE C13, 125.6754747 MHz
DECOUPLE H1, 499.8059905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec



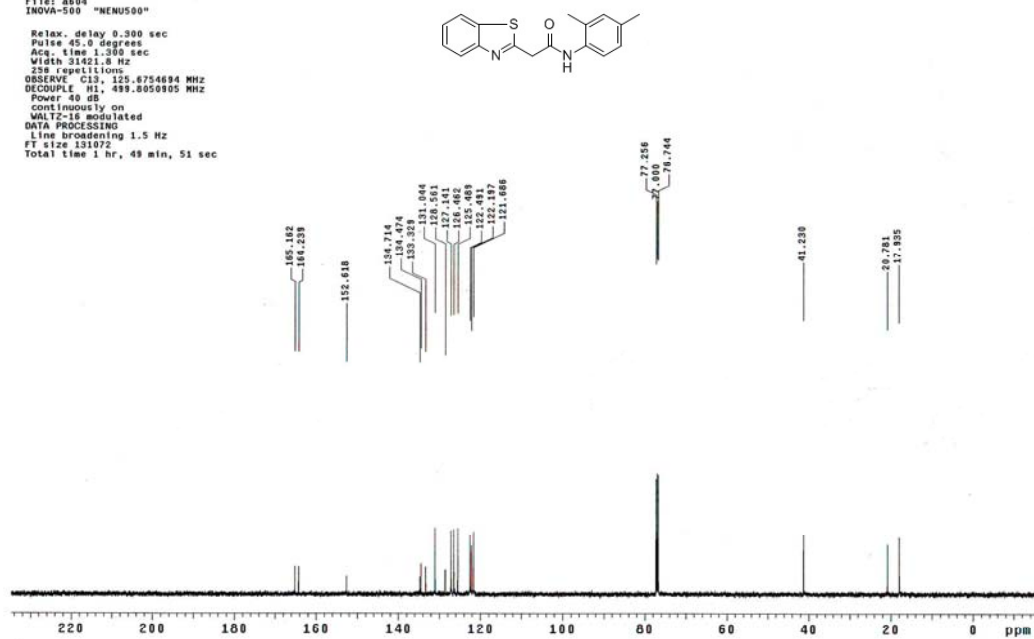
2e



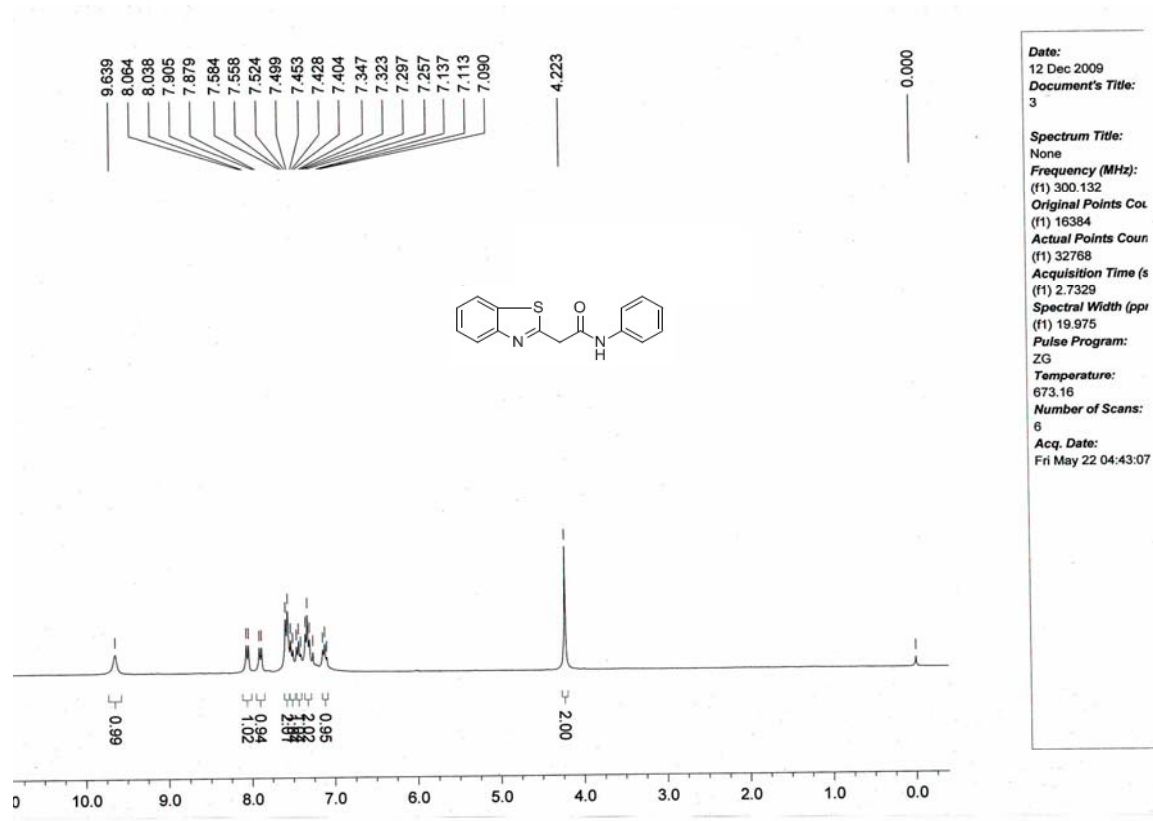
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 Spectrum Title: None
 Frequency (f1): 300.132
 Original Point (f1): 16384
 Actual Point (f1): 32768
 Acquisition (f1): 2.7329
 Spectral Width (f1): 19.975
 Pulse Program: zg
 Temperature: 673.16
 Number of: 5
 Acq. Date: Fri May 22 2009

STANDARD CARBON PARAMETERS

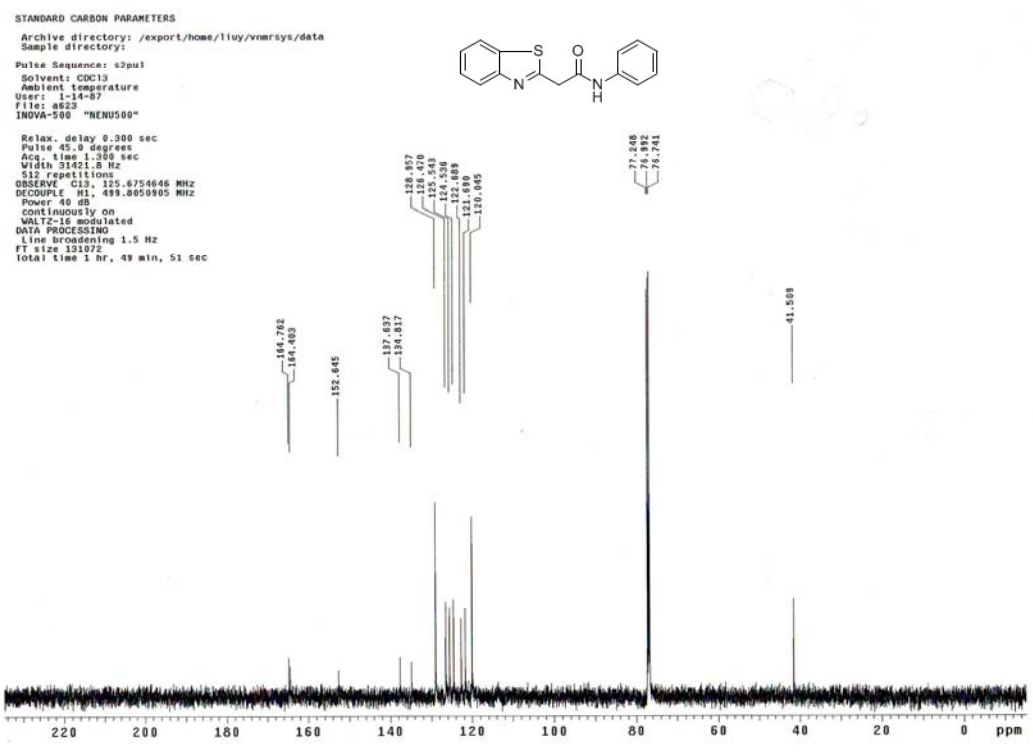
Archive directory: /export/home/lluy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 User: j-14-87
 File: s894
 INOVA-500 "HENU500"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.380 sec
 Width 31421.8 Hz
 256 repetitions
 OBSERVE C13, 125.6754694 MHz
 DECOUPLE H1, 499.8050305 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec



2f

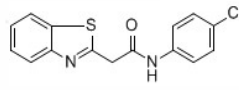
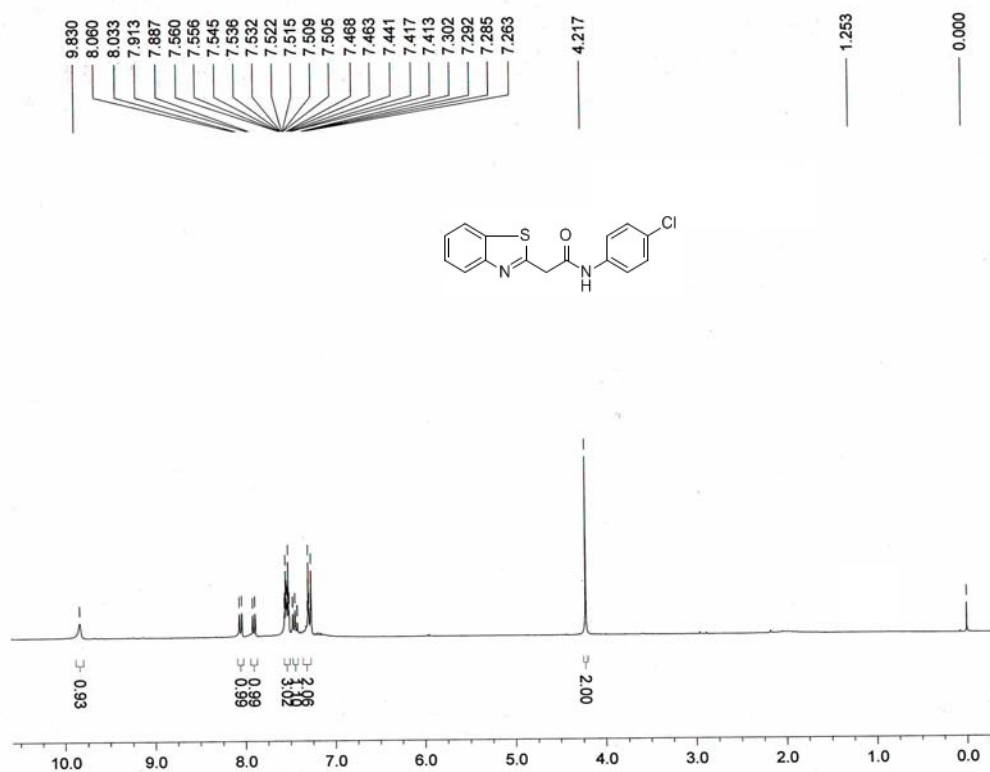


