

Supplementary Material

Convenient synthesis and characterization of new 1,3,4-thiadiazoles and thiazoles incorporating thiophene moiety

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Copies of the ^1H and ^{13}C NMR spectra of compounds **3**, **6a-i**, **10**, **12a-g** and of the IR and GCMS spectra of **3**, **6b**, **10**, **12b** :

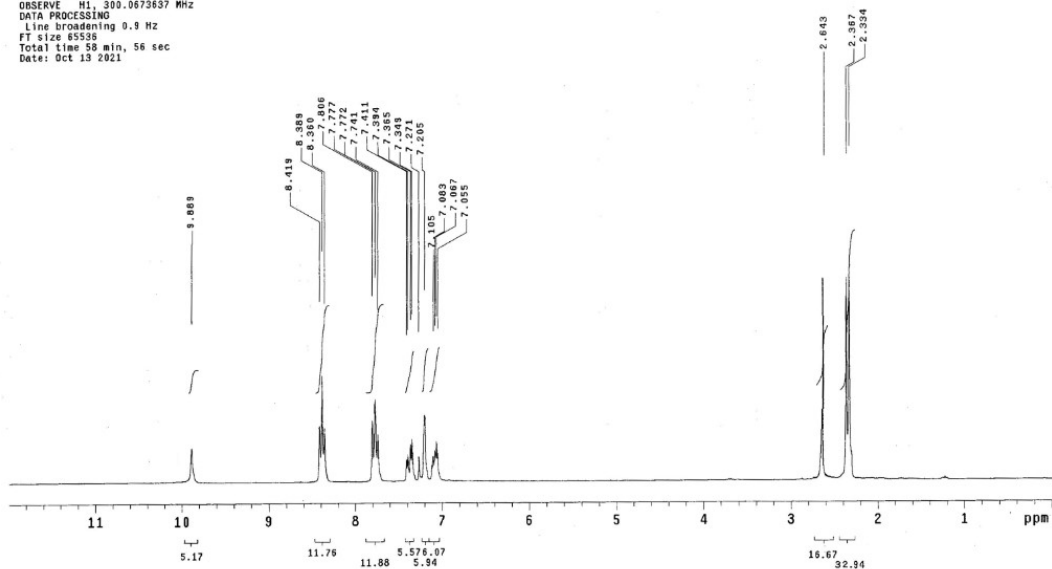
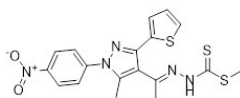
Compound 3	S2
Compounds 6a-i	S5
Compound 10	S16
Compounds 12a-g	S19

FatmaSaleh-H16-CDC13-H1

Archive directory: /export/home/vmr1/vmr/sys/data
 Sample directory: D05nm_test_12Mar2014-21:34:40
 File: PROTON

Pulse Sequence: s2pu1
 Solvent: CDC13
 Temp: 30.0 C / 303.1 K
 Mercury-3000S "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 65538
 Total time 58 min, 56 sec
 Date: Oct 13 2021

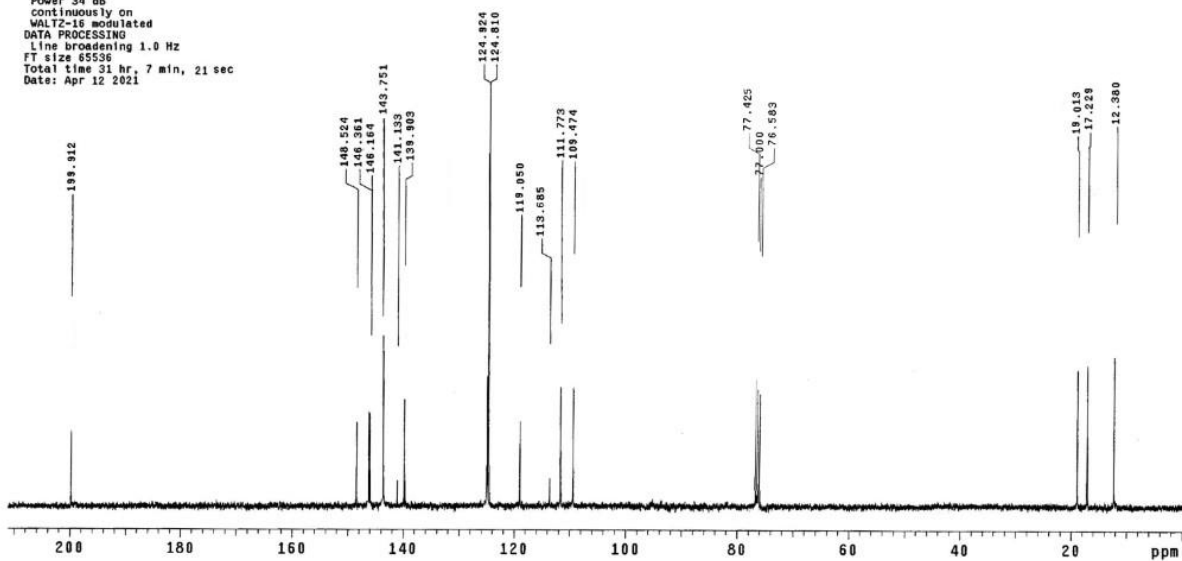
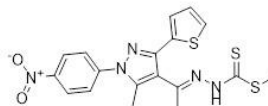


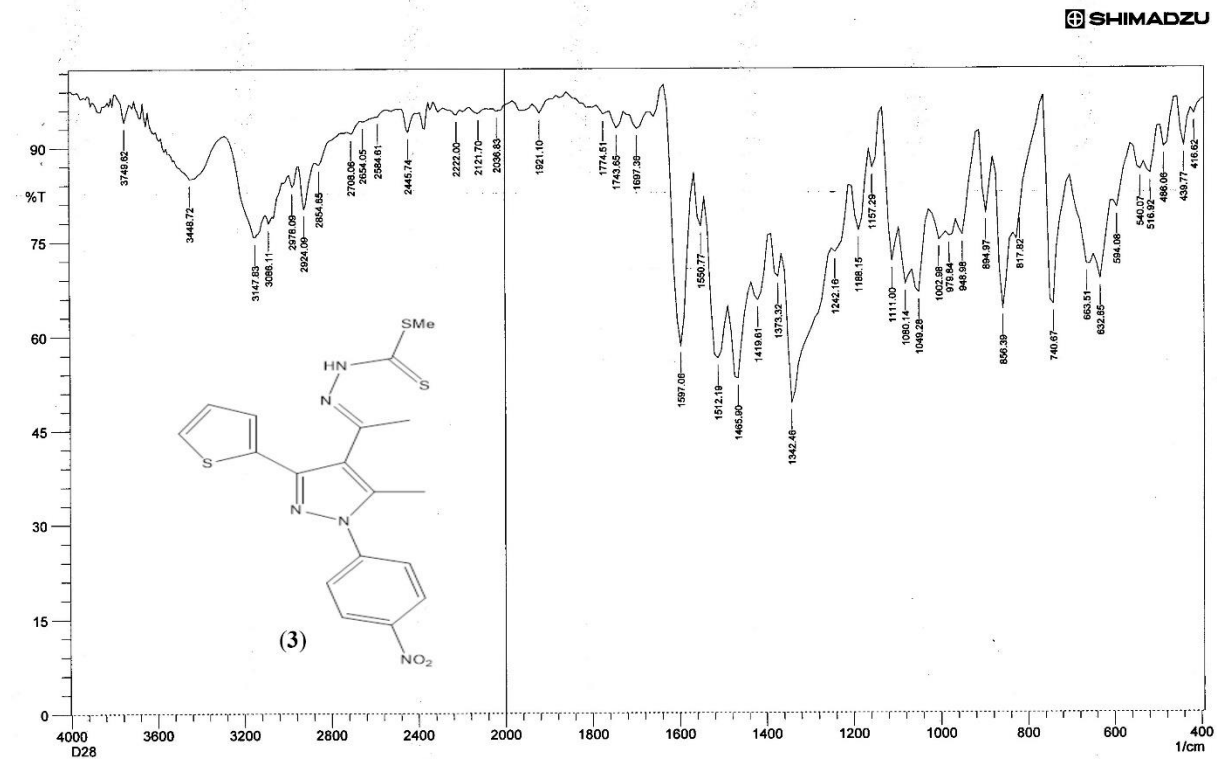
MernaTalat-H16-CDC13-C13

Archive directory: /export/home/vmr1/vmr/sys/data
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 File: PROTON

Pulse Sequence: s2pu1
 Solvent: CDC13
 Ambient temperature
 Mercury-3000S "NMR300"

Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 18761.7 Hz
 1312 repetitions
 OBSERVE C13, 75.4523914 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, 21 sec
 Date: Apr 12 2021





Comment;

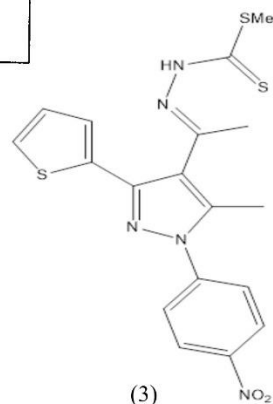
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**Cairo University
Micro Analytical Center**

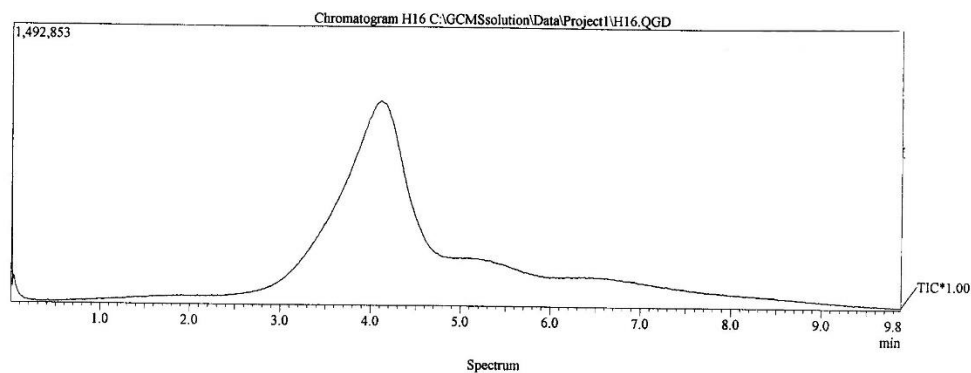
**DI Analysis
Shimadzu Qp-2010 Plus**

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 14/01/2007 10:14:47 ص
 Sample Name : H16
 Sample ID :
 Customer Name : Dr. Hamdy Hassanen- Science - Cairo
 Data File : C:\GCMSsolution\Data\Project\H16.QGD
 Org Data File : C:\GCMSsolution\Data\Project\H16.QGD
 Method File : C:\GCMSsolution\Data\Project\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
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 Modified : 14/01/2007 10:24:43 ص

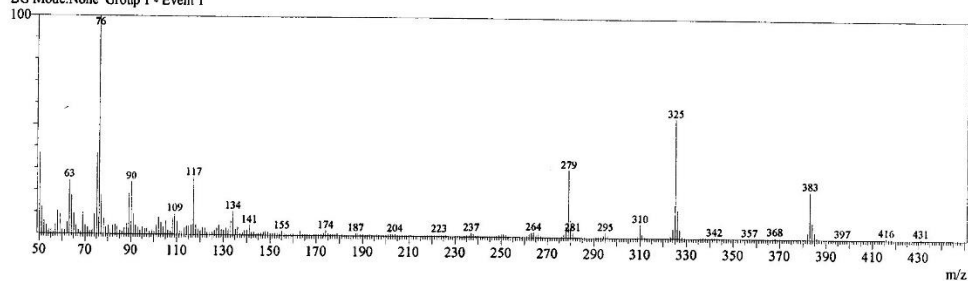
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 End Time : 10.00min
 ACQ Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1428
 Start m/z : 50.00
 End m/z : 700.00
 Electron Voltage : 70 eV
 Ionization Mode : EI



C:\GCMSsolution\Data\Project\H16.QGD



Line#:1 R.Time:4.2(Scan#:501)
 MassPeaks:265
 RawMode:Single 4.2(501) BasePeak:76(121024)
 BG Mode:None Group 1 - Event 1



Mass Table
 Line#:1 R.Time:4.2(Scan#:501)
 MassPeaks:265
 RawMode:Single 4.2(501) BasePeak:76(121024)
 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	44298	36.60	4	53.10	4905	4.05	7	56.05	1045	0.86
2	51.05	14812	12.24	5	54.10	2422	2.00	8	57.05	5305	4.38
3	52.05	7357	6.08	6	55.10	2679	2.21	9	58.00	12775	10.56

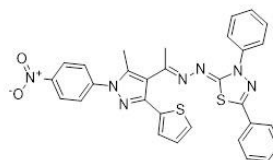
HandyHassanein-H19-CDC13-H1

Archive directory: /export/home/vmr1/vmrsys/data
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 File: PROTON

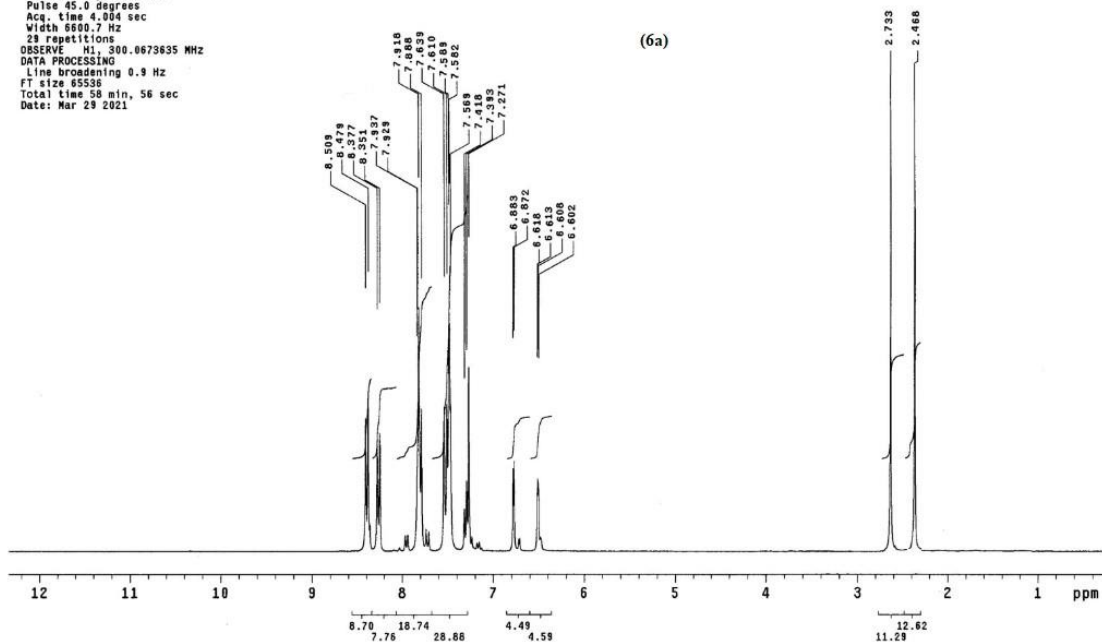
Pulse Sequence: s2pu1

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

Relax. delay 6.000 sec
 Pulse 45.0 degrees
 Acq. time 4.304 sec
 Width 6560.7 Hz
 28 Repetitions
 OBSERVE H1, 300.0673635 MHz
 DATA PROCESSING
 Line broadening 0.3 Hz
 FT size 65536
 Total time 58 min, 56 sec
 Date: Mar 29 2021



