

Synthesis and potent anti-pancreatic cancer activity of new pyrazole derivatives bearing chalcone, thiazol and thiadiazol moieties: Gene expression, DNA fragmentation and SAR

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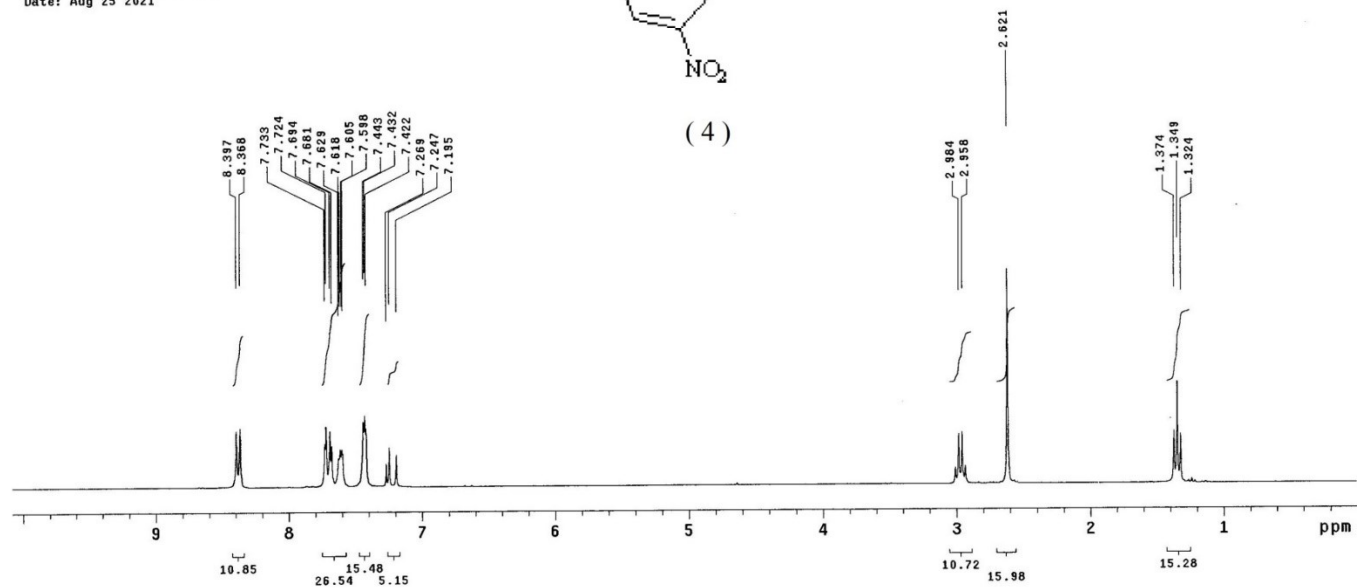
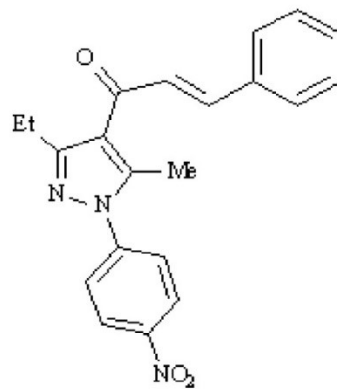
MernaTalat-M2-CDC13-H1

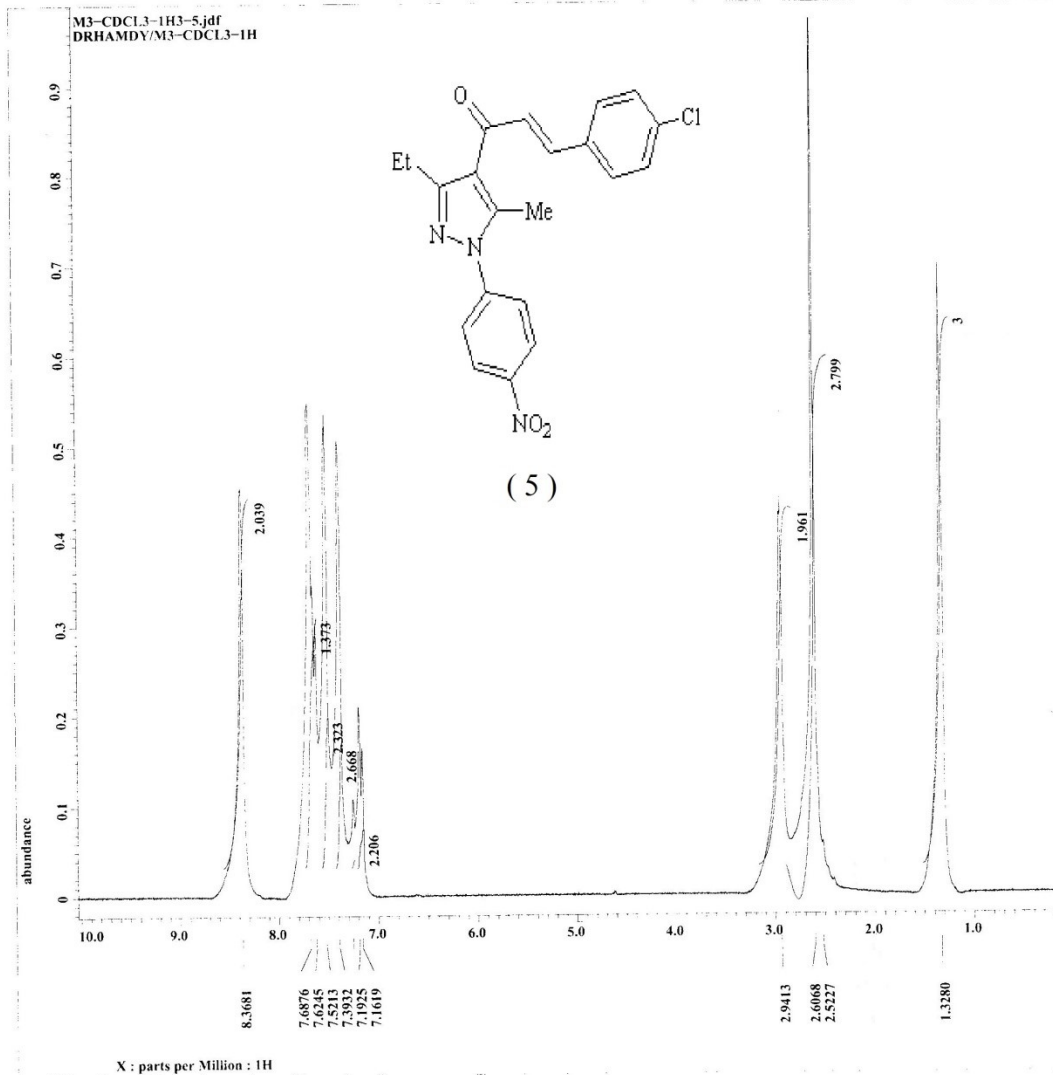
Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40

Pulse Sequence: s2pu1

Solvent: CDC13
Temp. 30.0 C / 303.1 K
File: MernaTalat-M2-CDC13-H1
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
10 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Aug 25 2021





JEOL

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Content         = DRHAMDY/M3-CDCL3
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Current_time    = 25-AUG-2021 11:2
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Dim_title       = 1H
Dim_units       = [ppm]
Dimensions      = X
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Machine         = scc
Revision_time   = 25-AUG-2021 11:2
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Site            = ECA500 (Datum BL)
Spectrometer    = DELTA2_NMR
Scans           = 16
Mod_return      = 1
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X_offset        = 5.0 [ppm]
X_freq          = 500.15991521 [MHz]
X_sweep         = 15.6641604 [kHz]
X_resolution    = 0.95606448 [Hz]
Irr_domain      = 1H
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Digital_filter  = TRUE
Filter_factor   = 8
Af_version      = 1
Delay_of_start  = 1.99999974 [s]
Actual_start_time = 25-AUG-2021 18:1
Acq_delay       = 7.94 [us]
Digital_filter_status = 2F
Clipped         = FALSE
Dc_balanced     = FALSE
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Tri90           = 10 [us]
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Sex90           = 10 [us]
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Non90           = 10 [us]
Dec90           = 10 [us]
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Irr90_hi        = 92 [us]
Tri90_hi        = 10 [us]
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Non90_hi        = 10 [us]
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X90_lo          = 92 [us]
Irr90_lo        = 92 [us]
Tri90_lo        = 10 [us]
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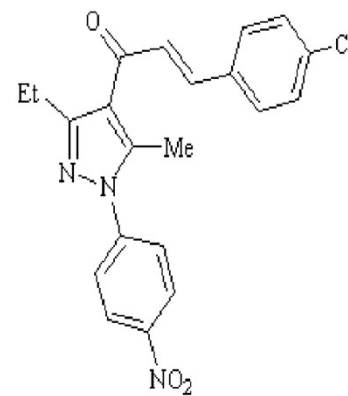
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HamdyHasaneen-M3-CDC13-C13

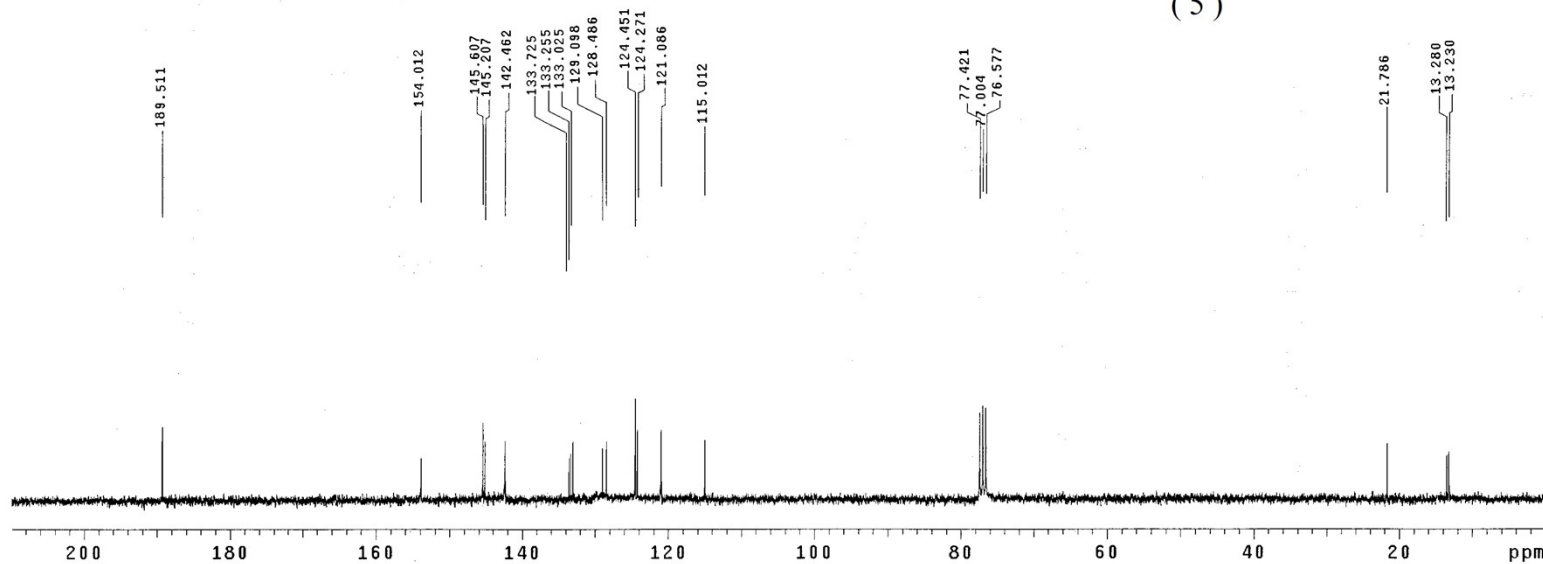
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Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1752 repetitions
OBSERVE C13, 75.4520074 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Dec 7 2021



(5)



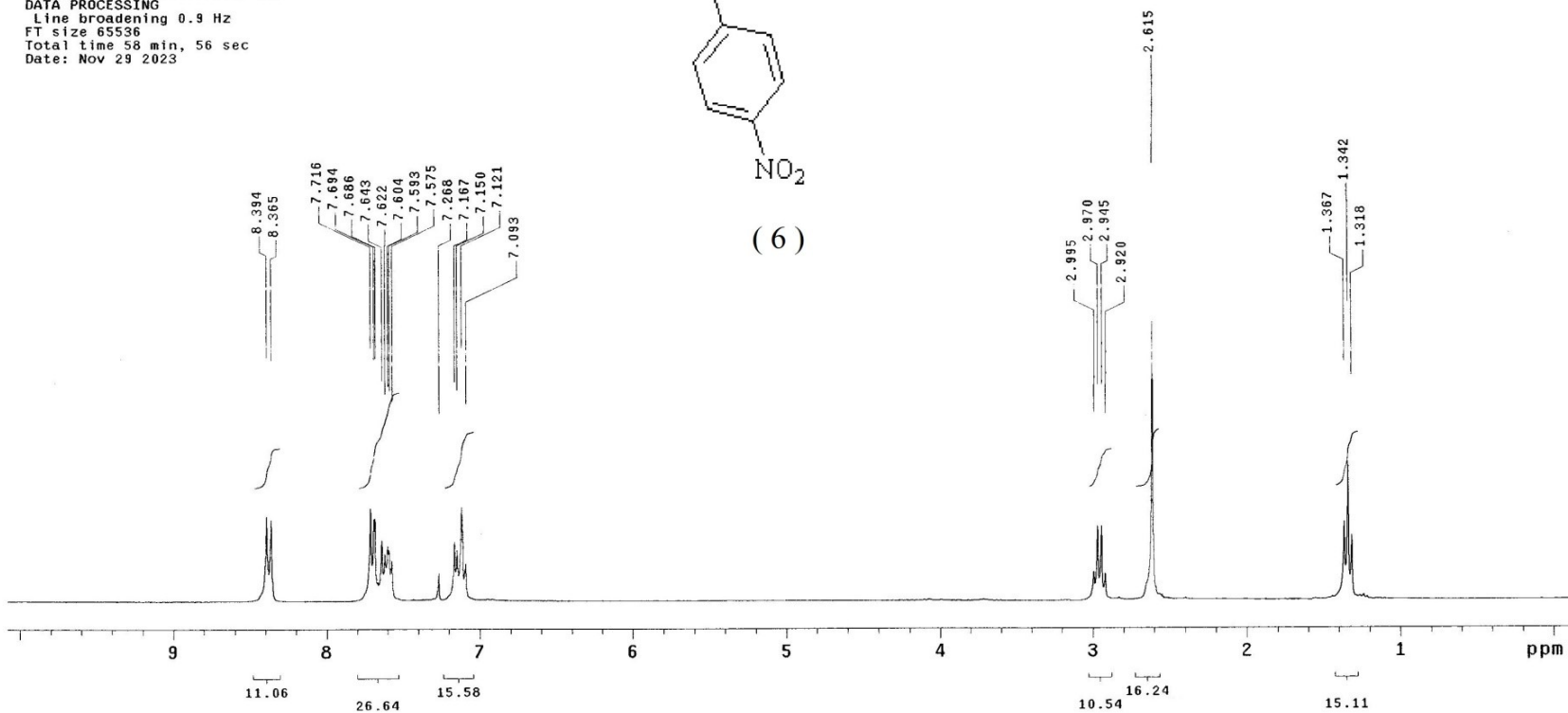
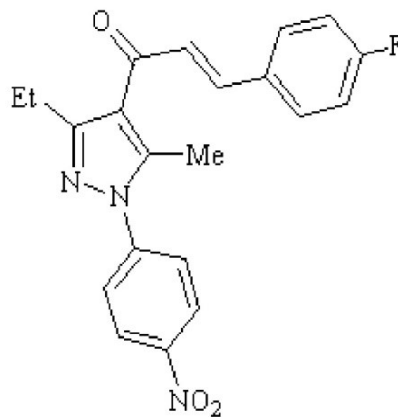
HamdyHasaneen-M13-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40

Pulse Sequence: s2pu1

Solvent: CDC13
Temp. 30.0 C / 303.1 K
File: HamdyHasaneen-M13-CDC13-H1
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
7 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Nov 29 2023

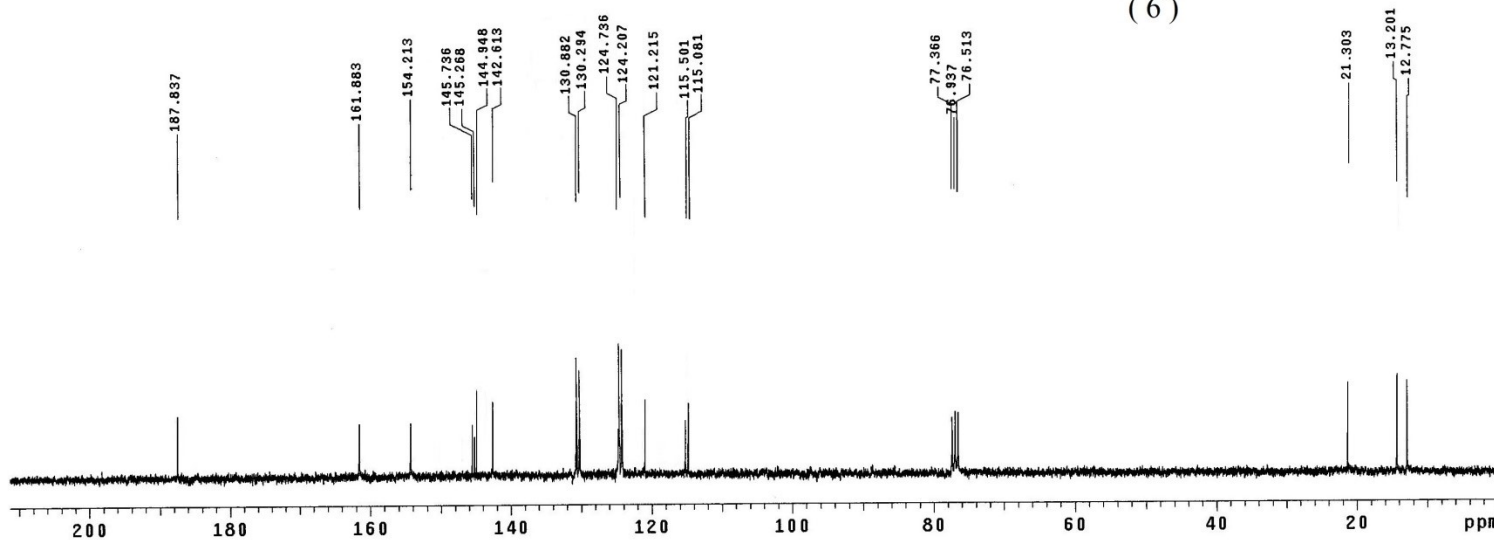
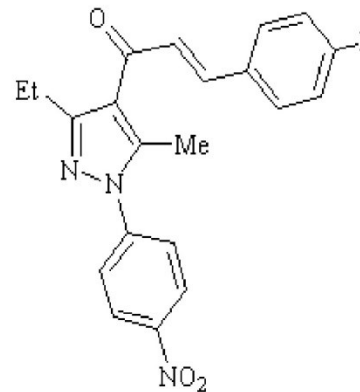


HamdyHasaneen-M13-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2088 repetitions
OBSERVE C13, 75.4520097 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 53 min, 46 sec
Date: Nov 30 2023

