

Supplementary Material

Microwave-promoted Heck and Suzuki coupling reactions of new 3-(5-bromobenzofuranyl)pyrazole in aqueous media

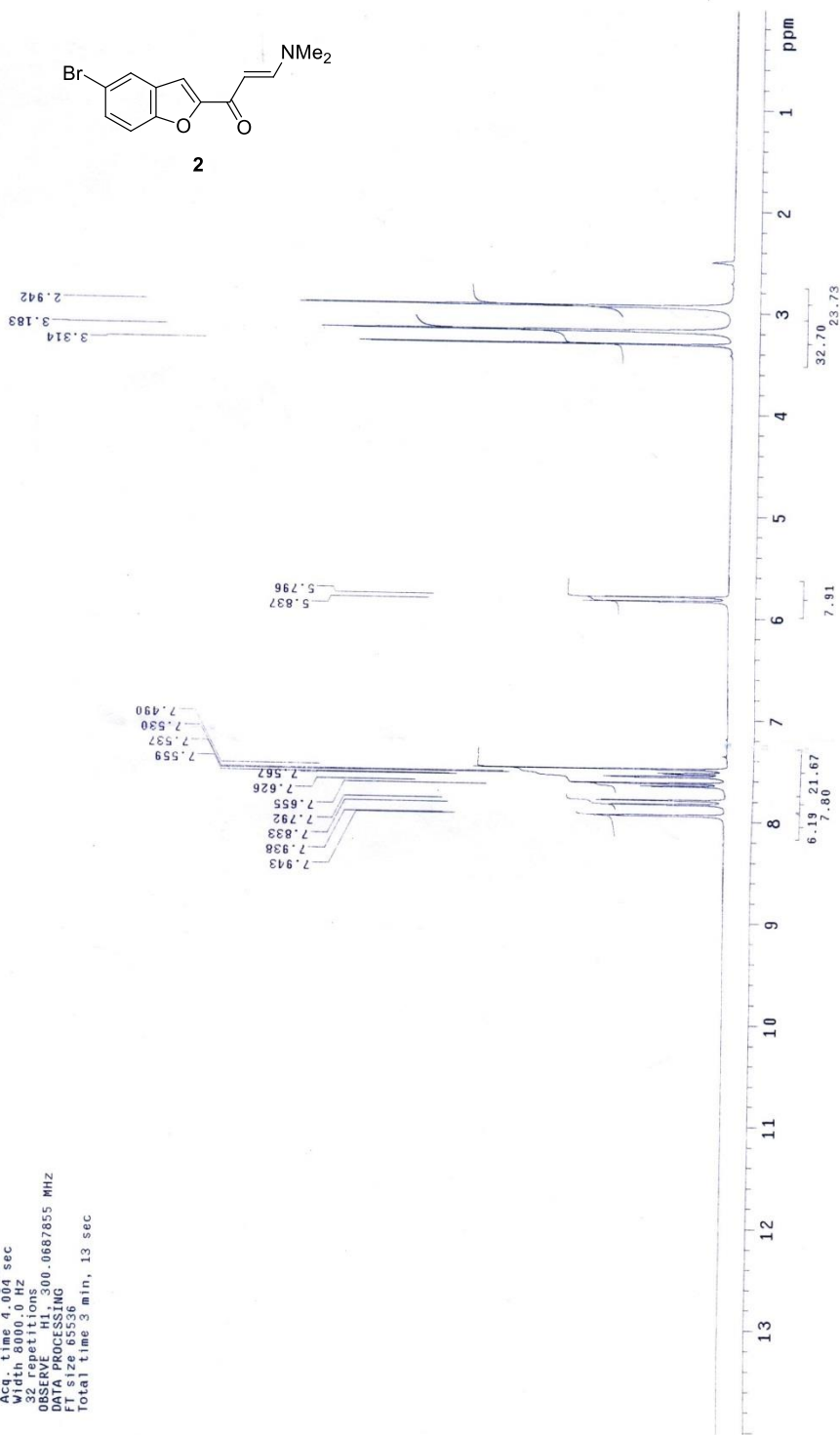
Kamal M. Dawood,* Ahmed F. Darweesh, Mohamed R. Shaaban and Ahmad M. Farag
Department of Chemistry, Faculty of Science, Cairo University, Giza 12613, Egypt

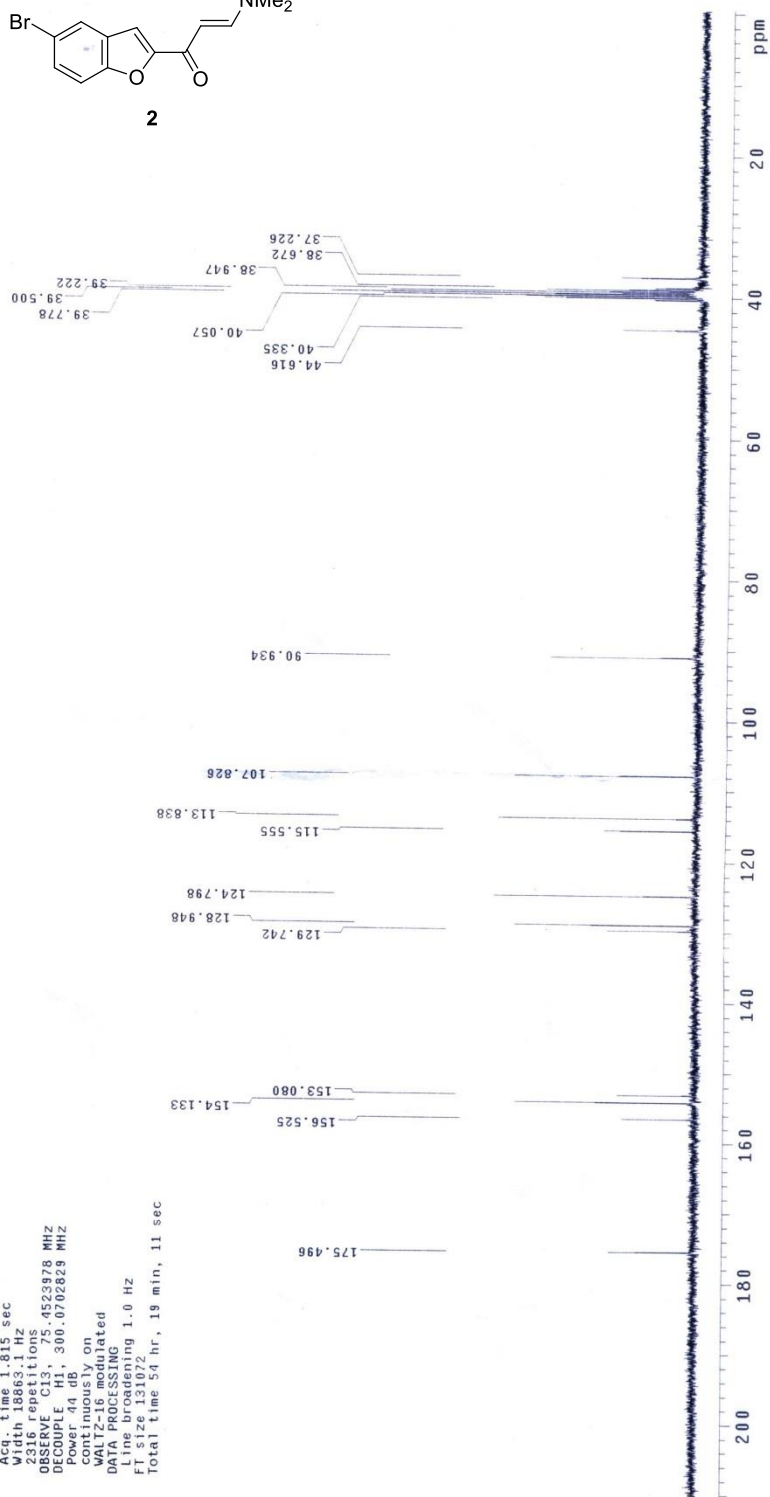
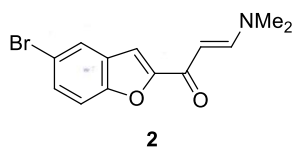
E-mail: dr_dawood@yahoo.com

Table of Contents

1. ¹ H NMR spectrum of compound 2	S2
2. ¹³ C NMR spectrum of compound 2	S3
3. ¹ H NMR spectrum of compound 3	S4
4. ¹³ C NMR spectrum of compound 3	S5
5. ¹ H NMR spectrum of compound 6	S6
6. ¹³ C NMR spectrum of compound 6	S7
7. ¹ H NMR spectrum of compound 7	S8
8. ¹³ C NMR spectrum of compound 7	S9
9. ¹ H NMR spectrum of compound 8	S10
10. ¹³ C NMR spectrum of compound 8	S11
11. ¹ H NMR spectrum of compound 9	S12
12. ¹³ C NMR spectrum of compound 9	S13
13. ¹ H NMR spectrum of compound 10	S14
14. ¹³ C NMR spectrum of compound 10	S15
15. ¹ H NMR spectrum of compound 11	S16
16. ¹³ C NMR spectrum of compound 11	S17
17. ¹ H NMR spectrum of compound 13	S18
18. ¹³ C NMR spectrum of compound 13	S19
19. ¹ H NMR spectrum of compound 14	S20
20. ¹³ C NMR spectrum of compound 14	S21
21. ¹ H NMR spectrum of compound 15	S22
22. ¹³ C NMR spectrum of compound 15	S23
23. ¹ H NMR spectrum of compound 16	S24
24. ¹³ C NMR spectrum of compound 16	S25

AhmadFathy-AFEA-DMSO-H1
Pulse Sequence: s2pul
Solvent: DMSO
Temperature: 303.1 K
Mercury-300BB "NMR300"
Relax. delay: 1.000 sec
Pulse: 74.1 degrees
Acq. time: 4.004 sec
Width: 8000.0 Hz
32 repetitions
Observed: 00.0687855 MHz
DATA PROCESSING
FT size: 65536
Total time: 3 min, 13 sec





AhmadFathy-AFEA-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrSYS/data
 Sample directory: NS00hy-4-13C-dmsO_06Jun2004
 File: CARBON

Pulse Sequence: s2pul

Solvent: DMSO
 Temp. 30.0 C / 303.1 K
 Mercury-3000BB "NMR300"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Width 1883.0 Hz
 Width 1883.0 Hz