(6a)



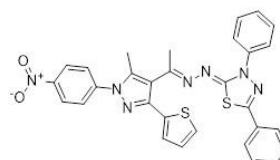
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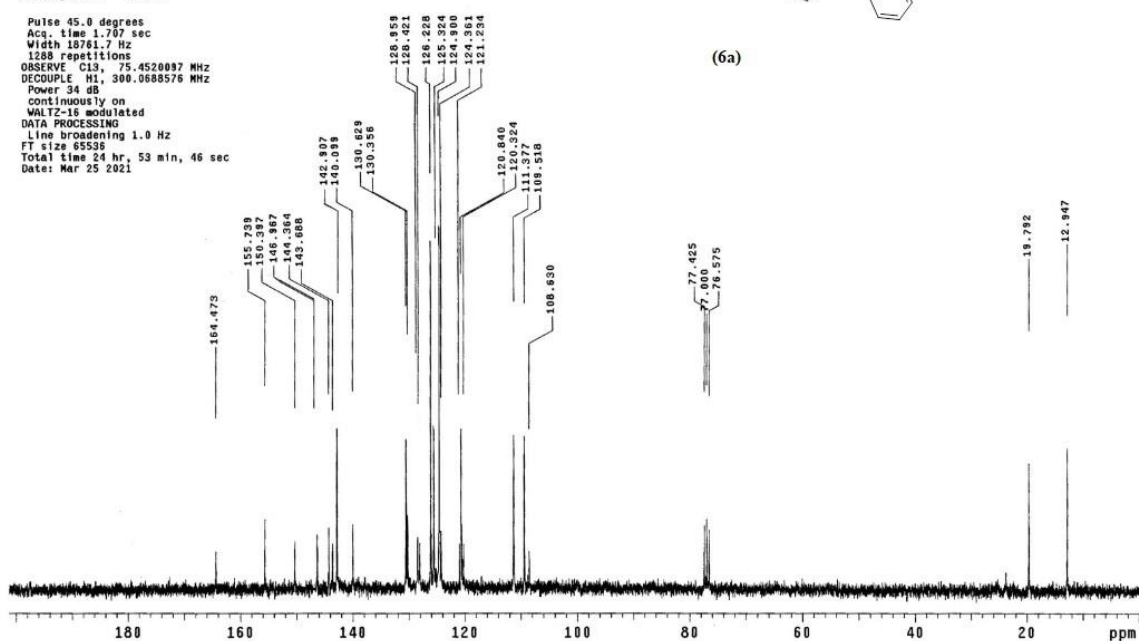
Pulse Sequence: s2pu1

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

Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 18761.7 Hz
 1288 repetitions
 OBSERVE C13, 75.4520087 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 25 2021



(6a)

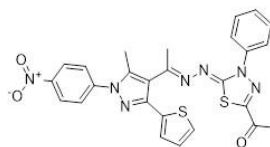


FatmaSaleh-H20-CDC13-H1

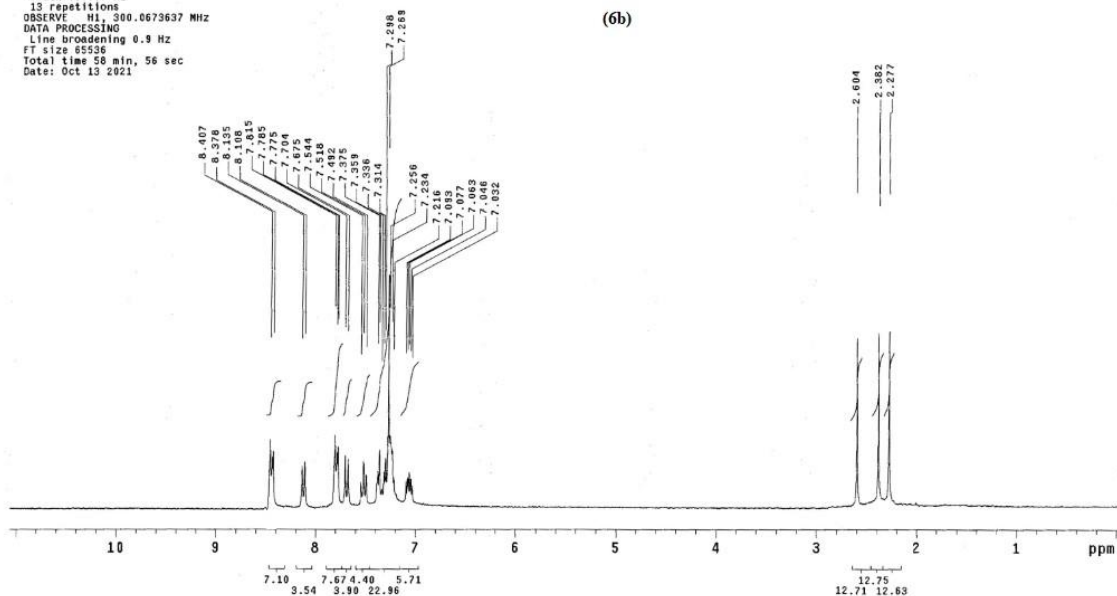
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 Sample directory: D05mm_test_12Mar2014-21:34:40
 File: PROTON

Pulse Sequence: s2pul
 Solvent: CDCl3
 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
 13 repetitions
 OBSERVE H1, 300.0673637 MHz
 DATA PROCESSING
 Line broadening 0.9 Hz
 FT size 65536
 Total time 58 min, 56 sec
 Date: Oct 13 2021



(6b)

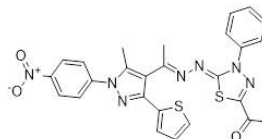


MohammedAbdulMoaty-H20-CDC13-C13

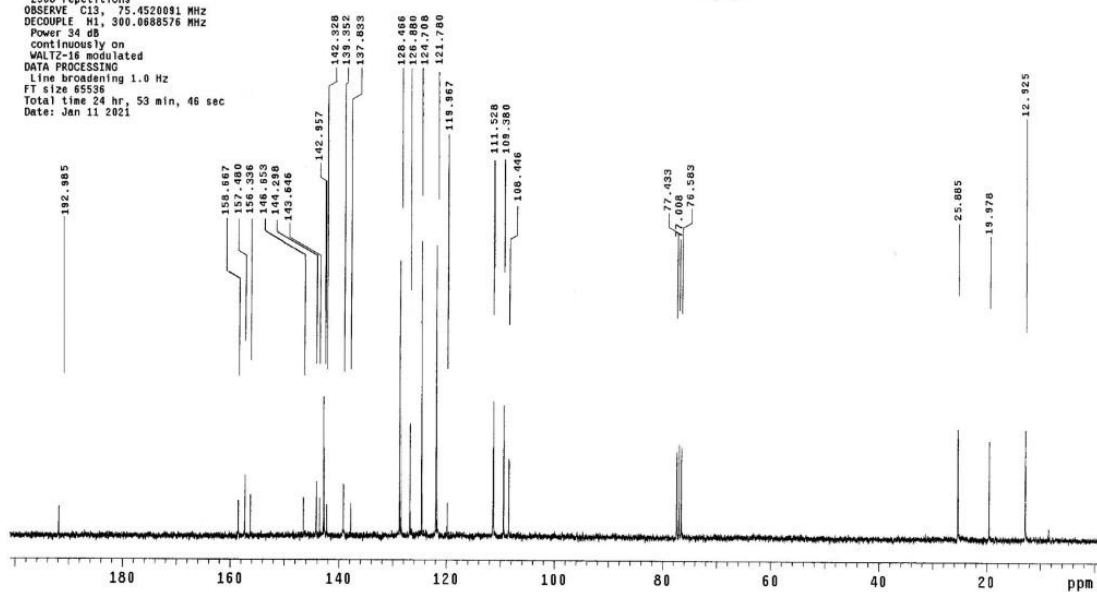
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 File: PROTON

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 Mercury-300BB "NMR300"

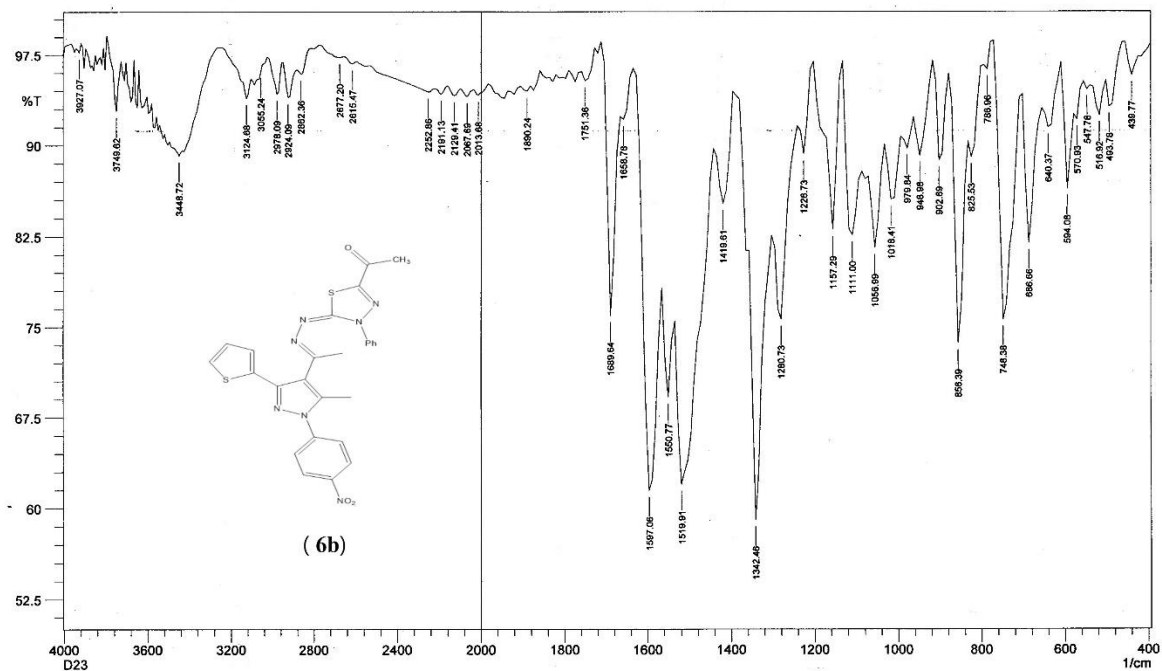
Pulse 45.0 degrees
 Acq. time 1.767 sec
 Width 18741.7 Hz
 2588 repetitions
 OBSERVE C13, 75.4520091 MHz
 DECOUPLE H1, 300.0688576 MHz
 Power 34 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 24 hr, 53 min, 46 sec
 Date: Jan 11 2021



(6b)



SHIMADZU



Comment;

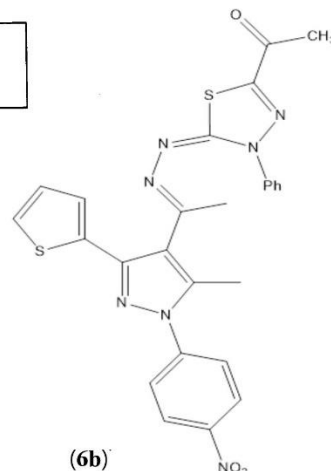
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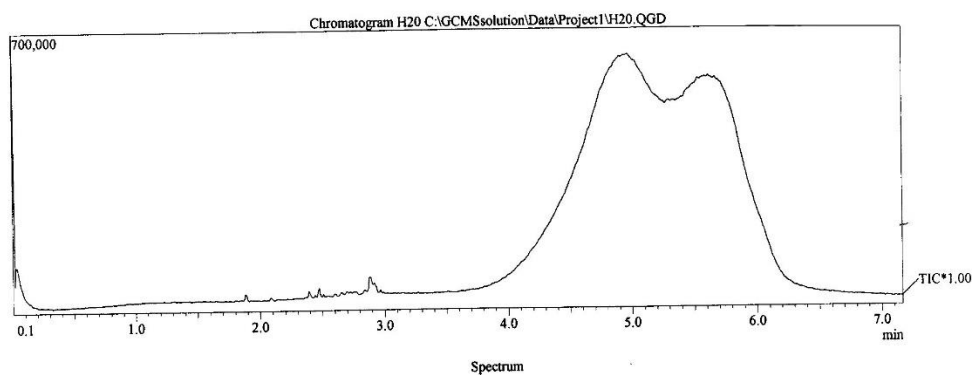
**DI Analysis
Shimadzu Qp-2010 Plus**

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 Analyzed : 31/01/2007 09:23:56
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 Sample ID :
 Customer Name : Dr. Hamdy Hassanen
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 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
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 Report File :
 Tuning File : C:\GCMSsolution\System1\Tune1_default.qgt
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 Modified : 31/01/2007 09:31:10

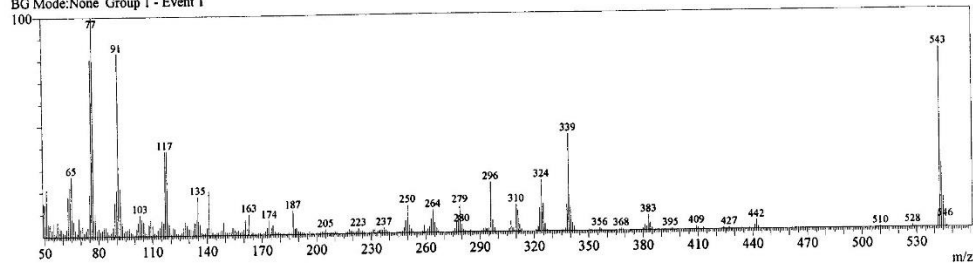
Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACQ Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1250
 Start m/z : 50.00
 End m/z : 650.00
 Electron Voltage : 70 eV
 Ionization Mode : EI



C:\GCMSsolution\Data\Project1\H2O.QGD



Line#: 1 R.Time: 5.0(Scan#: 595)
 MassPeaks: 280
 RawMode: Single 5.0(595) BasePeak: 77(43180)
 BG Mode: None Group 1 - Event 1



Mass Table
 Line#: 1 R.Time: 5.0(Scan#: 595)
 MassPeaks: 280
 RawMode: Single 5.0(595) BasePeak: 77(43180)
 BG Mode: None Group 1 - Event 1