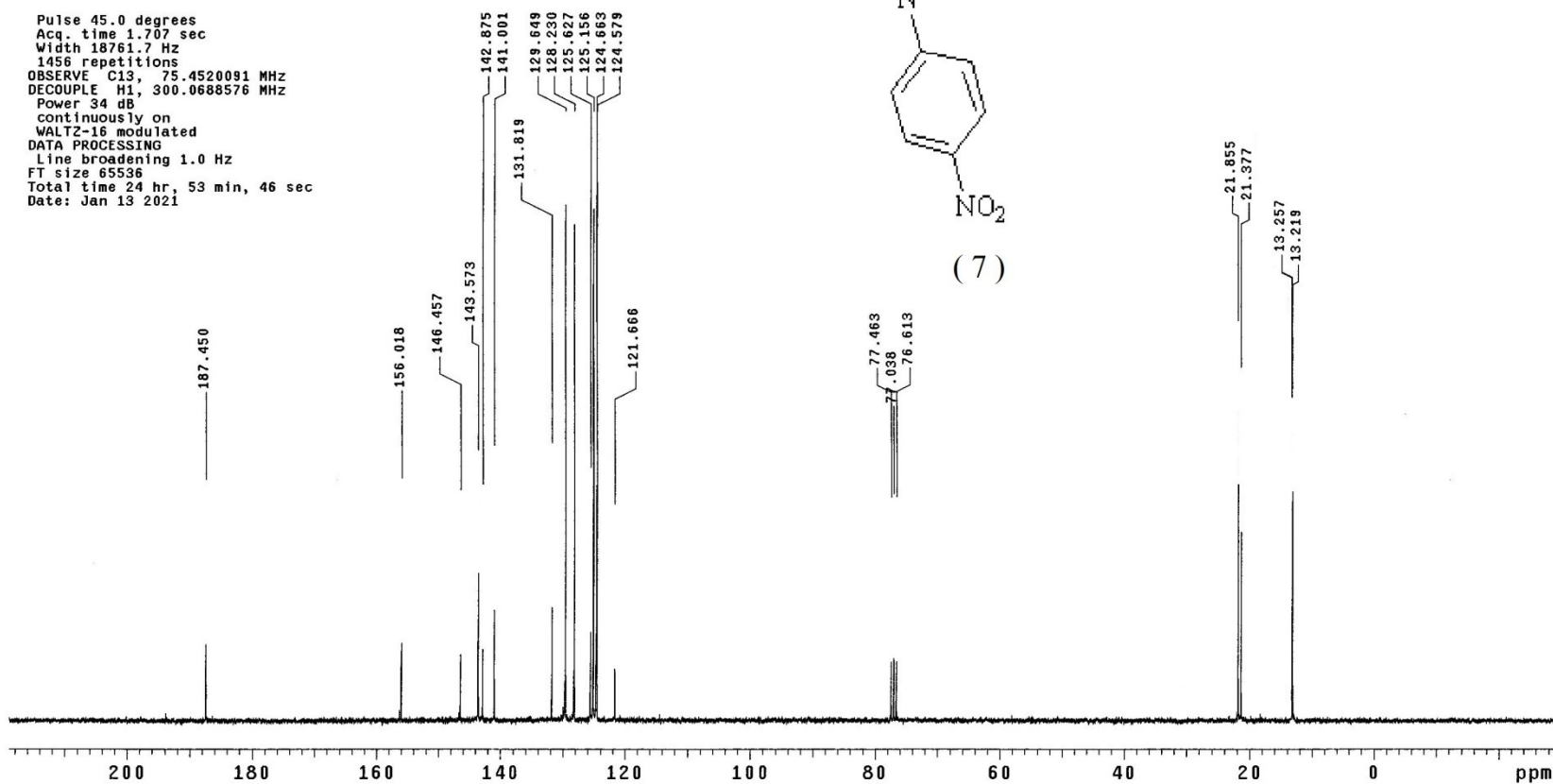
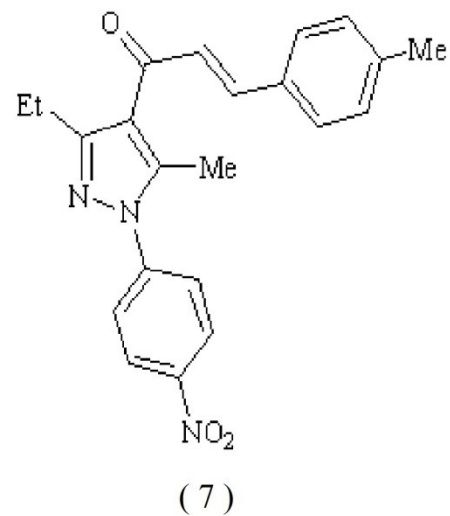


MohammadAbdulMoaty-M4-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1456 repetitions
OBSERVE C13, 75.4520091 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 53 min, 46 sec
Date: Jan 13 2021

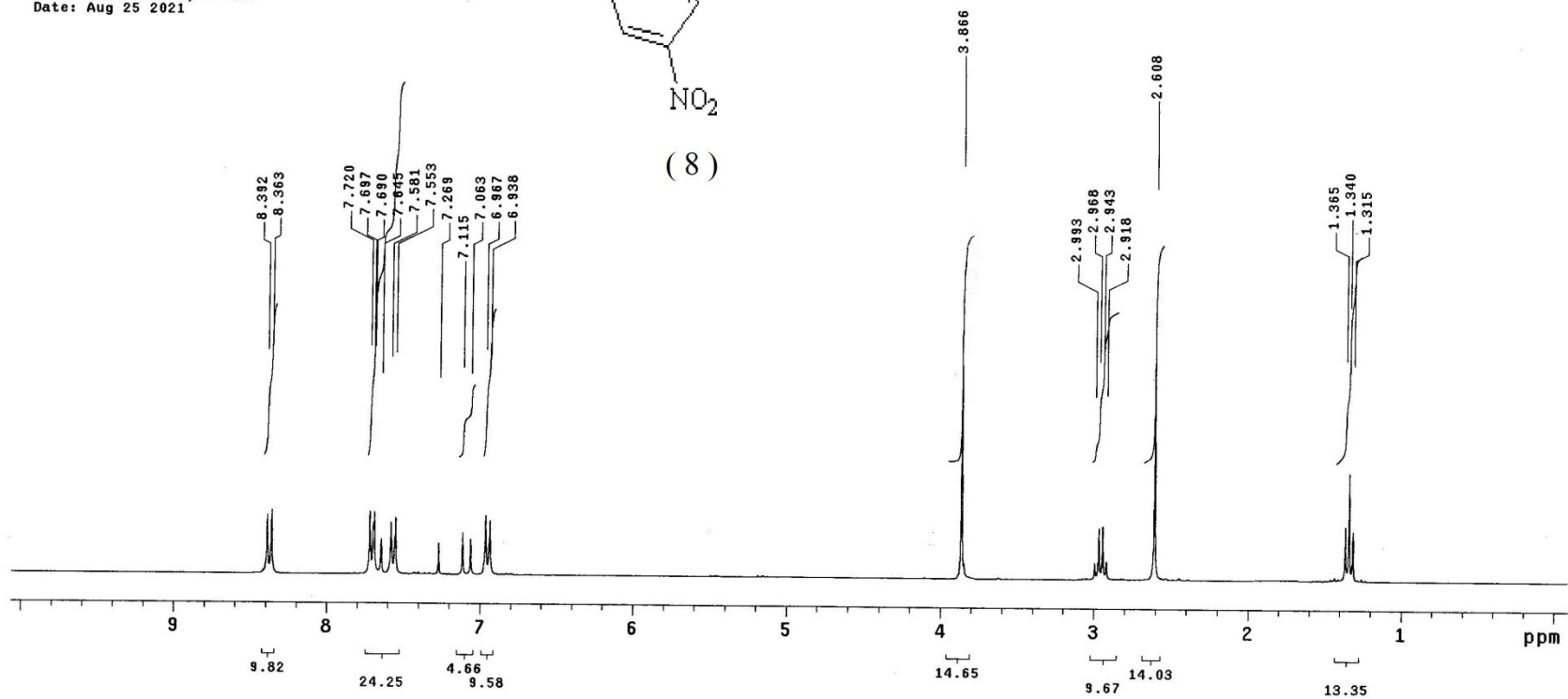
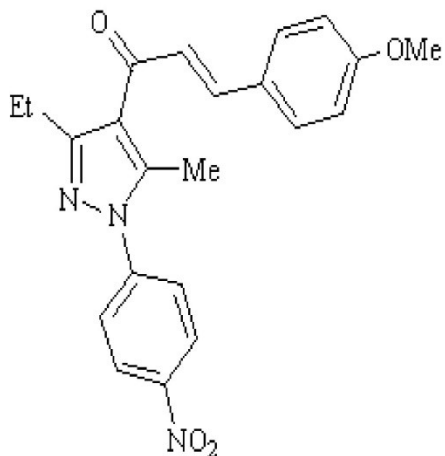


MernaTatlat-M5-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
14 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Aug 25 2021



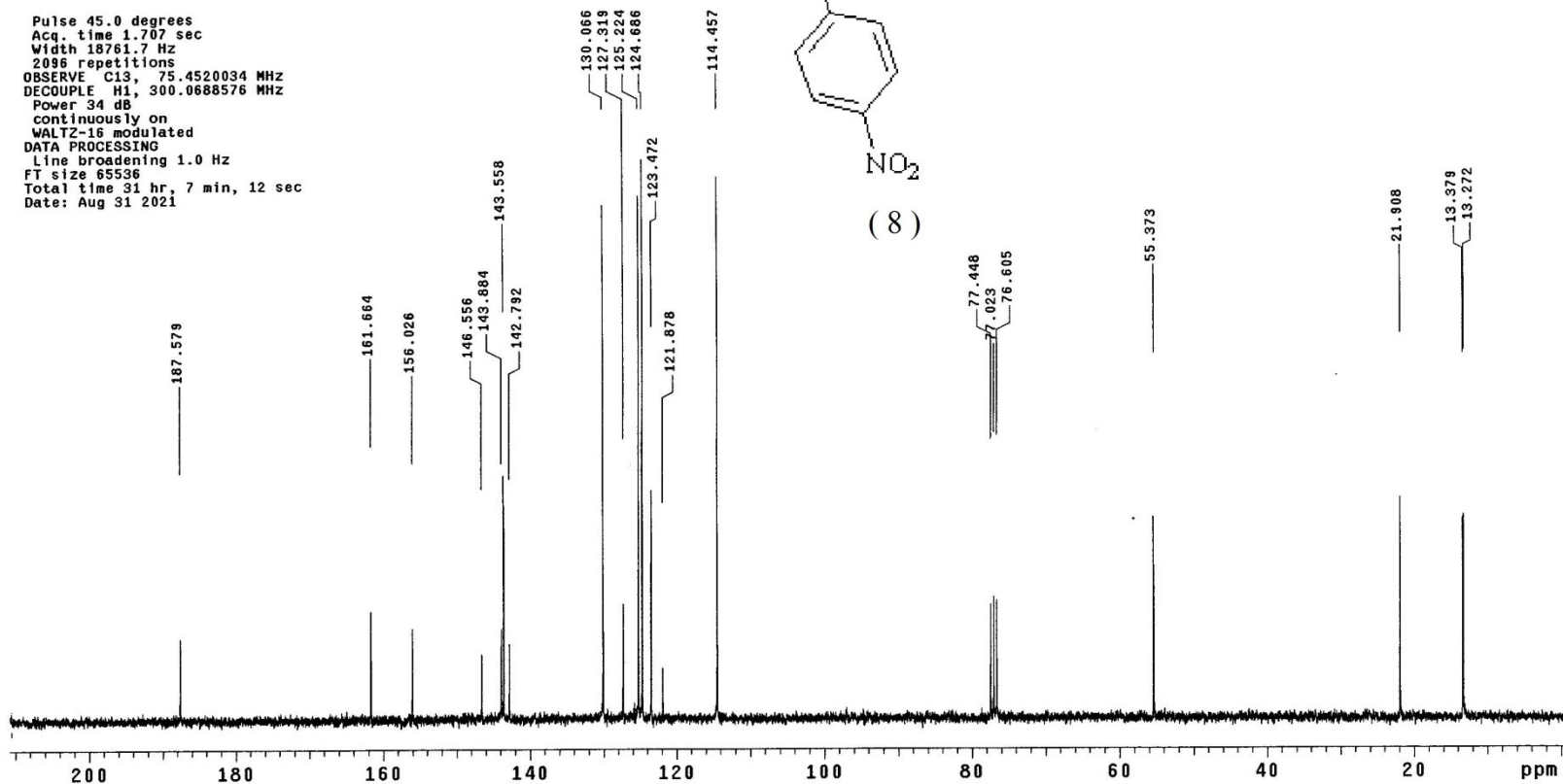
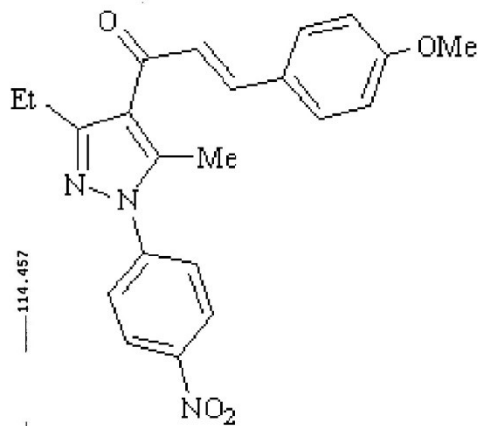
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Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2096 repetitions
OBSERVE C13, 75.4520034 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Aug 31 2021



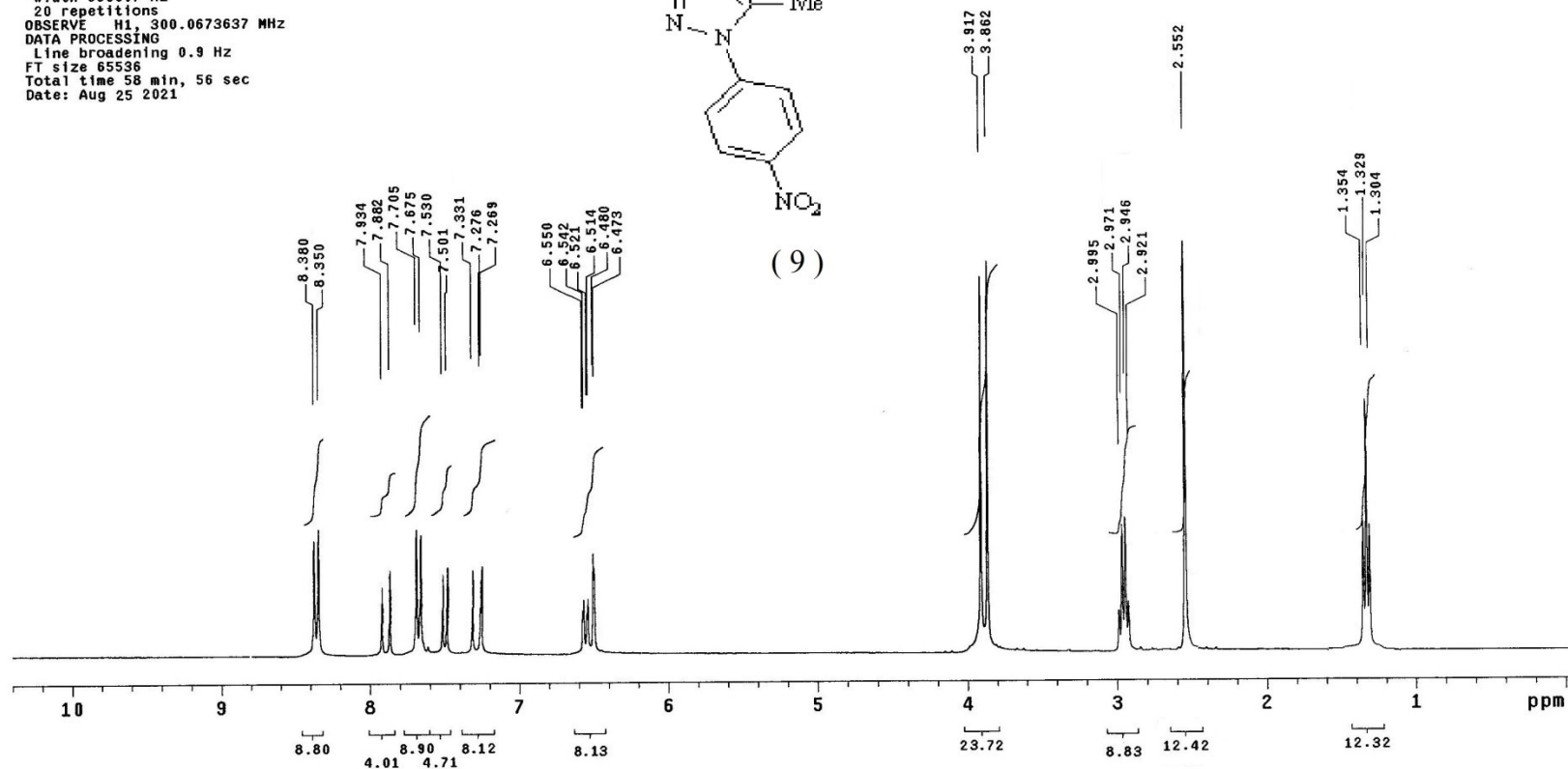
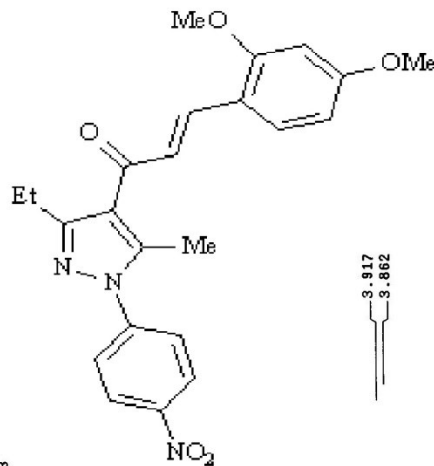
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Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40

Pulse Sequence: s2pu1

Solvent: CDC13
Temp. 30.0 C / 303.1 K
File: MernaTalat-A26-CDC13-H1
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
20 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Aug 25 2021

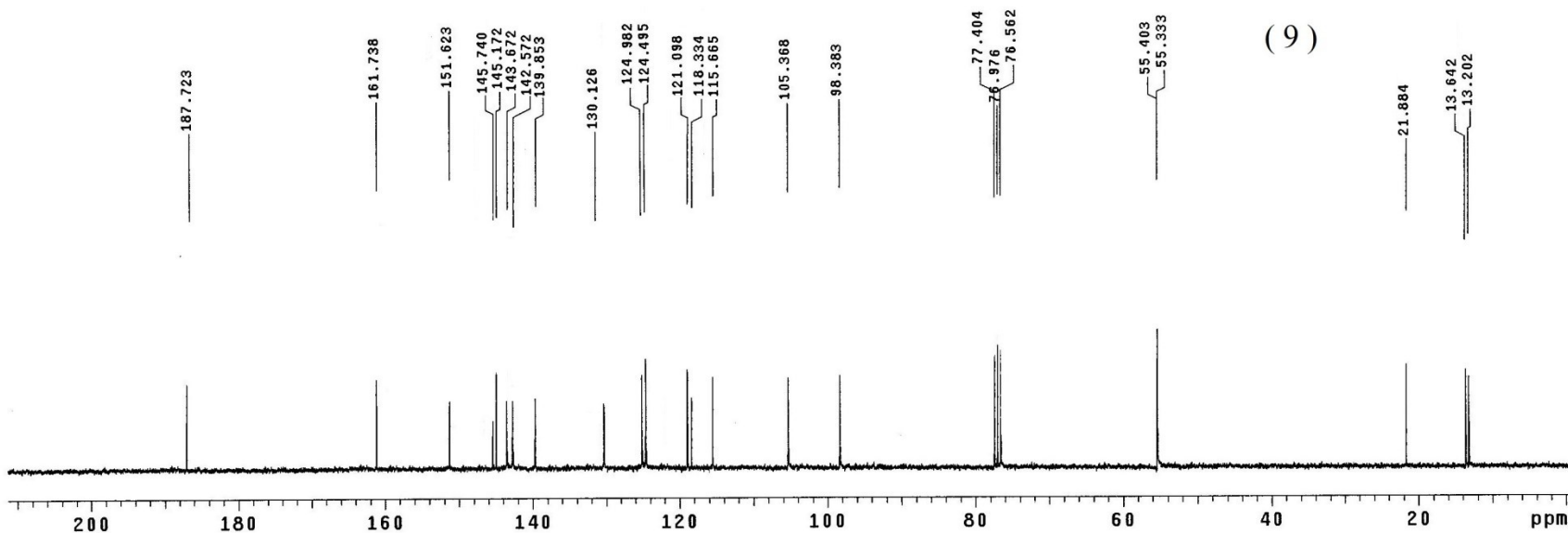
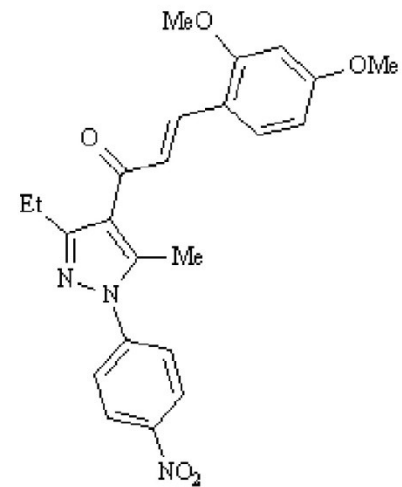


MernaTalaat-M6-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1360 repetitions
OBSERVE C13, 75.4520097 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 53 min, 46 sec
Date: Aug 26 2021