2316 repetitions

OBSERVE C13, 75.4523978 MHz

DECOUPLE H1, 300.0702829 MHz

Power 44 dB

Continuously on

Waltz16 decoupled

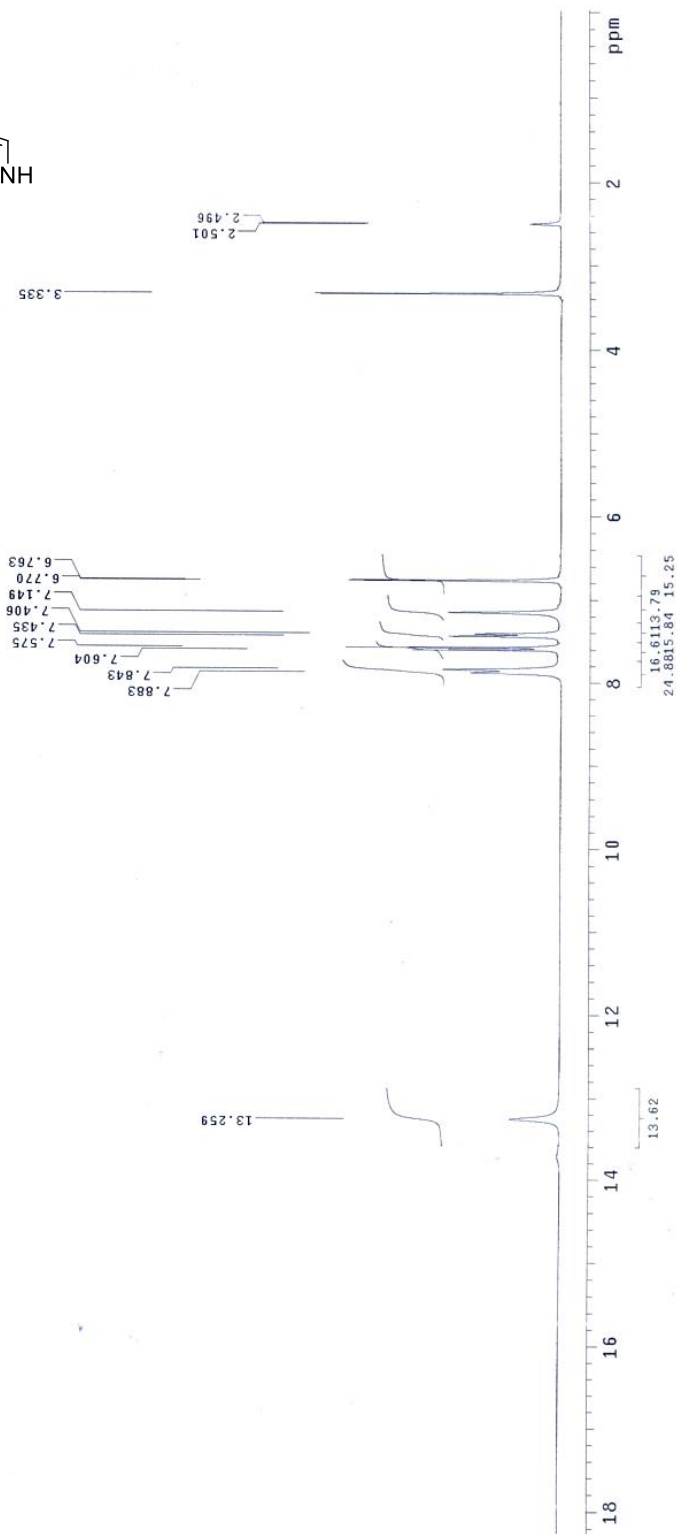
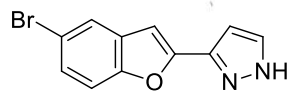
DATA PROCESSING

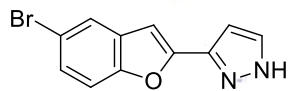
Line broadening 1.0 Hz

FT size 131072

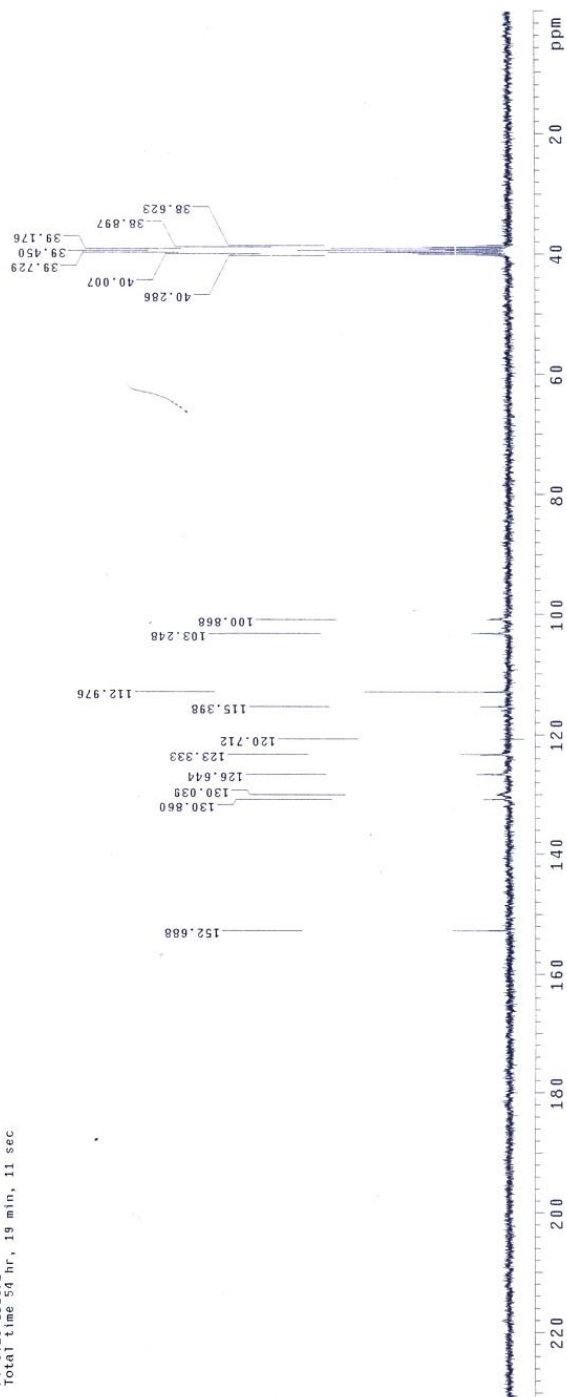
Total time 54 hr, 19 min, 11 sec

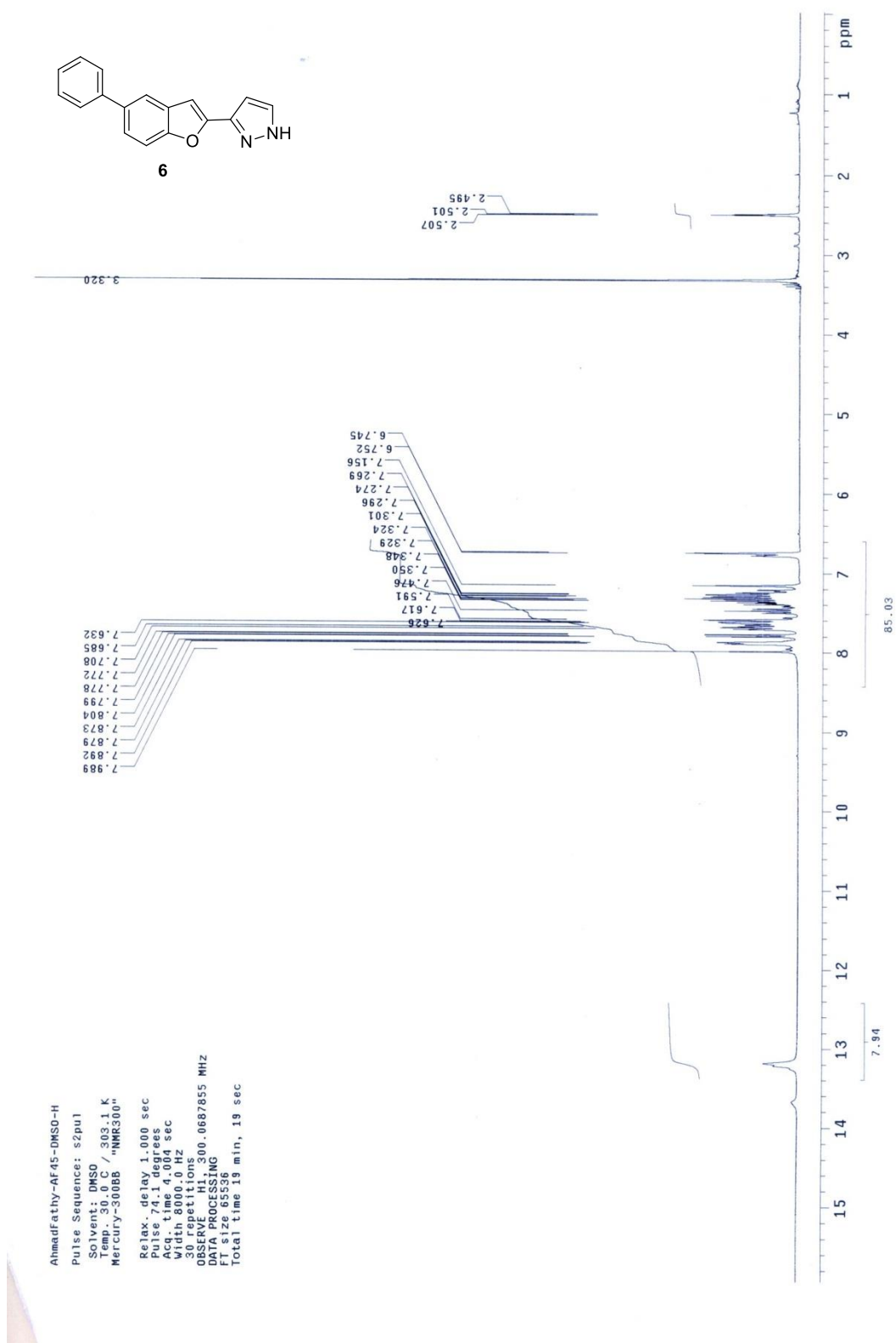
Ahmadfathy-ENIH-DMSO-H
Pulse Sequence: sZpu1
Solvent: DMSO
Temp.: 300.1 K
Mercury-300dB "NMR300"
Relax. delay: 1.000 sec
Pulse: 74.1 degree
Acq. time: 4.004 sec
Width: 8000.0 Hz
20 repetitions
OBSERVE: H1, 300.0687855 MHz
DATA PROCESSING
File size: 85932
Total time: 12 min, 53 sec