Date: 12 Dec 2009
 Document's Title: 3
 Spectrum Title: None
 Frequency (MHz): (f1) 300.132
 Original Points Co: (f1) 16384
 Actual Points Coun: (f1) 32768
 Acquisition Time (s): (f1) 2.7329
 Spectral Width (pp): (f1) 19.975
 Pulse Program: ZG
 Temperature: 673.16
 Number of Scans: 6
 Acq. Date: Fri May 22 04:43:07



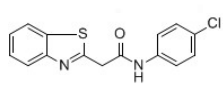
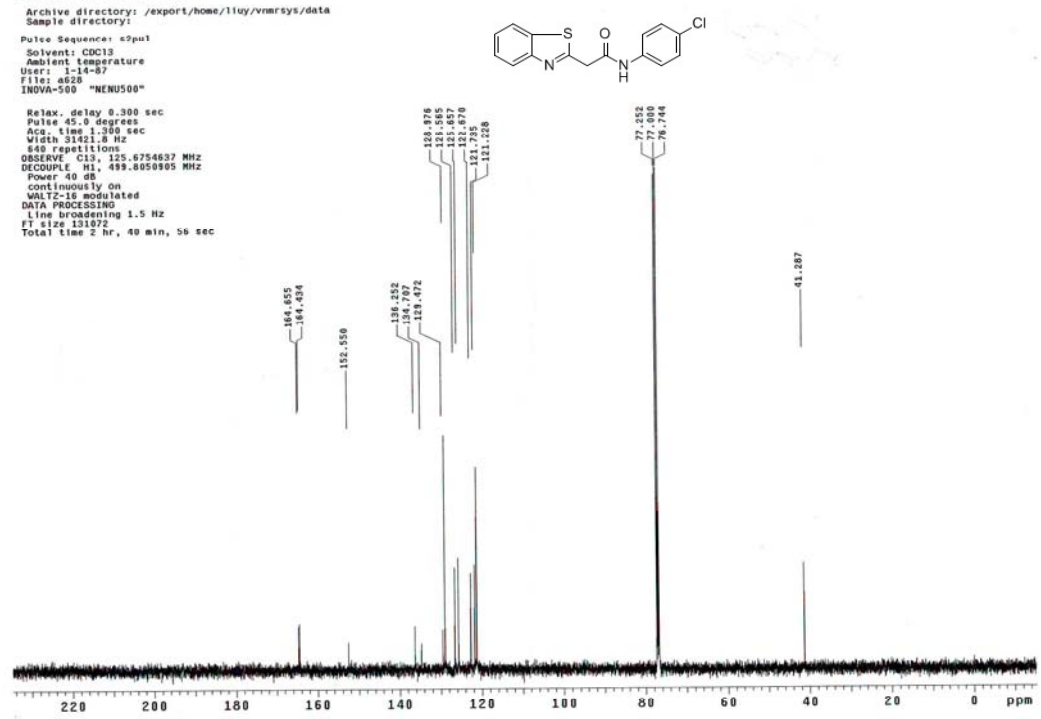
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 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 User: 1-14-07
 File: 4823
 INOVA-500 "NENUS00"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 SIZ repetitions
 OBSERVE C13, 125.6754646 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec

2g

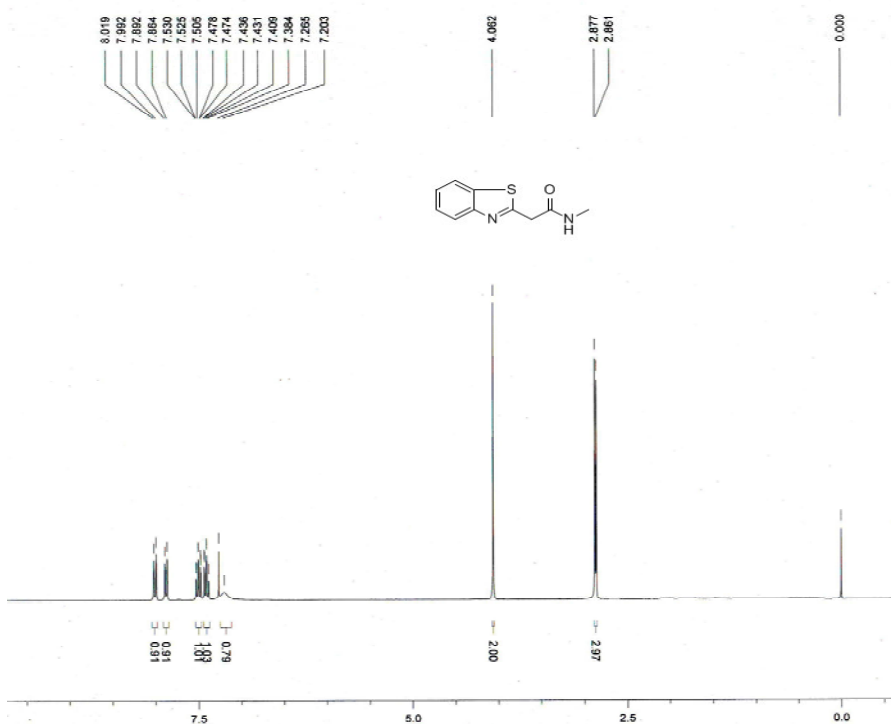


Date: 12 Dec 2009
 Document's 4
 Spectrum T1
 None
 Frequency (f1) 300.132
 Original Poi (f1) 16384
 Actual Poim (f1) 32768
 Acquisition (f1) 2.7329
 Spectral Wh (f1) 19.975
 Pulse Progr ZG
 Temperatur 673.16
 Number of : 6
 Acq. Date: Fri May 22 C

STANDARD CARBON PARAMETERS
 Archive directory: /export/home/liuy/vnmrsys/data
 Sample directory:
 Pulse Sequence: c9pul
 Solvent: CDCl3
 Ambient temperature
 User: i-14-87
 File: a628
 INOVA-500 "NENU500"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acc. time 1.300 sec
 Width 31421.0 Hz
 840 repetitions
 OBSERVE Ch1: 125.6754637 MHz
 DECOUPLE H1: 499.8050805 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 2 hr, 40 min, 56 sec

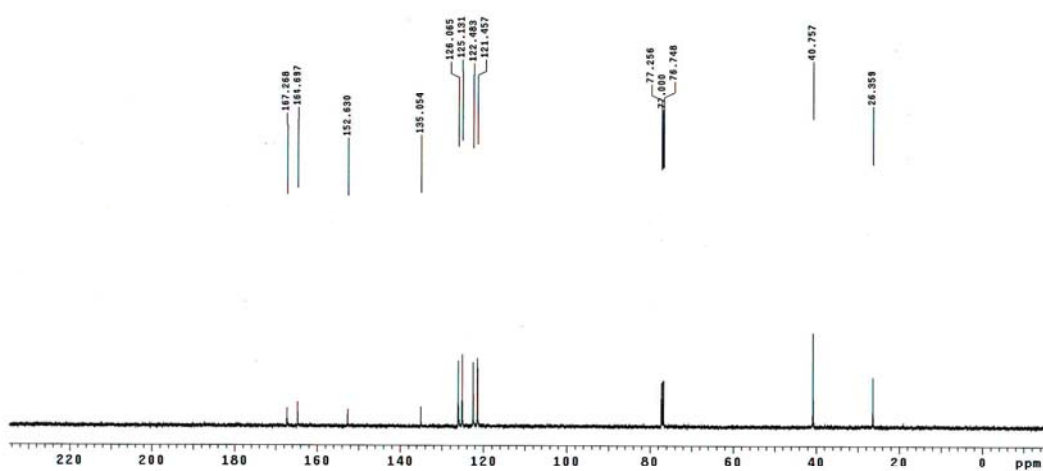


2h

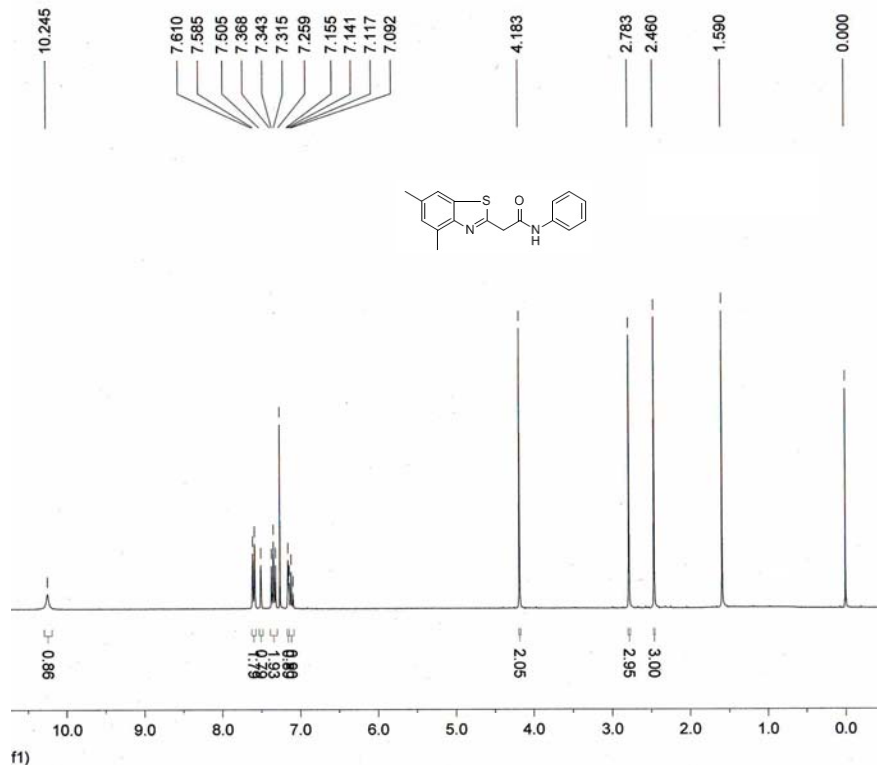


Date: 17 Jul 2009
 Document's Title: Mestre5
 Spectrum Title: None
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 Actual Points Count: (f1) 16384
 Acquisition Time (sec): (f1) 2.7329
 Spectral Width (ppm): (f1) 19.975
 Pulse Program: Unknown