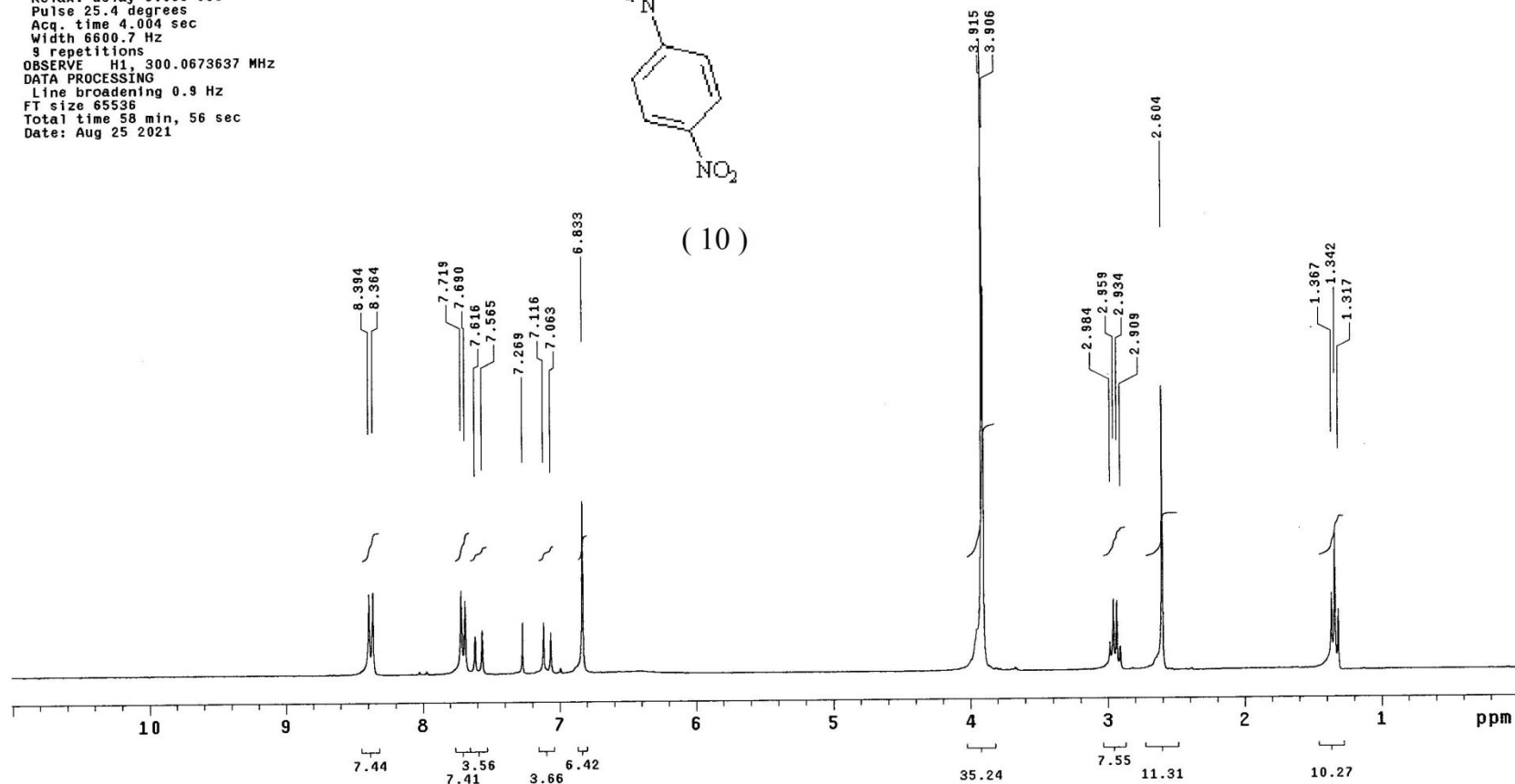
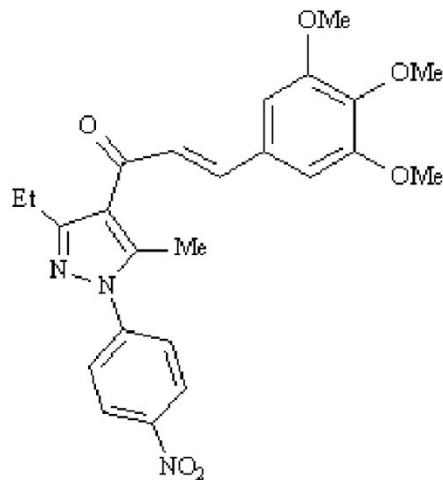
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Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
9 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Aug 25 2021

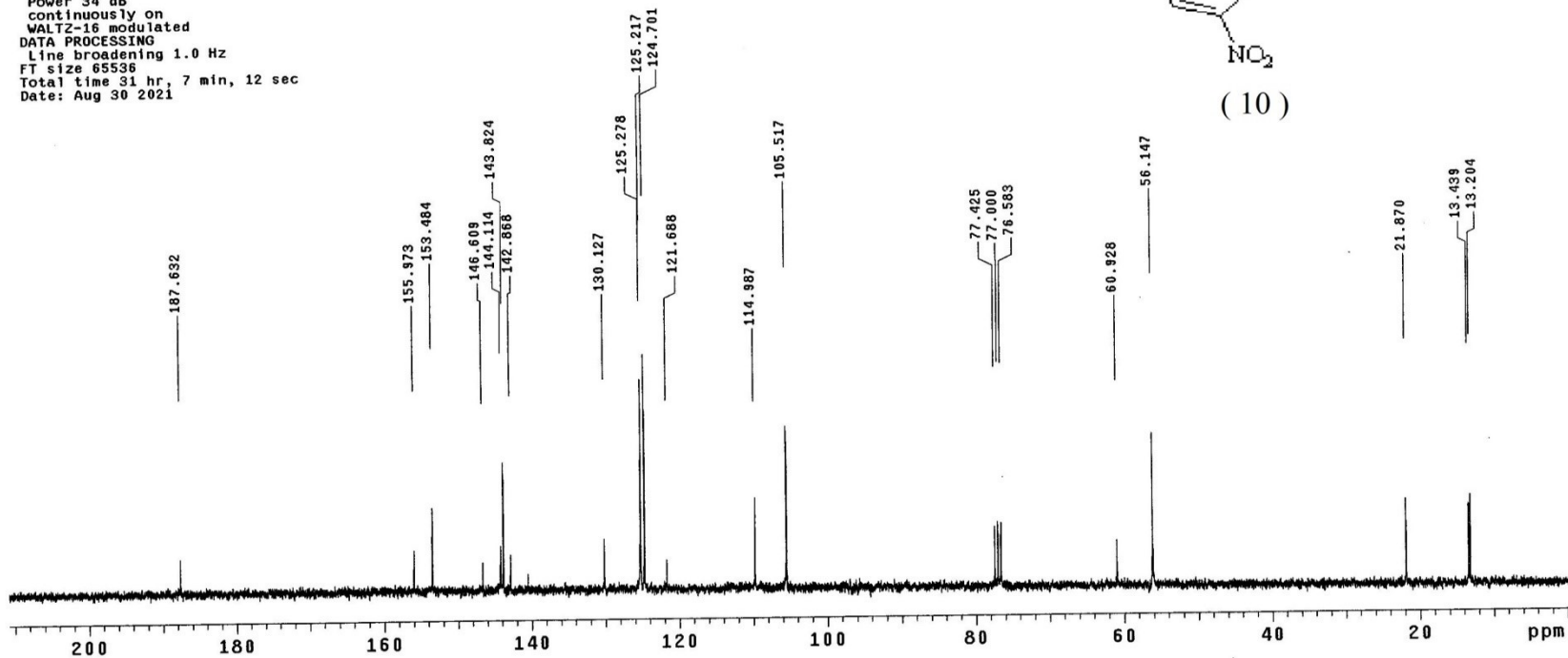
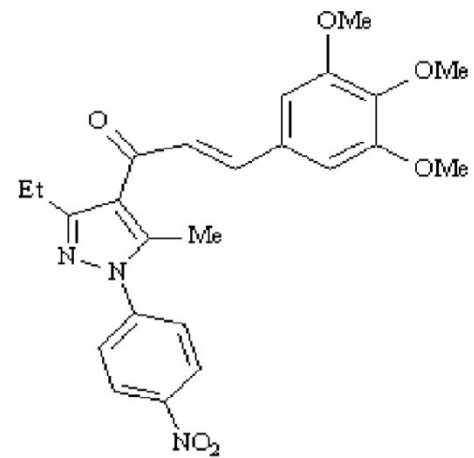


MernaTatlat-M7-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1312 repetitions
OBSERVE C13, 75.4520034 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Aug 30 2021



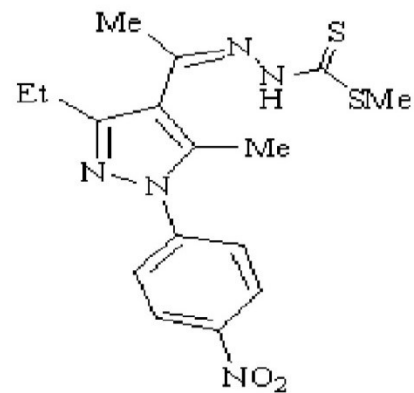
MernaTalaat-M9-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

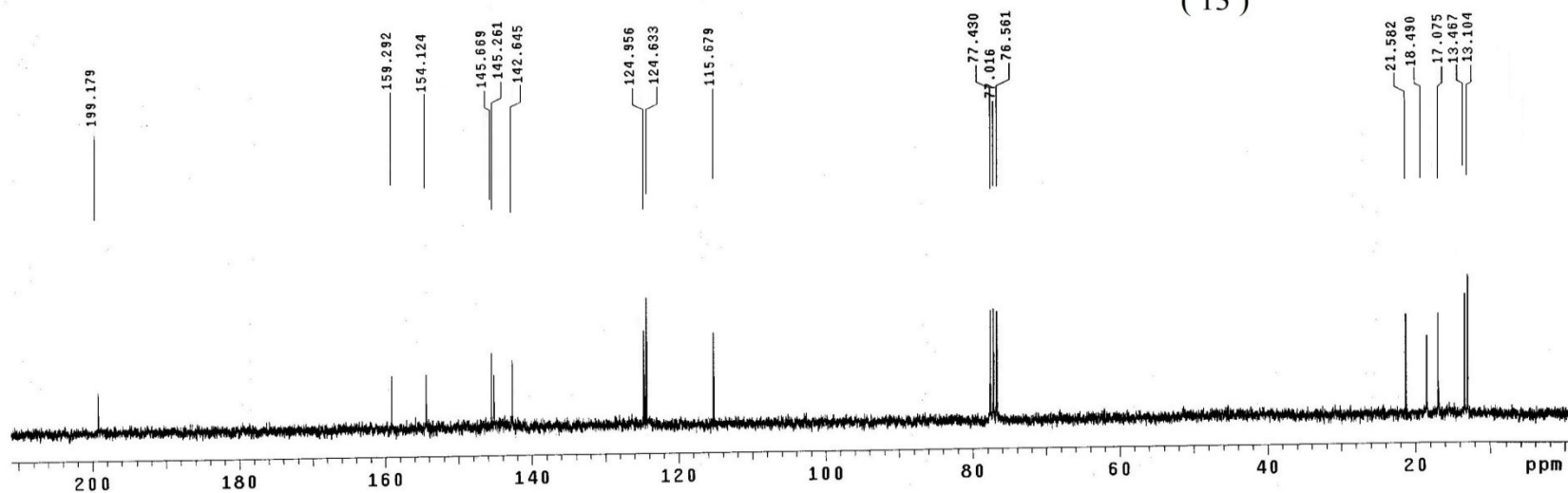
Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1160 repetitions
OBSERVE C13, 75.4523880 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Oct 13 2021



(13)



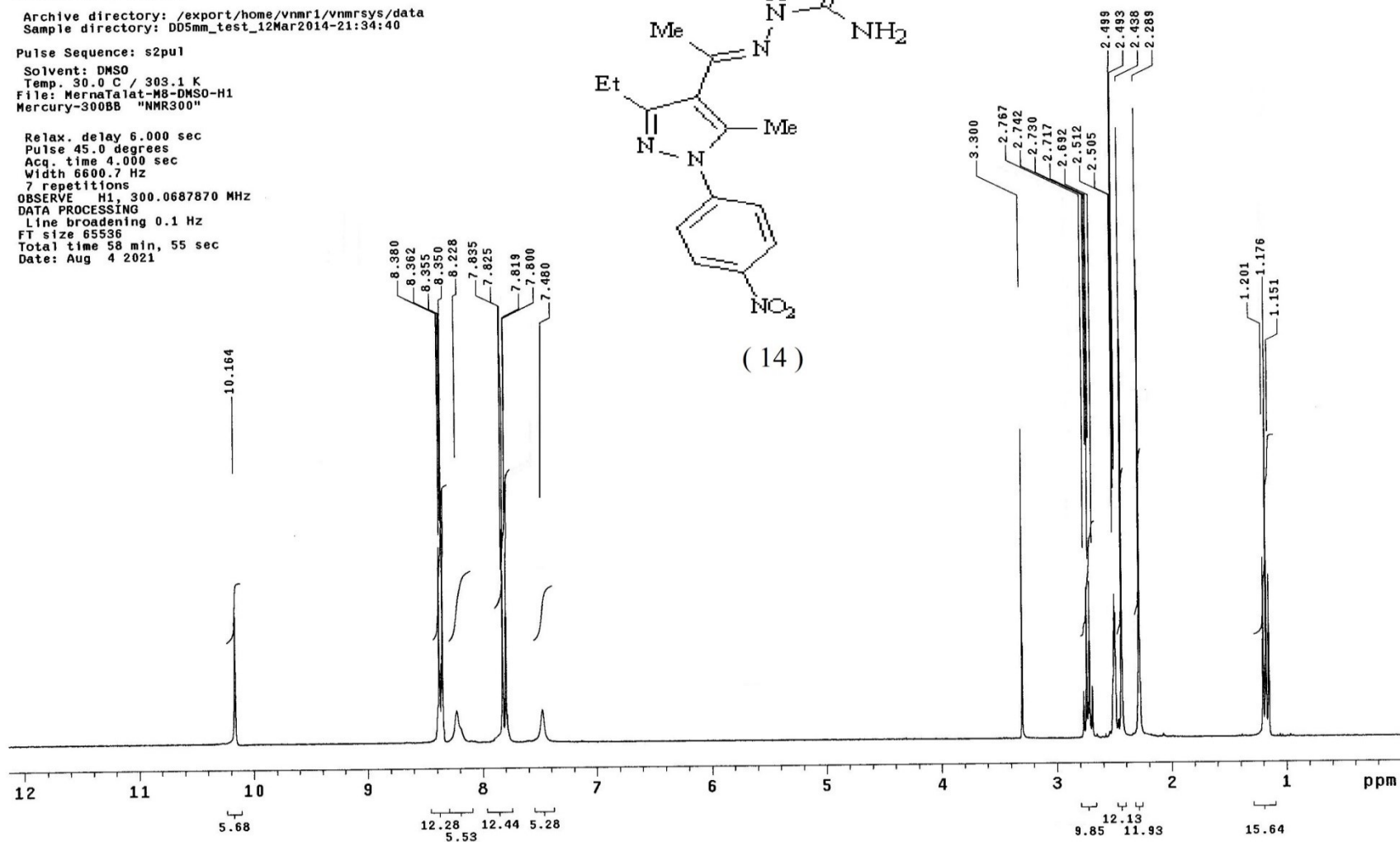
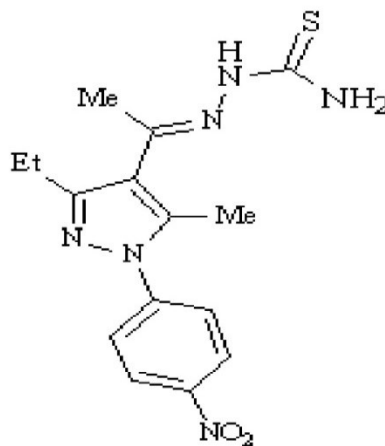
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Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40

Pulse Sequence: s2pul

Solvent: DMSO
Temp. 30.0 C / 303.1 K
File: MernaTalat-M8-DMSO-H1
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.000 sec
Width 6600.7 Hz
7 repetitions
OBSERVE H1, 300.0687870 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 6536
Total time 58 min, 55 sec
Date: Aug 4 2021

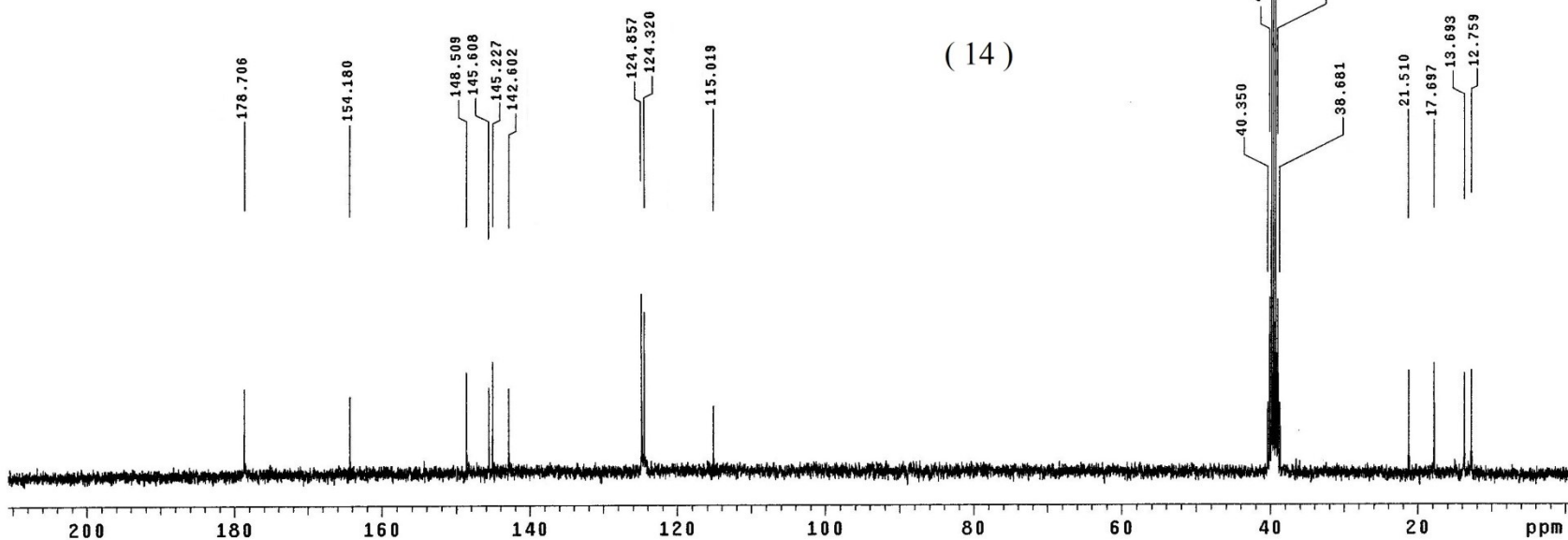
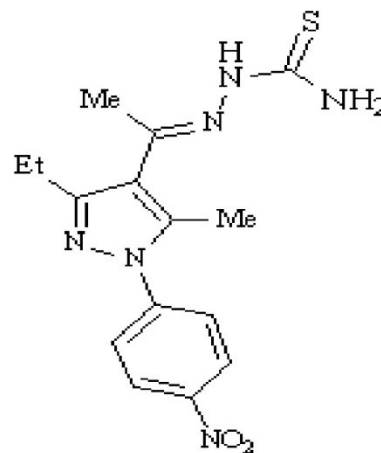


MernaTalaat-M8-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
3456 repetitions
OBSERVE C13, 75.4523885 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Aug 5 2021

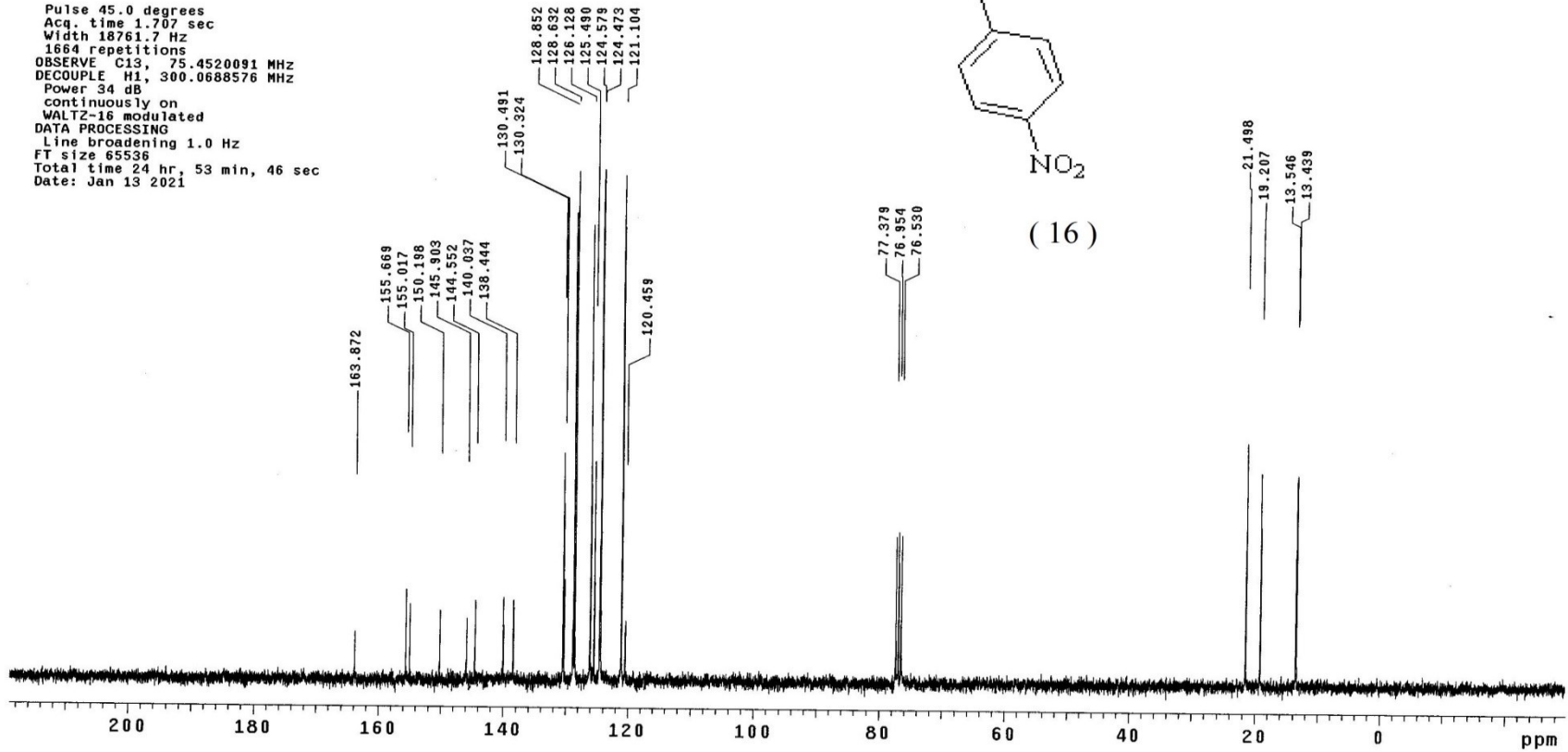
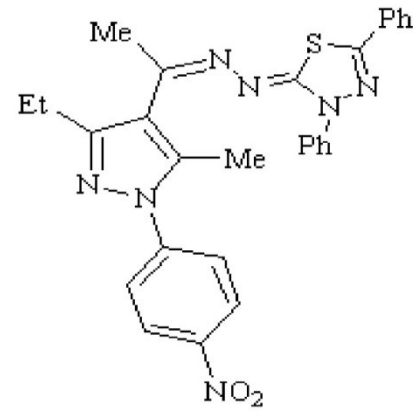