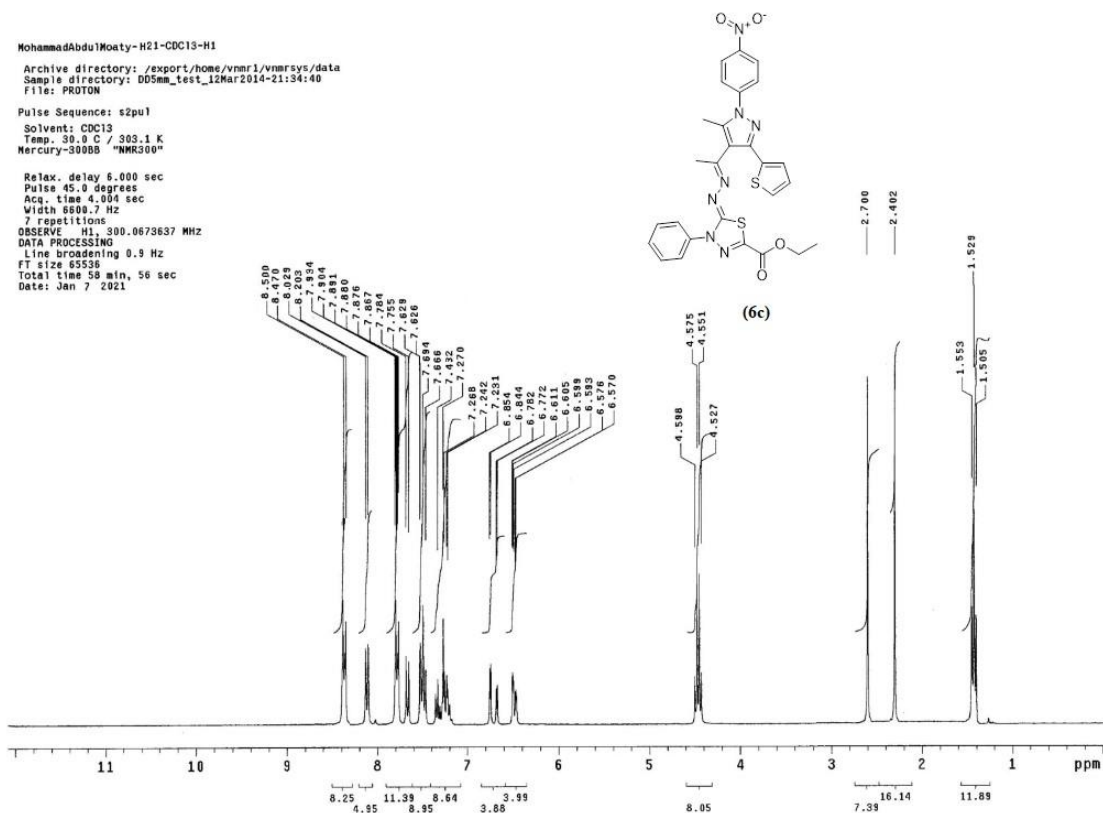
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	6314	14.62	4	53.05	2369	5.49
2	51.00	9279	21.49	5	54.00	1263	2.92
3	52.05	2435	5.64	6	55.05	2608	6.04
				7	56.10	769	1.78
				8	57.05	2874	6.66
				9	58.00	1809	4.19

MohammadAbdulMoaty-H21-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: 39.9 C / 303.1 K
Mercury-300BB "NMR300"

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.004 sec
Width 6500.7 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: Jan 7 2021

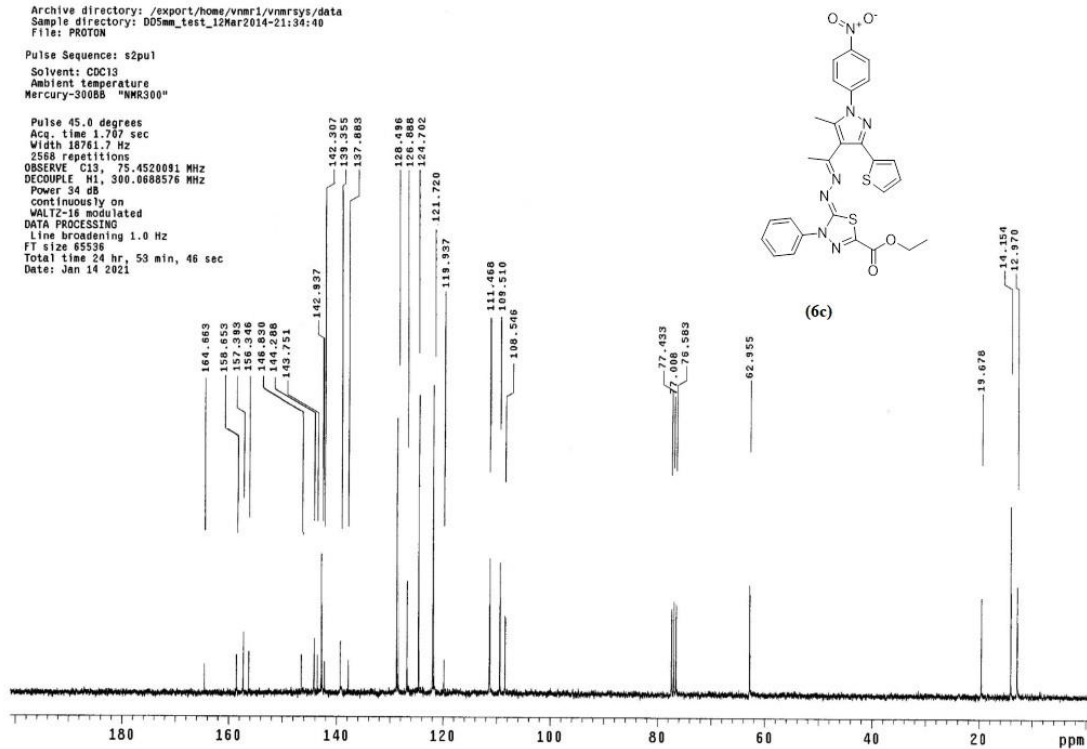


MohammadAbdulMoaty-H21-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05mm_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 16761.7 Hz
2556 repetitions
OBSERVE C13, 75.4520091 MHz
DECOUPLE H1, 300.0668576 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 14 2021

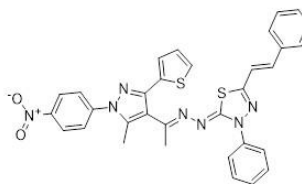


HandyHassanein-H24-CDCl3-H1

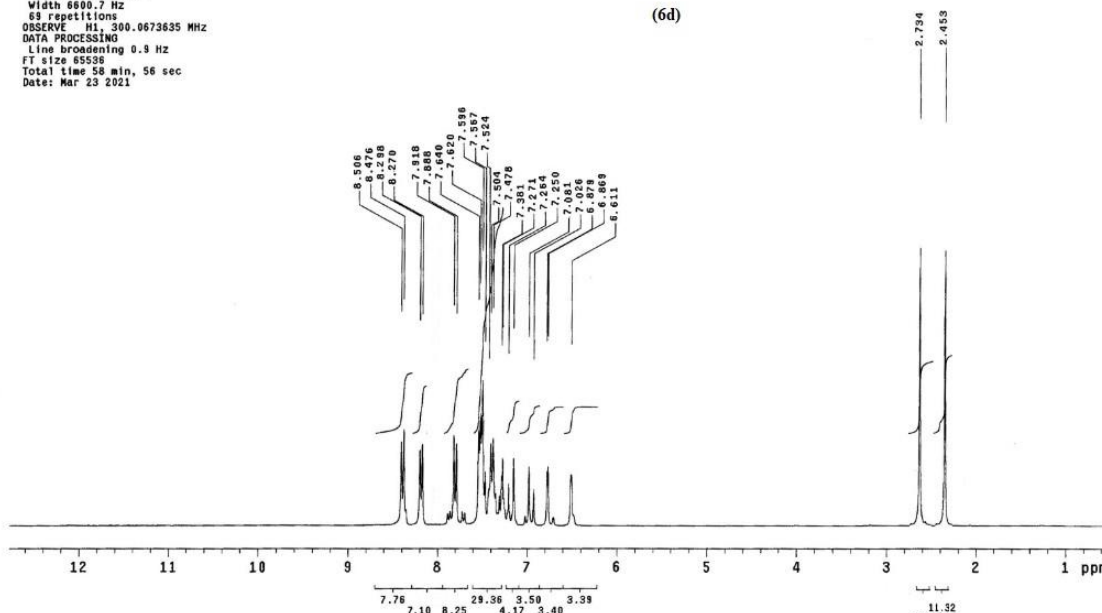
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 Sample directory: D05mm_test_12Mar2014-21:34:40
 File: PROTON

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Temp: 30.0 C / 303.1 K
 Mercury-3000B "NMR300"

Relax. delay 6.000 sec
 Pulse 45.0 degrees
 Acq. time 4.004 sec
 Width 6600.7 Hz
 63 repetitions
 OBSERVE HI, 300.0673635 MHz
 DATA PROCESSING
 Line broadening 0.9 Hz
 FT size 65538
 Total time 58 min, 56 sec
 Date: Mar 23 2021



(6d)

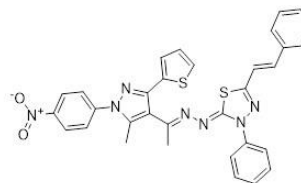


HandyHassanein-H24-CDCl3-C13

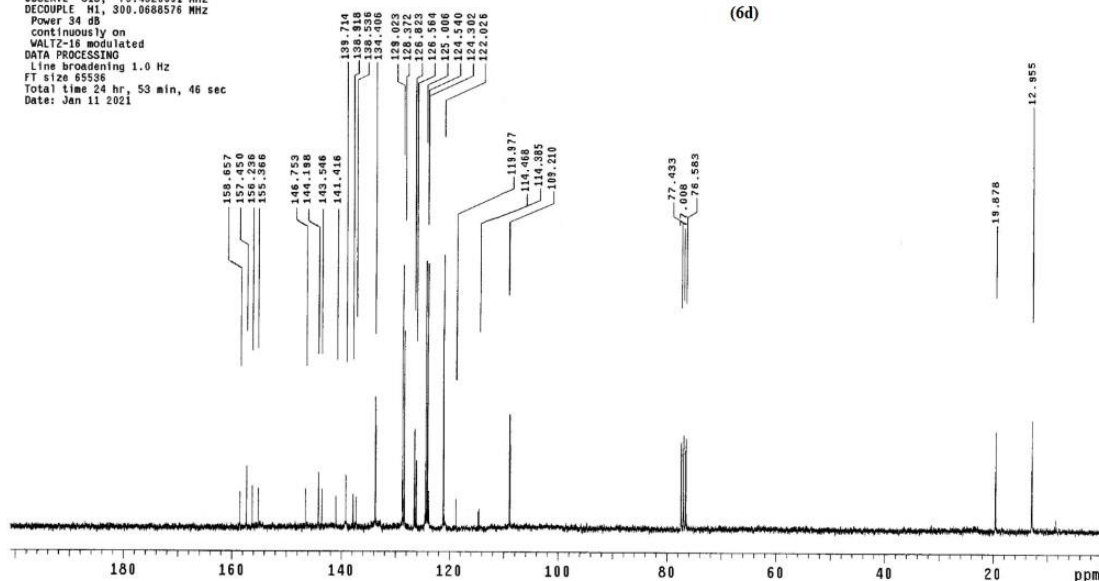
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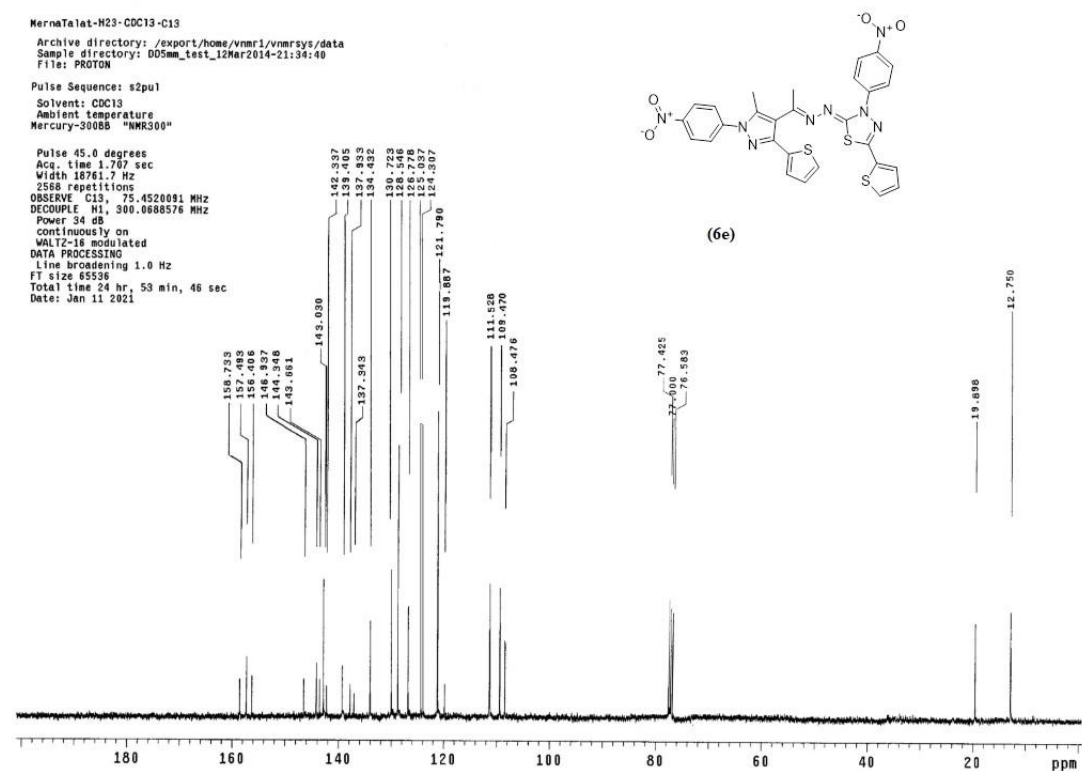
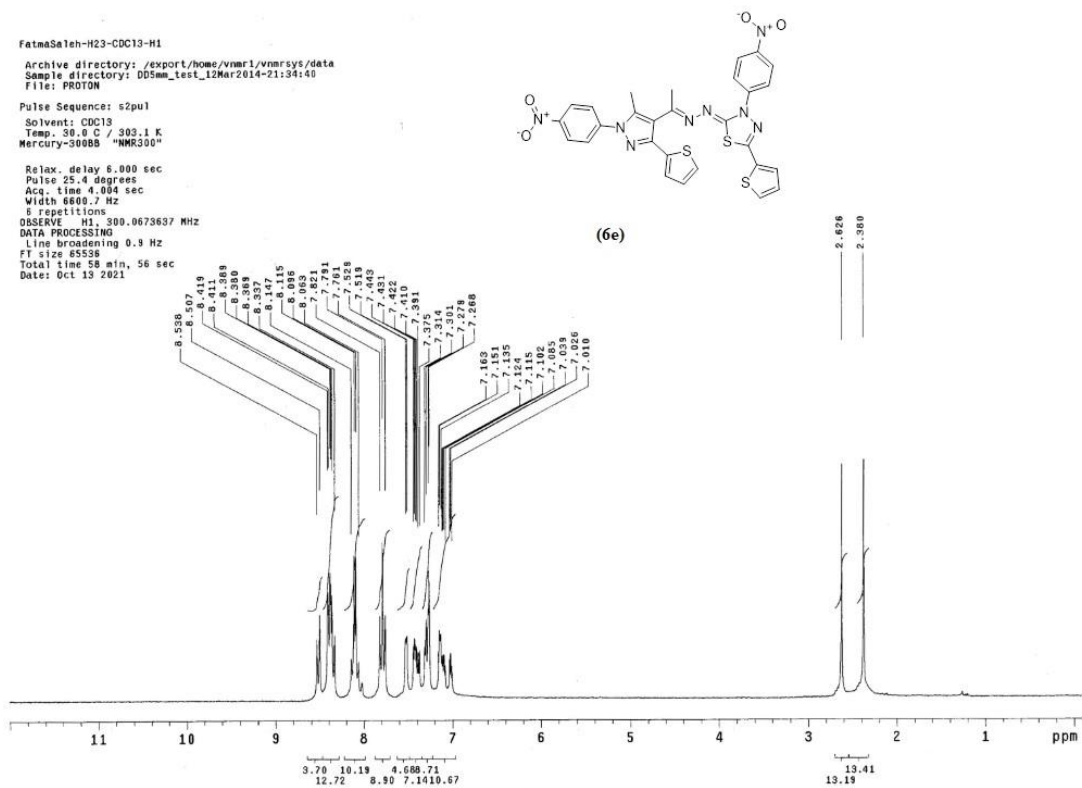
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 Solvent: CDCl3
 Ambient temperature
 Mercury-3000B "NMR300"

Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 18761.7 Hz
 2588 repetitions
 OBSERVE C13, 75.4520081 MHz
 DECOUPLE HI, 300.0686576 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 11 2021



(6d)



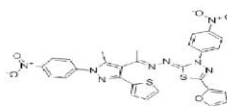


MernaTalat-H22-DMSO-H1

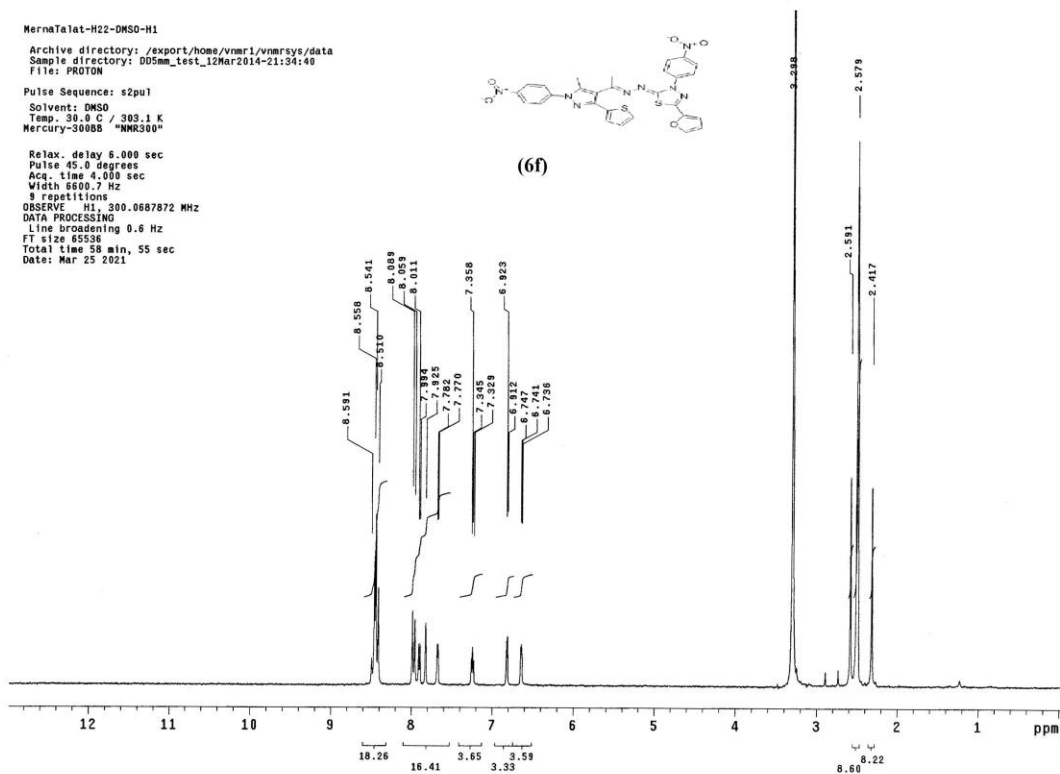
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Pulse Sequence: s2pu1
 Solvent: DMSO
 Temp: 30.0 C / 303.1 K
 Mercury-300BB "NMR300"

Relax. delay 6.000 sec
 Pulse 45.0 degrees
 Acq. time 4.000 sec
 Width 6600.7 Hz
 3 repetitions
 OBSERVE H1, 300.0687872 MHz
 DATA PROCESSING
 Line broadening 0.6 Hz
 FT size 65536
 Total time 58 min, 55 sec
 Date: Mar 25 2021



(6f)

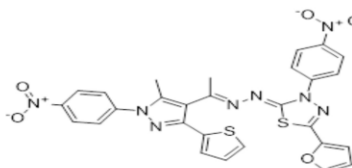


MernaTalat-H22-DMSO-C13

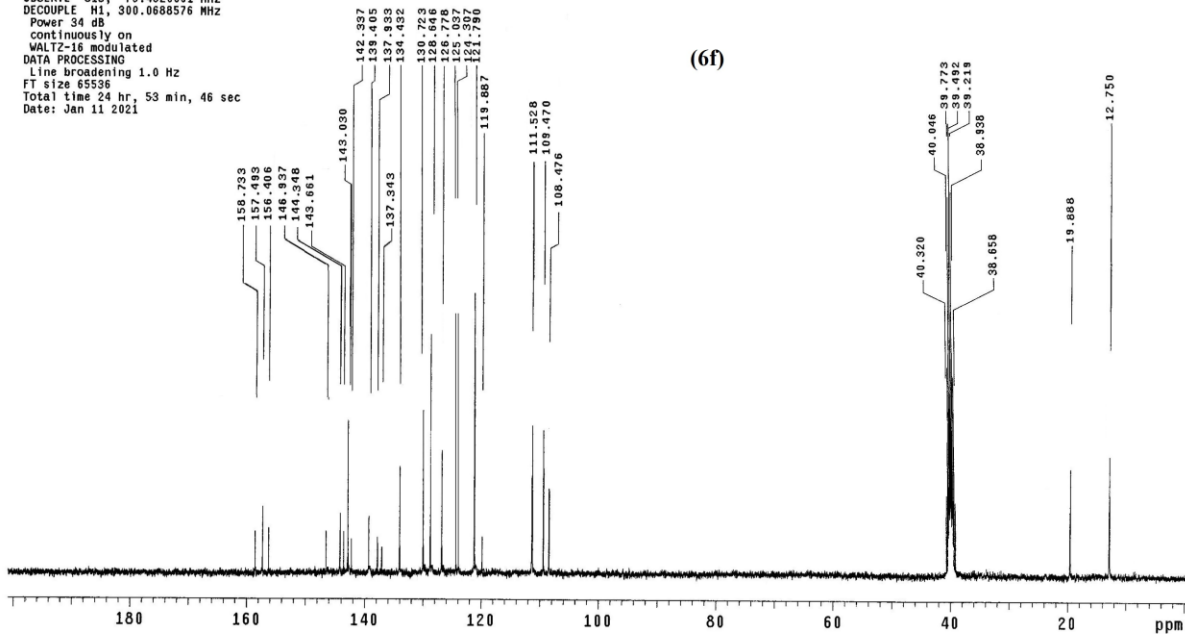
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 Sample directory: D05mm_test_12Mar2014-21:34:40
 File: PROTON

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

Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 18761.7 Hz
 2588 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 11 2021



(6f)

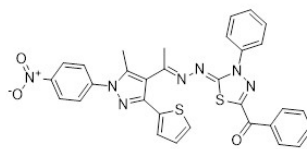


FatmaSaleh-H25-CDC13-H1

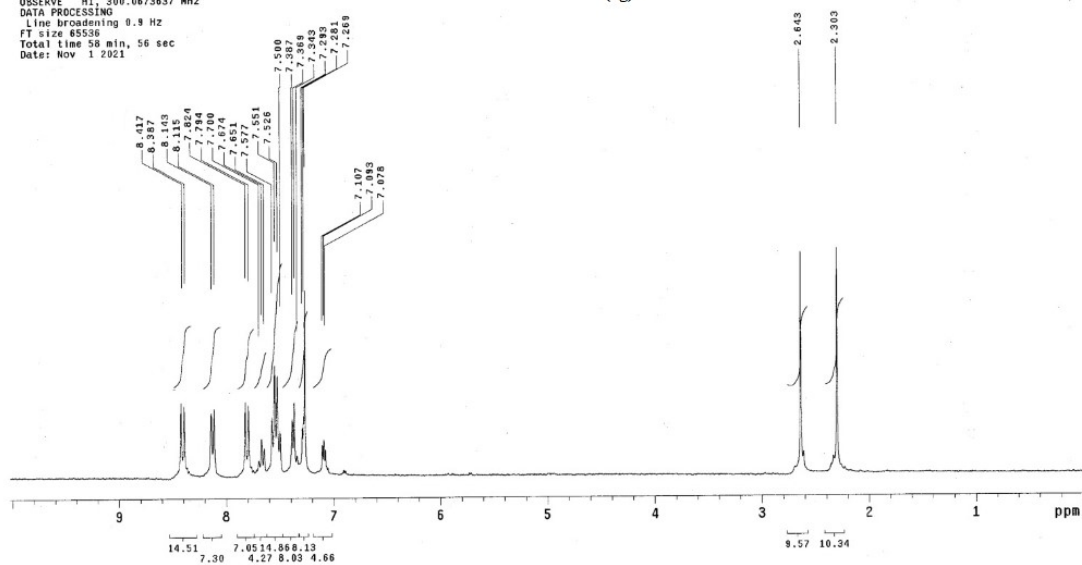
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 Sample directory: D05mm_test_12Mar2014-21:34:40
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Pulse Sequence: s2pu1
 Solvent: CDC13
 Temp: 30.0 C / 303.1 K
 Mercury-300BB "NMR300"

Relax. delay 6.000 sec
 Pulse 25.4 degrees
 Acq. time 4.004 sec
 Width 6590.7 Hz
 12 repetitions
 OBSERVE H1, 300.0673637 MHz
 DATA PROCESSING
 Line broadening 0.8 Hz
 FT size 65536
 Total time 56 min, 56 sec
 Date: Nov 1 2021



(6g)

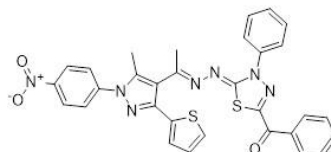


FatmaSaleh-H25-CDC13-C13

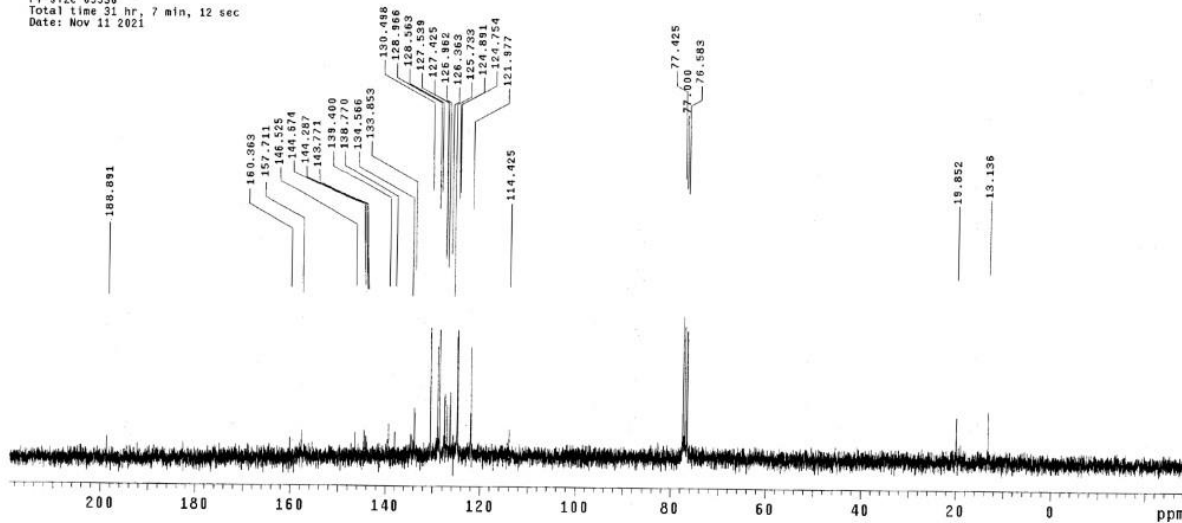
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 Sample directory: D05mm_test_12Mar2014-21:34:40

Pulse Sequence: s2pu1
 Solvent: CDC13
 Ambient temperature
 File: FatmaSaleh-H25-CDC13-C13
 Mercury-300BB "NMR300"

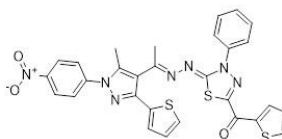
Pulse 45.0 degrees
 Acq. time 1.797 sec
 Width 18761.7 Hz
 1704 repetitions
 OBSERVE C13, 75.4520016 MHz
 DECOUPLE H1, 300.0668576 MHz
 Power 34 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 31 hr, 7 min, 12 sec
 Date: Nov 11 2021



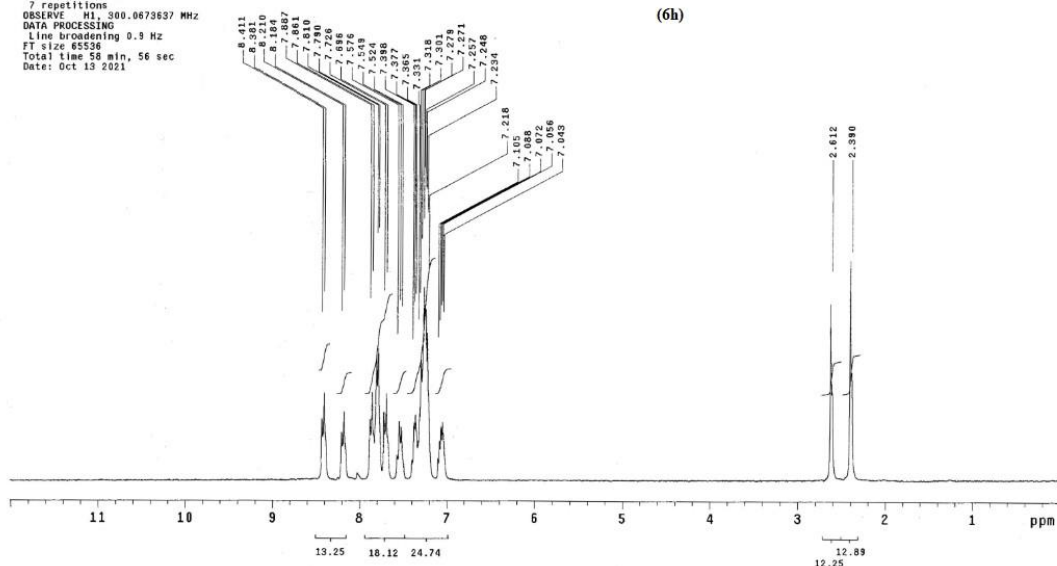
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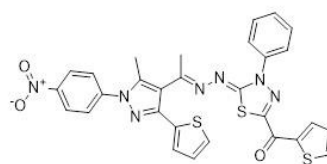
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Sample directory: D05mm_test_12Mar2014-21:34:40
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Solvent: CDC13
Temp: 30.0 C / 303.1 K
Mercury-300BB "NMR300"Relax. delay 6.000 sec
Pulse 25.4 degrees
Acq. time 4.004 sec
Width 6600.7 Hz
7 repetitions
OBSERVE N1 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 56 min, 56 sec
Date: Oct 13 2021