STANDARD CARBON PARAMETERS
 Archive directory: /export/home/lluy/vmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient Temperature
 User: 1-18-87
 File: s714
 INOVA-500 "MESTRE500"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 64 repetitions
 OBSERVE C13, 125.6754795 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power 40 dB
 continuously on
 MILT2-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec

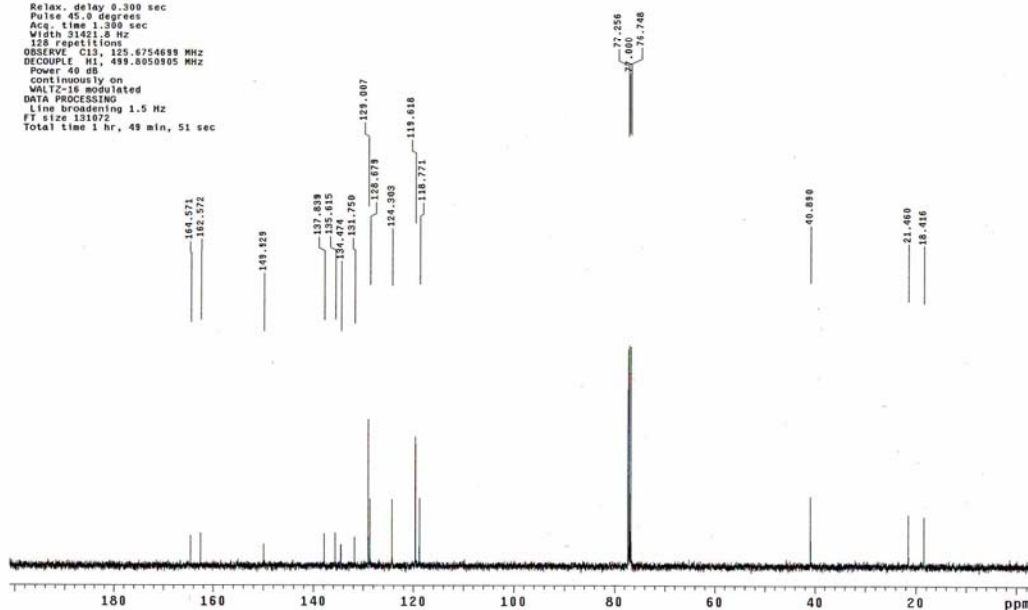
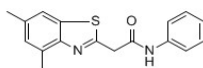


2j

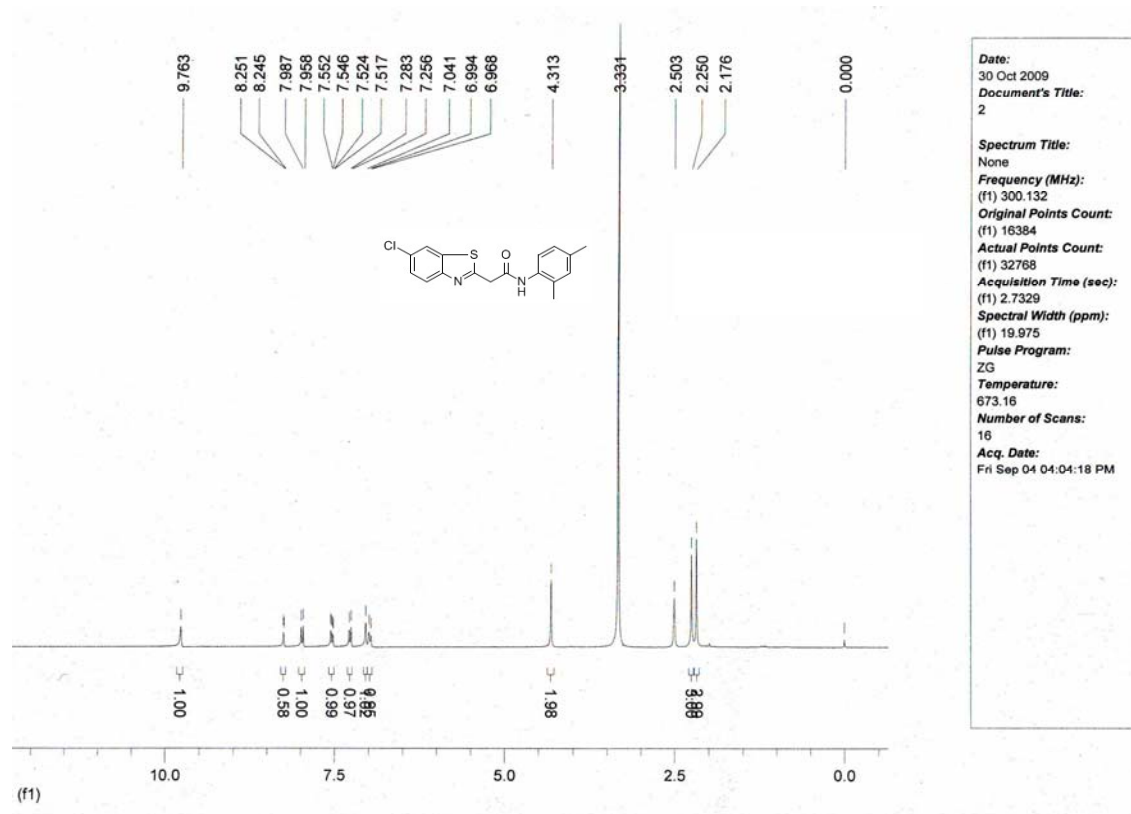


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 Original Points Count: (f1) 16384
 Actual Points Count: (f1) 32768
 Acquisition Time (sec): (f1) 2.7329
 Spectral Width (ppm): (f1) 19.975
 Pulse Program: ZG
 Temperature: 673.16
 Number of Scans: 4
 Acq. Date: Fri Jul 17 03:59:21 PM

STANDARD CARBON PARAMETERS
 Archive directory: /export/home/lluy/vnmrsys/data
 Sample directory:
 Pulse Sequence: e2pu1
 Solvent: CDCl3
 Ambient temperature
 User: i-14-87
 File: a887
 INOVA-500 "MNU500"
 Relax. delay 9.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.2 Hz
 128 Repetitions
 OBSERVE C13, 125.6750689 MHz
 DECOUPLE H1, 499.9059885 MHz
 Power 40 dB
 Continuous by on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec



2k



STANDARD CARBON PARAMETERS

Archive directory: /export/home/lluy/vnmrsys/data
Sample directory:

Pulse Sequence: s2pul

Solvent: DMSO

Ambient temperature

User: 1-14-87

File: s890

INNOVA-500 "MENU500"

Relax. delay 0.300 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 31421.8 Hz

259 repetitions

OBSERVE C13, 125.6780545 MHz

DECOUPLE H1, 499.8074646 MHz

Power 40 dB

continuous on

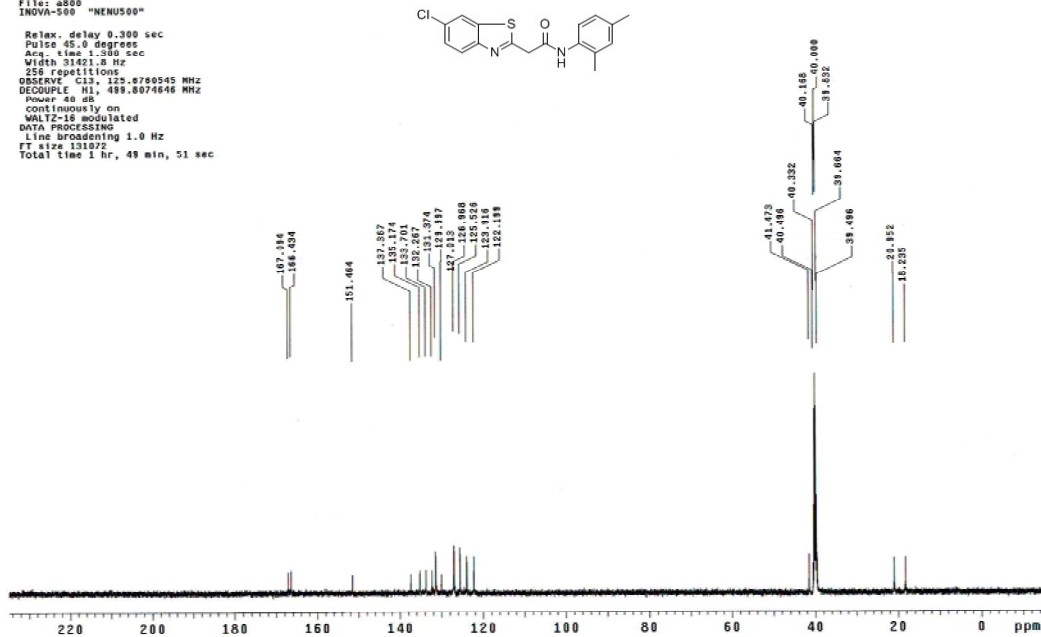
WALTZ-16 modulated

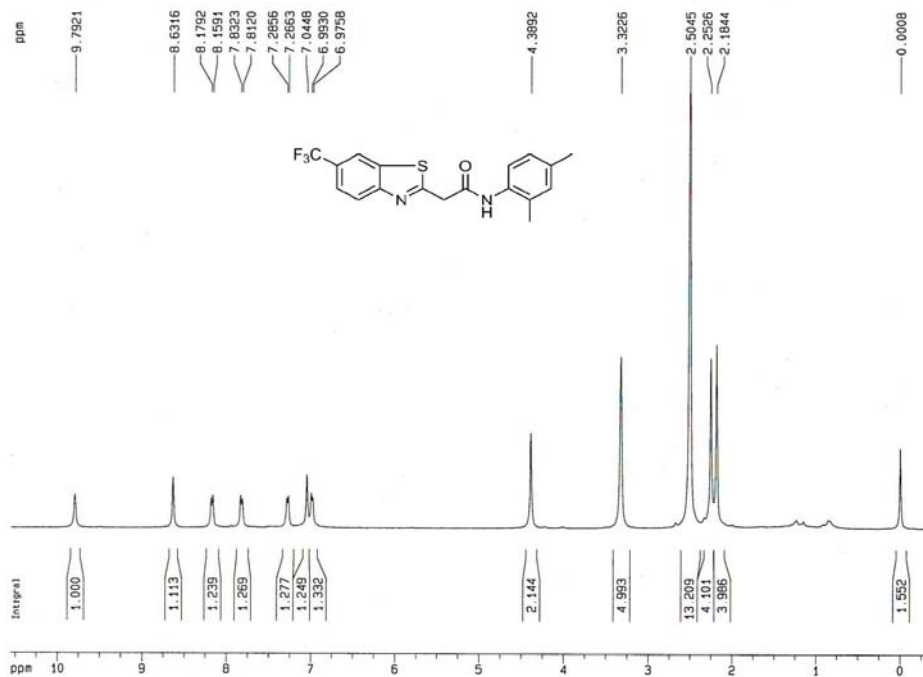
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 1 hr, 49 min, 51 sec