MohammadAbdulMoaty-M11-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1664 repetitions
OBSERVE C13, 75.4520091 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 53 min, 46 sec
Date: Jan 13 2021



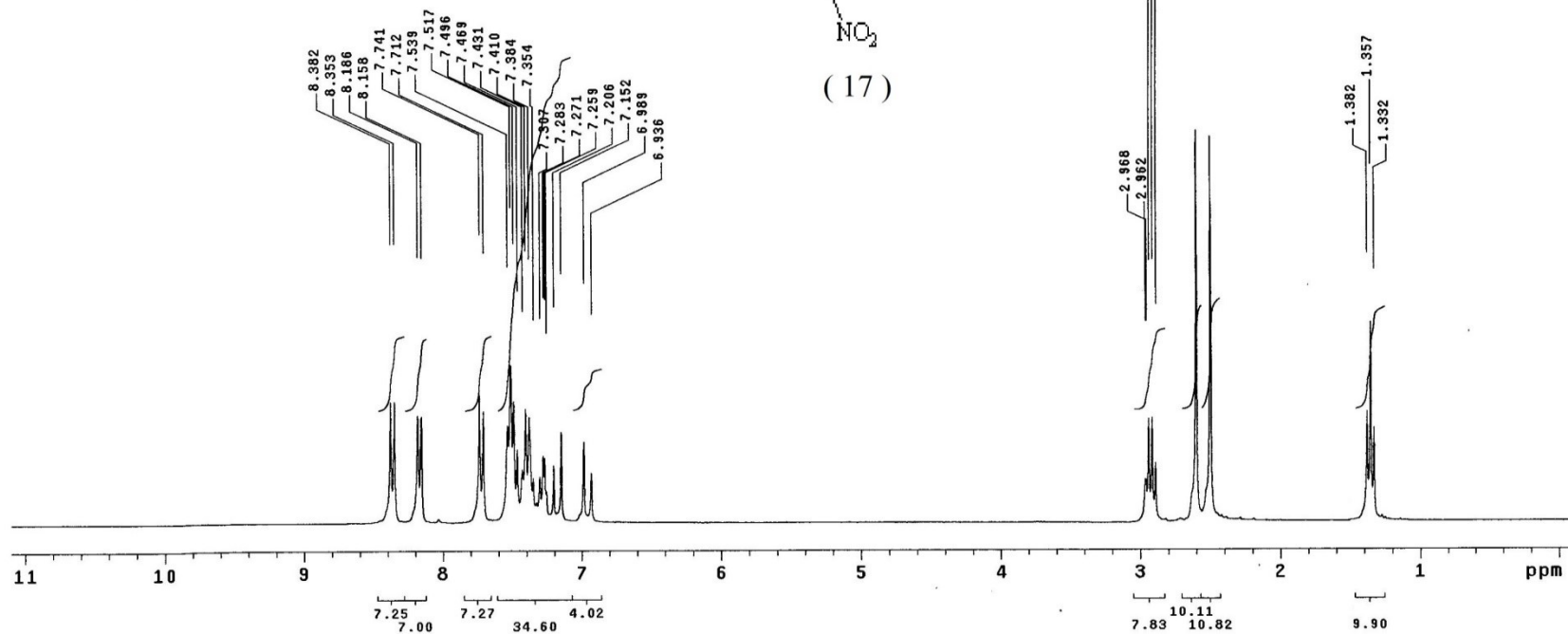
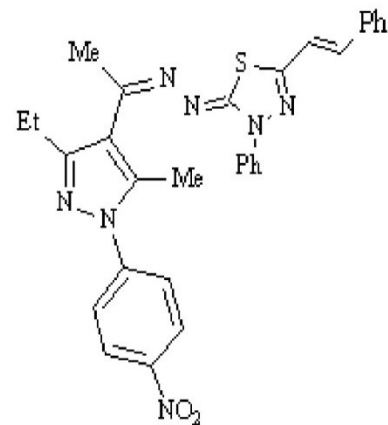
MernaTalat-M24-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
8 repetitions
OBSERVE H1, 300.0673635 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Mar 30 2021

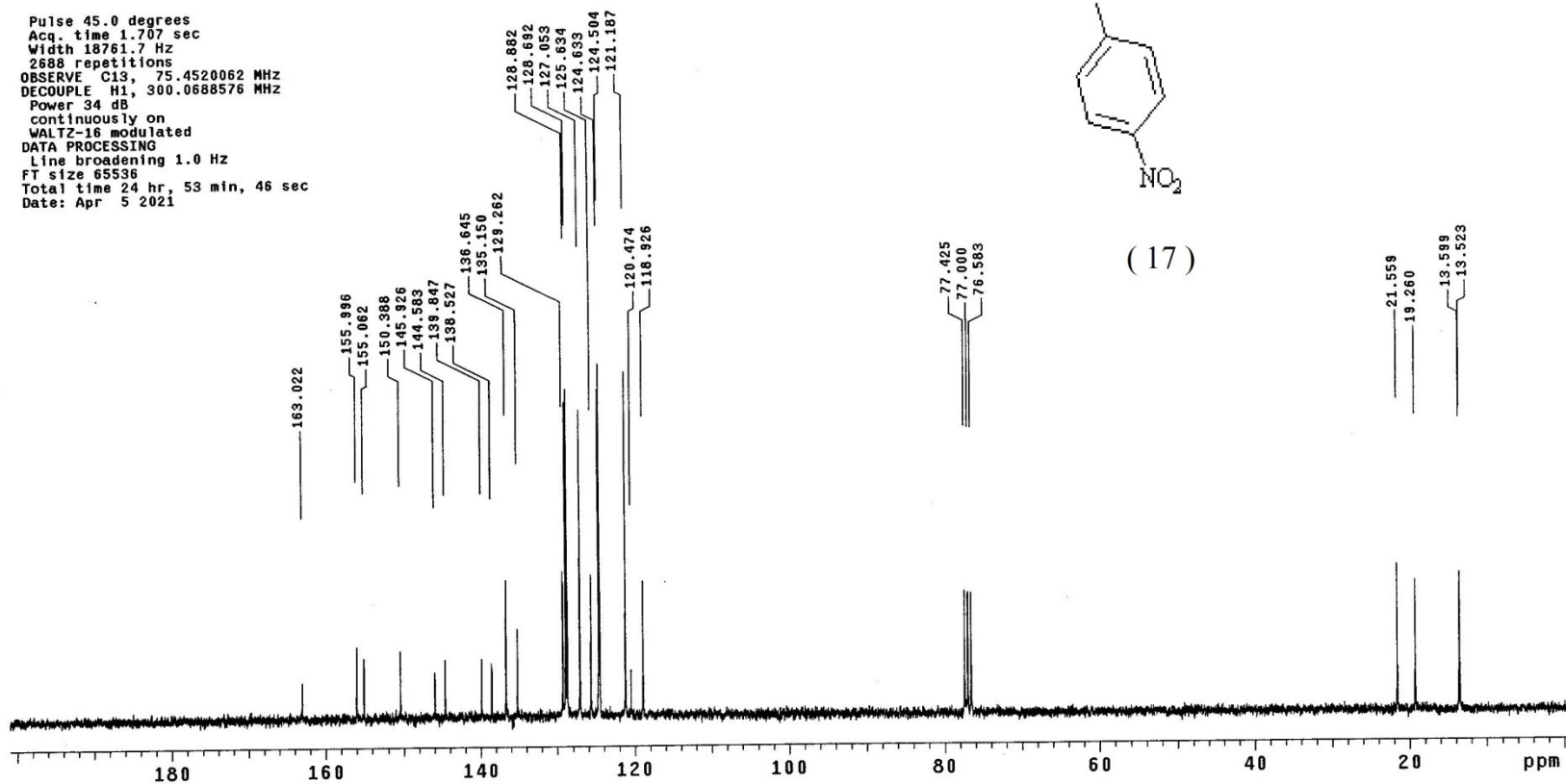


HamdyHasaneen-M24-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2688 repetitions
OBSERVE C13, 75.4520062 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 53 min, 46 sec
Date: Apr 5 2021

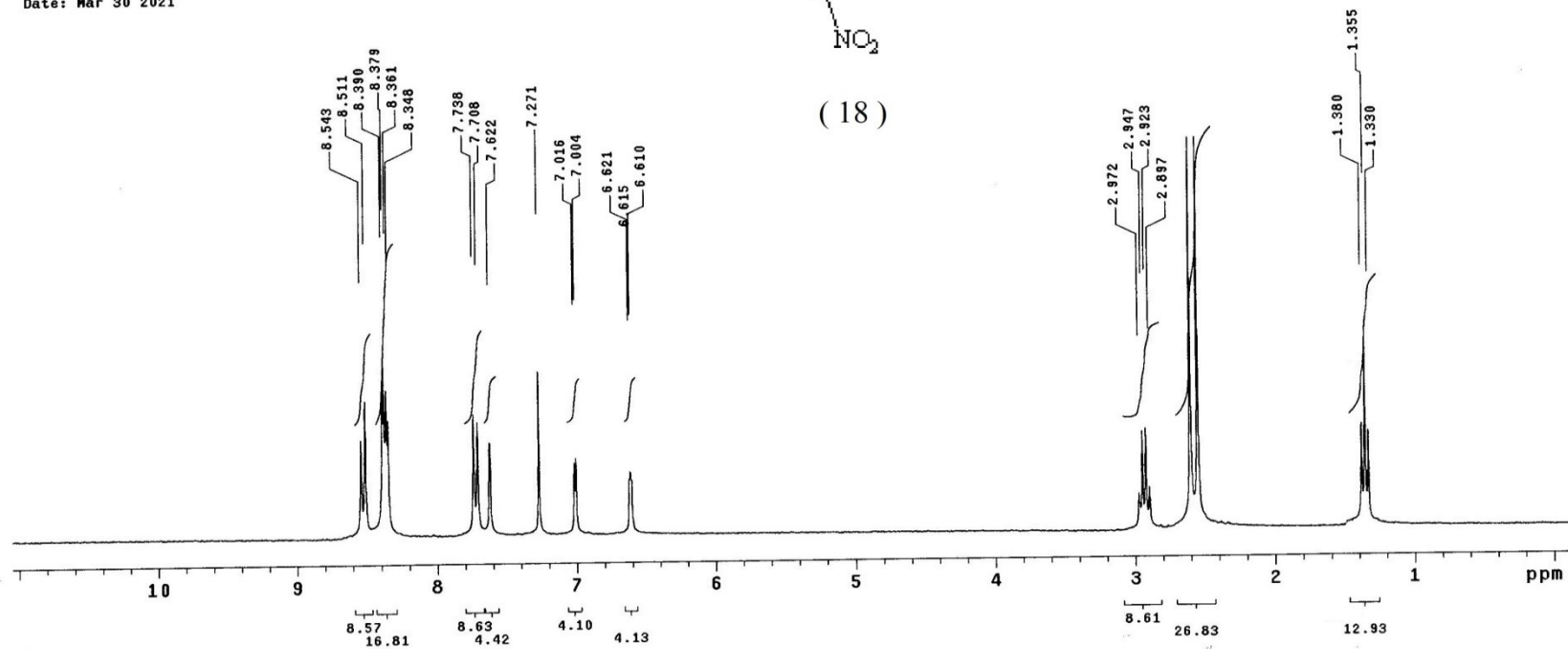
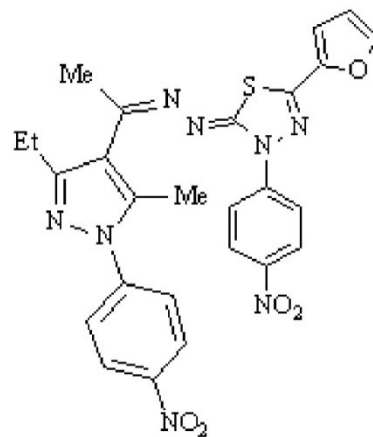


MernaTalat-M23-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
9 repetitions
OBSERVE H1, 300.0673635 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Mar 30 2021

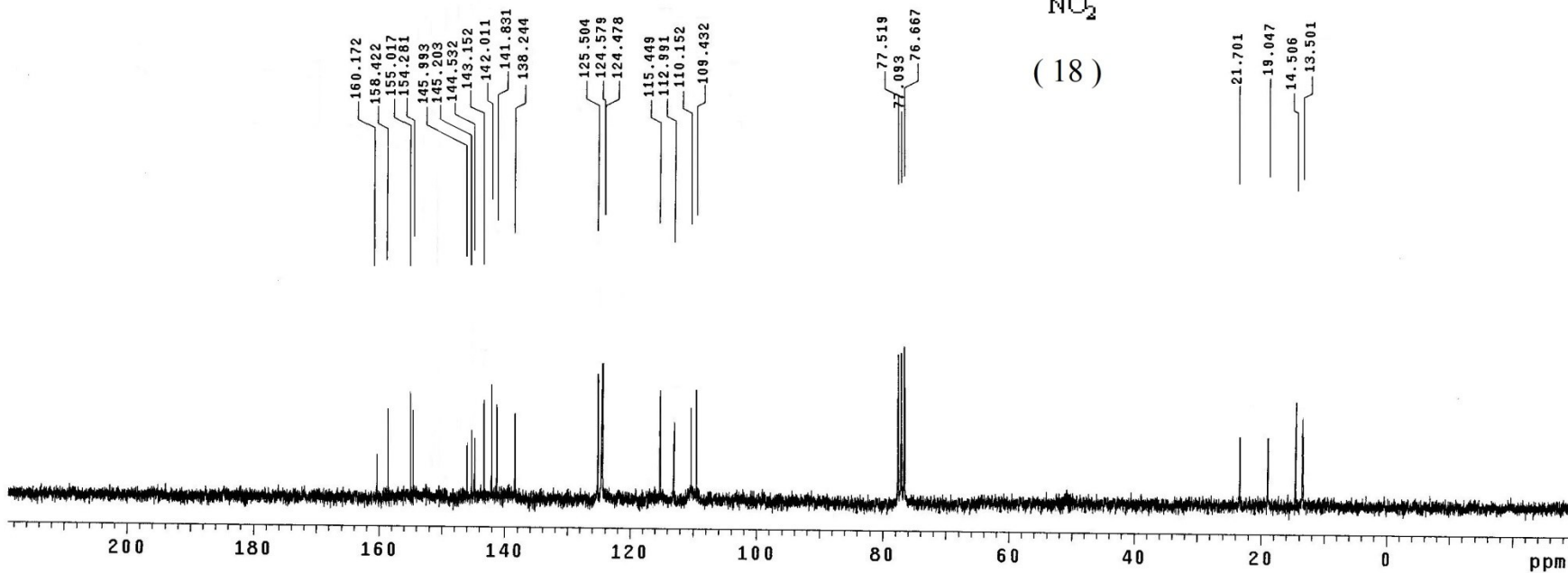
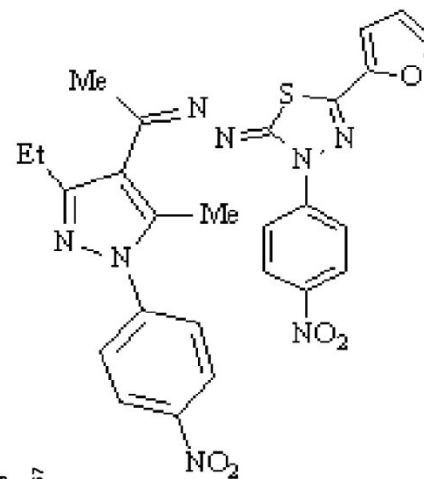


MernaTalat-M23-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2968 repetitions
OBSERVE C13, 75.4520074 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 53 min, 46 sec
Date: Apr 13 2021

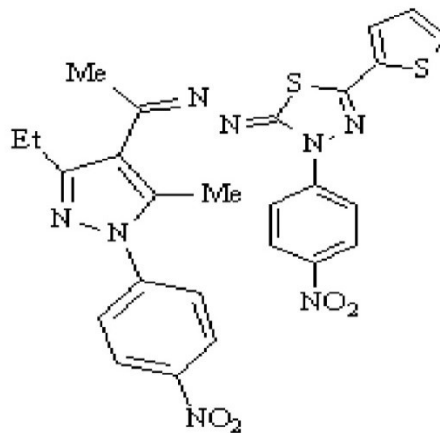


MernaTalat-M25-CDC13-H1

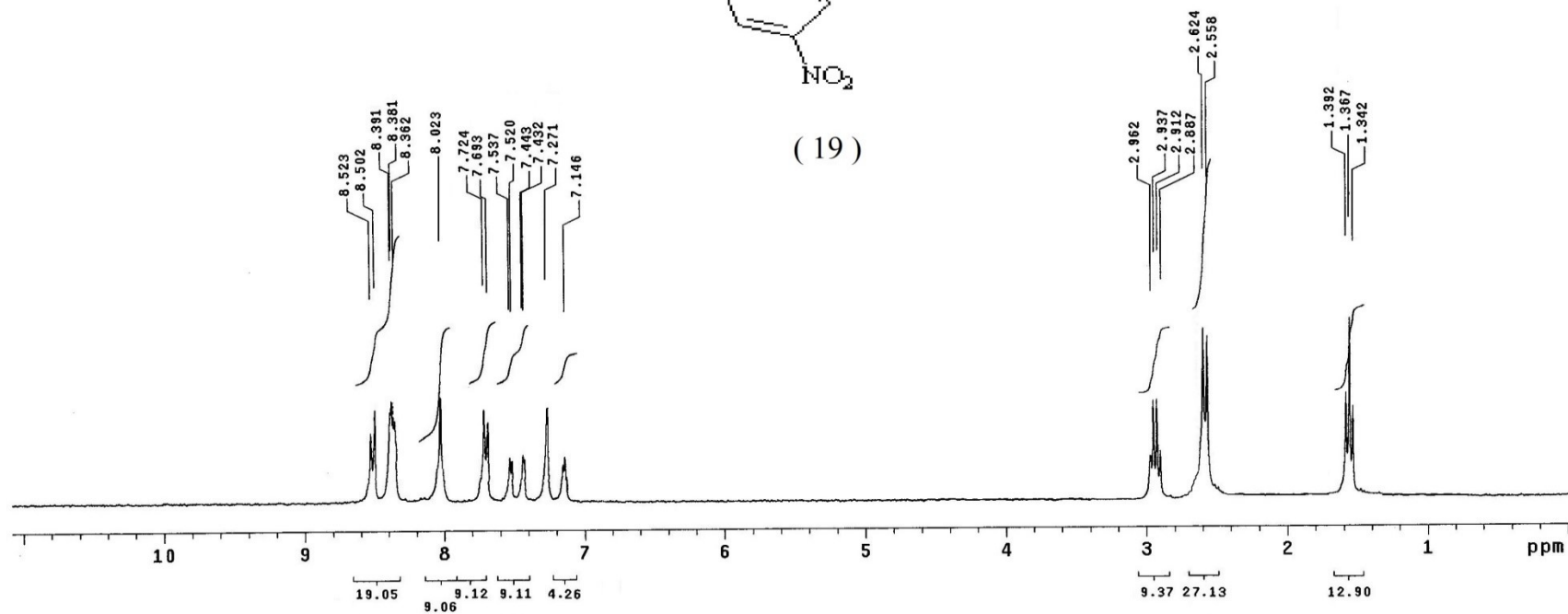
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
6 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Mar 30 2021



(19)

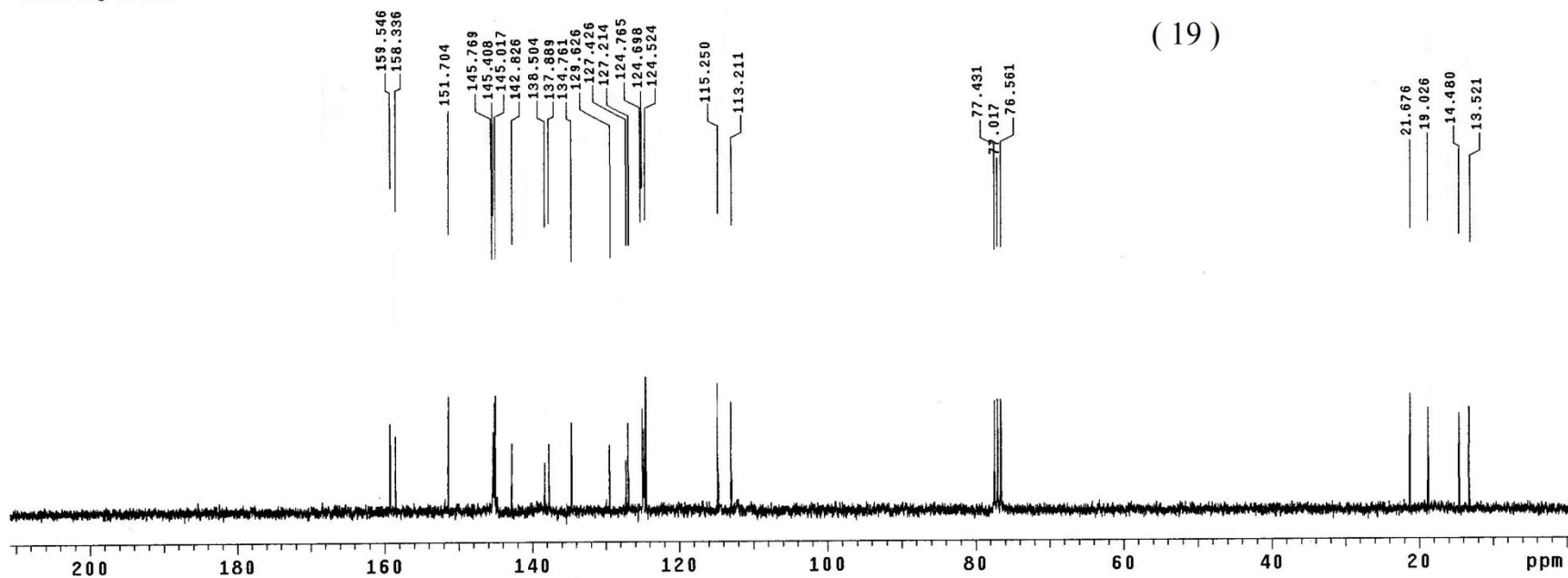
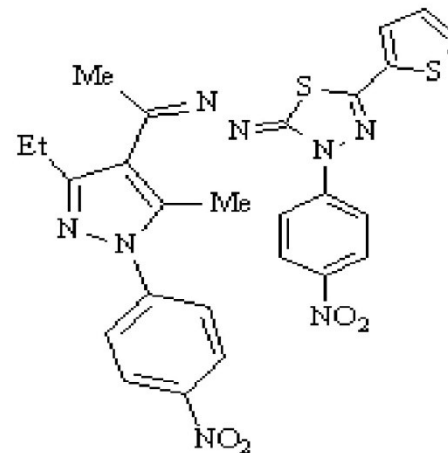