**3**

Ahmed:athy-ENHH-DMSO-C13
 Archive directory: /export/home/vnmr1/vnmr54/data
 Sample directory: NScbhy-4-130-dmsoc_06jun2004
 Pulse Sequence: s2pu1
 Solvent: DMSO
 Temp: 30.0 C / 303.1 K
 File: Ahmed:athy-ENHH-DMSO-C13
 Mercury-300BB -HRK300
 Relax. delay: 1.000 sec
 Pulse: 45.0 degrees
 Acq. time: 1.815 sec
 Width: 18863.1 Hz
 OBSERVED: C13, 75.4523958 MHZ
 DECOUPLE: H1, 300.0702829 MHZ
 Power: 44 dB
 Continuously on
 continuously gated
 DATA PROCESSING
 Line broadening: 1.0 Hz
 FT size: 131072
 Total time: 54 hr, 19 min, 11 sec



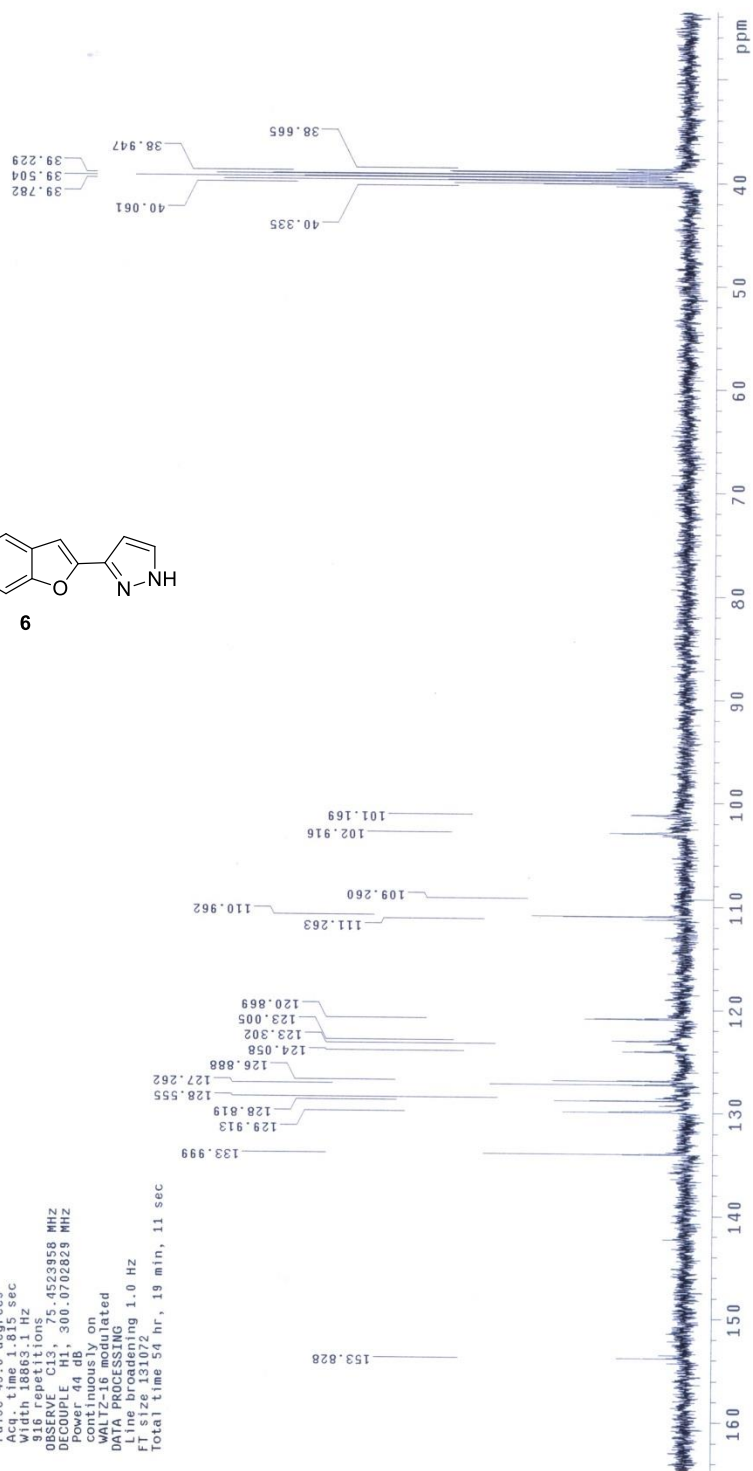
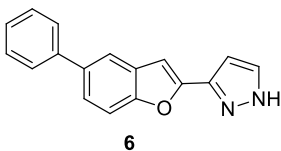


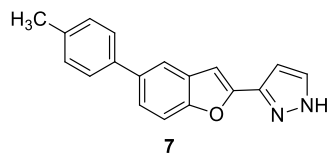
AhmadFathy-AF45-DMSO-C13
 Archive directory: /export/home/vnmr1/vnmr5ys/data
 Sample directory: MSobhy-4-13C-dmsd_163um2.004
 File: CARBON

Pulse Sequence: s2pul

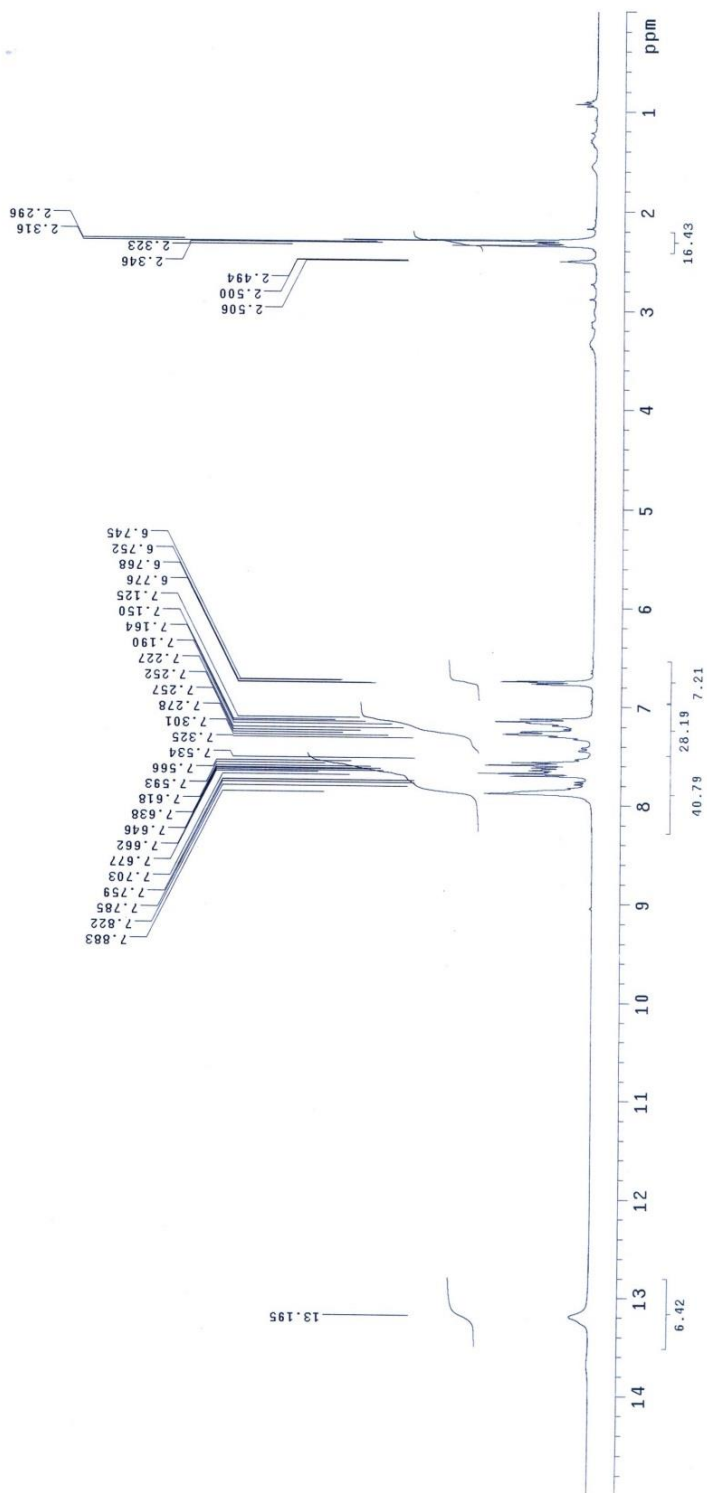
Solvent: DMSO
 Temp. 30.0 C / 303.1 K
 Mercury-300BB "NMR300"

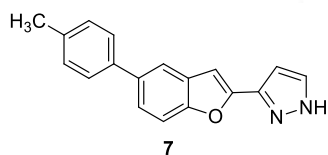
Relax. delay 1.000 sec
 Pulse prog zgpg30
 Acq time 1.000 sec
 Width 18863.1 Hz
 816 repetitions
 OBSERVE C13, 75.4523858 MHZ
 DECOUPLE H1, 300.0702829 MHZ
 Power delay continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 File size 131072
 Total time 58 hr, 19 min, 11 sec





AhmedFathy-AF49-DMSO-H1
 Pulse Sequence: s2pu1
 Solvent: DMSO
 Temp: 30.0 C / 303.1 K
 File: AhmedFathy-AF49-DMSO-H1
 Mercury-300BB NMR300
 Relax. delay: 1.000 sec
 Pulse: 74.1 degrees
 Acq. time: 4.004 sec
 Width: 8000.0 Hz
 28 Repetitions
 OBSERVE H1, 300.0687855 MHZ
 F1 F2 PROCESSING
 F1 F2 35-12
 Total time: 12 min, 53 sec





AhmadFathy-AF49-DMSO-C13-12-3-2009
 Archive directory: /export/home/vnmr1/vnmr5ys/data
 Sample directory: MSobhy-4-13C-dms0_06Jun2004
 File: CARBON

Pulse Sequence: s2pul

Solvent: DMSO
 Temp. 30.0 C / 303.1 K
 Mercury-300BB "NMR300"