HP-10-25-2

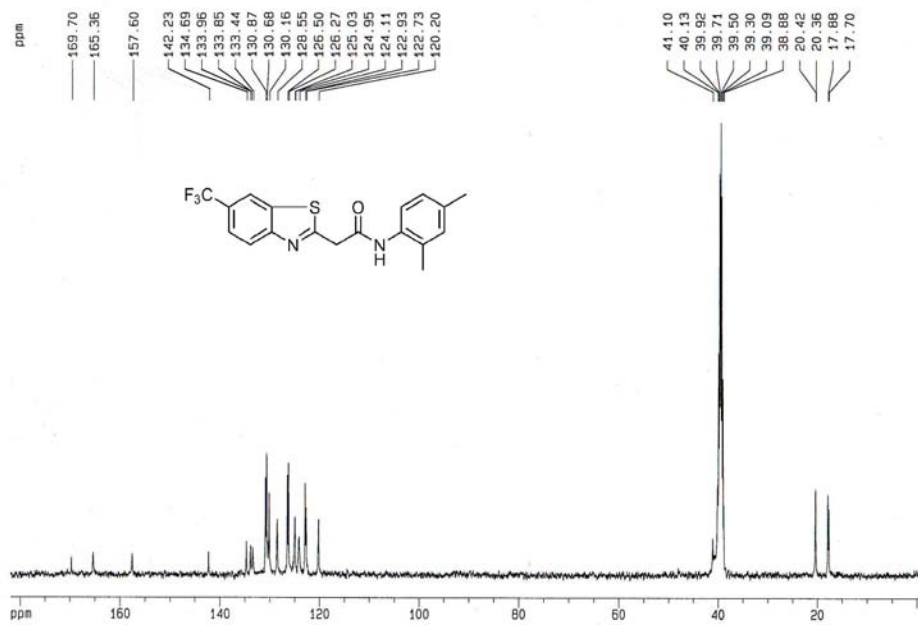
Current Data Parameters
 NAME HPeng
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
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 Time 18.49
 INSTRUM av400
 PROBHD 5 mm QNP 1H/13
 PULPROG zg
 TD 16384
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 5668.934 Hz
 FIDRES 0.345004 Hz
 AQ 1.4451188 sec
 RG 32
 DM 88.200 usec
 DE 6.00 usec
 TE 300.0 K
 D1 10.0000000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 6.50 usec
 PL1 -3.00 dB
 SF01 399.9525185 MHz

F2 - Processing parameters
 SI 65536
 SF 399.9500025 MHz
 WDW EM
 SSB 0
 LB 0.50 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 12.00 cm
 F1P 10.554 ppm
 F1 4220.93 Hz
 F2P -0.351 ppm
 F2 -140.31 Hz
 PPMCH 0.49566 ppm/c
 HZCM 198.23842 Hz/cm



HP1026-2

Current Data Parameters
 NAME HPeng
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20101026
 Time 18.41
 INSTRUM av400
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 16384
 SOLVENT DMSO
 NS 2143
 DS 0
 SWH 25062.656 Hz
 FIDRES 1.529703 Hz
 AQ 0.3269108 sec
 RG 8132
 DM 19.950 usec
 DE 6.00 usec
 TE 300.0 K
 D1 0.69999999 sec
 d11 0.03000000 sec

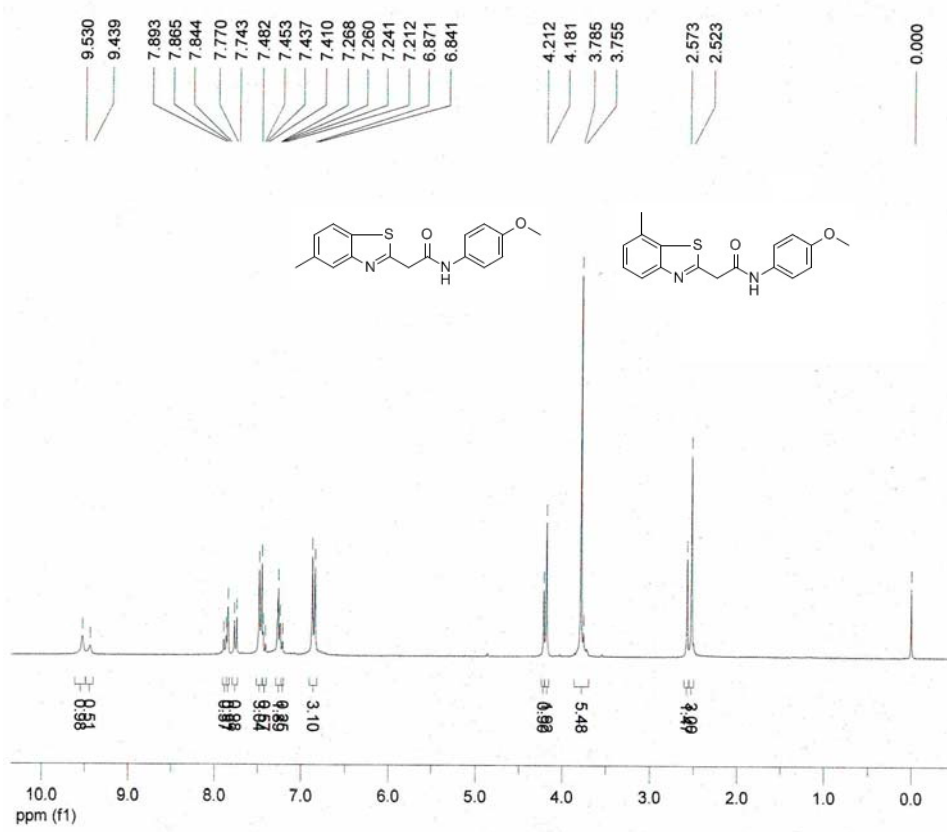
***** CHANNEL f1 *****
 NUC1 13C
 P1 2.80 usec
 PL1 -3.00 dB
 SF01 100.5785294 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -3.00 dB
 PL12 18.20 dB
 SF02 399.9515998 MHz

F2 - Processing parameters
 SI 65536
 SF 100.5679578 MHz
 WDW EM
 SSB 0
 LB 4.00 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 22.00 cm
 CY 10.00 cm
 F1P 181.934 ppm
 F1 18296.65 Hz
 F2P -1.062 ppm
 F2 -106.84 Hz
 PPMCH 8.31802 ppm/cm
 HZCM 836.52264 Hz/cm

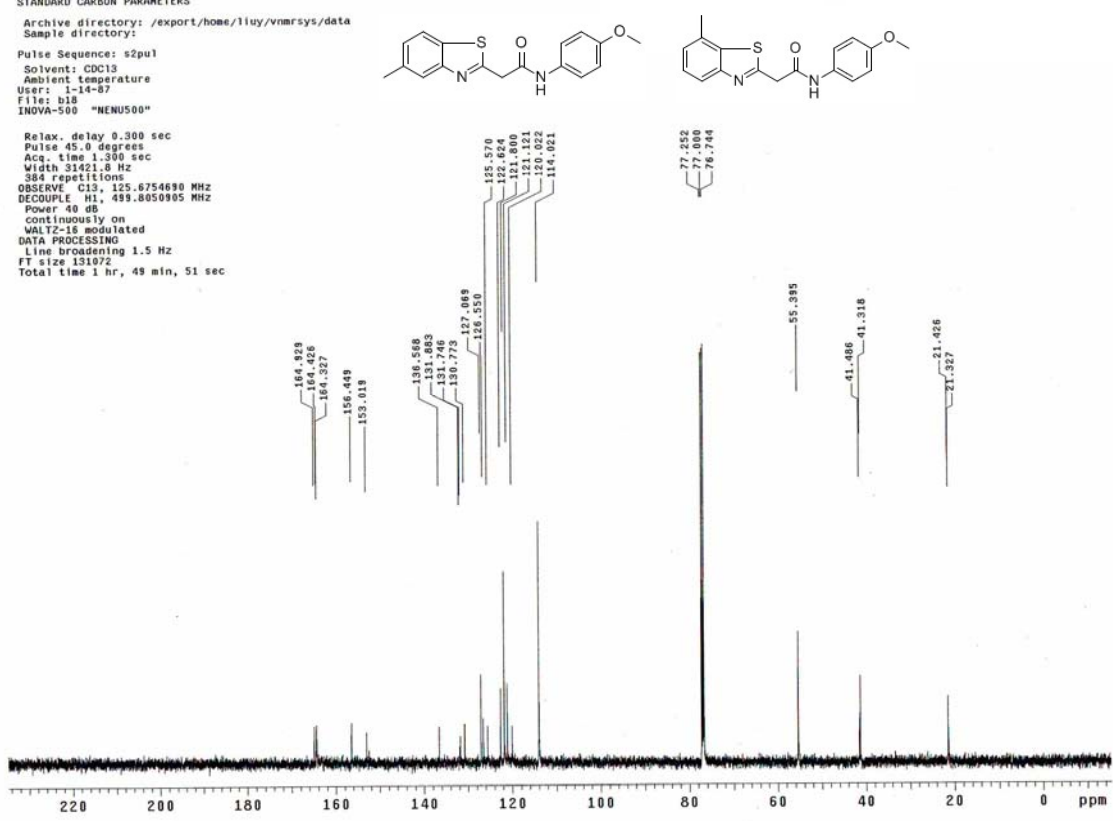
2n-1/2n-2(2:1)