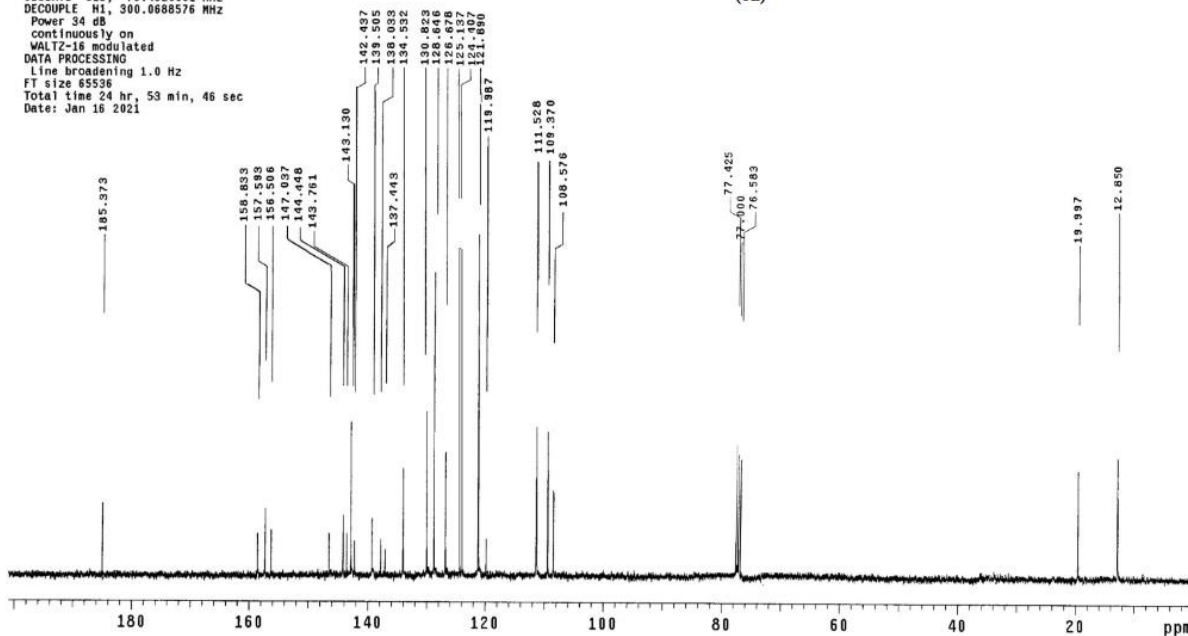
(6h)



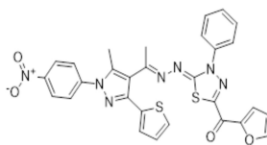
MernaTalat-H28-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTONPulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2588 repetitions
OBSERVE C13 75.4520081 MHz
DECOUPLE N1 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 16 2021

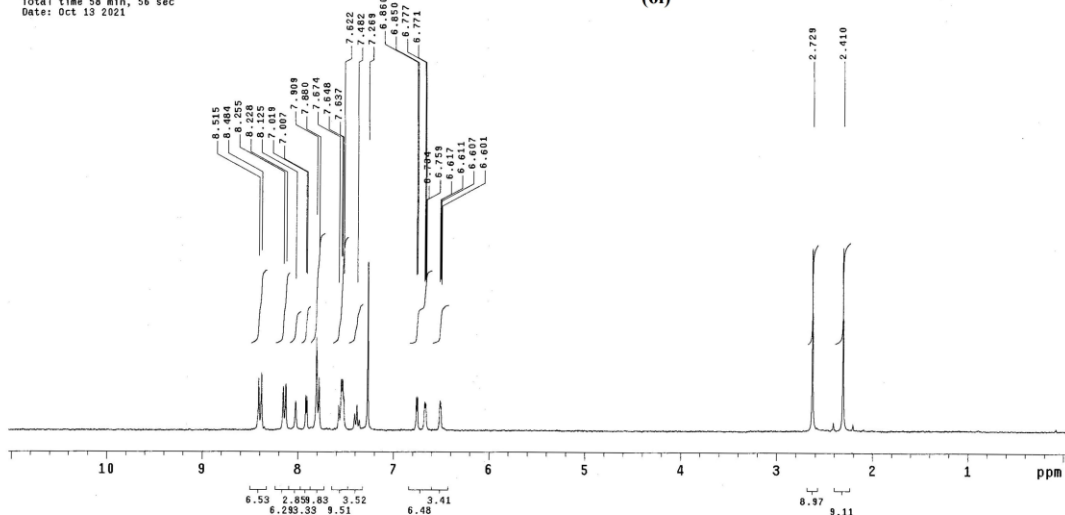
(6h)



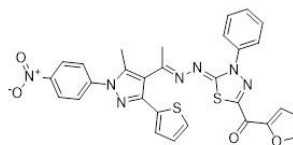
FatmaSaleh-H29-CDC13-H1

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTONPulse Sequence: s2pul
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
7 repetitions
OBSERVE H1: 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Oct 13 2021

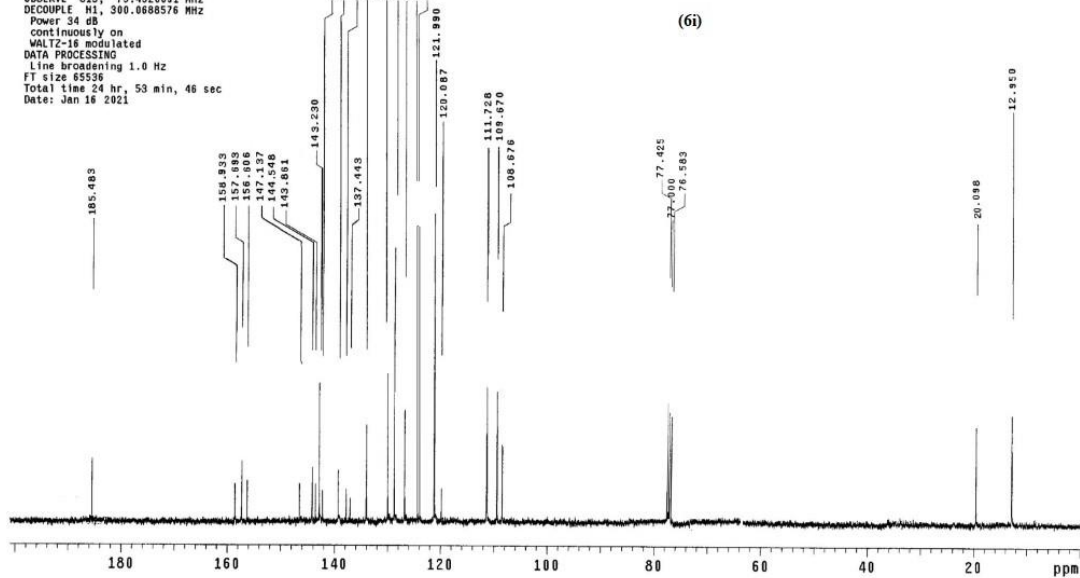
(6i)



MernaTalat-H29-CDC13-C13

Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTONPulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"Pulse 45.0 degrees
Acq. time 1.707 sec
Width 16761.7 Hz
2568 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 16 2021

(6i)

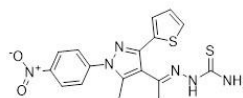


FatmaSaleh-H17-CDC13-H1

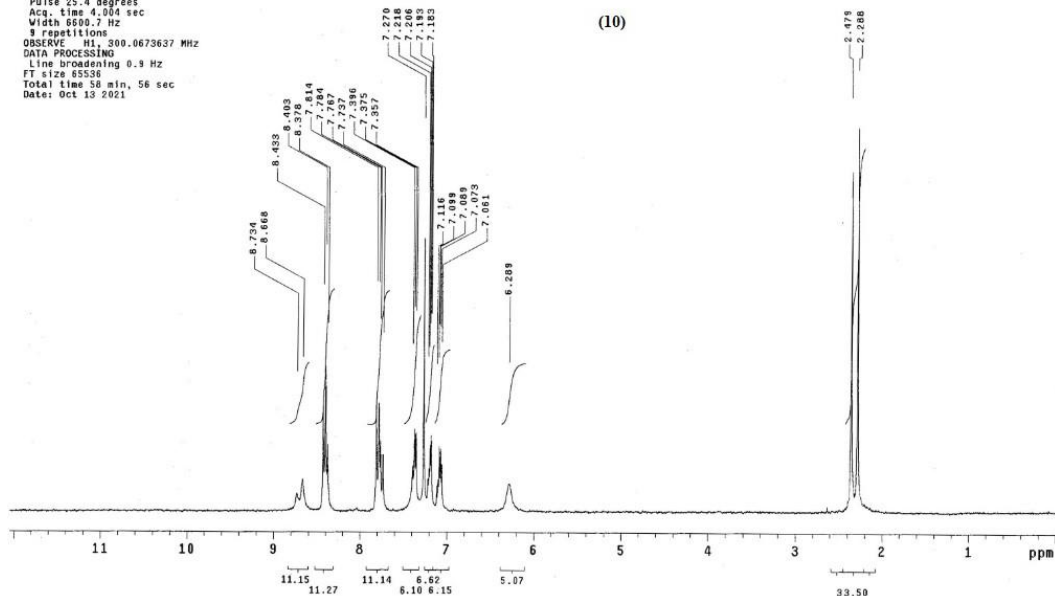
Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: D05mm_test_12Mar2014-21:34:40
 File: PROTON

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

Relax. delay 6.000 sec
 Pulse 25.4 degrees
 Acq. time 4.004 sec
 Width 6500.7 Hz
 8 repetitions
 OBSERVE H1, 300.0673637 MHz
 DATA PROCESSING
 Line broadening 0.9 Hz
 FT size 65536
 Total time 58 min, 56 sec
 Date: Oct 15 2021



(10)

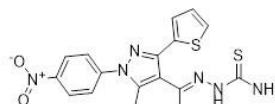


HernaTalat-H17-CDC13-C13

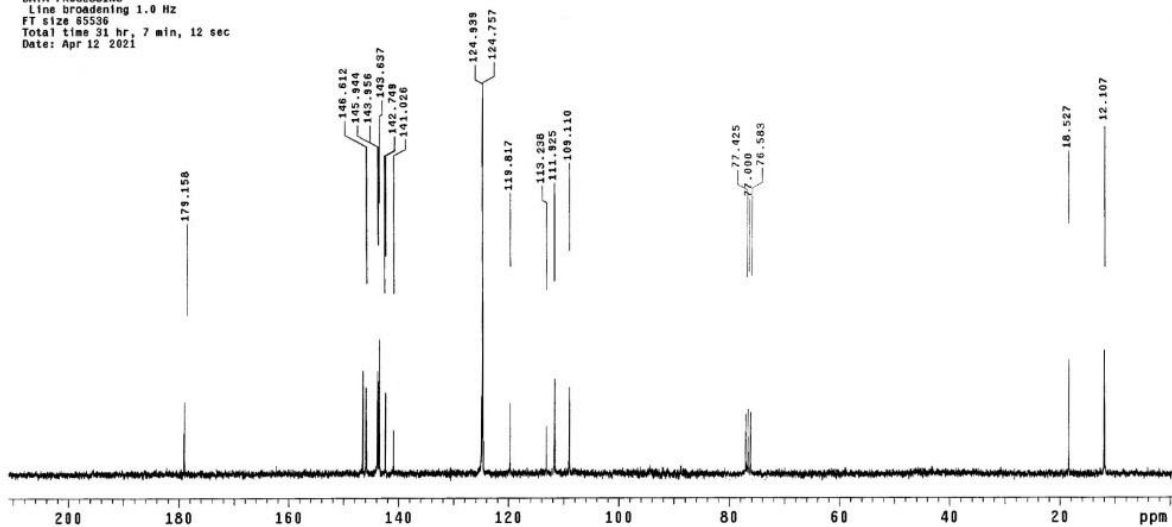
Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: D05mm_test_12Mar2014-21:34:40
 File: PROTON

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

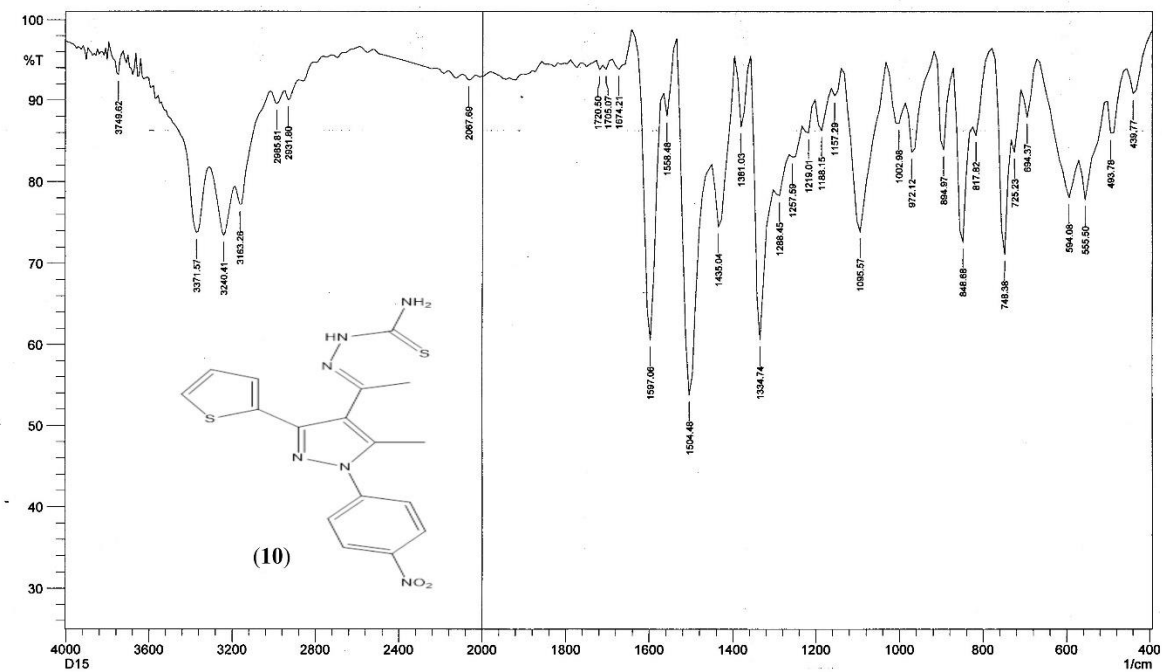
Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 18761.7 Hz
 680 repetitions
 OBSERVE C13, 75.4523891 MHz
 DECOUPLE H1, 300.0702830 MHz
 Power 34 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 31 hr, 7 min, 12 sec
 Date: Apr 12 2021



(10)



SHIMADZU



Comment;

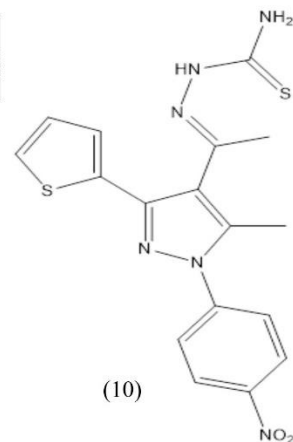
No. of Scans;
Resolution;Date/Time; 30/03/2021 11:41:50 AM
User; Administrator