Relax. delay 1.000 sec
 Pulse 15.0 degrees
 Width 18863.1 Hz

Width 18863.1 Hz
 2268 repetitions

OBSERVE C13, 75.4523970 MHz

DECOUPLE H1, 300.0702829 MHz

Power 44 dB

Modulation on

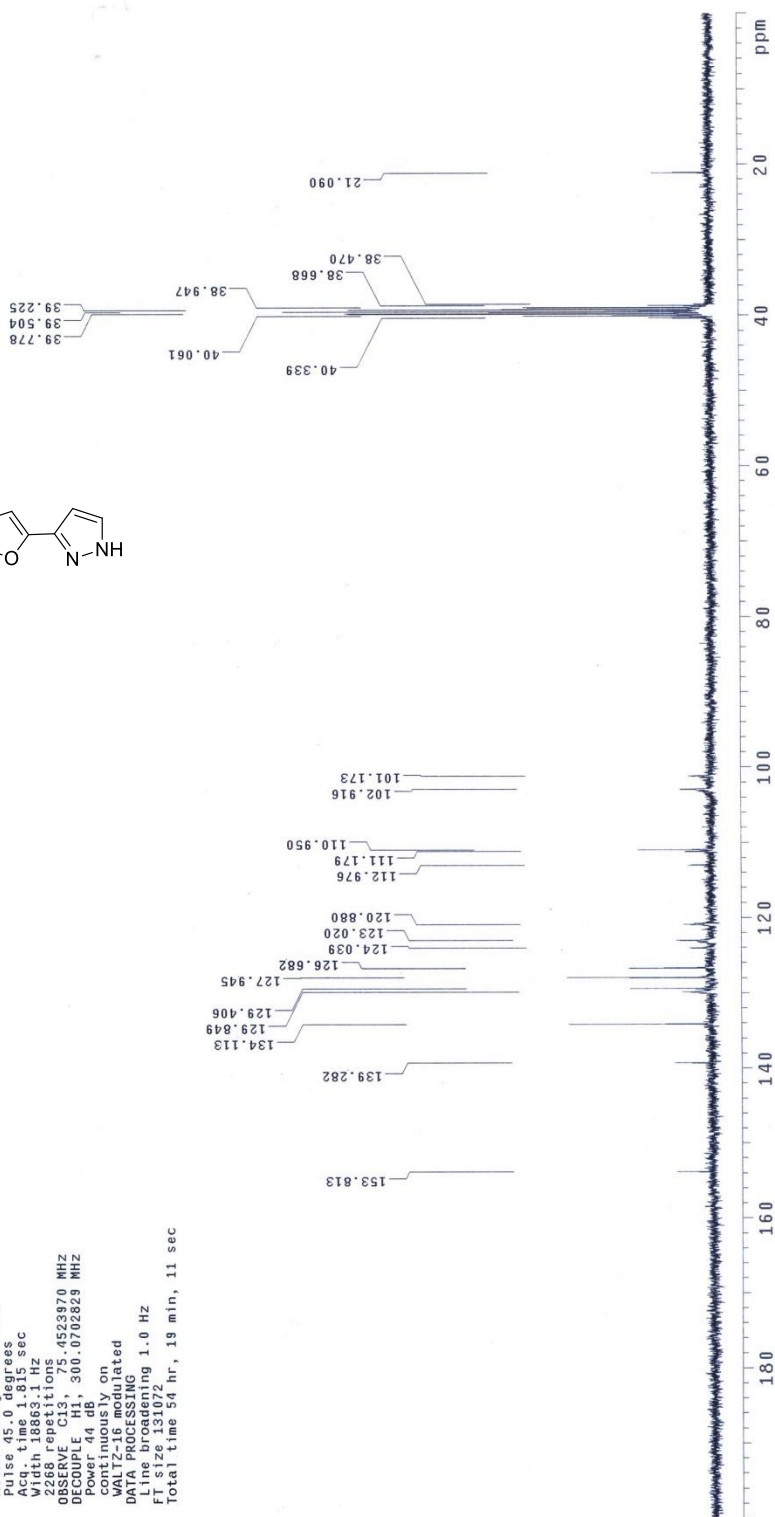
WALTZ16 modulated

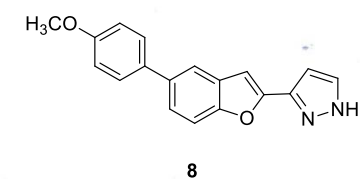
DATA PROCESSING

Line broadening 1.0 Hz

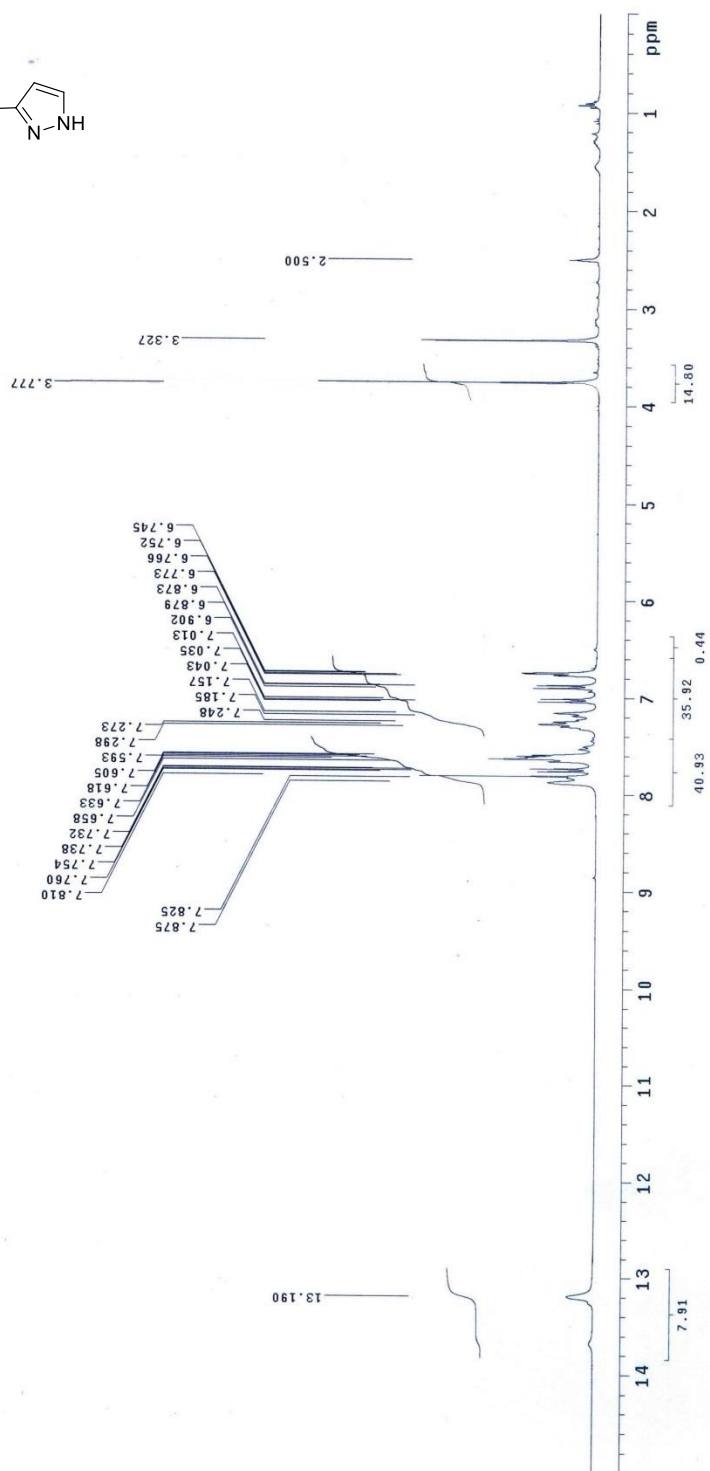
FT size 131072

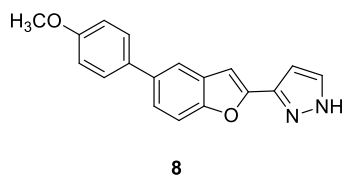
Total time 54 hr, 19 min, 11 sec



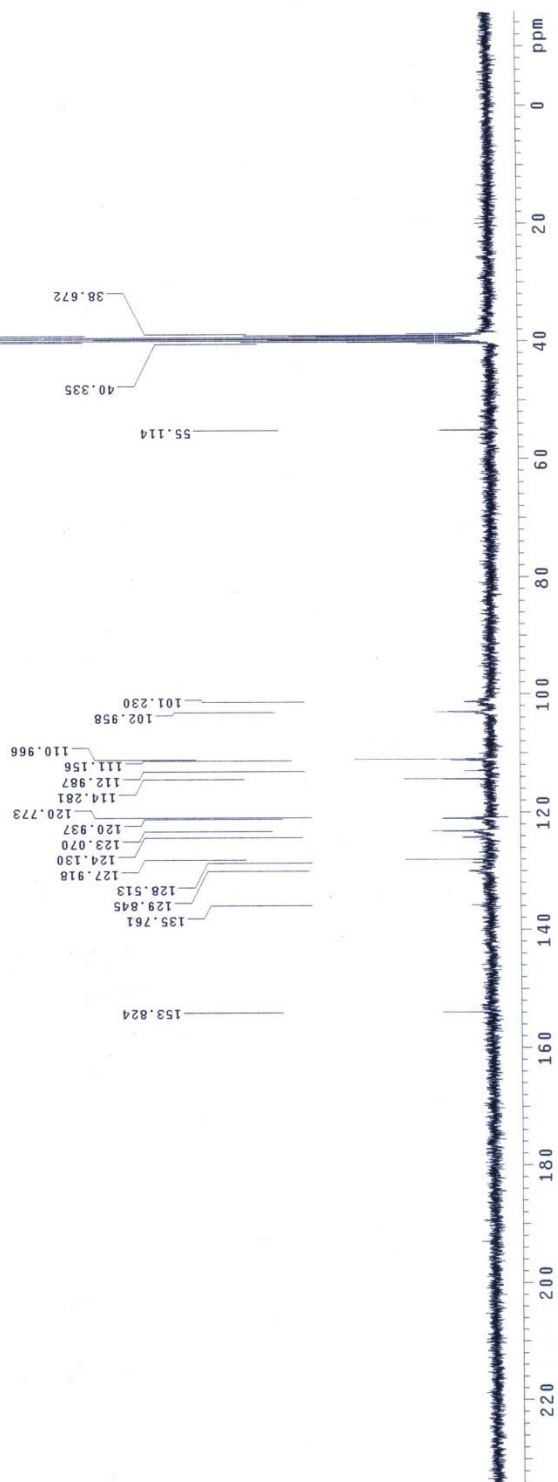


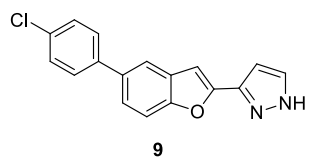
AhmadFathy-AF50-DMSO-H1
 Pulse Sequence: s2pu1
 Solvent: DMSO
 Temp: 300.1 K
 File: AhmadFathy-AF50-DMSO-H1
 Mercury-300BB "NMR300"
 Relax. delay 1.000 sec
 Pulse 74.1 degrees
 Acq. time 4.004 sec
 Width 8000.0 Hz
 OBSERVED: 13C
 OBSERVED: 1H 300.0687858 MHZ
 DATA PROCESSING
 FT size 65536
 Total time 12 min, 53 sec