MernaTalaat-M25-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
3064 repetitions
OBSERVE C13, 75.4520034 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Aug 30 2021

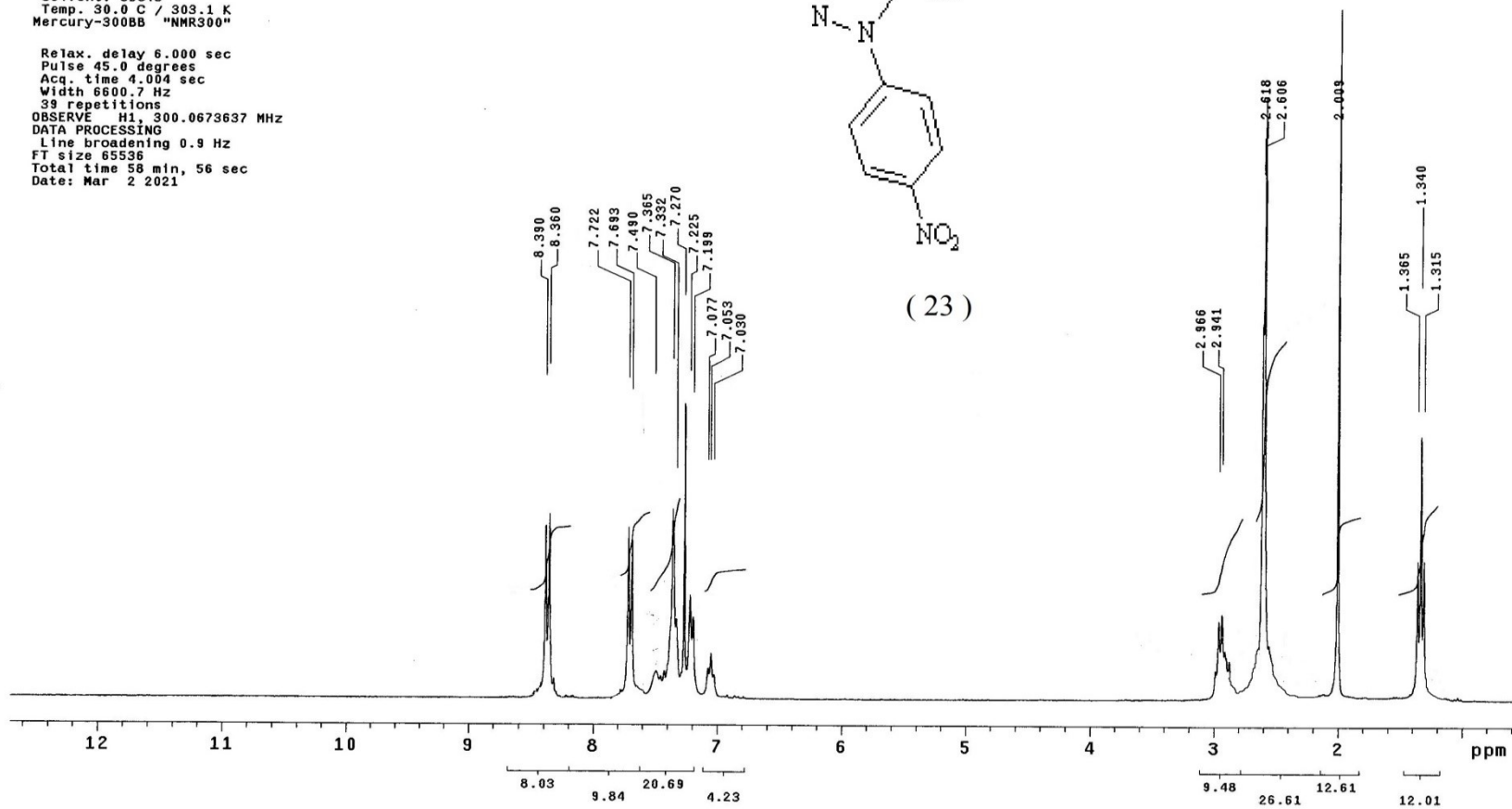
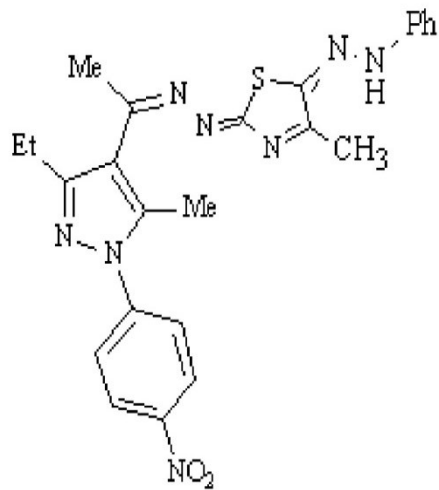


MonicaGameel-M27-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
39 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Mar 2 2021



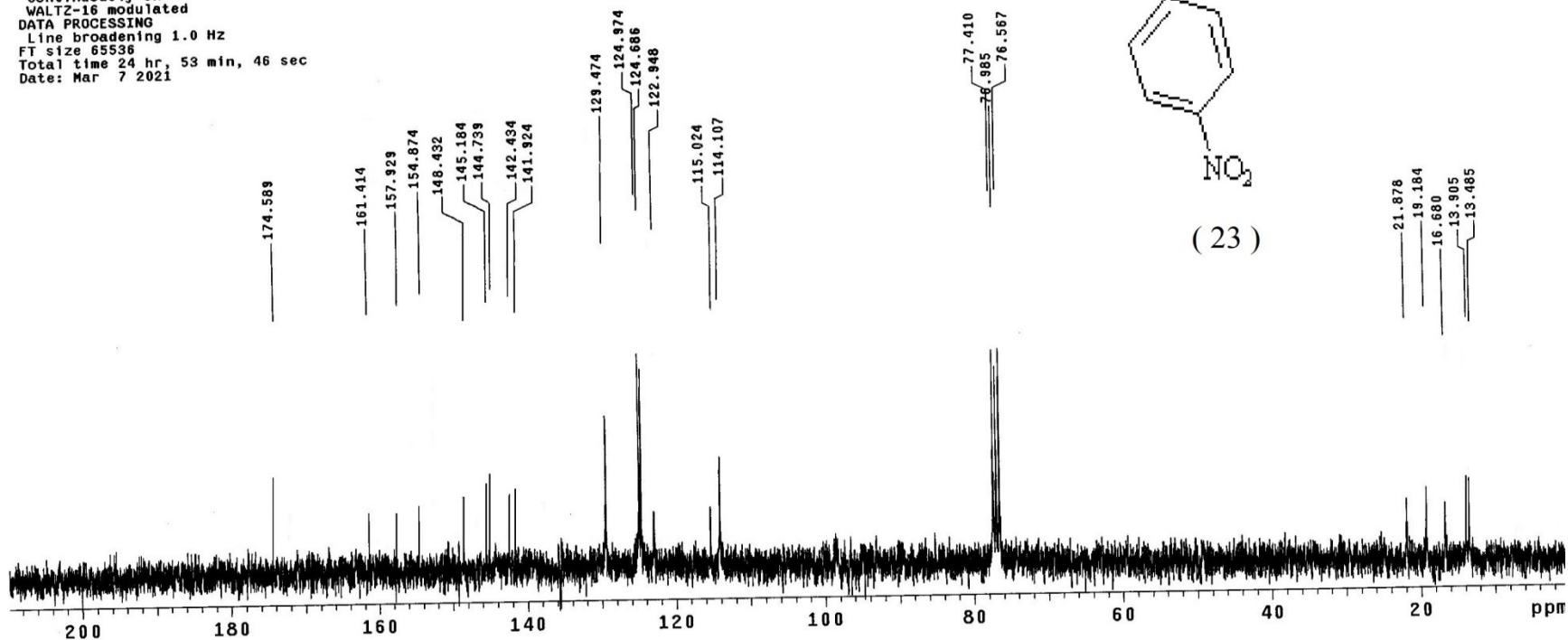
MonicaGamee1-M27-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: CDCl3
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2256 repetitions
OBSERVE C13, 75.4520022 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 53 min, 46 sec
Date: Mar 7 2021

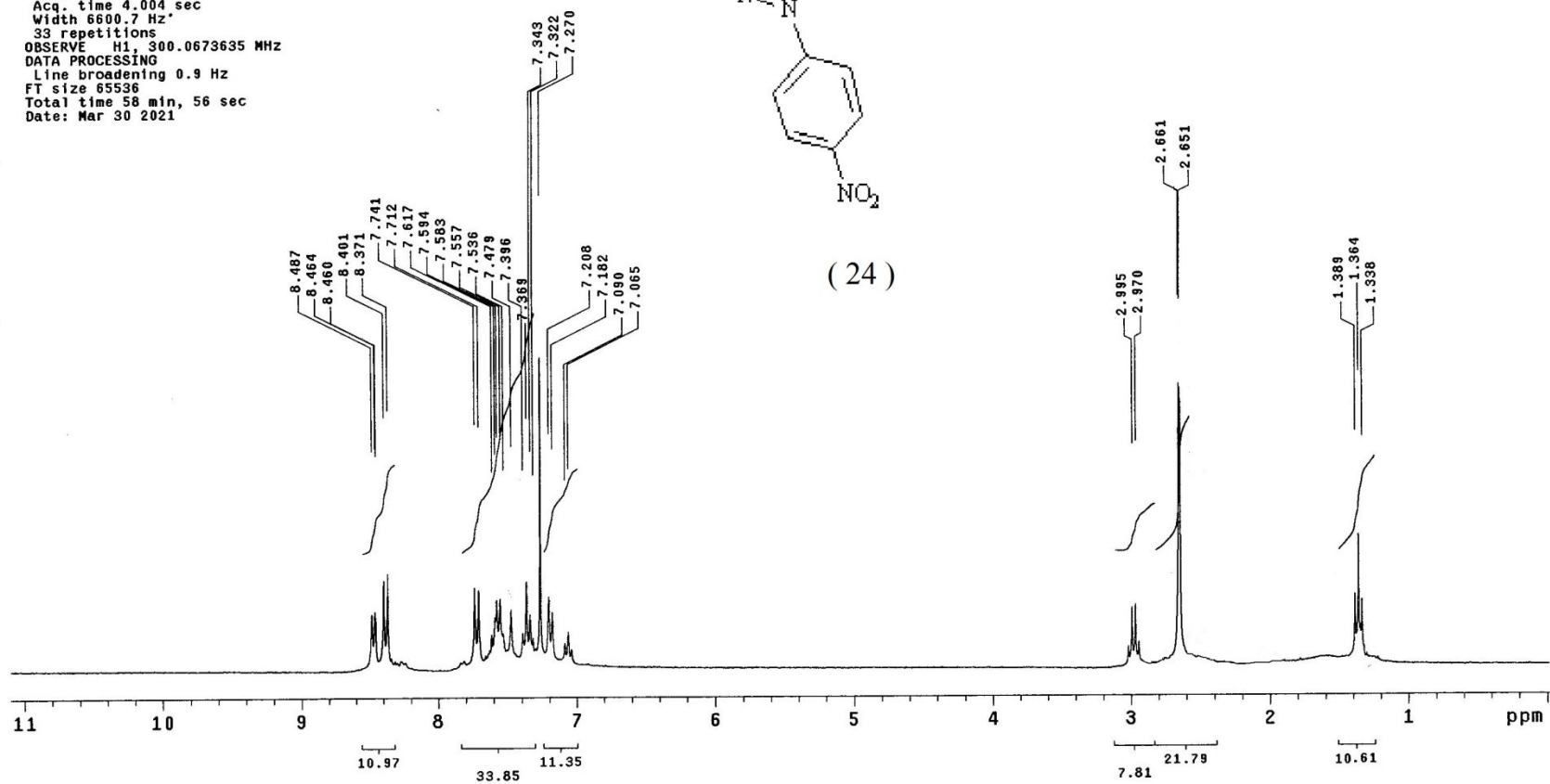
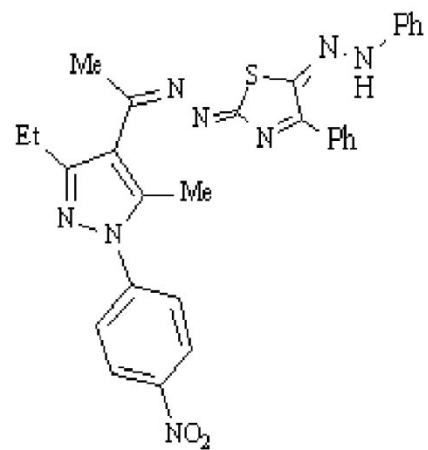


MernaTalat-M28-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
33 repetitions
OBSERVE H1, 300.0673635 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Mar 30 2021

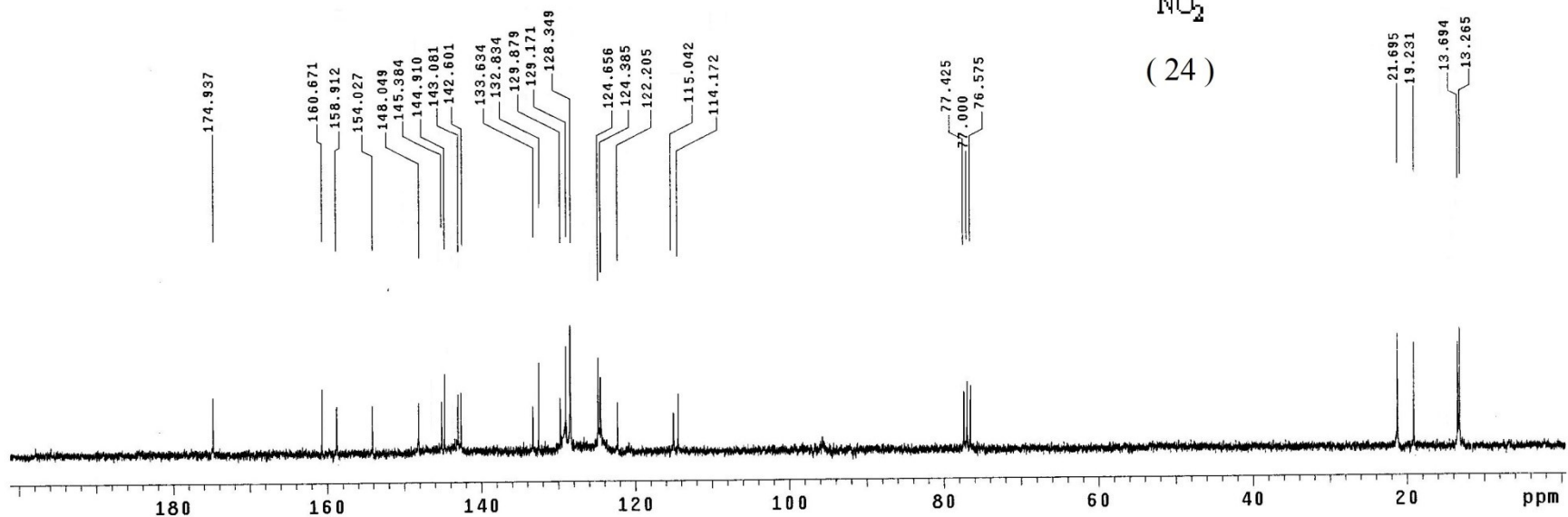
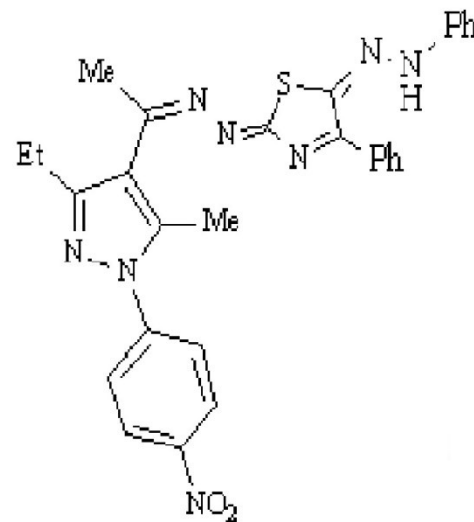


HamdyHasaneen-M28-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1488 repetitions
OBSERVE C13, 75.4520165 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Mar 31 2021

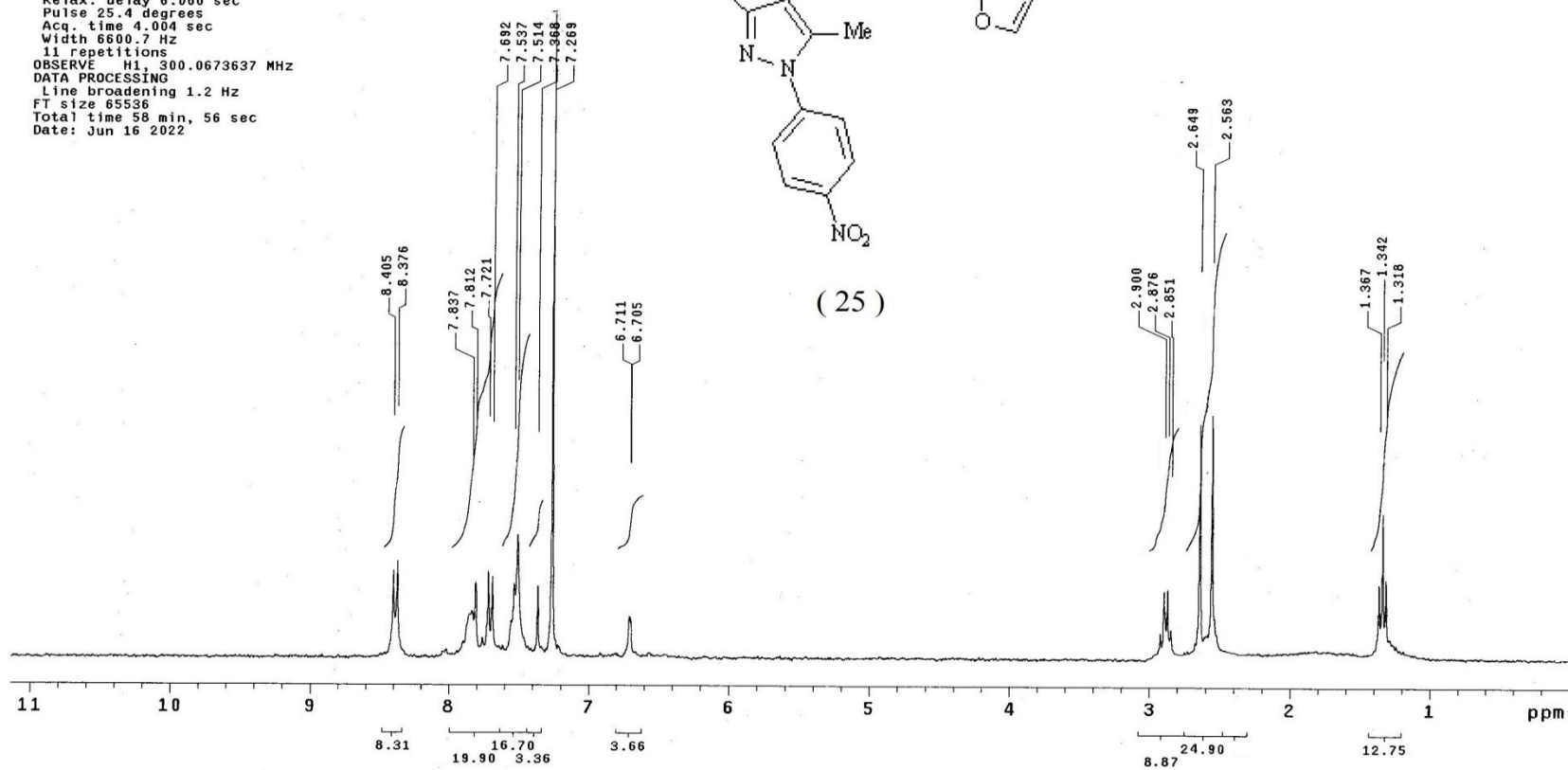
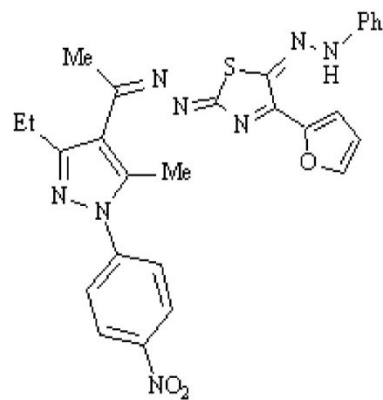