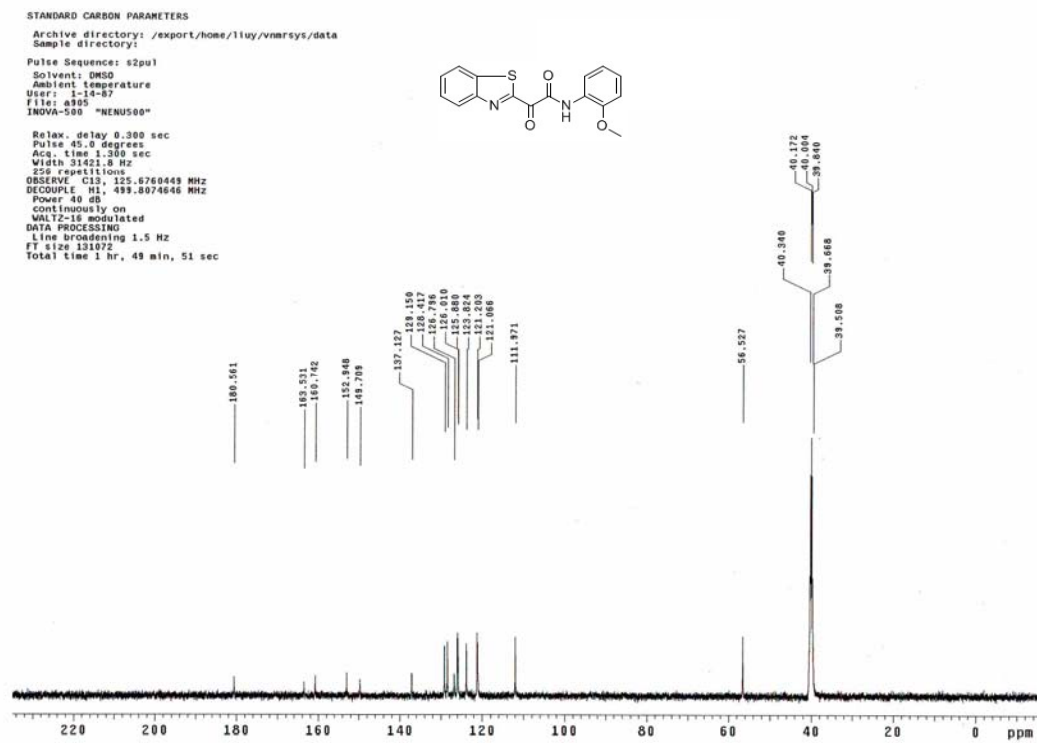
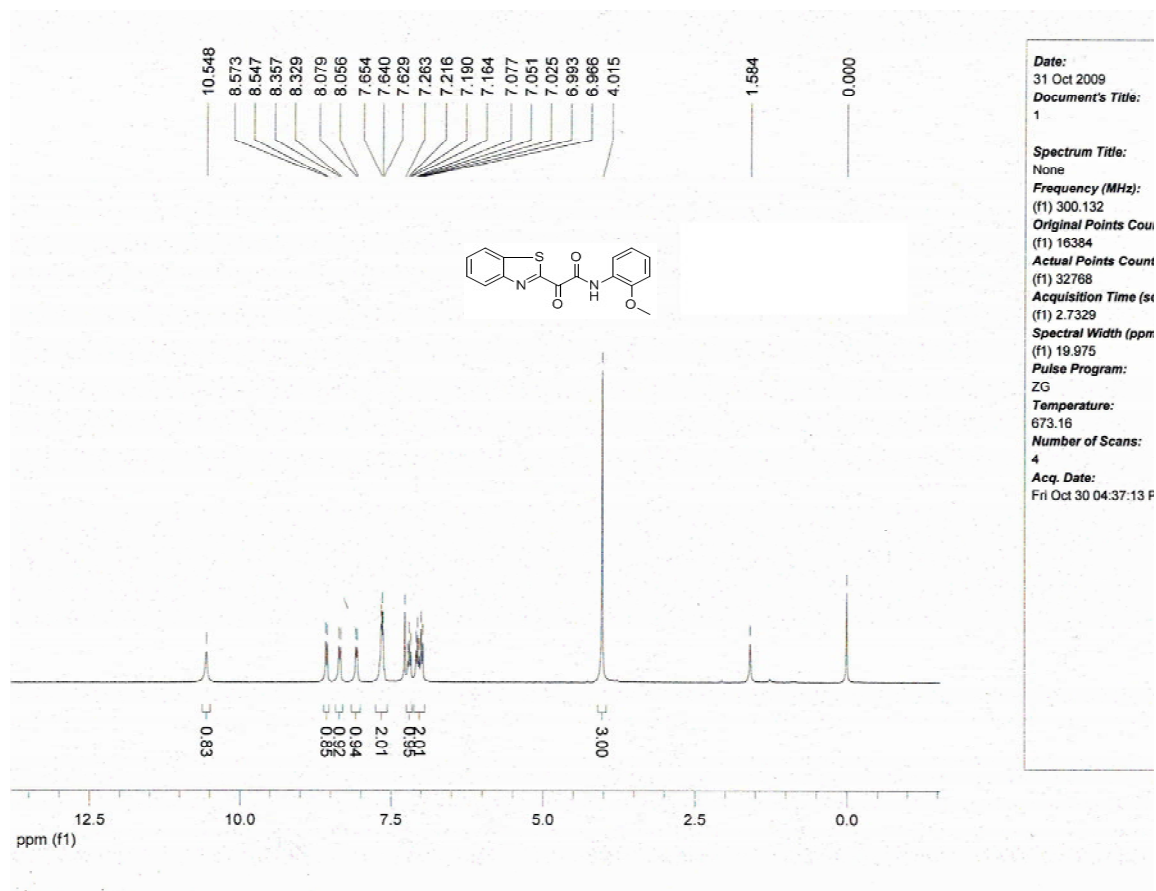
Date: 28 Nov 2009
 Document's Title: 1
 Spectrum Title: None
 Frequency (MHz): (f1) 300.132
 Original Points Co: (f1) 16384
 Actual Points Cour: (f1) 32768
 Acquisition Time (s): (f1) 2.7329
 Spectral Width (pp): (f1) 19.975
 Pulse Program: ZG
 Temperature: 673.16
 Number of Scans: 4
 Acq. Date: Fri Nov 27 04:28:08

STANDARD CARBON PARAMETERS
 Archive directory: /export/home/liuy/vnmrSYS/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 User: 1-14-87
 File: b19
 INOVA-500 "MENU500"

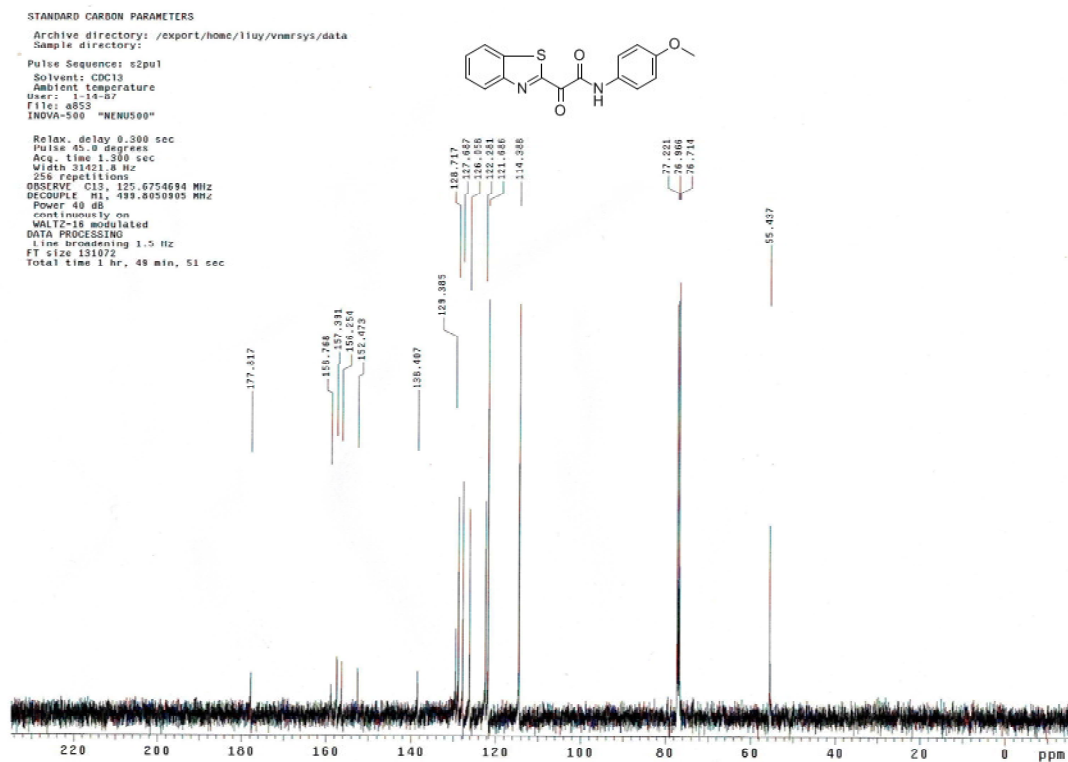
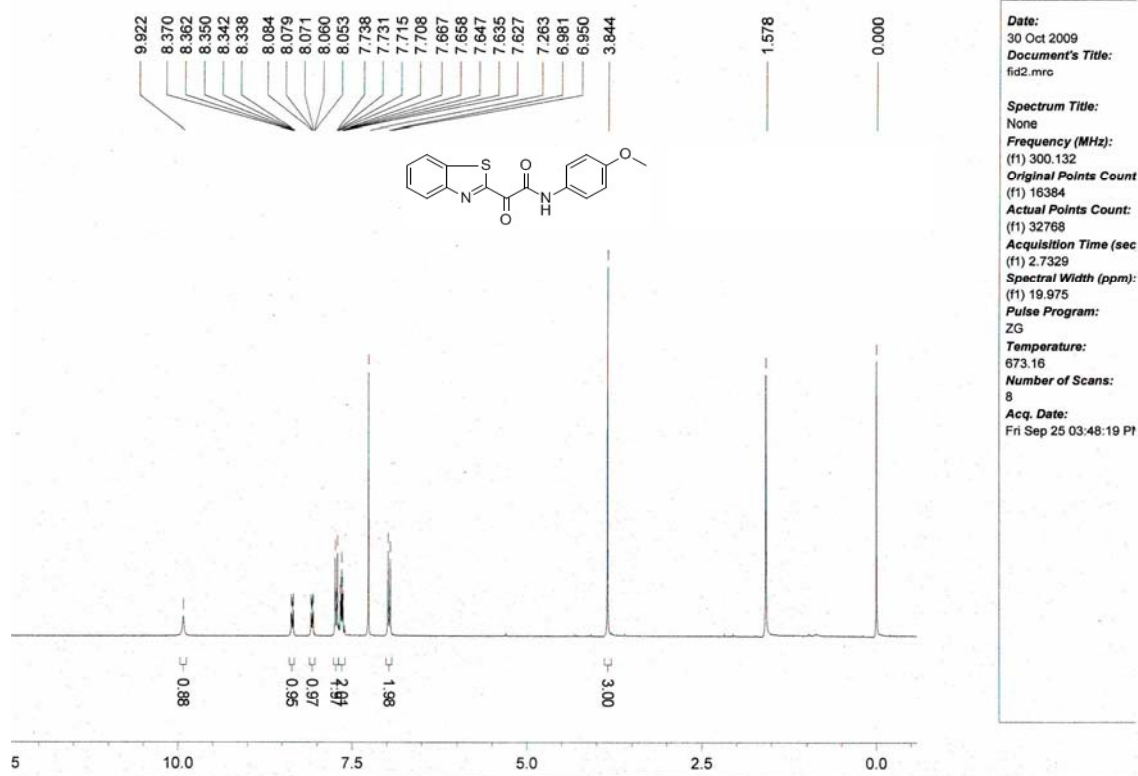
Relax. delay 9.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.0 Hz
 384 repetitions
 OBSERVE C13, 125.6754690 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power 40 dB
 continuously on
 MALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec