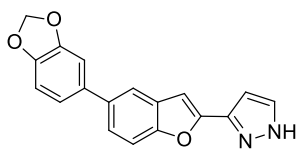
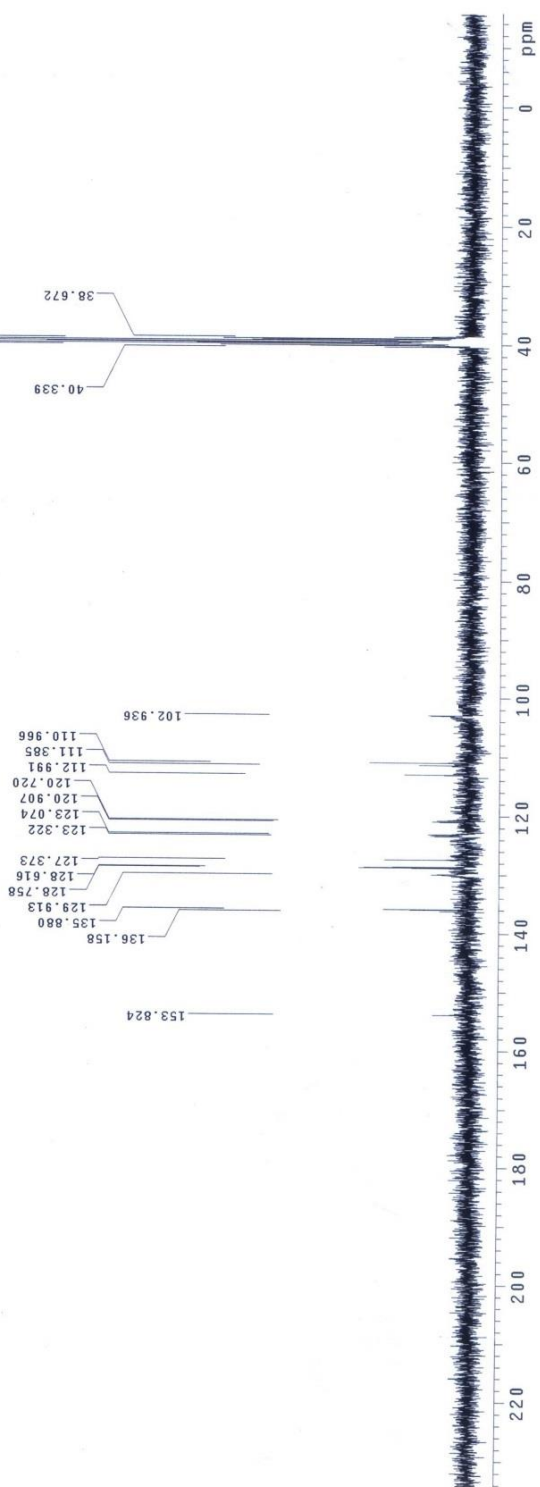
AhmadFathy-AF50-DMSO-C13
 Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: MSobhy-4-13C-dms0_06Jun2004
 File: C13001
 Pulse Sequence: szpu1
 Solvent: DMSO
 Temp: 30.0 C / 303.1 K
 Mercury-300BB "NMR300"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.815 sec
 Width 18863.1 Hz
 Observed F1 300.1362829 MHz
 OBSERVE F2 75.4523958 MHz
 DECOUPLE H1 300.0702829 MHz
 Power 44 dB
 continuously on
 WALTZ-16 modulated
 Data Processing
 File Processing 1.0 Hz
 FT size 131072
 Total time 54 hr, 19 min, 11 sec



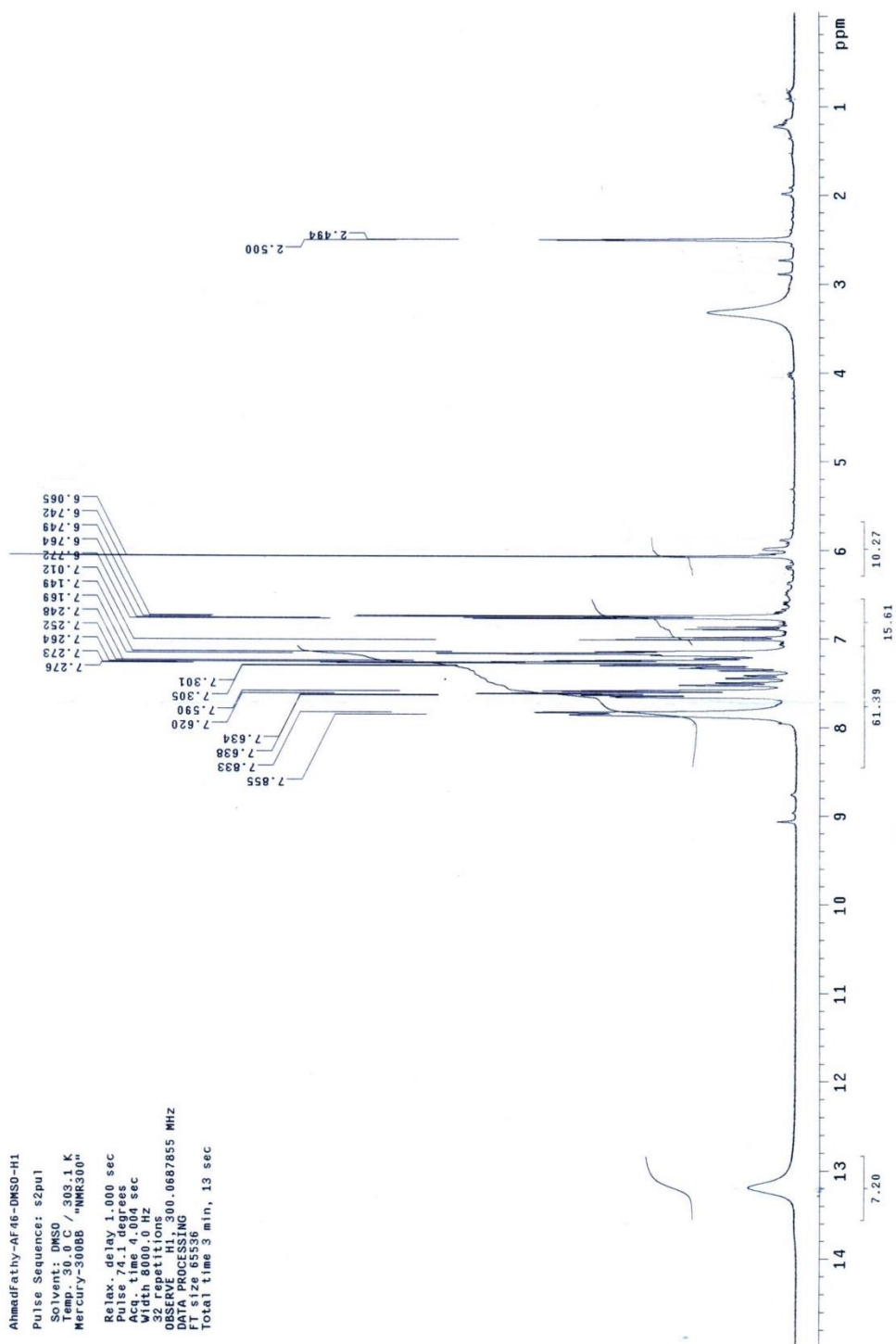


6

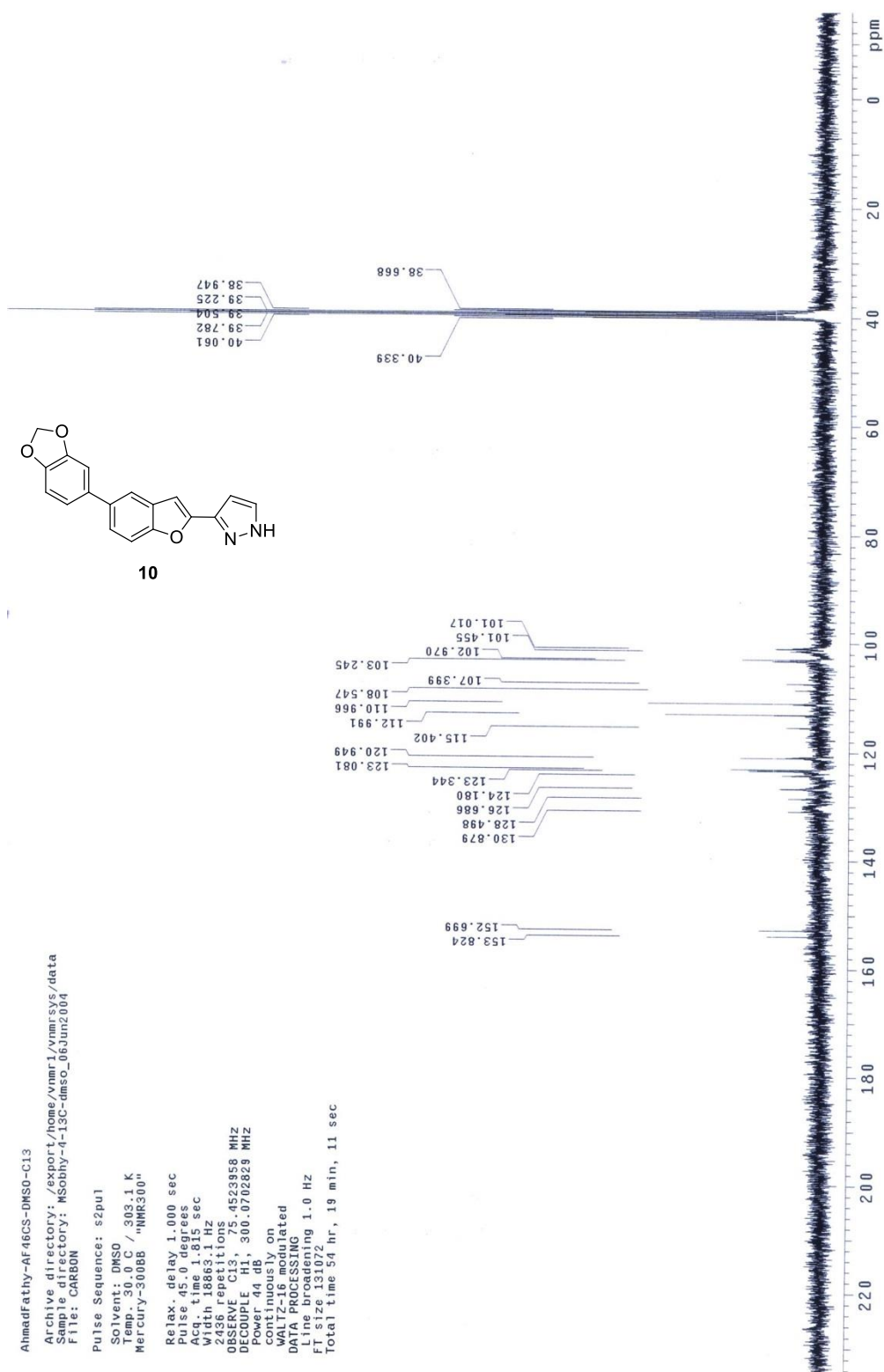
AhmedFathy-AF48-DMSO-C13
 Archive directory: /export/home/vnmr1/vnmrSYS/data
 Sample directory: MSobhy-4-13C-dmsO_06Jun2004
 Pulse Sequence: s2pul
 Solvent: DMSO
 Temp: 300.1 K
 File: AhmedFathy-AF48-DMSO-C13
 Mercury-300BB "NMR300"
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.815 sec
 Width 18863.1 Hz
 OBSERVE CH3
 REPEATS 1
 DECOUPLE CH1, 300.0702829 MHz
 Power 44 dB, continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 F2 size 131072
 Total time 54 hr, 19 min, 11 sec