MohammadAbdulMoaty-M29-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
11 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 1.2 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Jun 16 2022

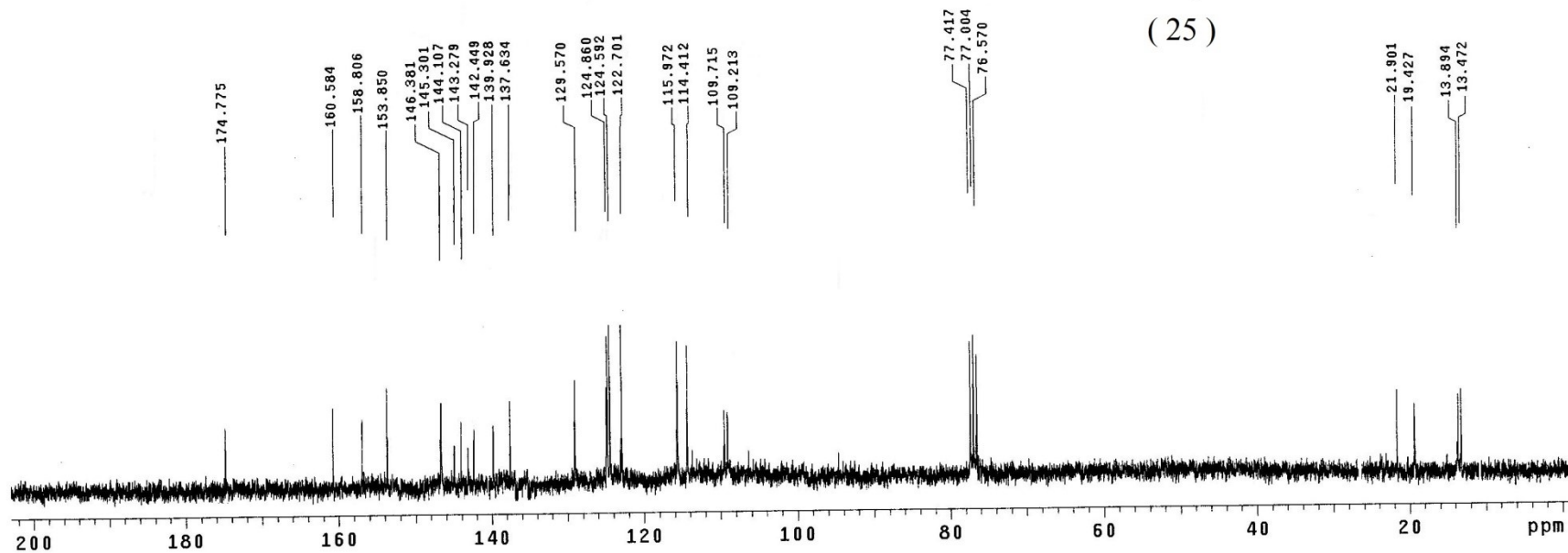
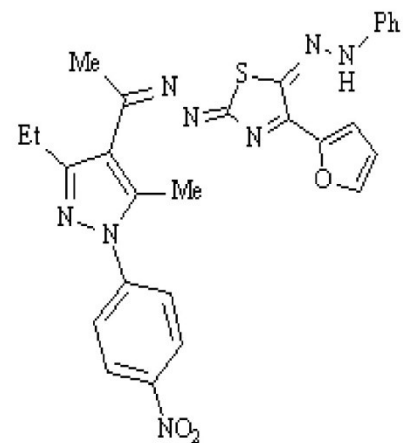


HamdyHasaneen-M29-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2472 repetitions
OBSERVE C13, 75.4520034 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Oct 6 2021

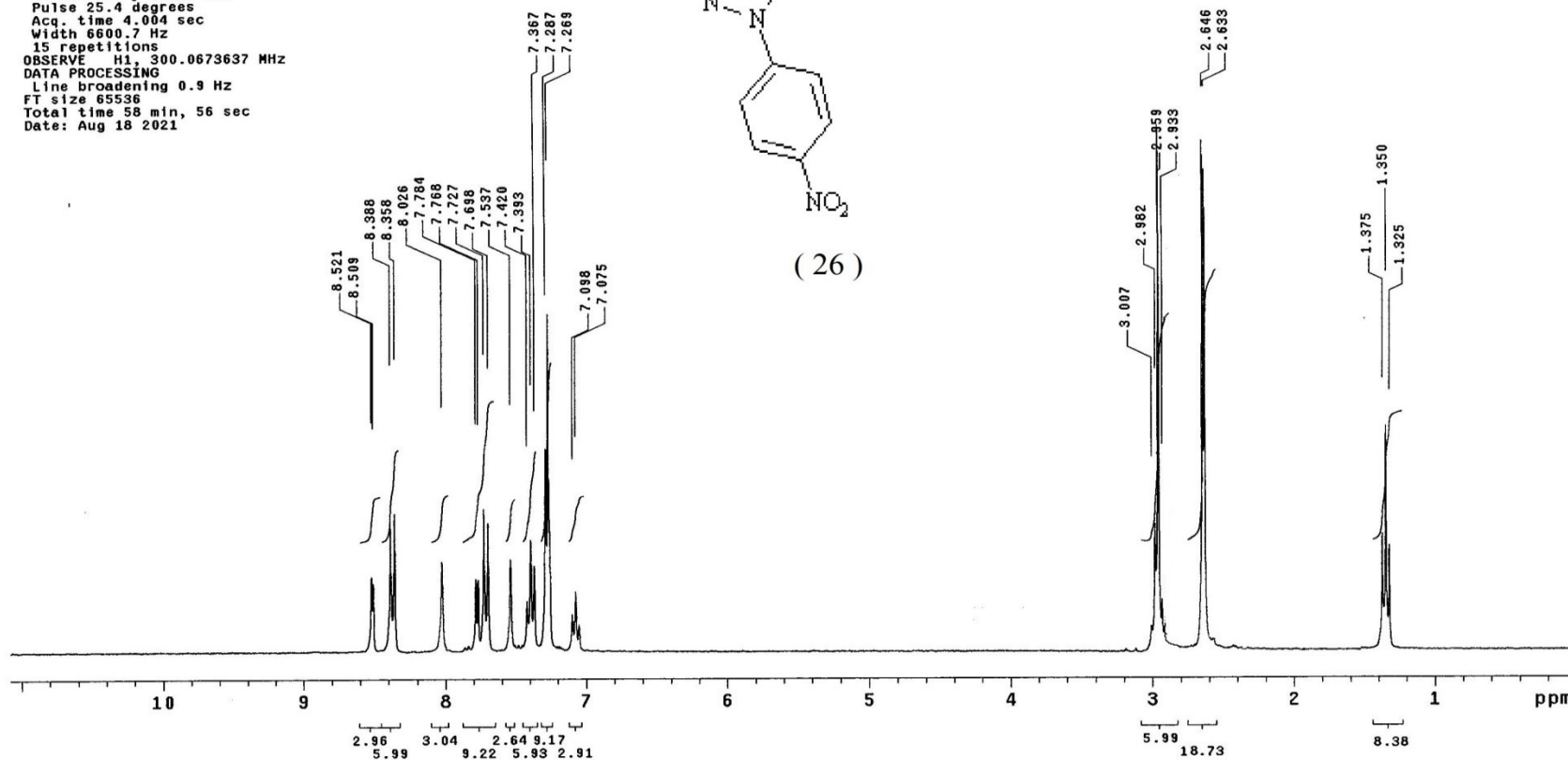
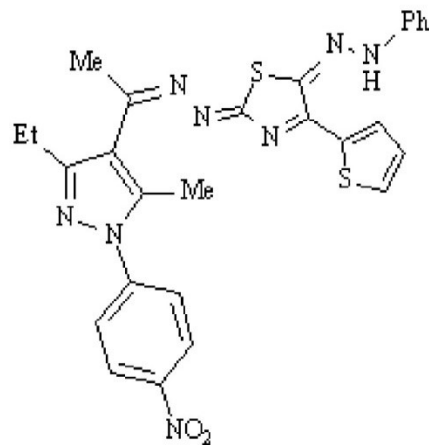


MernaTalat-M40-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1
Solvent: CDC13
Temp. 30.0 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
15 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Aug 18 2021



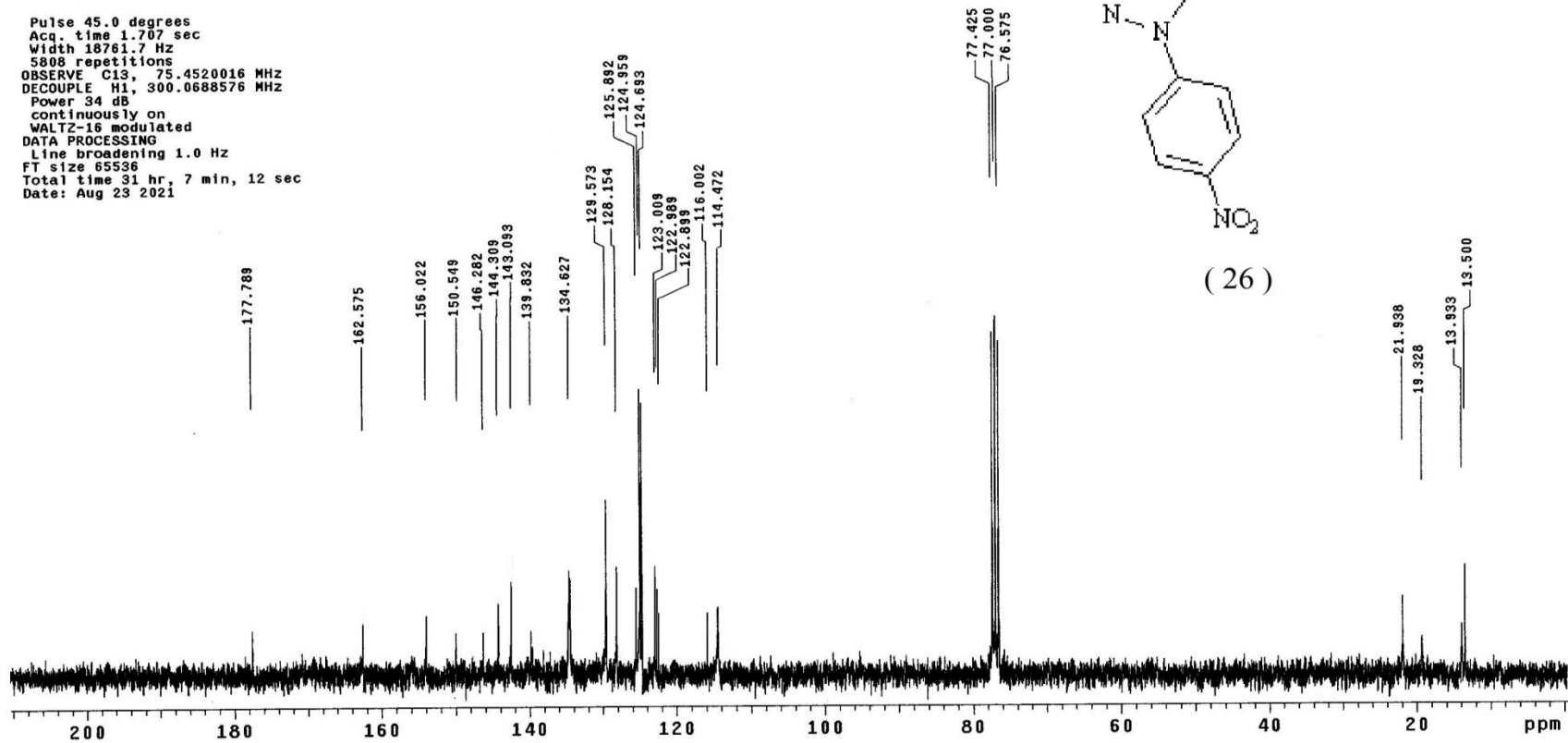
MernaTalat-M40-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTON

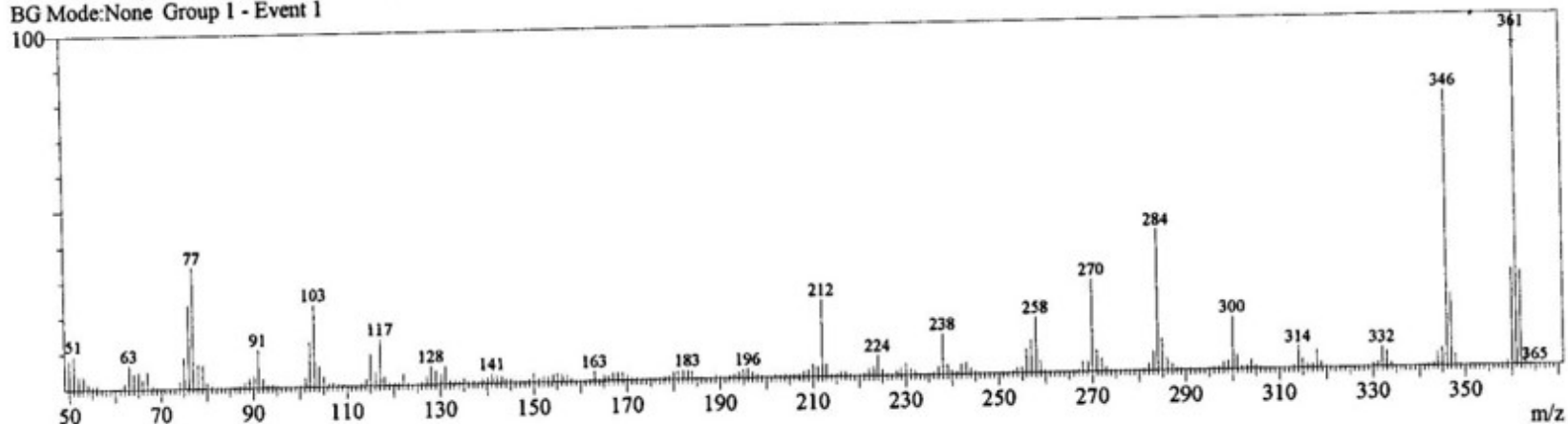
Pulse Sequence: s2pu1

Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"

Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
5808 repetitions
OBSERVE C13, 75.4520016 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Aug 23 2021



Line#:1 R.Time:3.9(Scan#:464)
 MassPeaks:313
 RawMode:Single 3.9(464) BasePeak:361(5033470)
 BG Mode:None Group 1 - Event 1



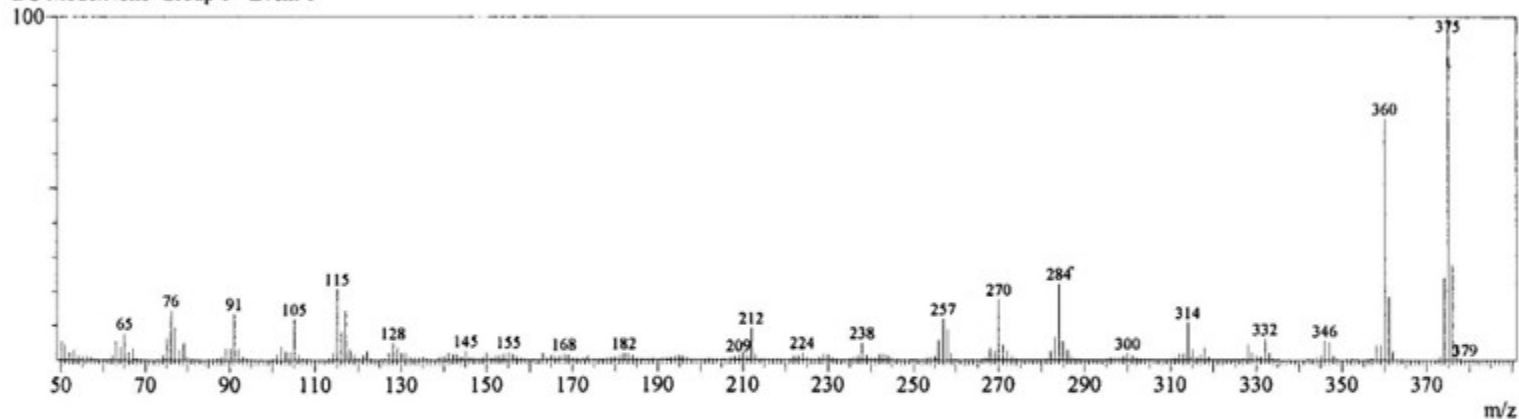
Mass Table

Line#:1 R.Time:3.9(Scan#:464)
 MassPeaks:313
 RawMode:Single 3.9(464) BasePeak:361(5033470)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	403995	8.03	4	53.05	180497	3.59	7	56.05	55906	1.11
2	51.00	482354	9.58	5	54.05	82369	1.64	8	57.10	18018	0.36
3	52.05	189657	3.77	6	55.05	52016	1.03	9	58.05	2991	0.06

Mass spectrometry of compound 4.

Line#:1 R.Time:2.5(Scan#:306)
 MassPeaks:328
 RawMode:Single 2.5(306) BasePeak:375(2324311)
 BG Mode:None Group 1 - Event 1



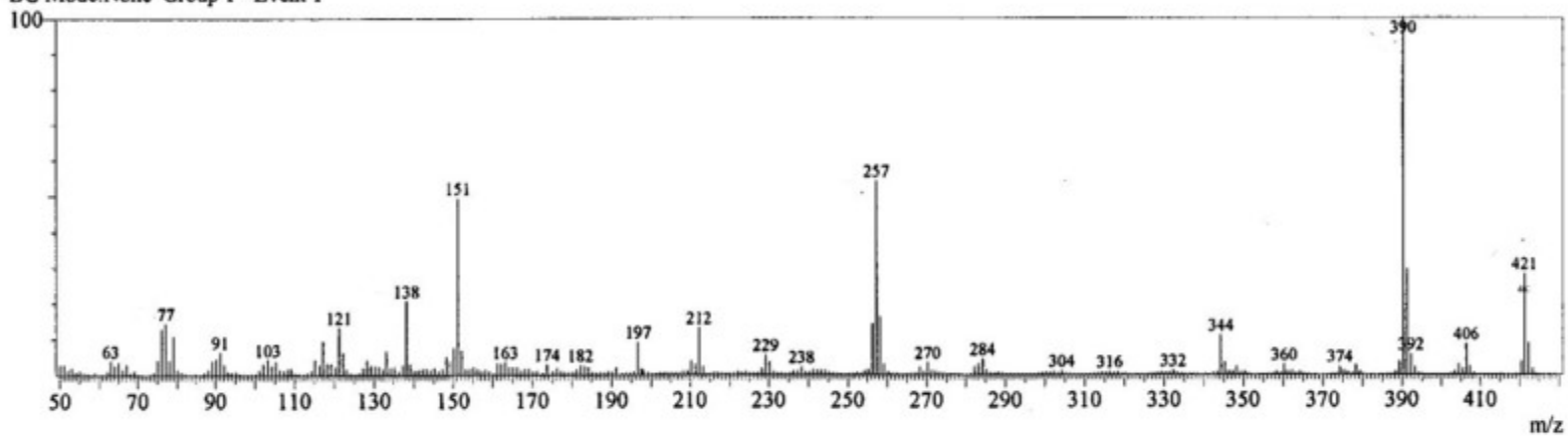
Mass Table

Line#:1 R.Time:2.5(Scan#:306)
 MassPeaks:328
 RawMode:Single 2.5(306) BasePeak:375(2324311)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	130298	5.61	4	53.05	68307	2.94	7	56.10	26516	1.14
2	51.05	102015	4.39	5	54.10	32065	1.38	8	57.10	19106	0.82
3	52.05	55471	2.39	6	55.05	29480	1.27	9	58.00	4439	0.19

Mass spectrometry of compound 7.

Line#:1 R.Time:3.2(Scan#:381)
 MassPeaks:366
 RawMode:Single 3.2(381) BasePeak:390(6439162)
 BG Mode:None Group 1 - Event 1



Mass Table

Line#:1 R.Time:3.2(Scan#:381)

MassPeaks:366

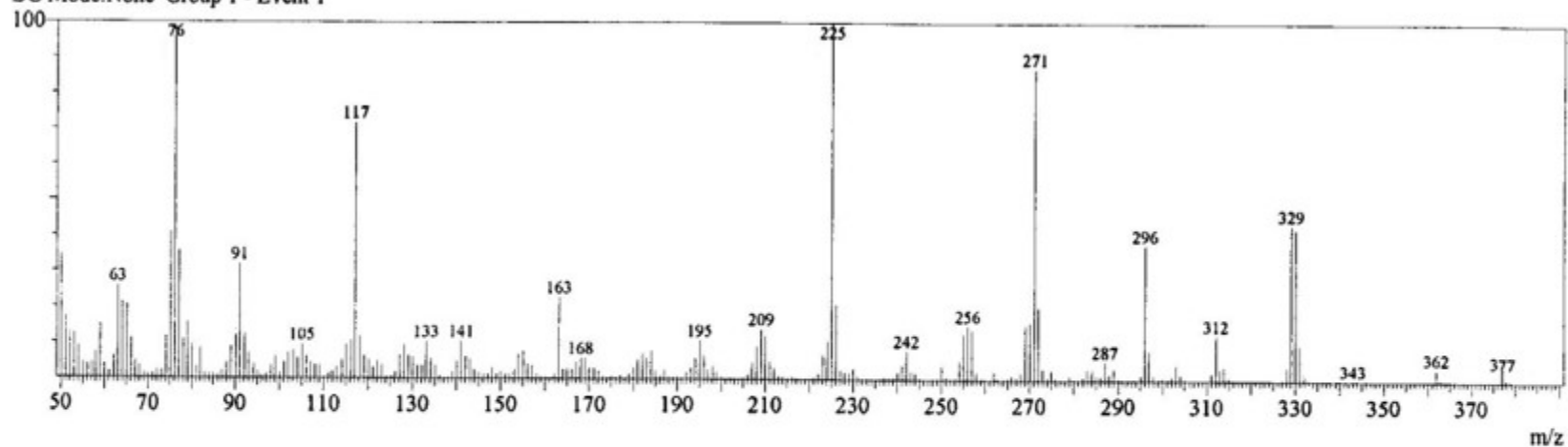
RawMode:Single 3.2(381) BasePeak:390(6439162)

BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	171915	2.67	4	53.10	113916	1.77	7	56.10	39190	0.61
2	51.05	179539	2.79	5	54.10	52082	0.81	8	57.10	25751	0.40
3	52.10	83591	-1.30	6	55.05	77956	1.21	9	58.15	4574	0.07

Mass spectrometry of compound 9.