**Cairo University
Micro Analytical Center**

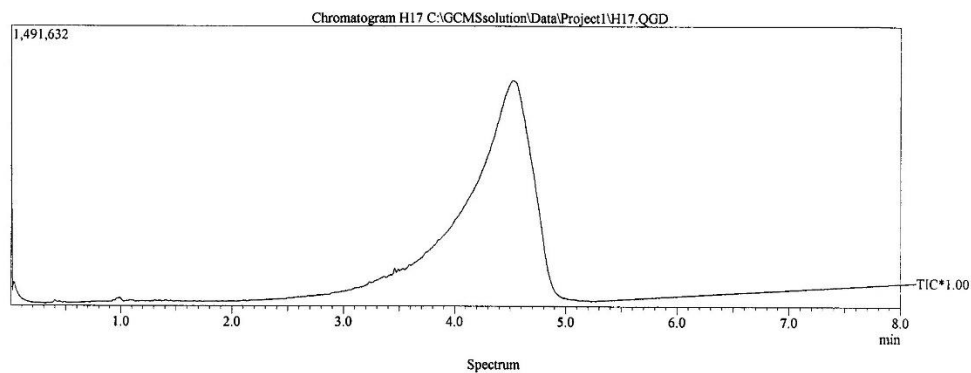
**DI Analysis
Shimadzu Qp-2010 Plus**

Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 14/01/2007 10:32:17
 Sample Name : H17
 Sample ID :
 Customer Name : Dr. Hamdy Hassanen- Science - Cairo
 Data File : C:\GCMSsolution\Data\Project1\H17.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\H17.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
 \$Endf\$Modified by : Dr. Mai Younis
 Modified : 14/01/2007 10:37:34

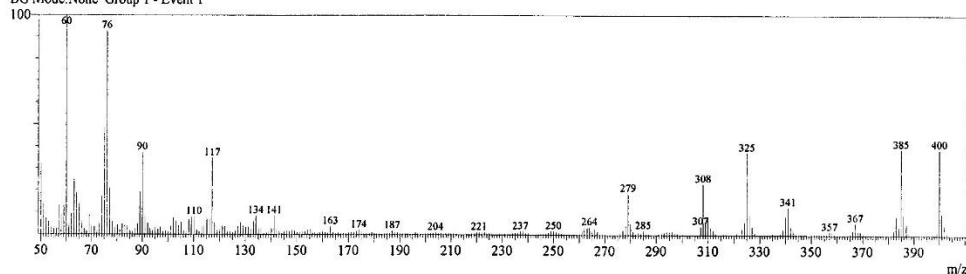
Method
 Analytical Line 1
 IonSourceTemp : 250.00 °C
 [MS Table]
 --Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACQ Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1428
 Start m/z : 50.00
 End m/z : 700.00
 Electron Voltage : 70 eV
 Ionization Mode : EI



C:\GCMSsolution\Data\Project1\H17.QGD



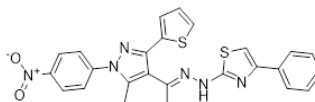
Line#:1 R.Time:4.5(Scan#:541)
 MassPeaks:289
 RawMode:Single 4.5(541) BasePeak:60(94306)
 BG Mode:None Group 1 - Event 1



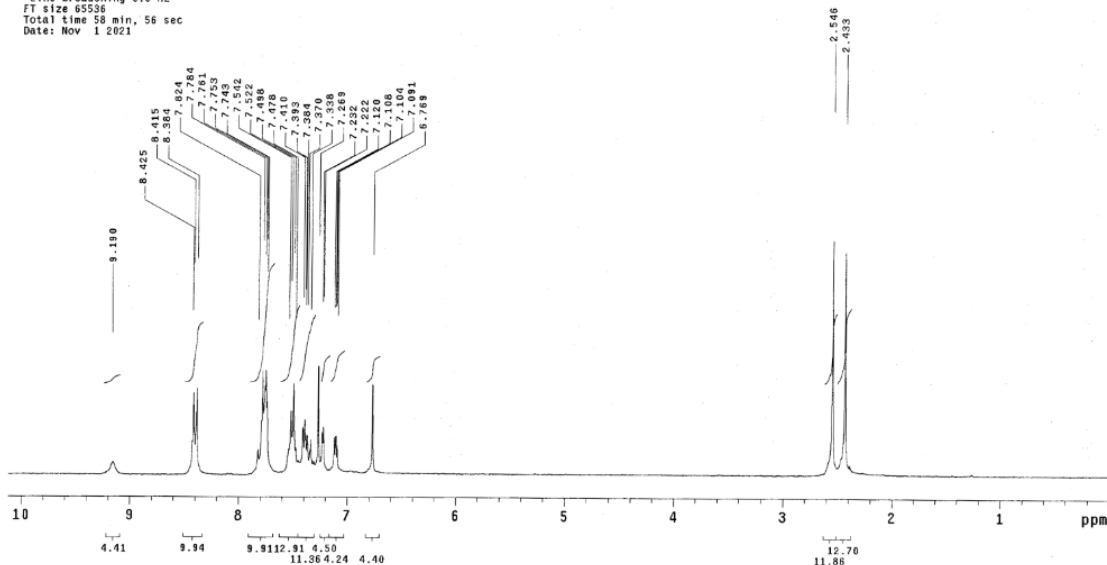
Mass Table
 Line#:1 R.Time:4.5(Scan#:541)
 MassPeaks:289
 RawMode:Single 4.5(541) BasePeak:60(94306)
 BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	30231	32.06	4	53.10	5463	5.79	7	56.10	2518	2.67
2	51.05	12981	13.76	5	54.05	3085	3.27	8	57.10	12284	13.03
3	52.05	6995	7.42	6	55.10	2353	2.50	9	58.05	8408	8.92

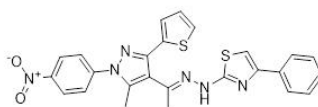
FatmaSaleh-H36-CDC13-H1

Archive directory: /export/home/vmr1/vmr/sys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTONPulse 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 0.9 Hz
FT size 65536
Total time 58 min, 56 sec
Date: Nov 1 2021

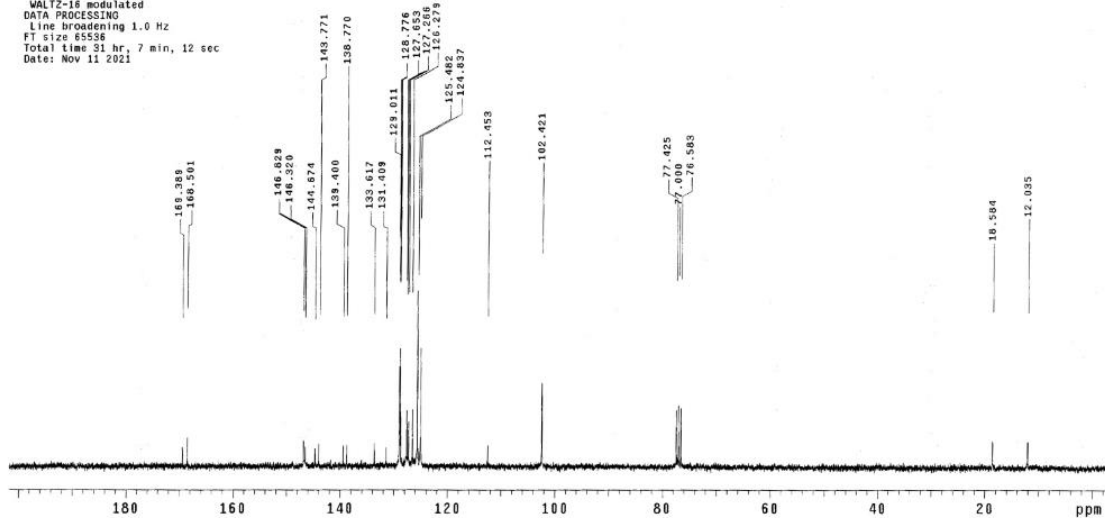
(12a)



FatmaSaleh-H36-CDC13-C13

Archive directory: /export/home/vmr1/vmr/sys/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: FatmaSaleh-H36-CDC13-C13Pulse Sequence: s2pu1
Solvent: DMSO
Ambient Temperature
File: FatmaSaleh-H36-CDC13-C13
Mercury-300BB "NMR300"Pulse 45.0 degrees
Acq. time 1.737 sec
Width 18761.7 Hz
1328 repetitions
OBSERVE C13, 75.4520079 MHz
DECOUPLE H1, 300.0702850 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: Nov 11 2021

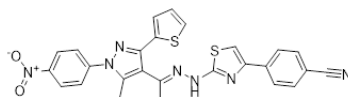
(12a)



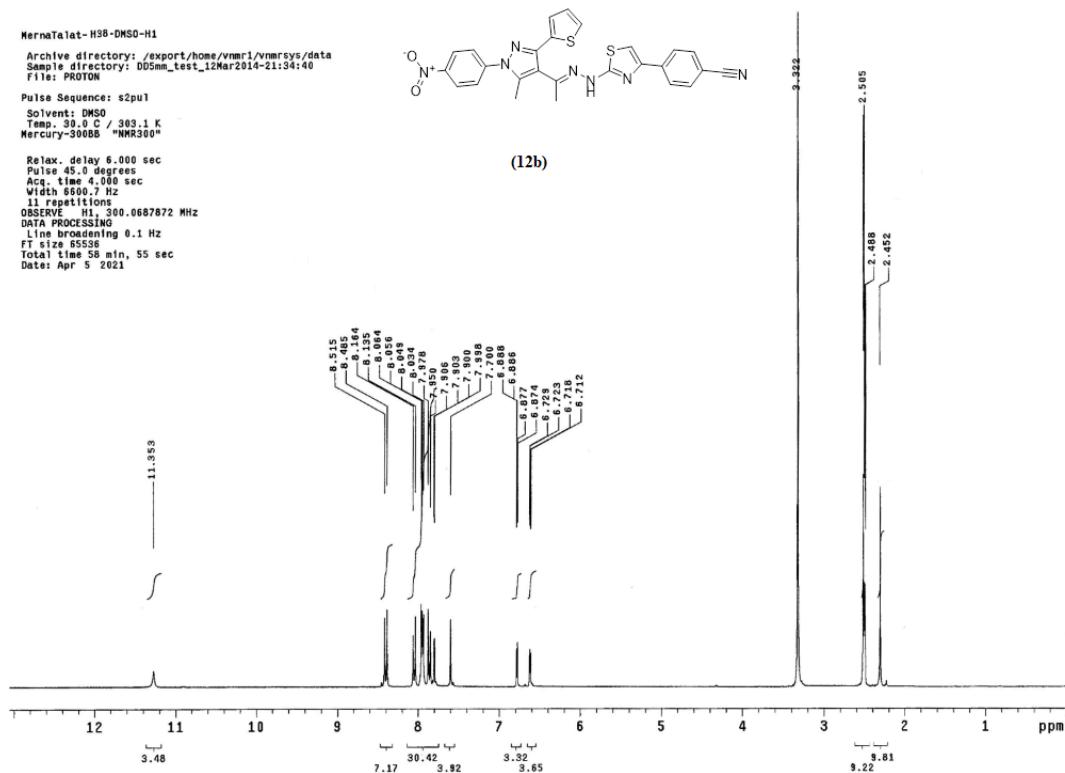
MernaTalat-H38-DMSO-H1

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

Pulse Sequence: s2pu1

Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-300BB "NMR300"Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.900 sec
Width 6600.7 Hz
11 repetitions
OBSERVE H1, 300.0687872 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 85536
Total time 38 min, 55 sec
Date: Apr 5 2021

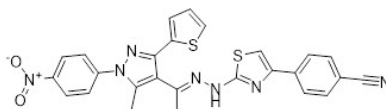
(12b)



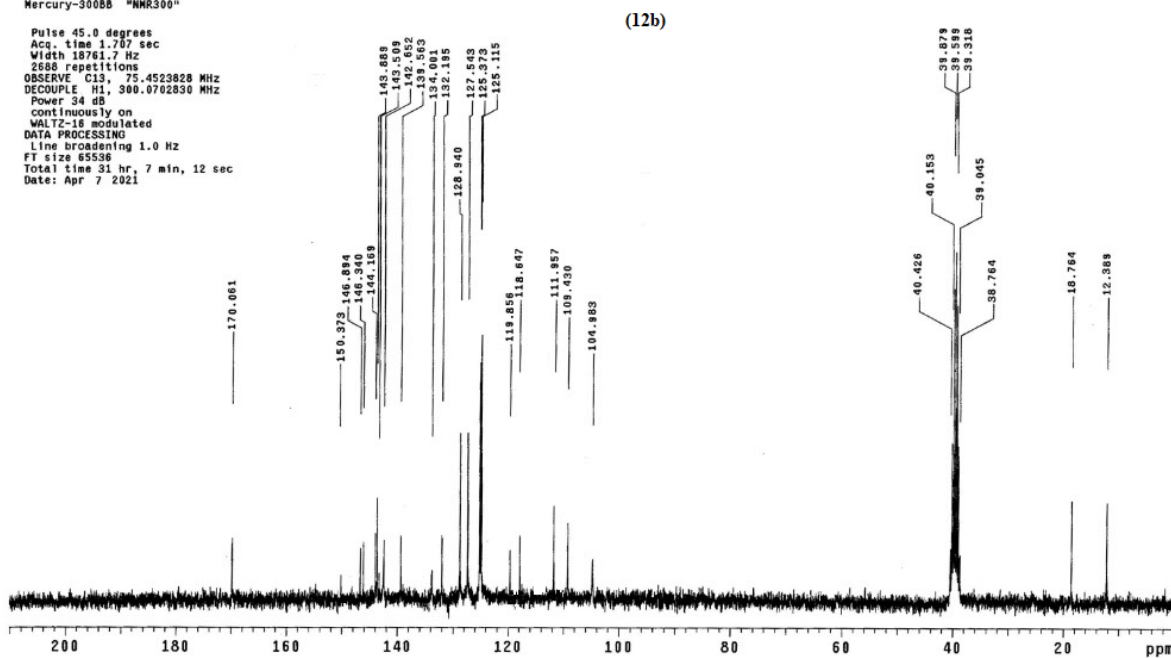
MernaTalat-H38-DMSO-C13

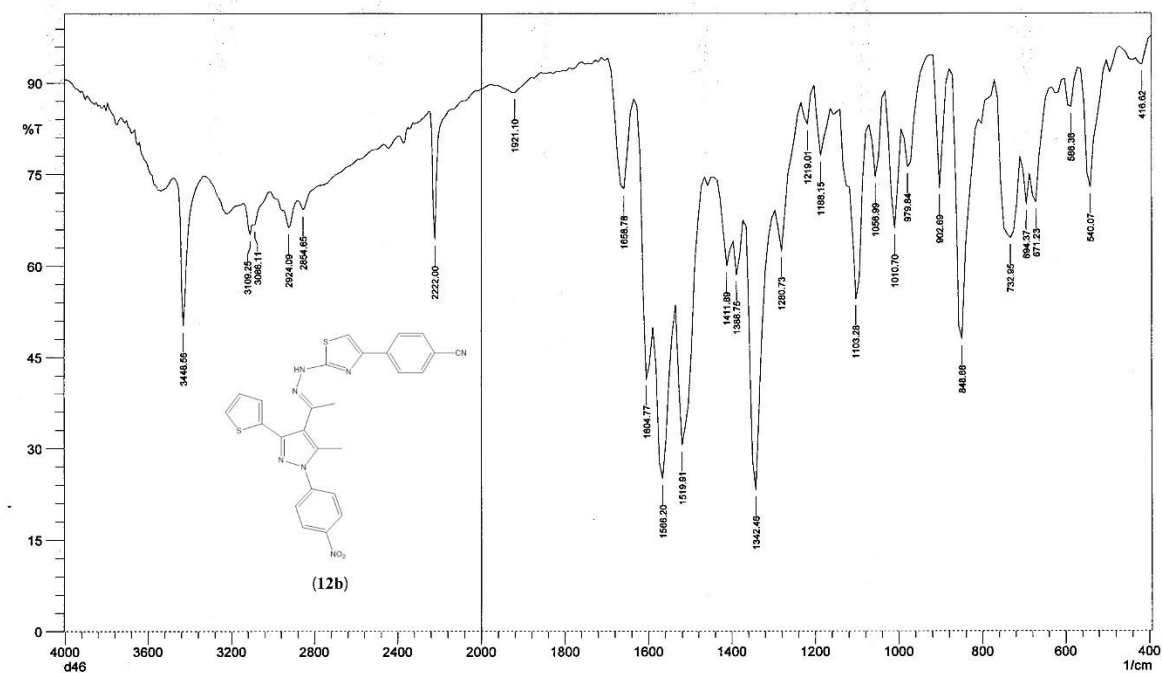
Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory: D05mm_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300BB "NMR300"Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
2688 repetitions
OBSERVE C13, 75.4523828 MHz
DECOUPLE H1, 300.0702830 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 85536
Total time 31 hr, 7 min, 12 sec
Date: Apr 7 2021