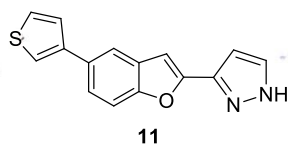


10

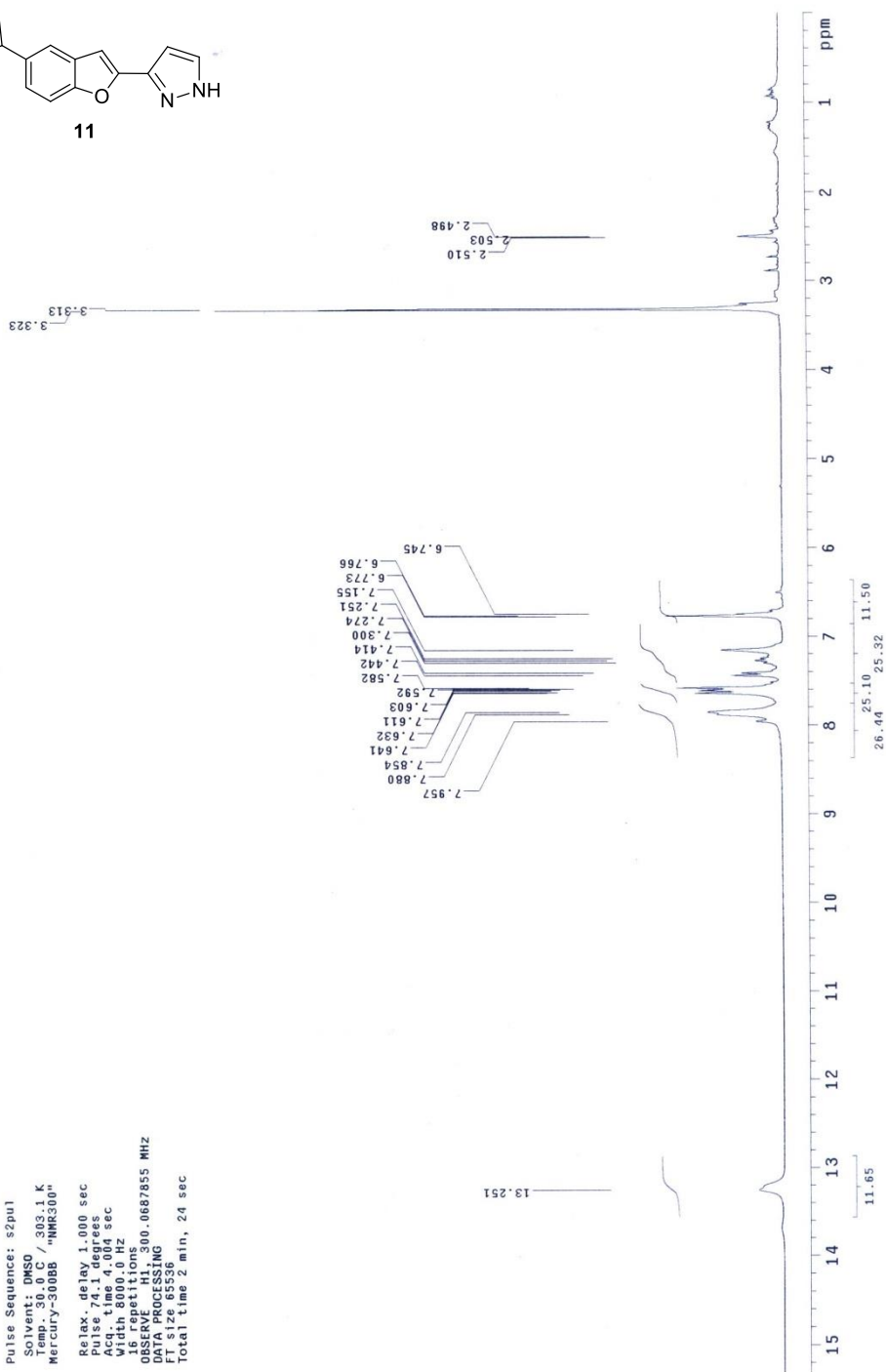


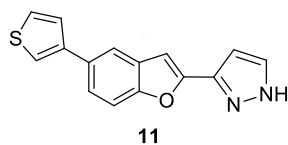
AhmadFathy-AF46-DMSO-H1
 Pulse Sequence: s2pul
 Solvent: DMSO
 Temp: 303.1 K
 Mercury-300BB "NMR300"
 Relax. delay 1.000 sec
 Pulse 74.1 degrees
 Acq. time 4.004 sec
 Width 8000.0 Hz
 32 repetitions
 0.0687855 MHz
 DATA PROCESSING
 FT size 65536
 Total time 3 min, 13 sec





AhmadFathy-AF47CS-DMSO-H
Pulse Sequence: s2pu1
Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-300BBB "NMR300"
Relax. delay 1.000 sec
Pulse width 4.000 sec
Pulse program 1.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE F1, 300.0687855 MHz
DATA ACQUISITION
F1 F2 65536
Total time 2 min, 24 sec

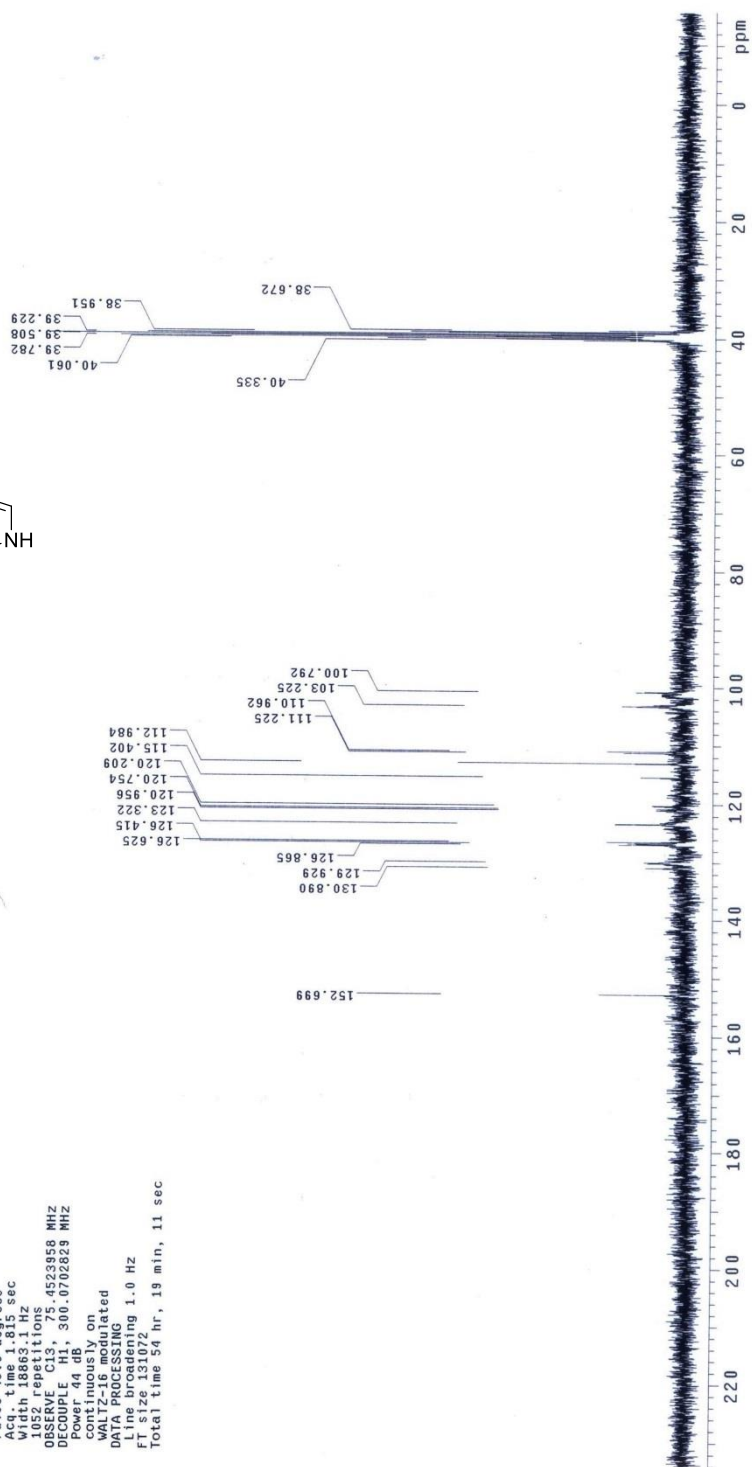


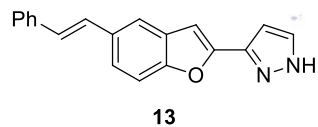


AhmadFathy-AF47-DMSO-C13
 Archive directory: /export/home/vnmr1/vnmrSYS/data
 Sample directory: MSobhy-4-13C-dms0_06Jun2004
 File: CARBON

Pulse Sequence: s2pul
 Solvent: DMSO
 Temp: 30.0 C / 303.1 K
 Mercury-300BB "NMR300"

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 8.815 sec
 Wct. time 8.815 sec
 1052 repetitions
 OBSERVE C13, 75.4523958 MHZ
 DECOUPLE H1, 300.0702829 MHZ
 Power 44 dB
 Continuously on
 Wct. time 8.815 sec
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
 Total time 54 hr, 19 min, 11 sec