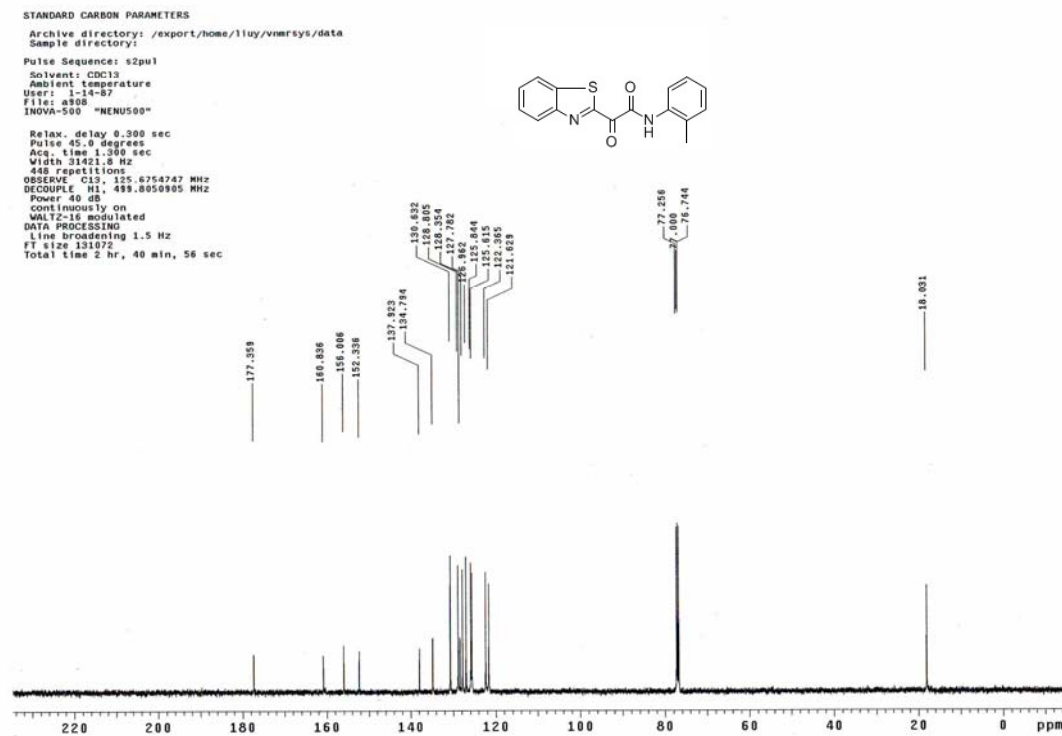
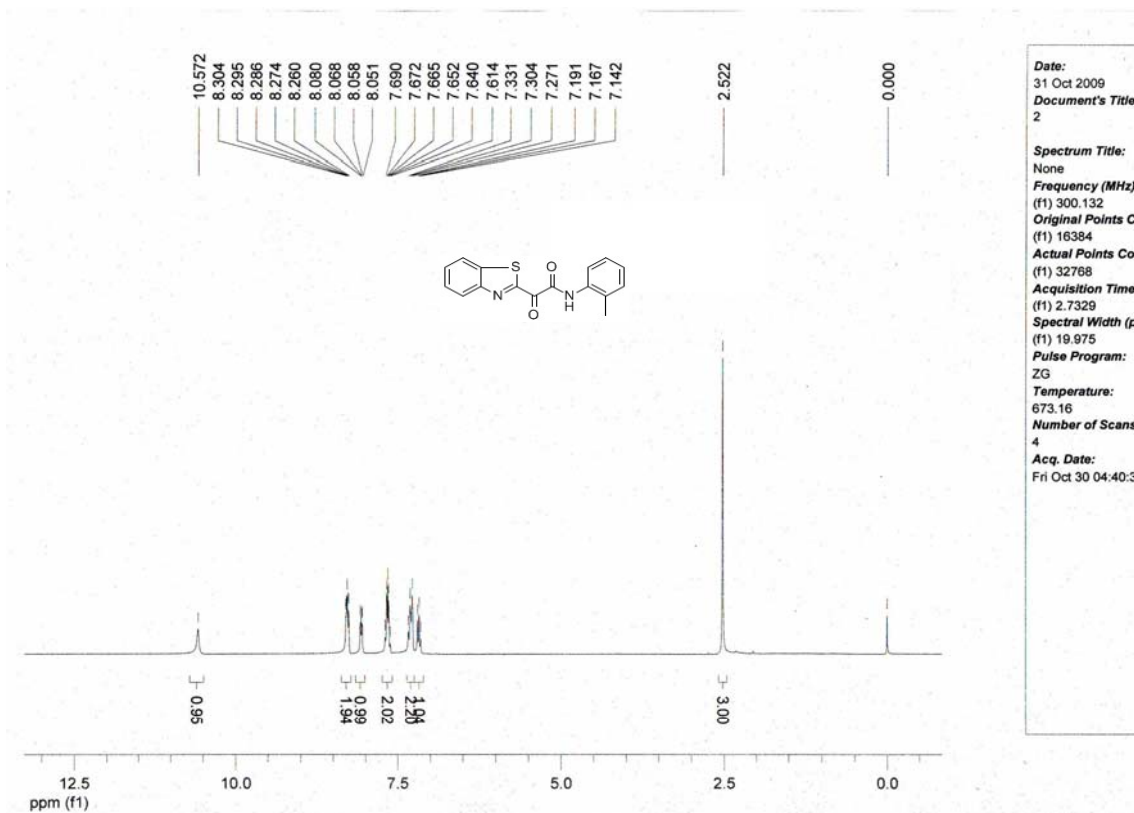
3a