Line#:1 R.Time:2.1(Scan#:255)
 MassPeaks:279
 RawMode:Single 2.1(255) BasePeak:225(289166)
 BG Mode:None Group 1 - Event 1



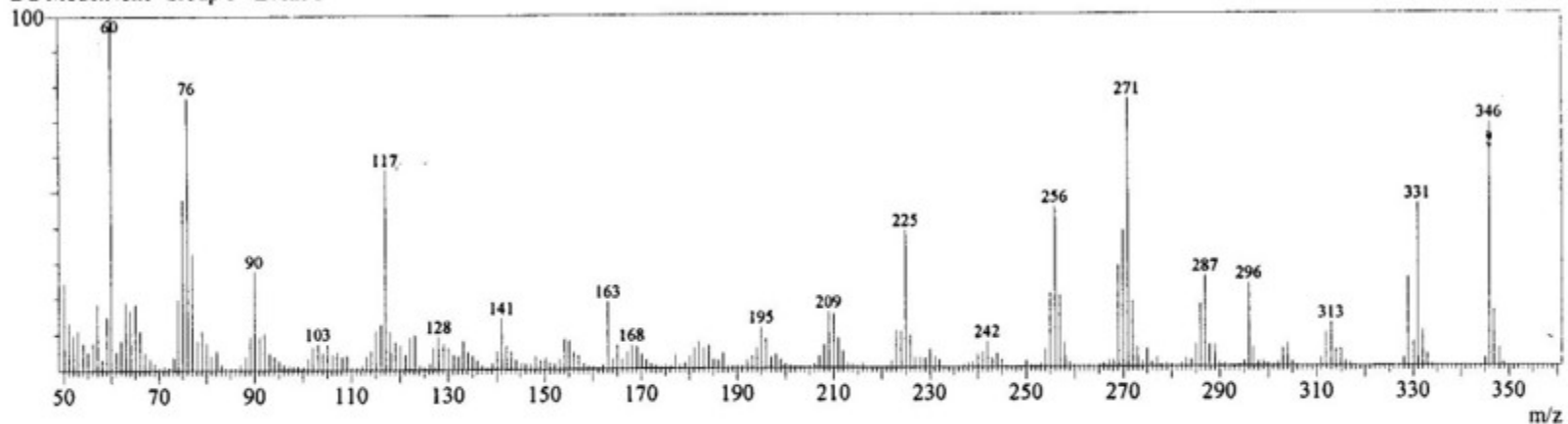
Mass Table

Line#:1 R.Time:2.1(Scan#:255)
 MassPeaks:279
 RawMode:Single 2.1(255) BasePeak:225(289166)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	100018	34.59	4	53.05	36340	12.57	7	56.10	11215	3.88
2	51.05	49651	17.17	5	54.05	26017	9.00	8	57.05	12186	4.21
3	52.05	37384	12.93	6	55.10	13516	4.67	9	58.00	20849	7.21

Mass spectrometry of compound 13.

Line#:1 R.Time:2.1(Scan#:254)
 MassPeaks:289
 RawMode:Single 2.1(254) BasePeak:60(423030)
 BG Mode:None Group 1 - Event 1



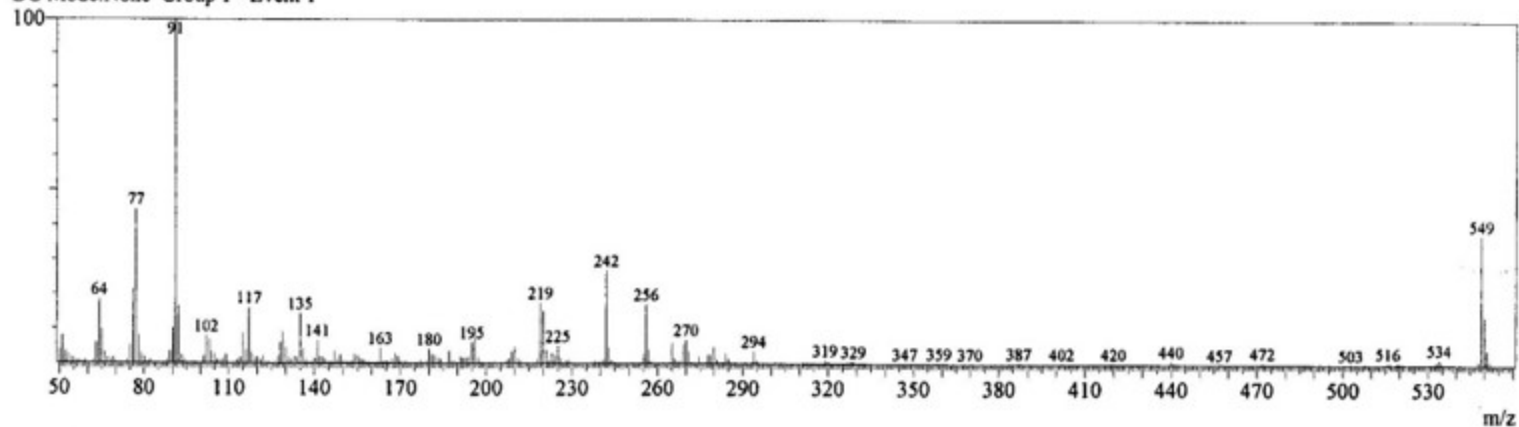
Mass Table

Line#:1 R.Time:2.1(Scan#:254)
 MassPeaks:289
 RawMode:Single 2.1(254) BasePeak:60(423030)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	103272	24.41	4	53.05	47124	11.14	7	56.10	32281	7.63
2	51.05	56509	13.36	5	54.05	31940	7.55	8	57.05	78022	18.44
3	52.05	40823	9.65	6	55.10	21977	5.20	9	58.05	13451	3.18

Mass spectrometry of compound 14.

Line#:1 R.Time:3.6(Scan#:429)
 MassPeaks:332
 RawMode:Single 3.6(429) BasePeak:91(452497)
 BG Mode:None Group 1 - Event 1



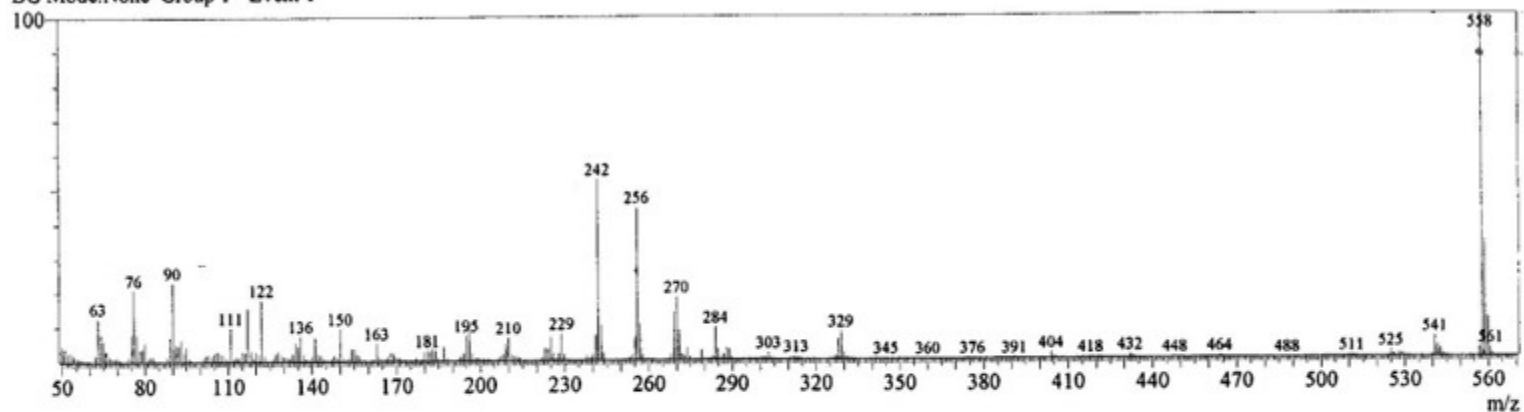
Mass Table

Line#:1 R.Time:3.6(Scan#:429)
 MassPeaks:332
 RawMode:Single 3.6(429) BasePeak:91(452497)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	17536	3.88	4	53.05	11440	2.53	7	56.10	4516	1.00
2	51.05	35963	7.95	5	54.05	7970	1.76	8	57.05	3855	0.85
3	52.05	15270	3.37	6	55.05	6859	1.52	9	58.05	1760	0.39

Mass spectrometry of compound 17.

Line#:1 R.Time:3.8(Scan#:451)
 MassPeaks:458
 RawMode:Single 3.8(451) BasePeak:558(1674935)
 BG Mode:None Group 1 - Event 1



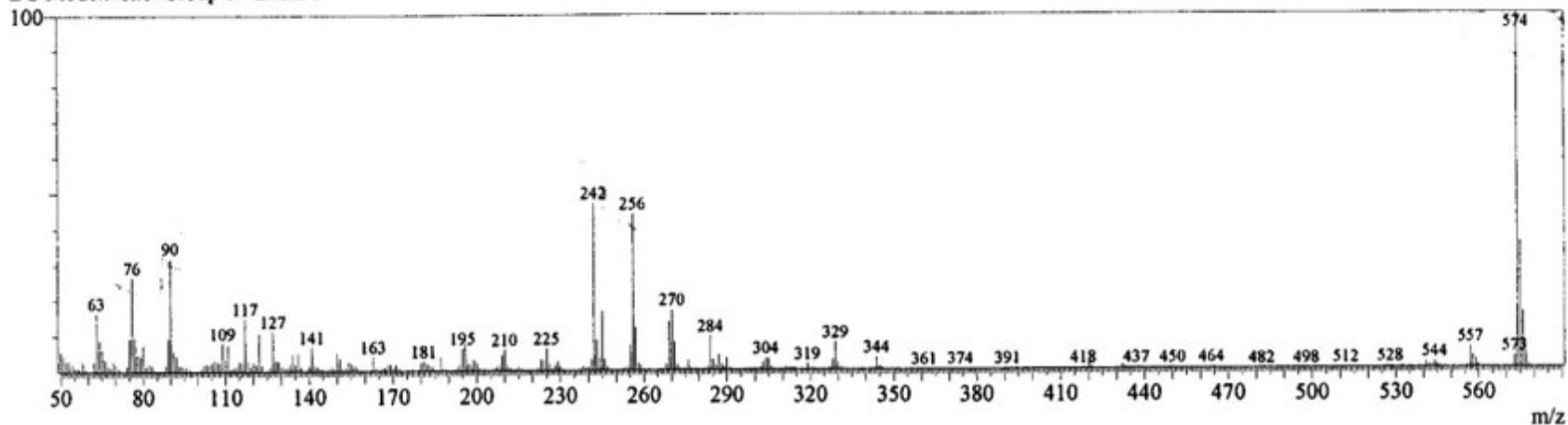
Mass Table

Line#:1 R.Time:3.8(Scan#:451)
 MassPeaks:458
 RawMode:Single 3.8(451) BasePeak:558(1674935)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	73865	4.41	4	53.05	46038	2.75
2	51.05	61739	3.69	5	54.05	28966	1.73
3	52.05	40734	2.43	6	55.05	22633	1.35
				7	56.05	14331	0.86
				8	57.05	11224	0.67
				9	58.00	7087	0.42

Mass spectrometry of compound 18.

Line#:1 R.Time:3.9(Scan#:465)
 MassPeaks:479
 RawMode:Single 3.9(465) BasePeak:574(1105230)
 BG Mode:None Group 1 - Event 1



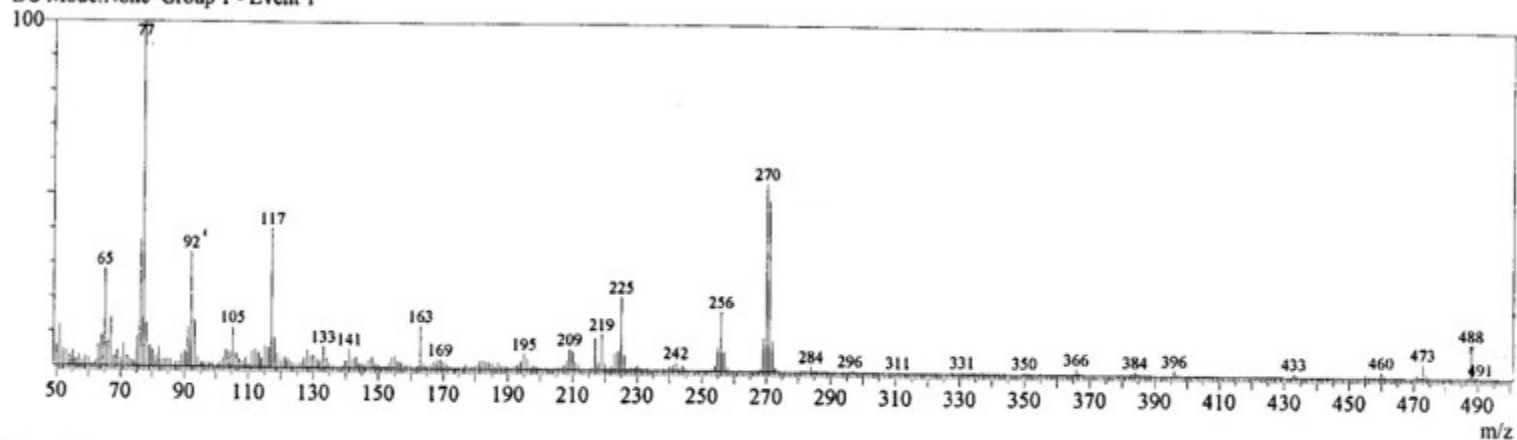
Mass Table

Line#:1 R.Time:3.9(Scan#:465)
 MassPeaks:479
 RawMode:Single 3.9(465) BasePeak:574(1105230)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	60149	5.44	4	53.05	34412	3.11	7	56.10	10642	0.96
2	51.05	48788	4.41	5	54.10	23186	2.10	8	57.05	9888	0.89
3	52.05	34338	3.11	6	55.10	13017	1.18	9	58.00	33687	3.05

Mass spectrometry of compound 19.

Line#:1 R.Time:2.4(Scan#:290)
 MassPeaks:289
 RawMode:Single 2.4(290) BasePeak:77(167234)
 BG Mode:None Group 1 - Event 1



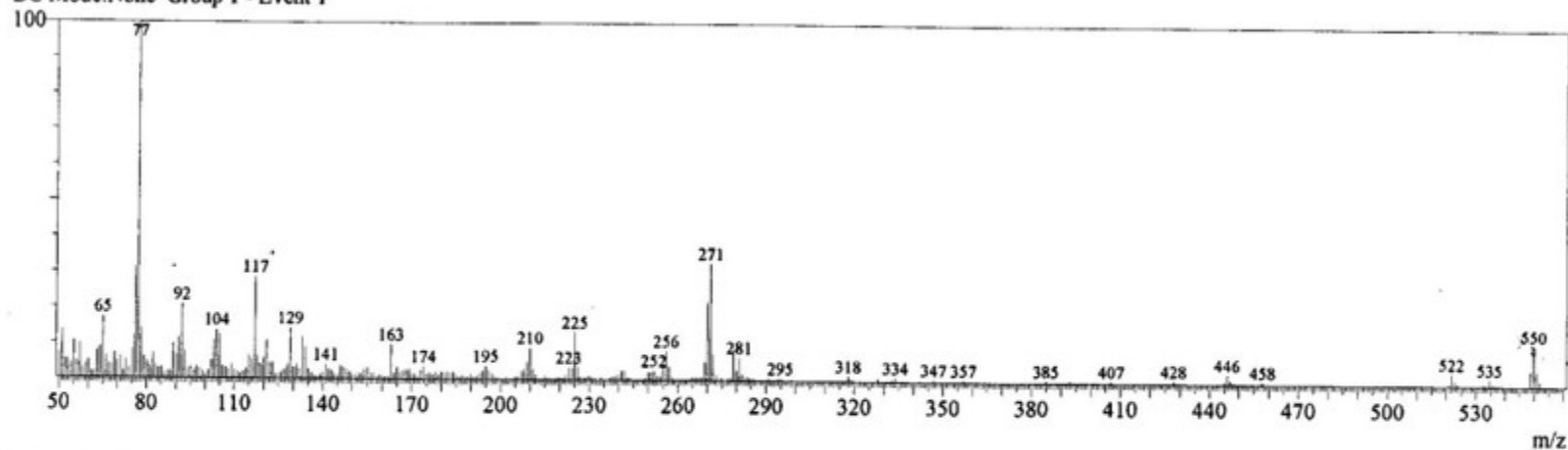
Mass Table

Line#:1 R.Time:2.4(Scan#:290)
 MassPeaks:289
 RawMode:Single 2.4(290) BasePeak:77(167234)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	9914	5.93	4	53.05	7429	4.44	7	56.05	3812	2.28
2	51.00	20022	11.97	5	54.05	5722	3.42	8	57.05	5633	3.37
3	52.05	8420	5.03	6	55.05	7386	4.42	9	58.05	2613	1.56

Mass spectrometry of compound 23.

Line#:1 R.Time:4.1(Scan#:495)
 MassPeaks:245
 RawMode:Single 4.1(495) BasePeak:77(55143)
 BG Mode:None Group 1 - Event 1



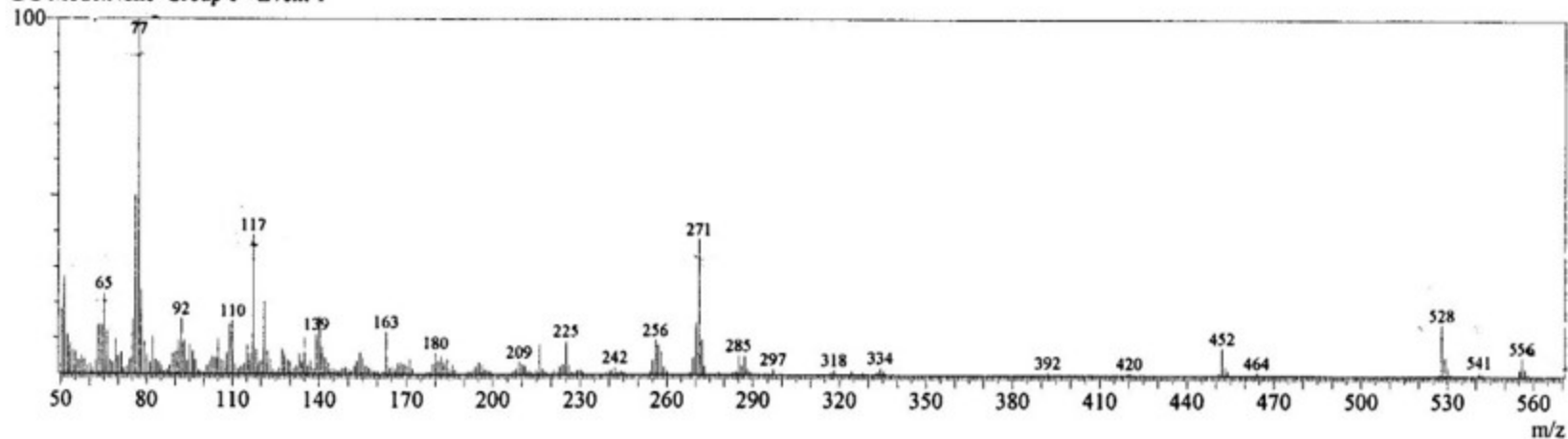
Mass Table

Line#:1 R.Time:4.1(Scan#:495)
 MassPeaks:245
 RawMode:Single 4.1(495) BasePeak:77(55143)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	3937	7.14	4	53.05	2886	5.23	7	56.05	2674	4.85
2	51.00	7417	13.45	5	54.05	2471	4.48	8	57.05	5387	9.77
3	52.05	2978	5.40	6	55.05	5769	10.46	9	58.05	1615	2.93

Mass spectrometry of compound 24.