AhmedFathy-AF-52-DMSO-H

Pulse Sequence: s2pul

Solvent: DMSO
Temp: 30.0 C
F1: AhmedFathy-AF-52-DMSO-H
Mercury-300BB "NMR300"

Relax. delay 1.000 sec

Pulse 74.1 degrees

Acq. time 4.004 sec

Width 8000.0 Hz

32 repetitions

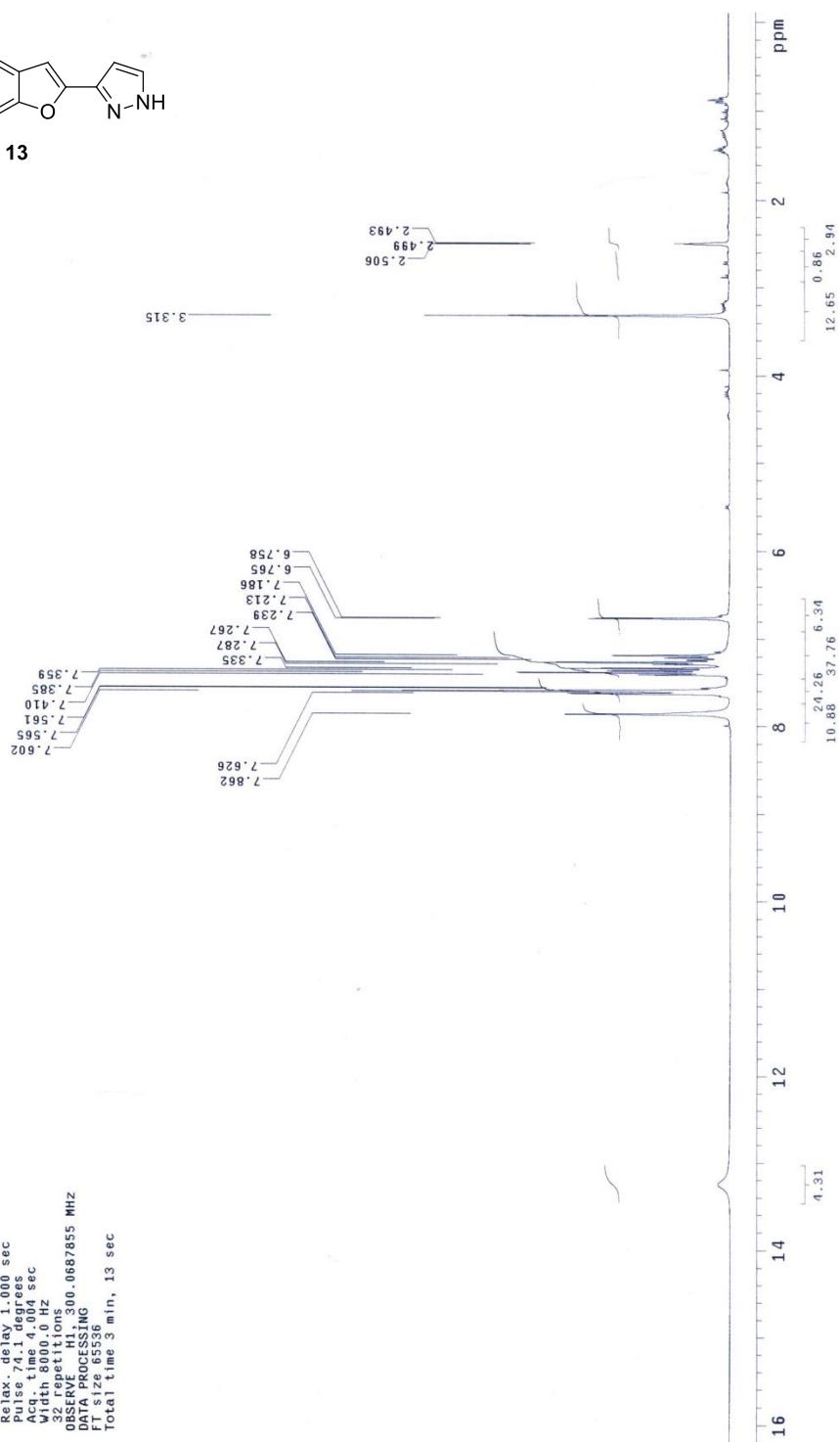
032 REPTITION

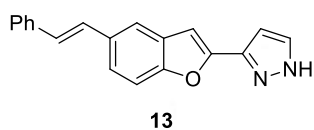
000.0687855 MHZ

DATA PROCESSING

FT size 65536

Total time 3 min, 13 sec





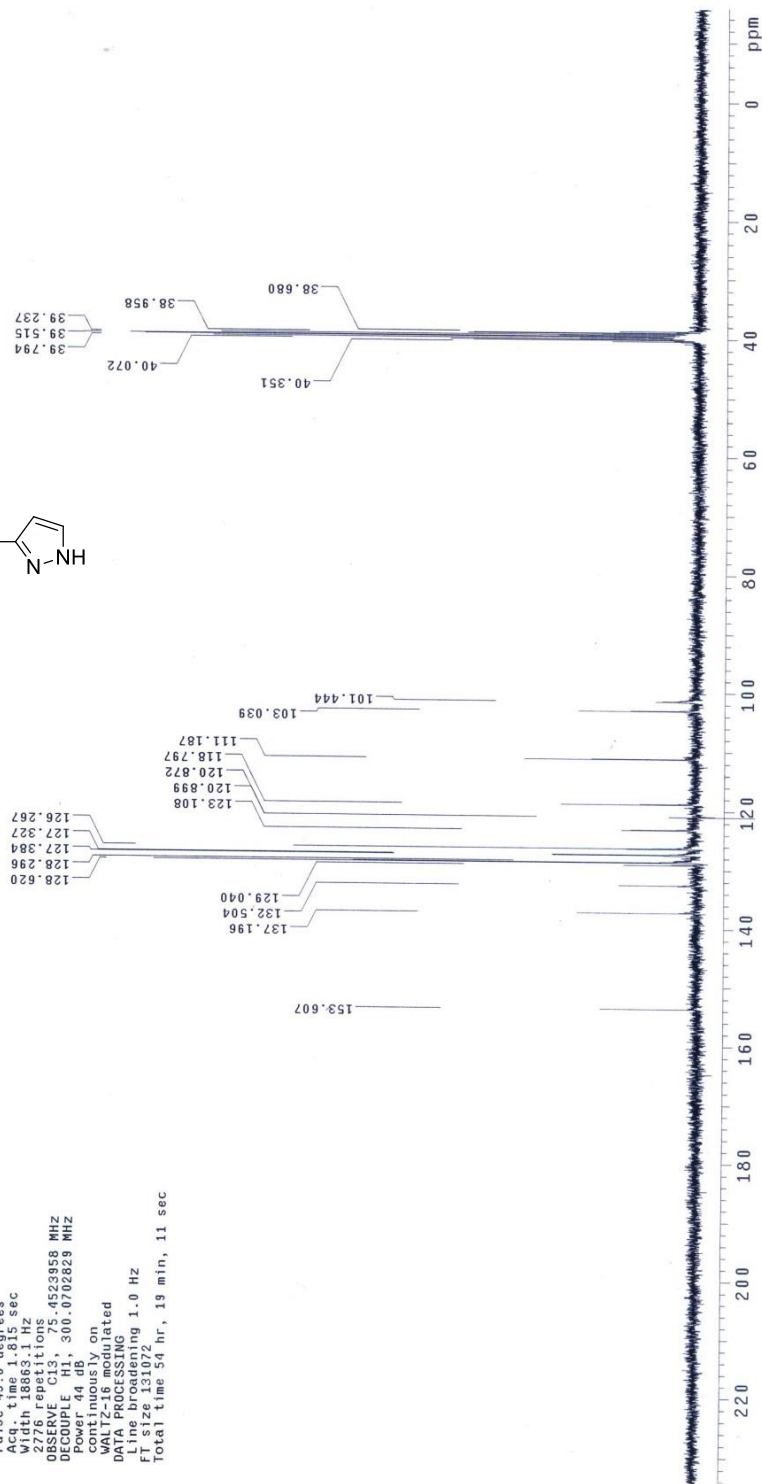
AhmedFathy-AF52-DMSO-C13

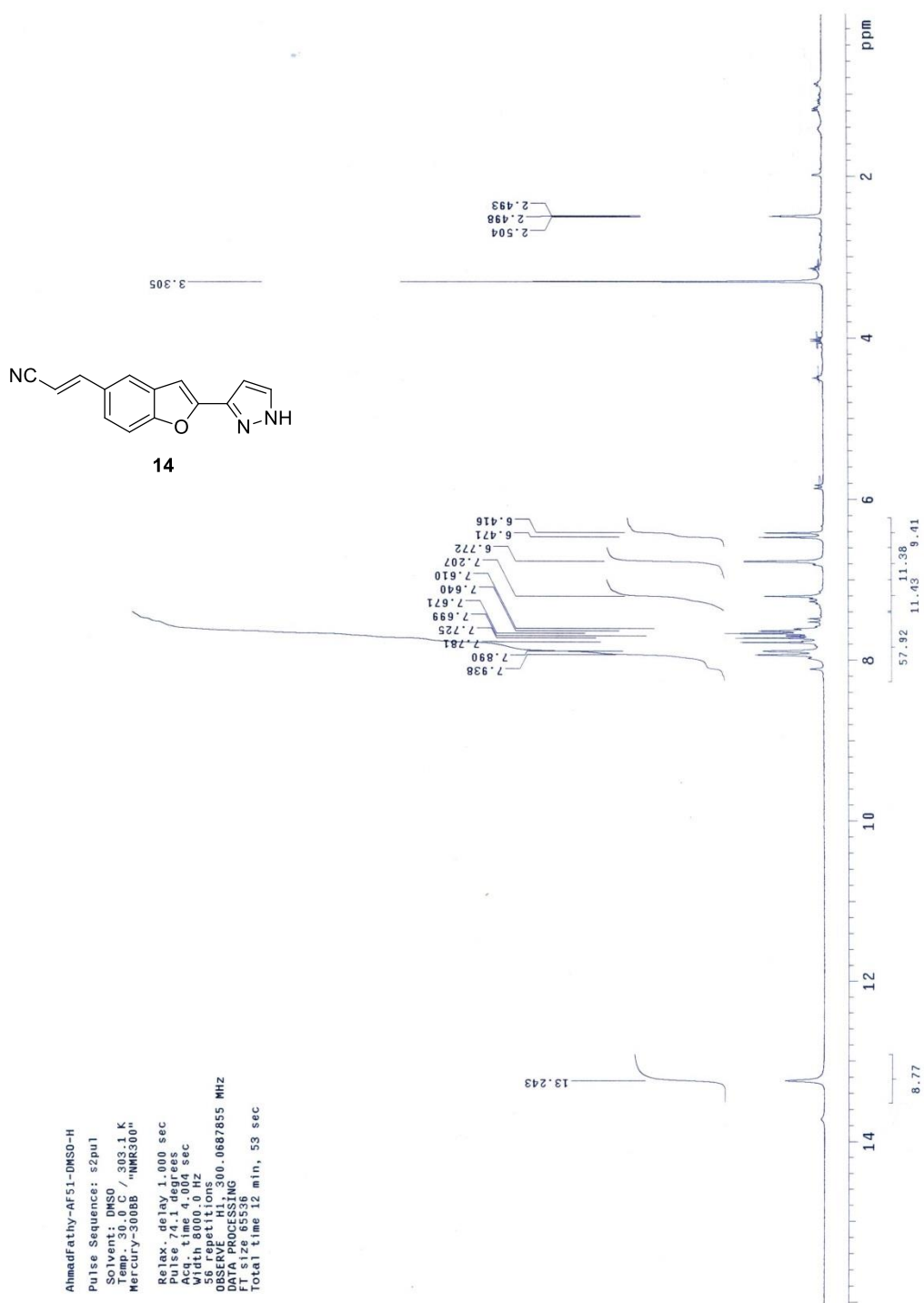
Archive directory: /export/home/vnmr1/vnmrSYS/data
 Sample directory: NSobhy-4-13C-dmsO_06Jun2004
 File: CARBON