(12b)





Comment;

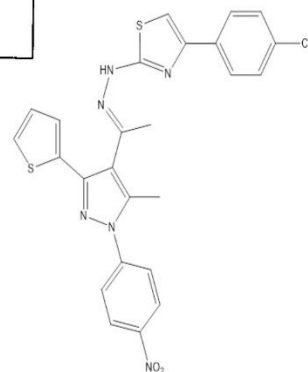
No. of Scans;
Resolution;Date/Time; 14/07/2021 12:26:19 PM
User; Administrator

**Cairo University
Micro Analytical Center**

**DI Analysis
Shimadzu Qp-2010 Plus**

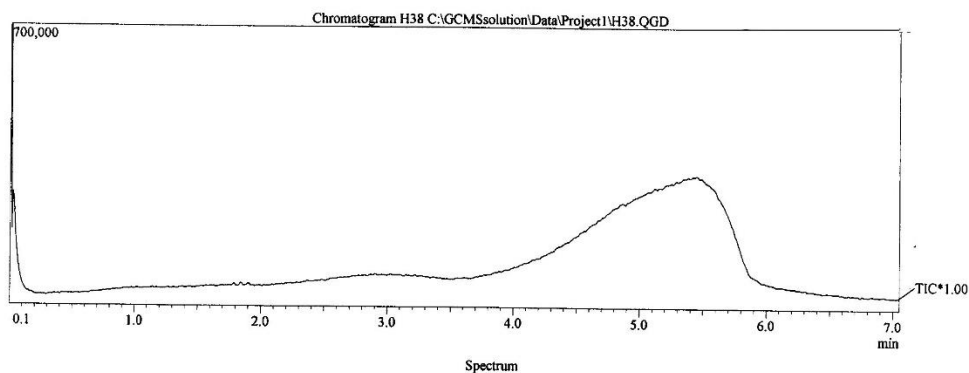
Sample Information
 Analyzed by : Dr. Mai Younis
 Analyzed : 09/02/2007 10:48:58
 Sample Name : H38
 Sample ID :
 Customer Name : Dr. Hamdy Hassanen- Science - Cairo
 Data File : C:\GCMSsolution\Data\Project1\H38.QGD
 Org Data File : C:\GCMSsolution\Data\Project1\H38.QGD
 Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
 Report File :
 Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
 \$Endl\$Modified by : Dr. Mai Younis
 Modified : 09/02/2007 10:56:04

Method
 Analytical Line 1
 [MS Table]
 -Group 1 - Event 1--
 Start Time : 0.00min
 End Time : 10.00min
 ACQ Mode : Scan
 Event Time : 0.50sec
 Scan Speed : 1428
 Start m/z : 50.00
 End m/z : 700.00
 Electron Voltage : 70 eV
 Ionization Mode : EI

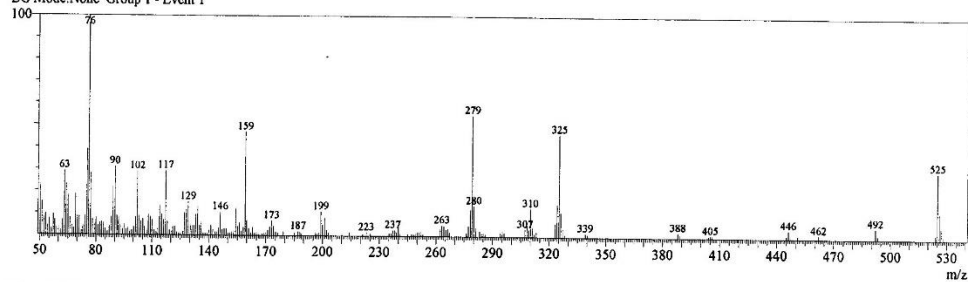


(12b)

C:\GCMSsolution\Data\Project1\H38.QGD



Line#: 1 R.Time: 5.3(Scan#: 637)
 MassPeaks: 210
 RawMode: Single 5.3(637) BasePeak: 76(23047)
 BG Mode: None Group 1 - Event 1



Mass Table

Line#: 1 R.Time: 5.3(Scan#: 637)

MassPeaks: 210

RawMode: Single 5.3(637) BasePeak: 76(23047)

BG Mode: None Group 1 - Event 1

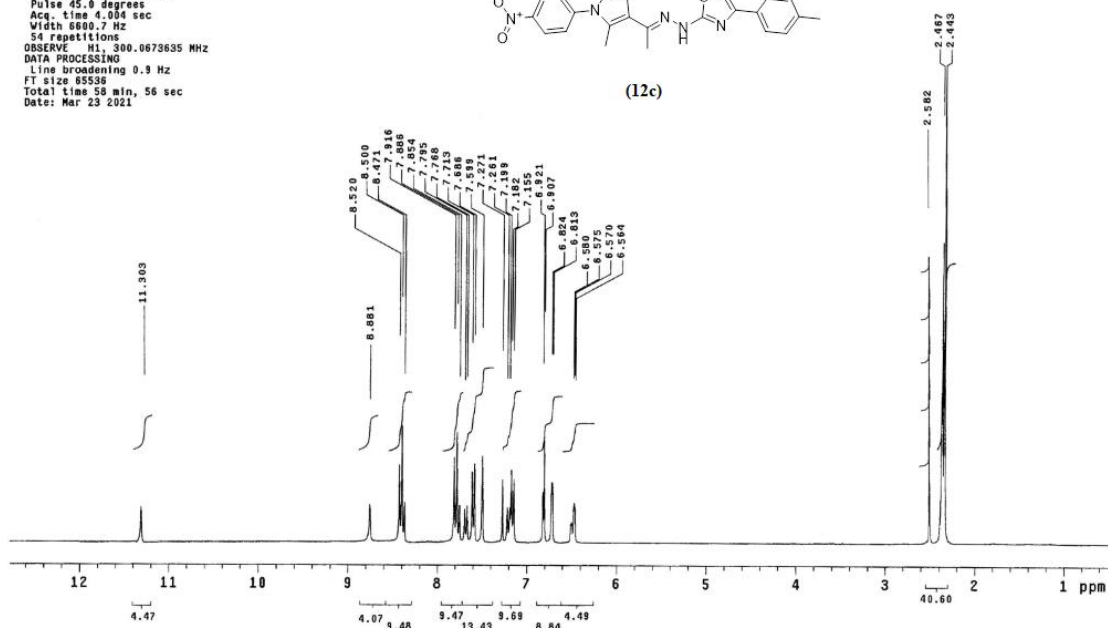
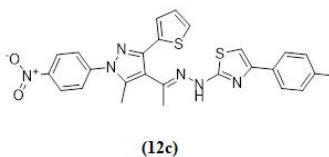
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.10	5327	23.11	4	53.05	2204	9.56	7	56.10	692	3.00
2	51.05	3483	15.11	5	54.05	961	4.17	8	57.10	2134	9.26
3	52.05	1822	7.91	6	55.05	1956	8.49	9	58.00	1639	7.11

HandyHassaneIn-H41-CDC13-H1

Archive directory: /export/home/vmr1/vmrsys/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 4.054 sec
 Width 6580.7 Hz
 54 repetitions
 OBSERVE H1, 300.0673635 MHz
 DATA PROCESSING
 Line broadening 0.3 Hz
 FT size 65538
 Total time 58 min, 56 sec
 Date: Mar 23 2021

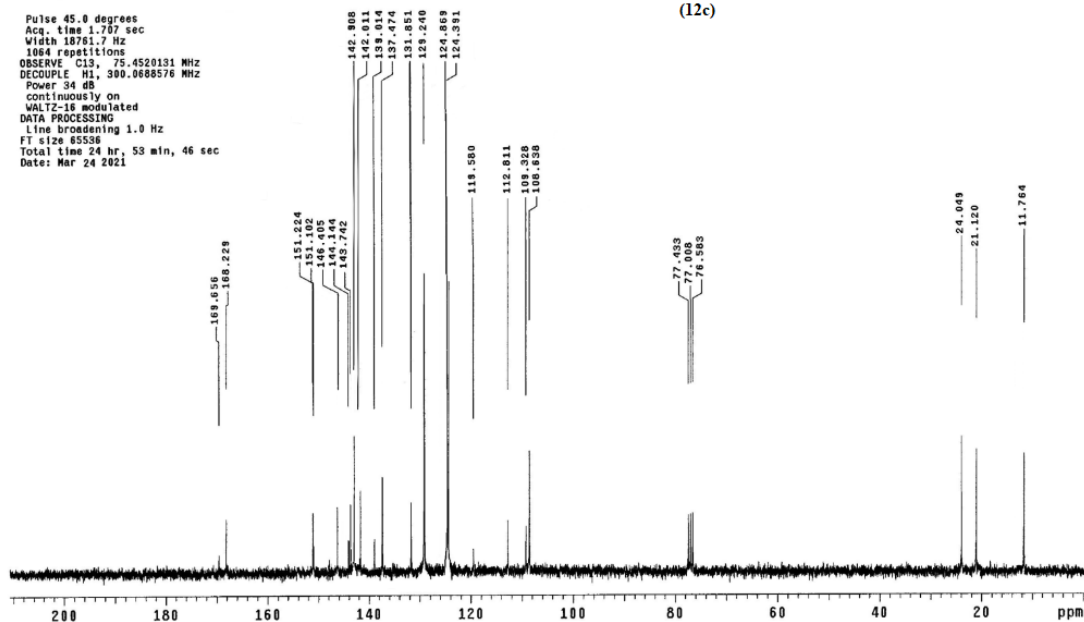
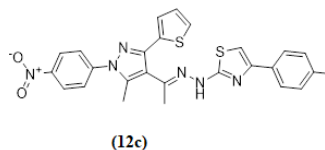


MernaTalat-H41-CDC13-C13

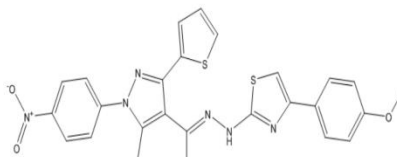
Archive directory: /export/home/vmr1/vmrsys/data
 Sample directory: DD5mm_test_12Mar2014-21:34:40
 File: PROTON

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

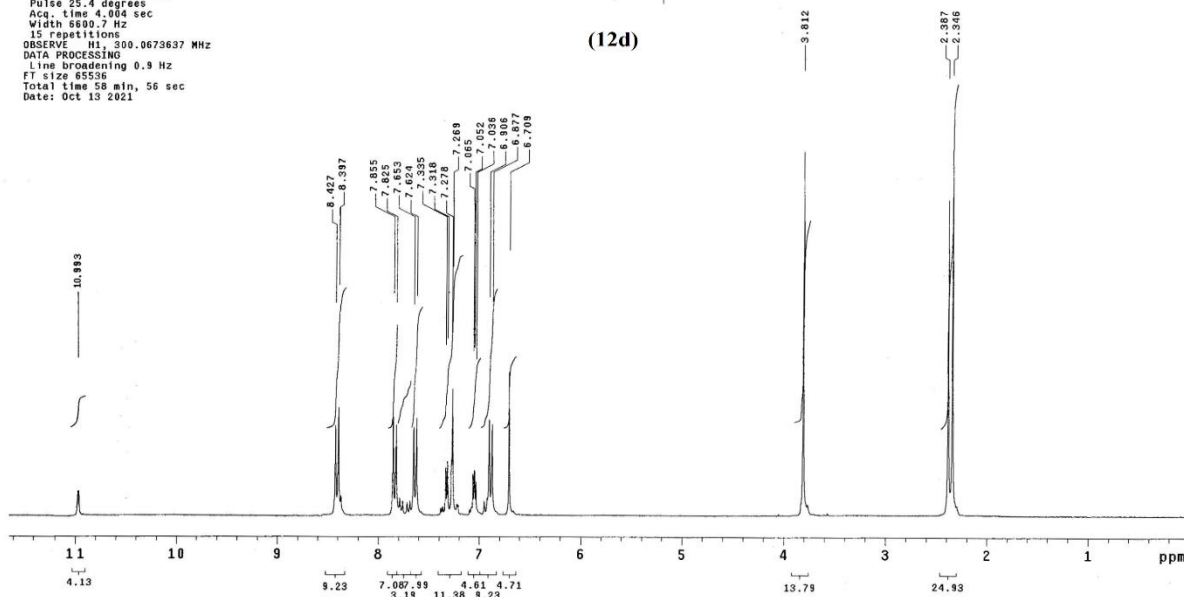
Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 10761.7 Hz
 1084 repetitions
 OBSERVE C13, 75.4520131 MHz
 DECOUPLE H1, 300.0668576 MHz
 Power 54 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65538
 Total time 24 hr, 53 min, 46 sec
 Date: Mar 24 2021



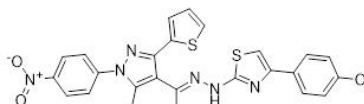
FatmaSaleh-H42-CDC13-H1

Archive directory: /export/home/vmr1/vmr/sys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTONPulse 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 5900.7 Hz
15 repetitions
OBSERVE H1, 300.0673637 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 85536
Total time 56 min, 56 sec
Date: Oct 13 2021