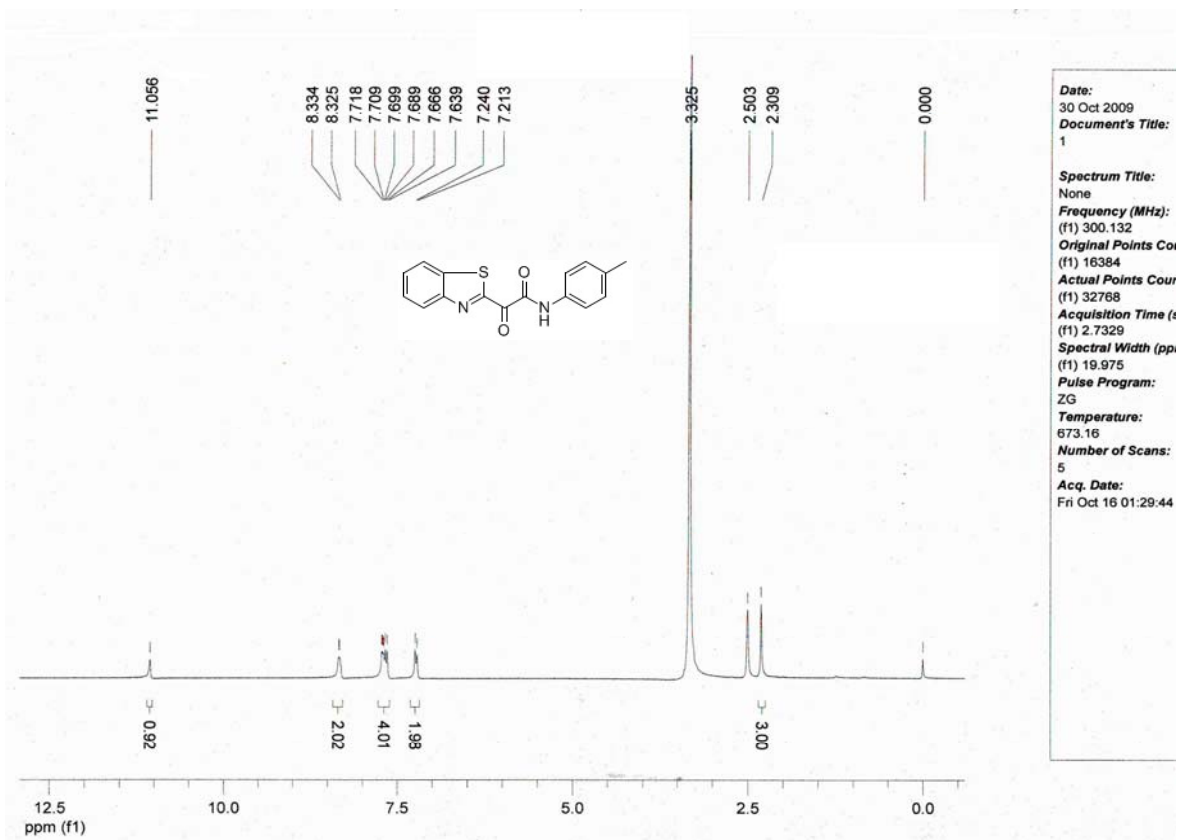
3b



3c

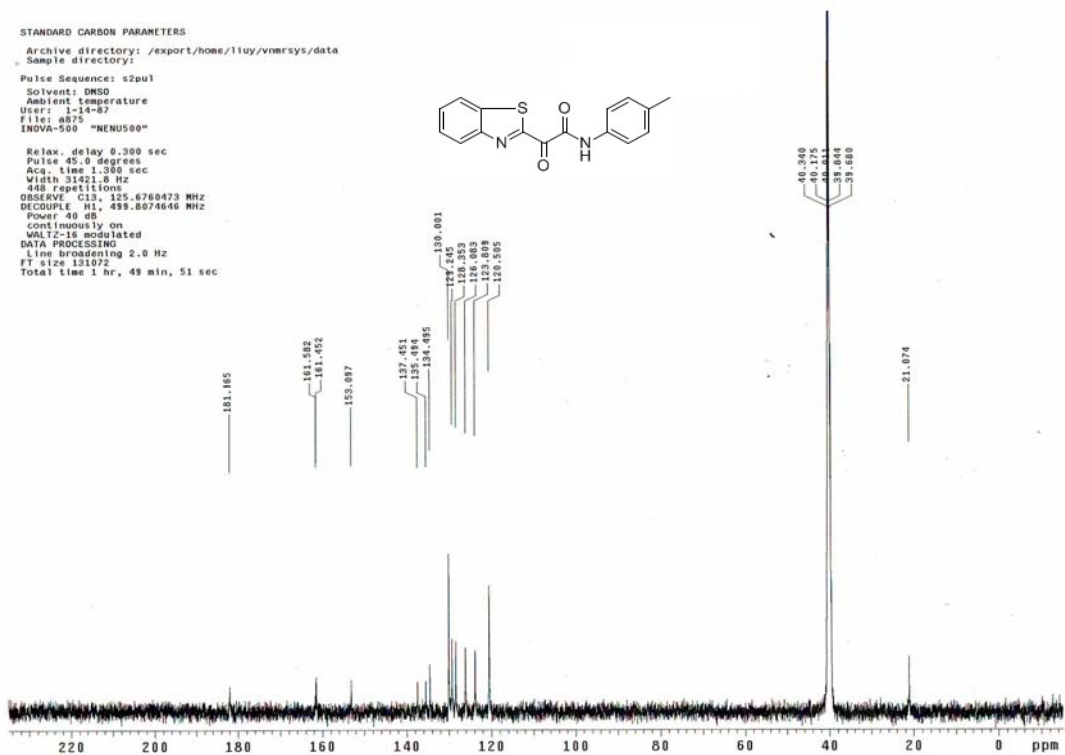


3d



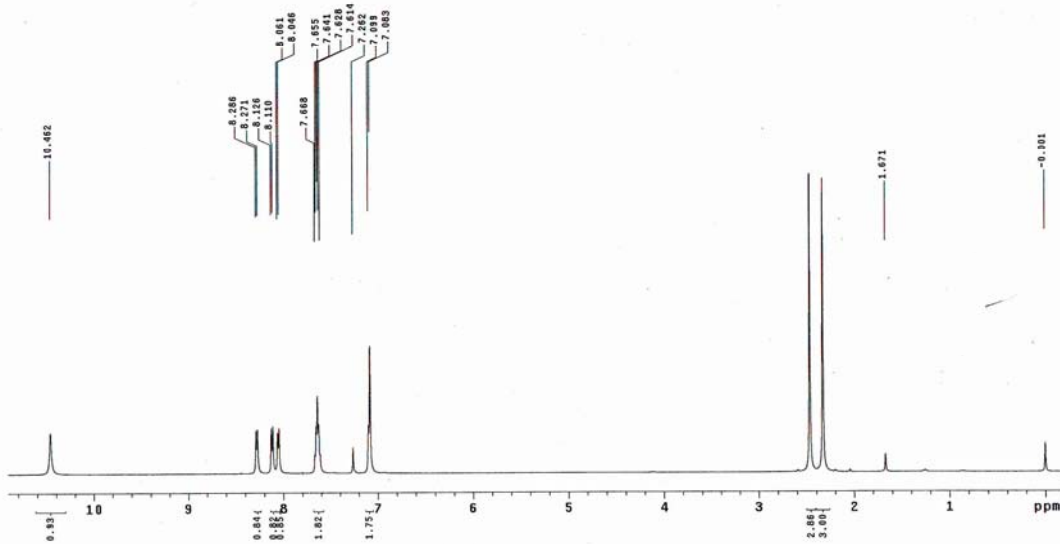
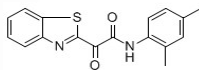
STANDARD CARBON PARAMETERS
 Archive directory: /export/home/11uy/vnmrsys/data
 Sample directory:
 Pulse Sequence: s2pul
 Solvent: DMSO
 Ambient temperature
 User: i-14-57
 File: a875
 INOVA-500 "MENSU00"

Relax. delay 6.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 21421.8 Hz
 448 repetitions
 OBSERV: C13, 125.6760473 MHz
 DECOUPLE H1, 499.8074846 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 131092
 Total time 1 hr, 49 min, 51 sec

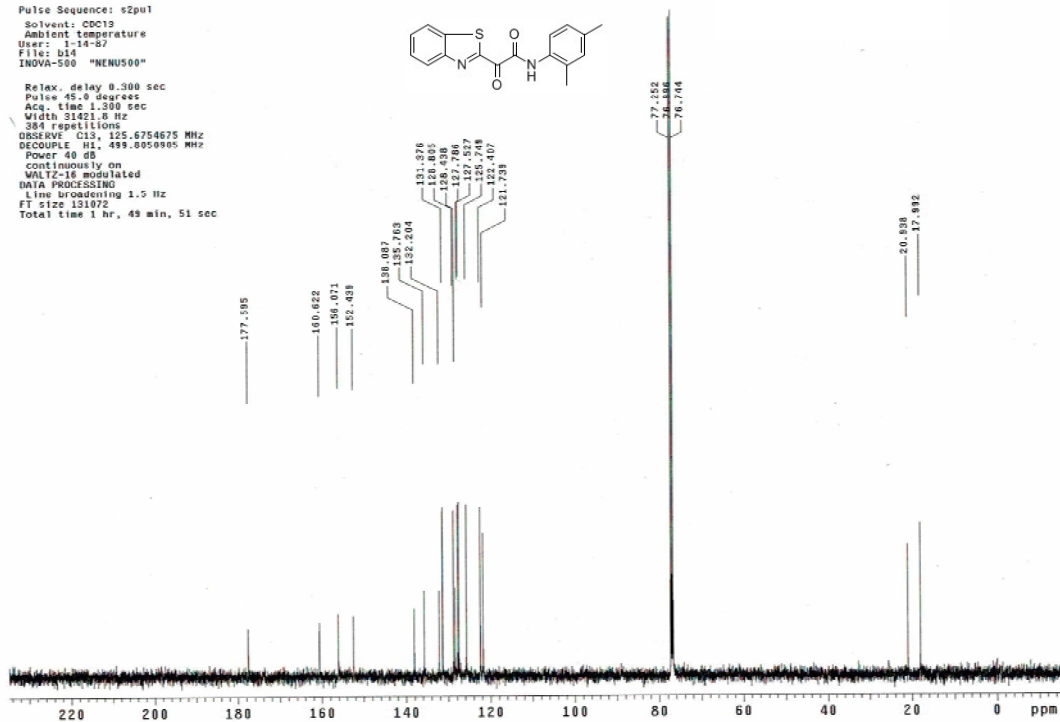
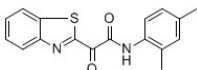