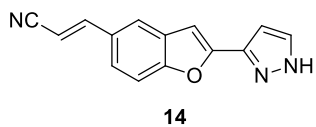
Pulse Sequence: s2pu1

Solvent: DMSO
 Temp.: 30.0 C / 303.1 K
 Mercury-300BB "NMR300"

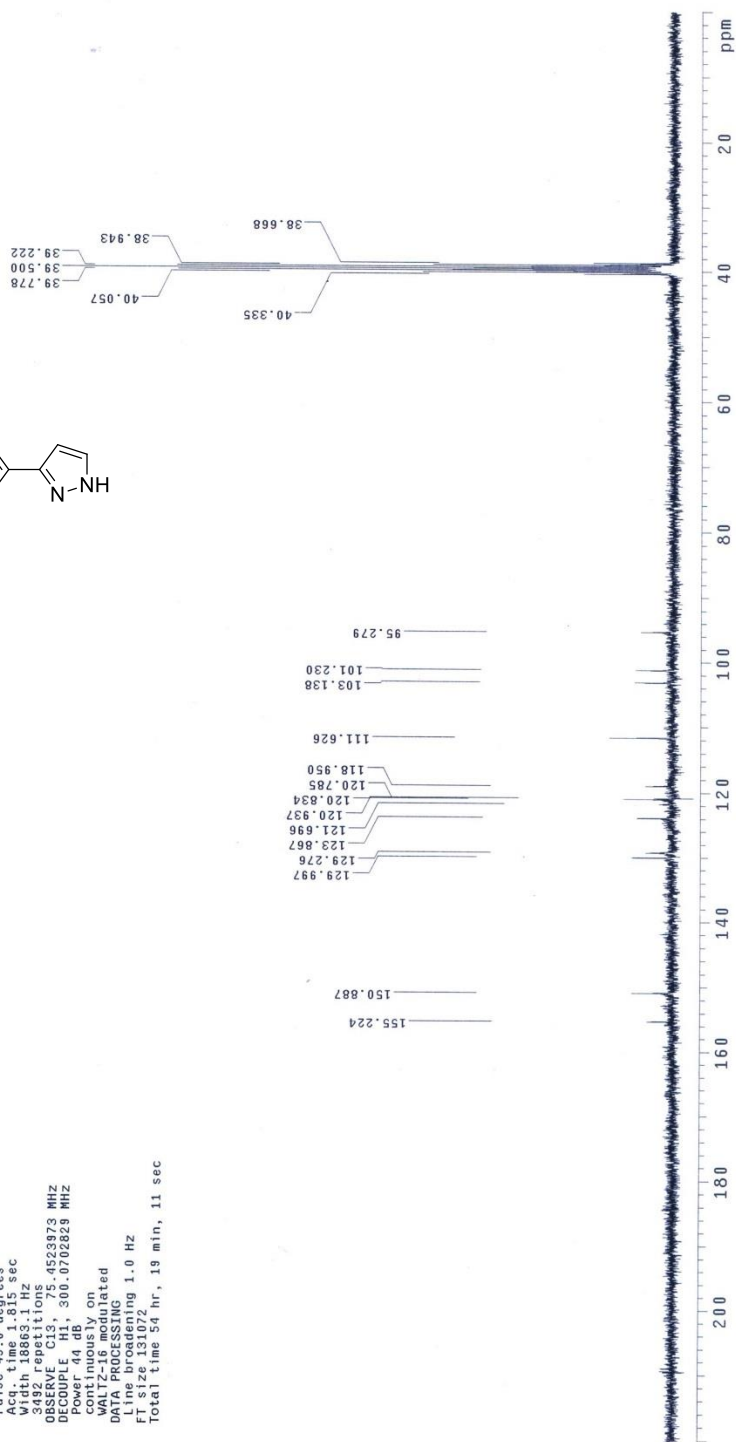
Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.015 sec
 Wdr time 1.015 sec
 2776 repetitions
 OBSERVE C13, 75.4523958 MHZ
 DECOUPLE H1, 300.0702829 MHZ
 Power 44 dB
 Continuously on
 Watergate gated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
 Total time 54 hr, 19 min, 11 sec

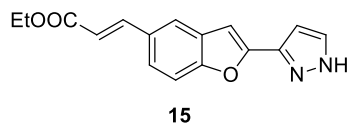




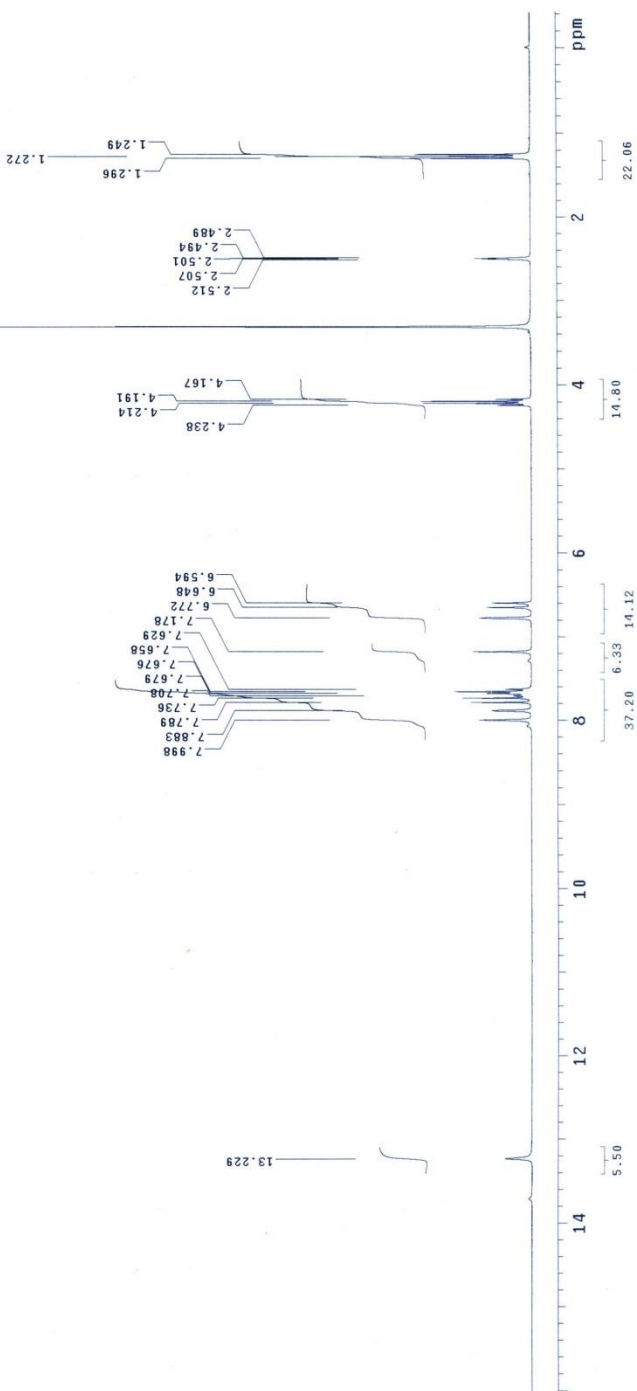


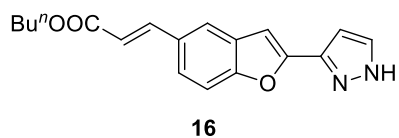
AhmadFathy-AF51-DMSO-C13-4-3-2009
 Archive directory: /export/home/vmar1/vmar1sus/data
 Sample directory: NS00by-4-13C-dms0_06Jun2004
 File: CARBON
 Pulse Sequence: szpu1
 Solvent: DMSO
 Temp.: 30.06 / 303.1 K
 Mercury-300BS -NMR300M
 Relax. delay: 1.000 sec
 Pulse: 45.0 degrees
 Acq. time: 1.815 sec
 Width: 18863.1 Hz
 S42: Repetitions: 452873
 DECOUPLE: CH, 300.0762823 MHz
 Power: 44 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING: 1.0 Hz
 FT Size: 131072
 Total time: 54 hr, 19 min, 11 sec





AhmaudFathy-AF14-DMSO-H1
 Pulse Sequence: s2pul
 Solvent: DMSO
 Temp: 30.0 C / 303.1 K
 Mercury-300BBB / NMR300P
 Relax. delay 1.000 sec
 Pulse 74.1 degrees
 Acq. time 4.004 sec
 Width 8000.0 Hz
 Observed F1 on 300.0687855 MHz
 DATA PROCESSING
 FT size 65536
 Total time 3 min, 13 sec





AhmedFathy-AF53-DMSO-H1
 Pulse Sequence: s2pul
 Solvent: DMSO
 Temp: 303.1 K
 Mercury-300BB "NMR300"
 Relax. delay 1.000 sec
 Pulse 74.1 degrees
 Acq. time 4.004 sec
 Width 8000.0 Hz
 OBSERVED F1: 300.0687855 MHz
 DATA PROCESSING
 FT size 65536
 Total time 12 min, 53 sec