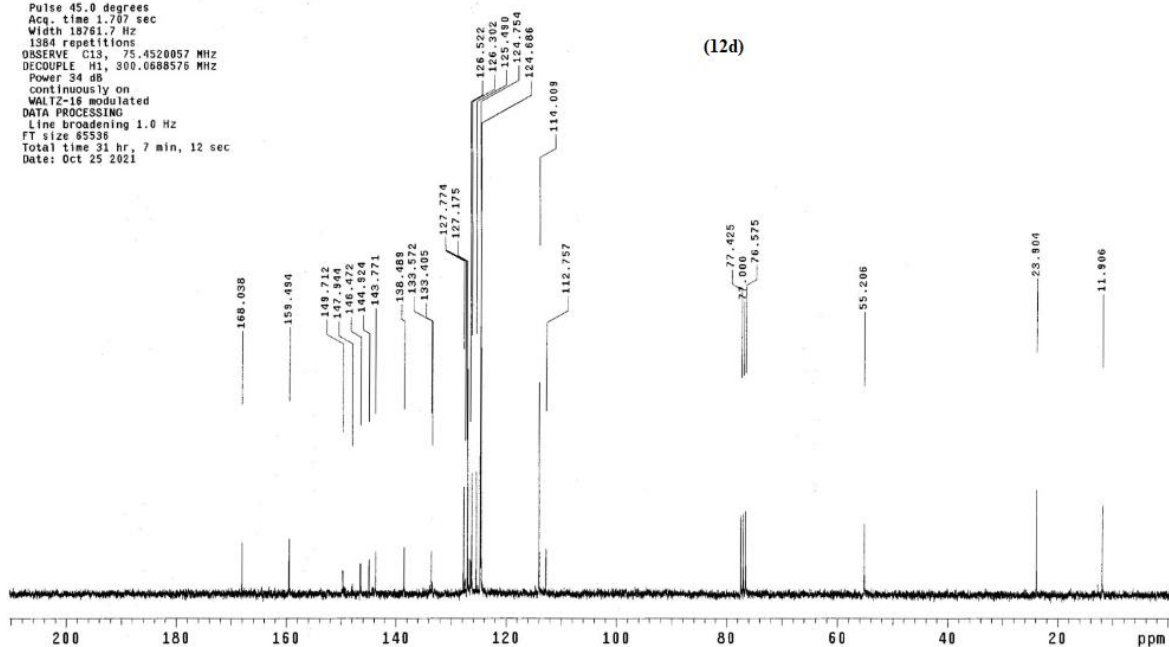
(12d)



FatmaSaleh-H42-CDC13-C13

Archive directory: /export/home/vmr1/vmr/sys/data
Sample directory: DD5mm_test_12Mar2014-21:34:40
File: PROTONPulse Sequence: s2pu1
Solvent: CDC13
Ambient temperature
Mercury-300BB "NMR300"Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18761.7 Hz
1384 repetitions
OBSERVE C13, 75.4520057 MHz
DECOUPLE H1, 300.0688576 MHz
Power 34 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 85536
Total time 31 hr, 7 min, 12 sec
Date: Oct 25 2021

(12d)

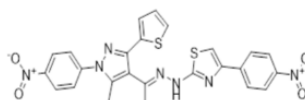


FatmaSaleh-H37-CDCl3-H1

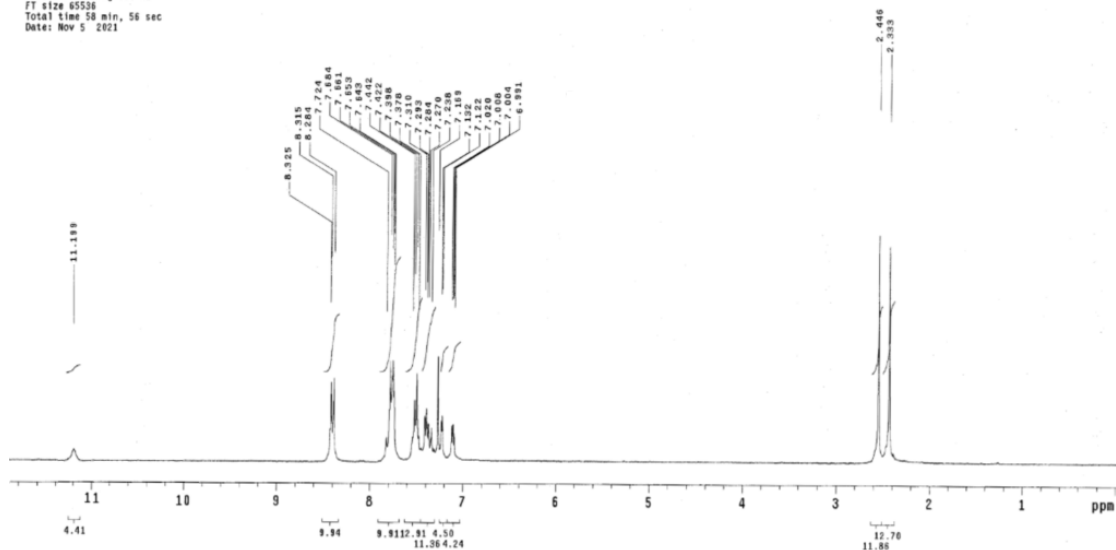
Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: D05mm_test_12Mar2014-21:34:48
 File: PSD09

Pulse Sequence: s2pul
 Solvent: CDCl3
 Temp: 30.0 C / 303.1 K
 Mercury-300BB "NMR300"

Relax. delay 6.000 sec
 Pulse 25.4 degrees
 Acq. time 4.034 sec
 Width 6600.7 Hz
 11 repetitions
 OBSERVE H1, 300.0673937 MHz
 DATA PROCESSING
 Line broadening 0.8 Hz
 FT size 65538
 Total time 58 min, 56 sec
 Date: Nov 5 2021



(12e)

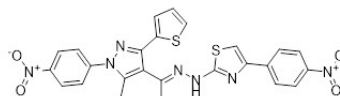


FatmaSaleh-H37-CDCl3-C13

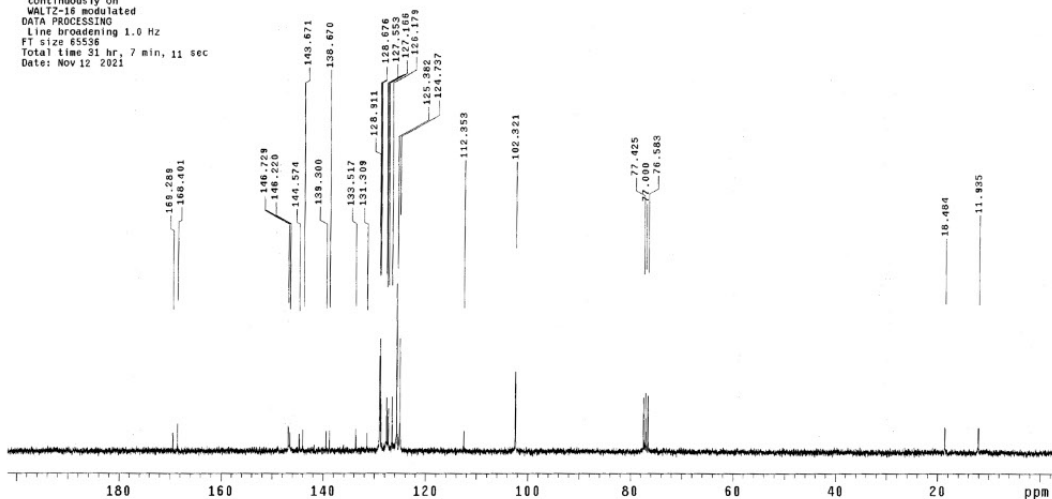
Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: D05mm_test_12Mar2014-21:34:40

Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 File: FatmaSaleh-H37-CDCl3-C13
 Mercury-300BB "NMR300"

Pulse 45.0 degrees
 Acq. time 1.707 sec
 Width 18761.7 Hz
 1928 repetitions
 OBSERVE C13, 75.4520079 MHz
 DECOUPLE H1, 300.0702830 MHz
 Power 34 dB
 continuously on
 WALTZ-18 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65538
 Total time 51 hr, 7 min, 11 sec
 Date: Nov 12 2021



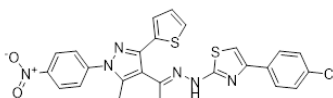
(12e)



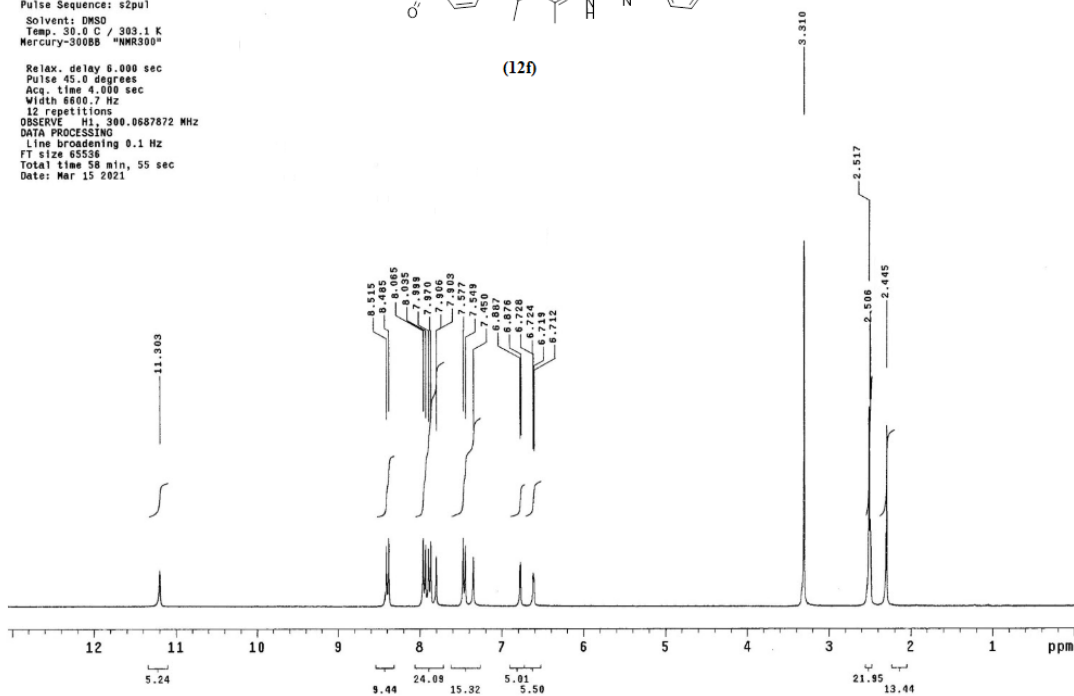
MernaTalat-H39-DMSO-H1

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05ma_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Temp: 30.0 C / 303.1 K
Mercury-300SB "NMR300"Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 4.008 sec
Width 6600.7 Hz
12 repetitions
OBSERVE H1 300.068782 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 65536
Total time 58 min, 55 sec
Date: Mar 15 2021

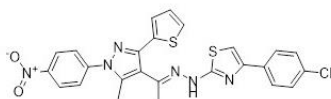
(12f)



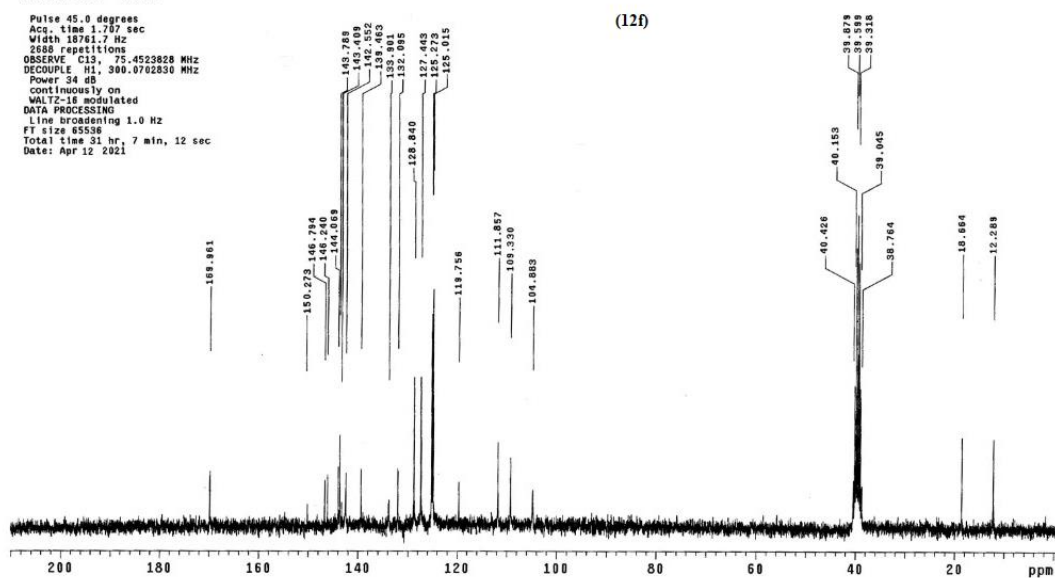
MernaTalat-H39-DMSO-C13

Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory: D05ma_test_12Mar2014-21:34:40
File: PROTON

Pulse Sequence: s2pu1

Solvent: DMSO
Ambient temperature
Mercury-300SB "NMR300"Pulse 45.0 degrees
Acq. time 1.707 sec
Width 18741.7 Hz
2888 repetitions
OBSERVE C13 75.4523858 MHz
DECOUPLE H1 300.0762830 MHz
Power 34 dB
continuous on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 31 hr, 7 min, 12 sec
Date: Apr 12 2021

(12f)

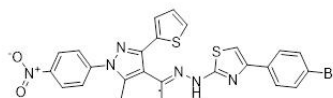


MohammadAbdulMoathy-H40-CDC13-H1

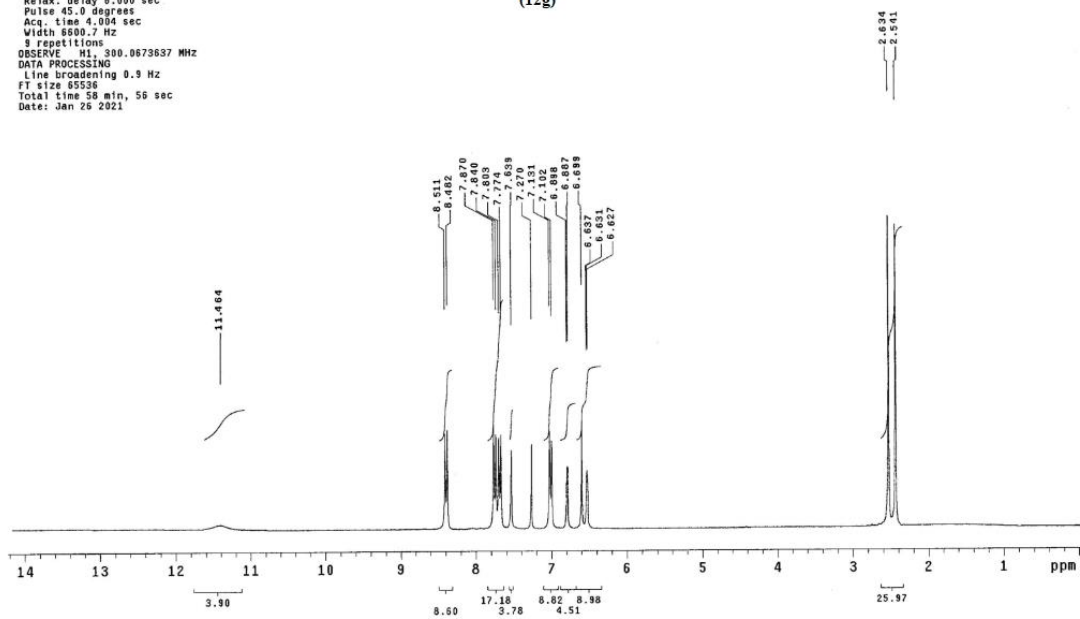
Archive directory: /export/home/vnmr1/vnmrsys/data
 Sample directory: DD5mm_test_12Mar2014-21:34:40
 File: PROTON

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 8900.7 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: Jan 26 2021



(12g)

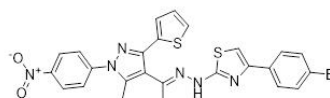


MohammadAbdulMoathy-H40-CDC13-C13

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 16761.7 Hz
 1688 repetitions
 OBSERVE C13, 75.4520045 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: Feb 24 2021



(12g)