Line#:1 R.Time:2.2(Scan#:268)
 MassPeaks:218
 RawMode:Single 2.2(268) BasePeak:77(35302)
 BG Mode:None Group 1 - Event 1

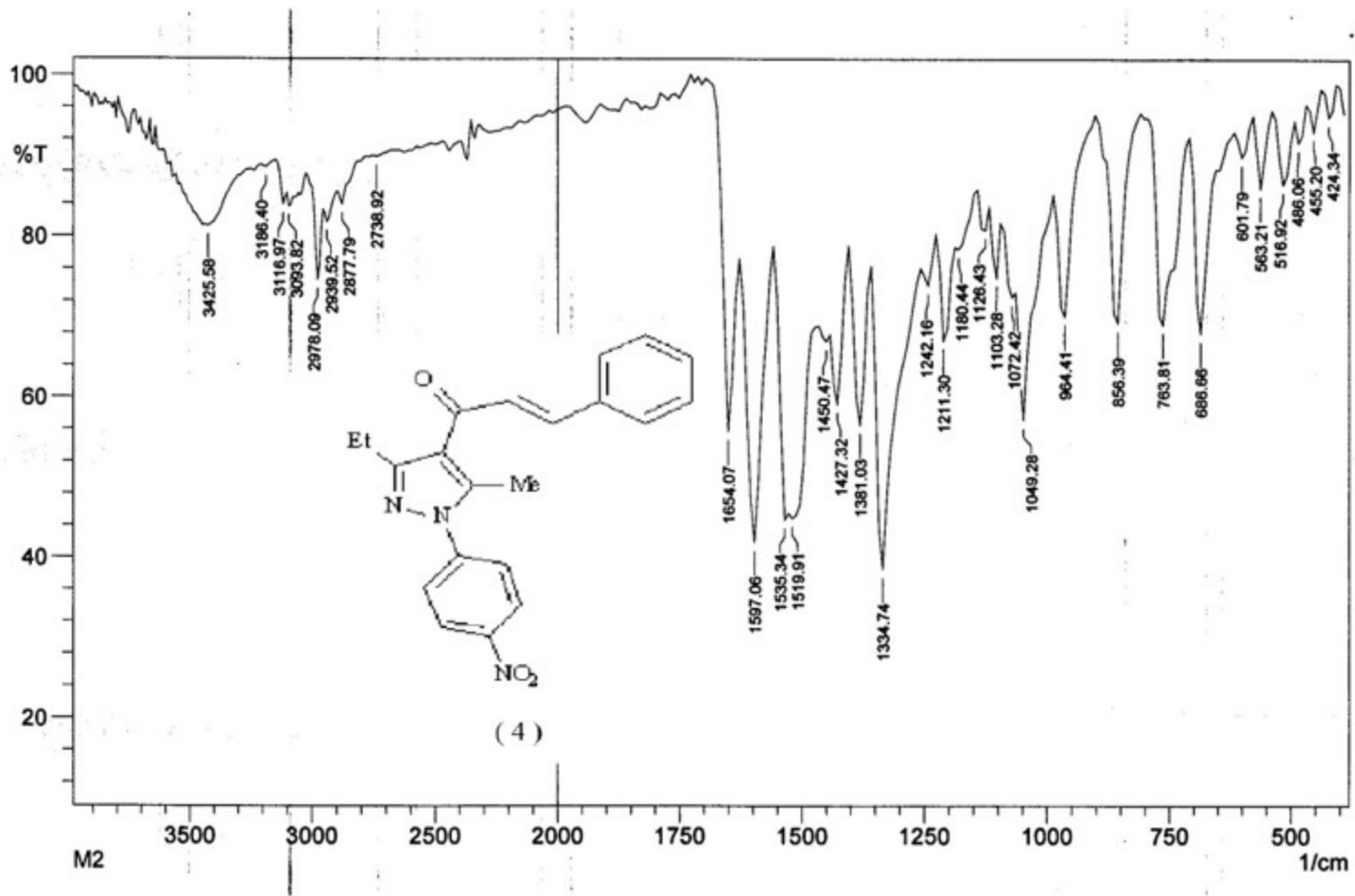


Mass Table

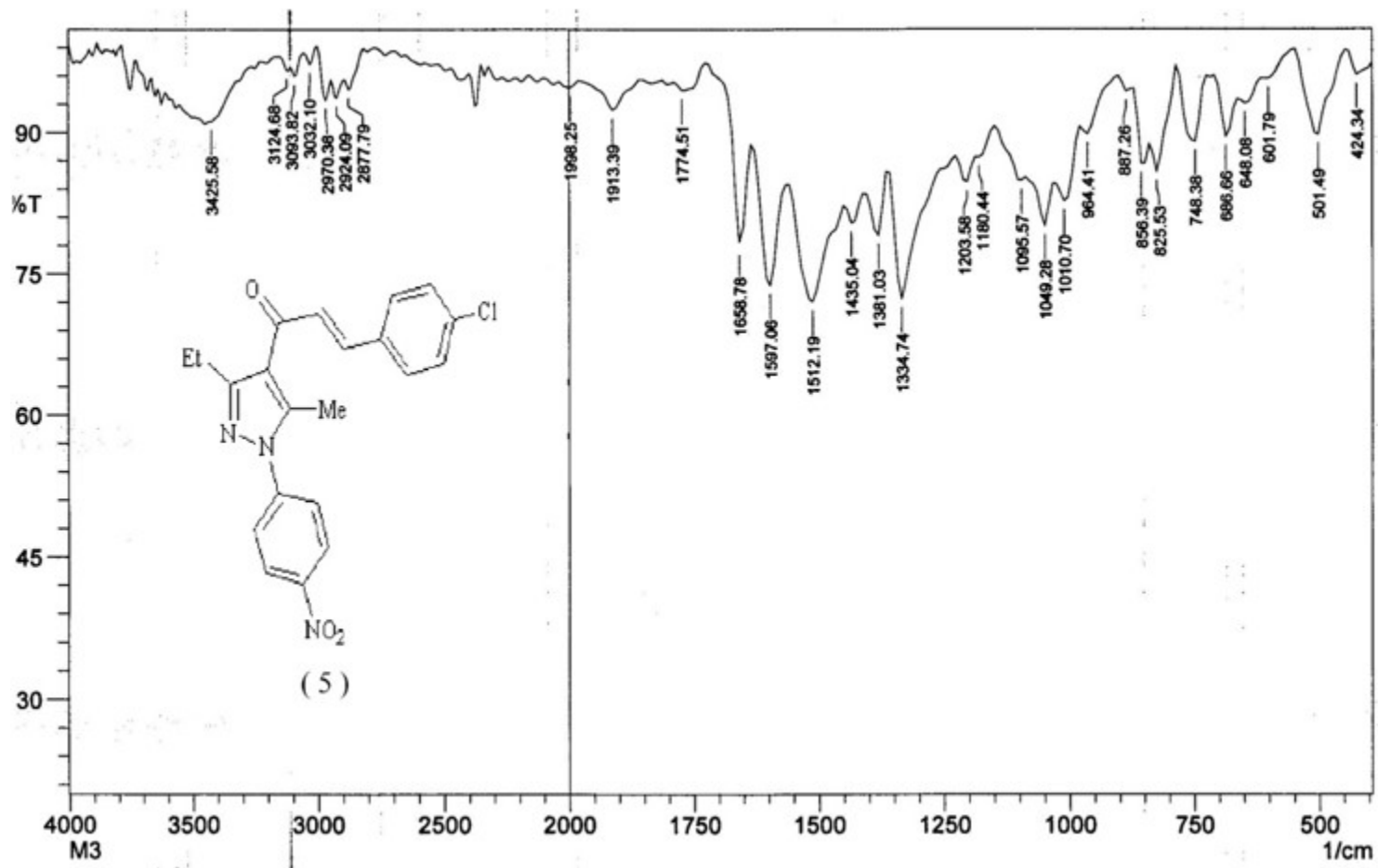
Line#:1 R.Time:2.2(Scan#:268)
 MassPeaks:218
 RawMode:Single 2.2(268) BasePeak:77(35302)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	6456	18.29	4	53.05	2993	8.48	7	56.10	1398	3.96
2	51.05	9674	27.40	5	54.05	2328	6.59	8	57.05	1777	5.03
3	52.10	3879	10.99	6	55.05	2291	6.49	9	58.00	1623	4.60

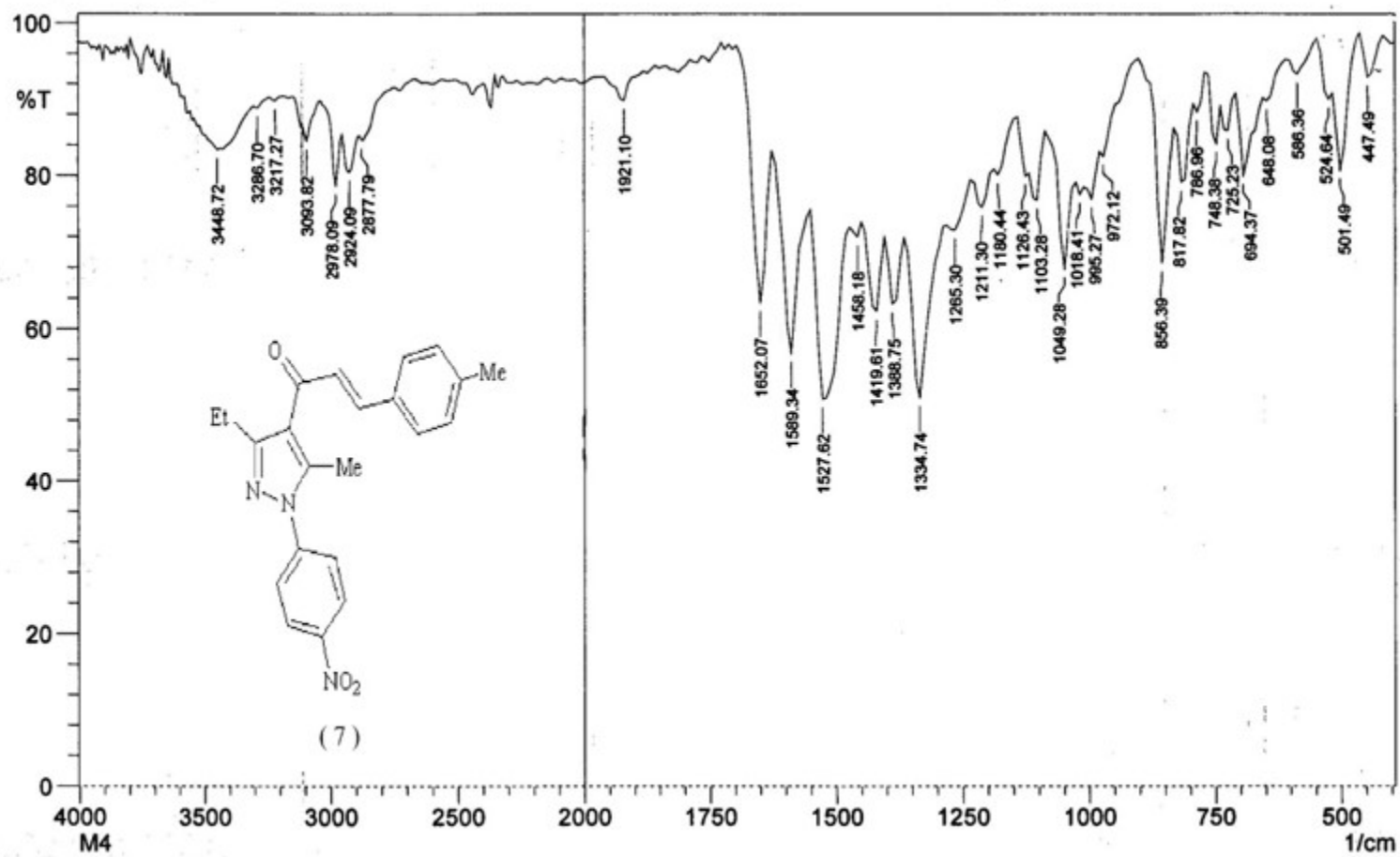
Mass spectrometry of compound 26.



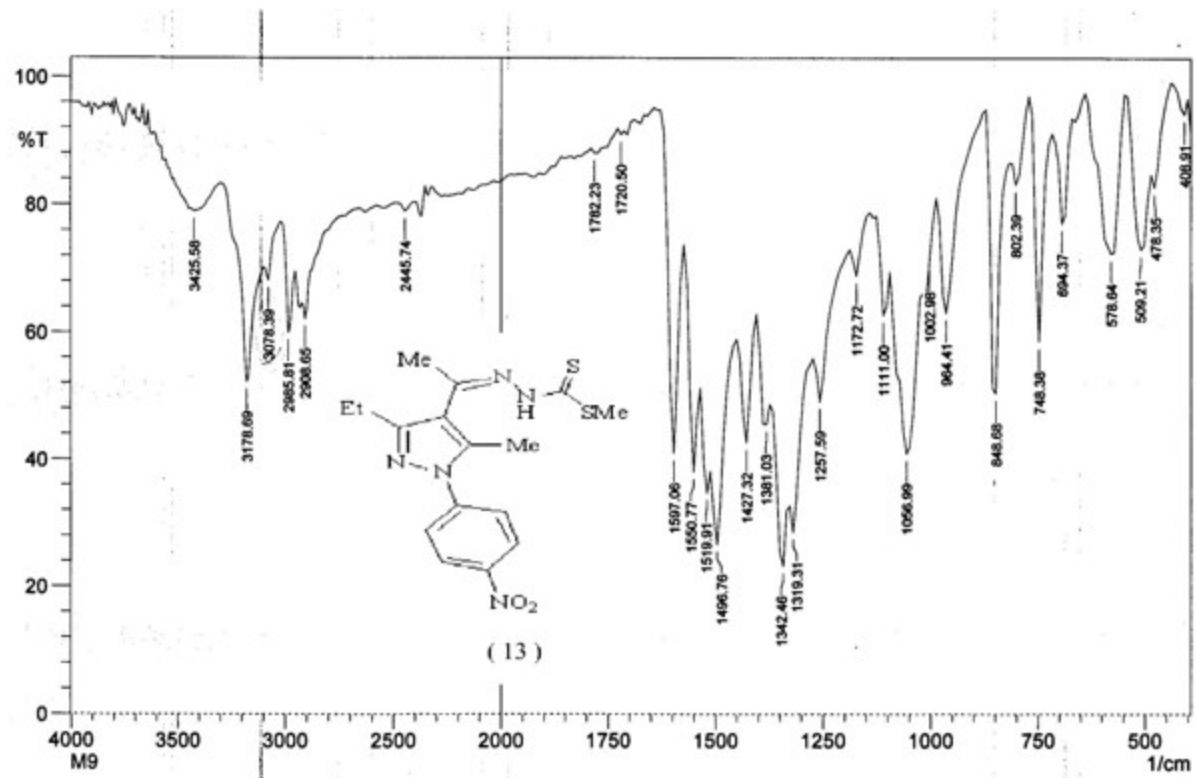
IR spectrum of compound 4.



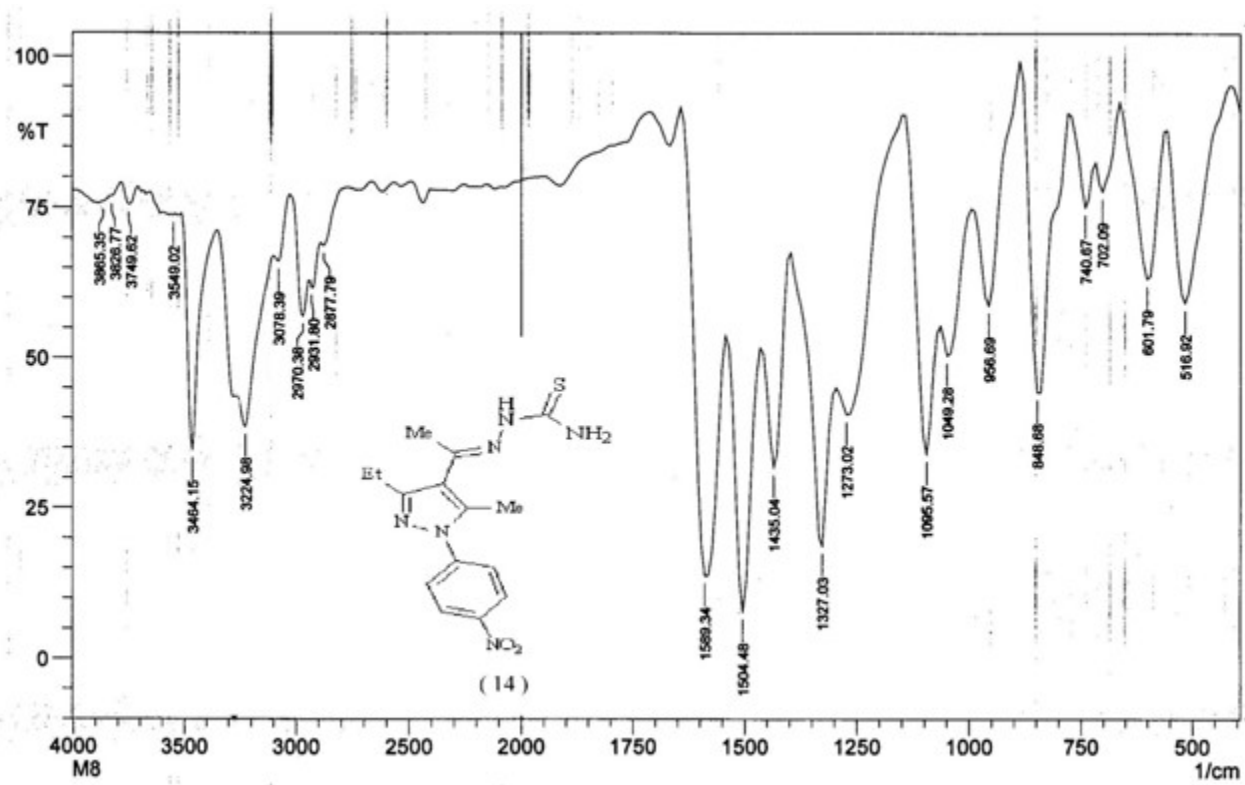
IR spectrum of compound 5.



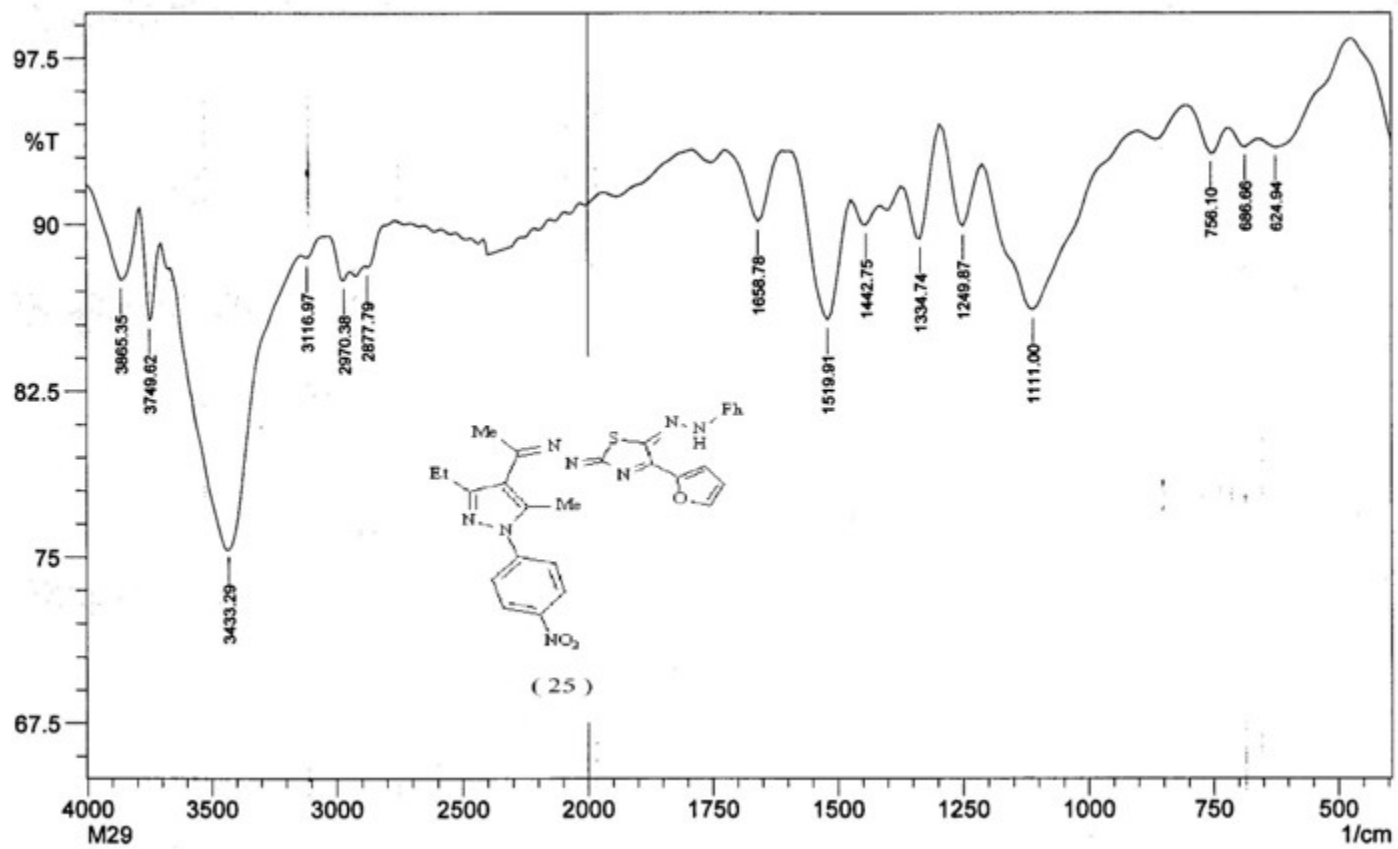
IR spectrum of compound 7.



IR spectrum of compound 13.



IR spectrum of compound 14.



IR spectrum of compound 25.