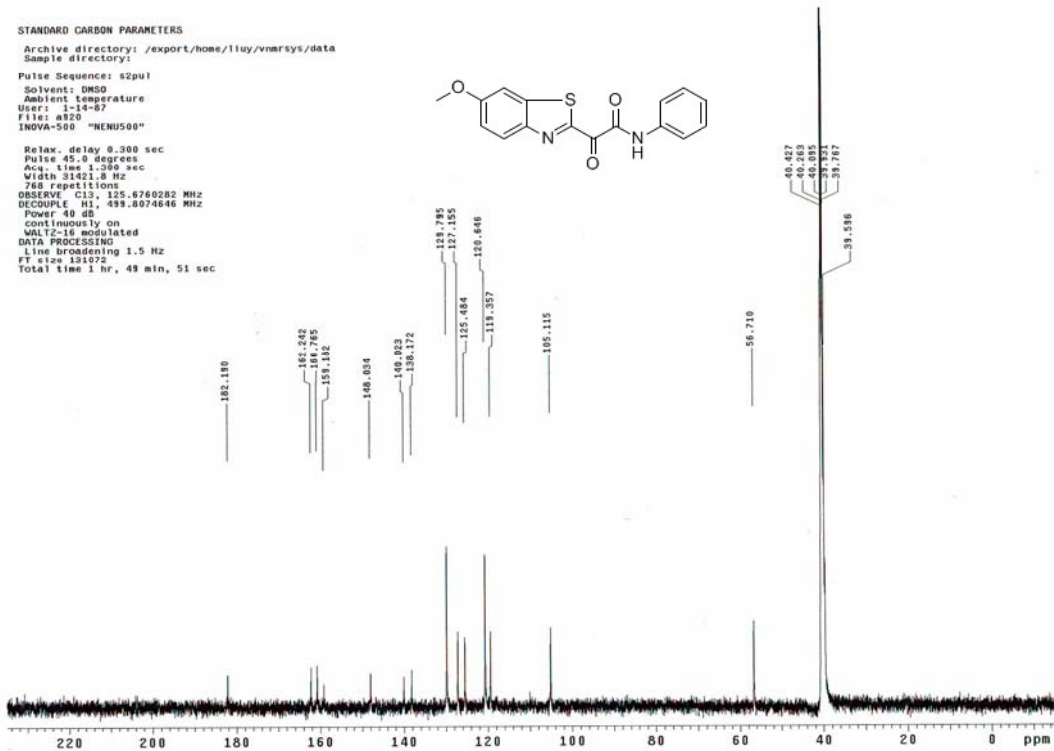
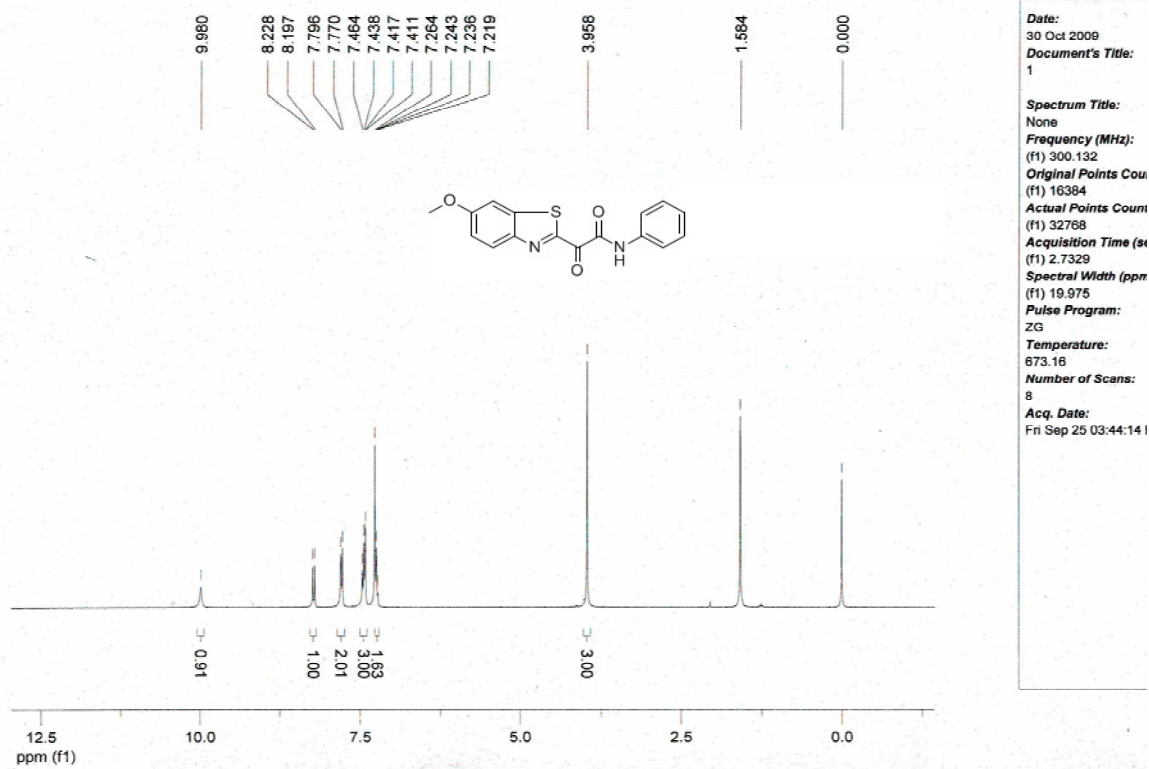
3e

STANDARD PROTON PARAMETERS
 Archive directory: /export/home/11uy/vnmrSYS/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient Temperature
 File: b13
 INOVA-500 "NENUS00"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.092 sec
 Width 8471.9 Hz
 0 repetitions
 OBSERVE H1, 499.8025907 MHz
 DATA PROCESSING
 FT size 65536
 Total time 0 min, 23 sec

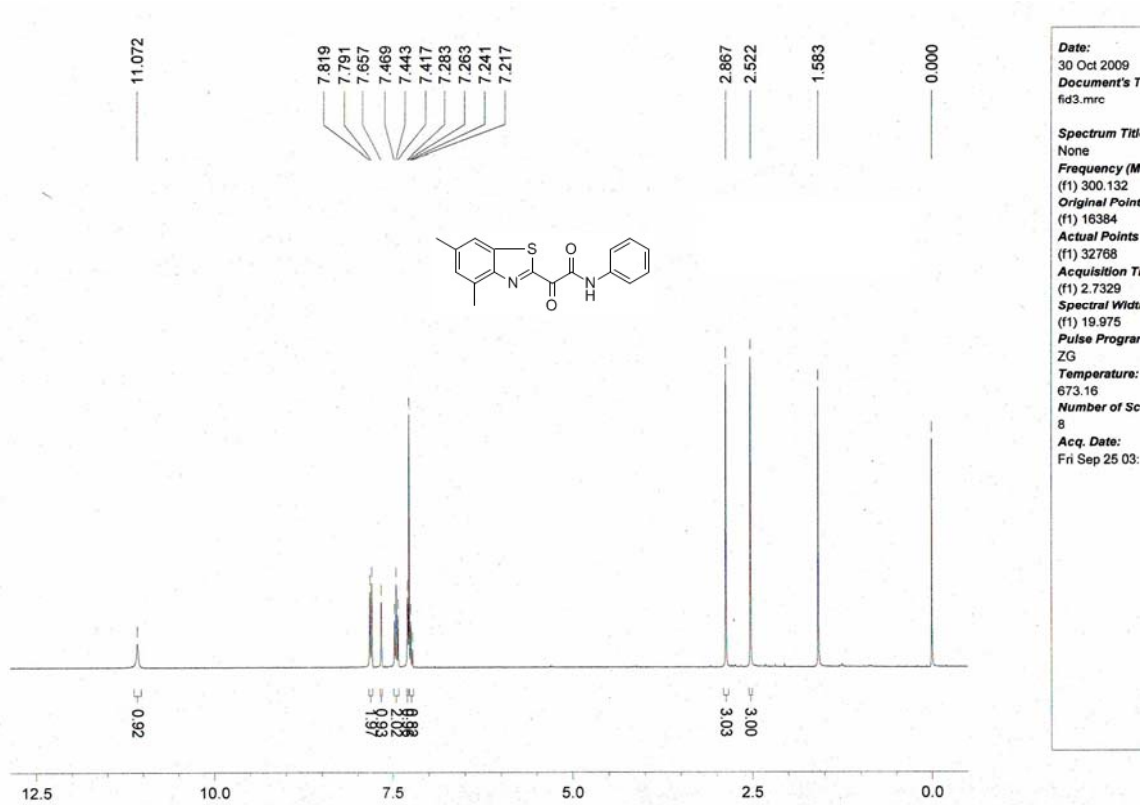


STANDARD CARBON PARAMETERS
 Archive directory: /export/home/11uy/vnmrSYS/data
 Sample directory:
 Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 User: 1-14-87
 File: b14
 INOVA-500 "NENUS00"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 384 repetitions
 OBSERVE C13, 125.6754675 MHz
 DECOUPLE H1, 499.8050905 MHz
 Power 48 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec

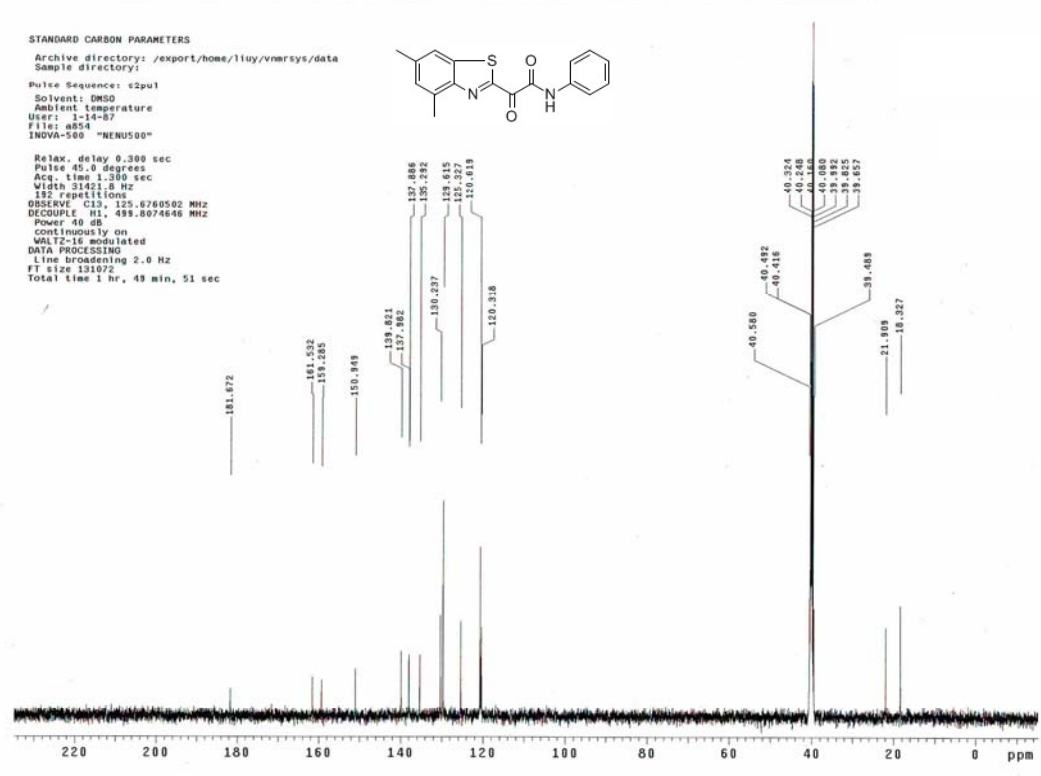




3j



Date: 30 Oct 2009
 Document's T: fid3.mrc
 Spectrum Title: None
 Frequency (M): (f1) 300.132
 Original Point: (f1) 16384
 Actual Points: (f1) 32768
 Acquisition Time: (f1) 2.7329
 Spectral Width: (f1) 19.975
 Pulse Program: ZG
 Temperature: 673.16
 Number of Scans: 8
 Acq. Date: Fri Sep 25 03:



STANDARD CARBON PARAMETERS
 Archive directory: /export/home/lluy/vnmrsys/data
 Sample directory:
 Pulse Sequence: cspul
 Solvent: DMSO
 Ambient temperature
 User: 1-14-87
 File: a854
 INOVA-500 "NENU500"
 Relax. delay 0.300 sec
 Pulse 45.0 degrees
 Acq. time 1.300 sec
 Width 31421.8 Hz
 182 repetitions
 OBSERVE C13, 125.6760562 MHz
 DECOUPLE N1, 499.8074646 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 131072
 Total time 1 hr, 49 min, 51 sec

3k

