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SUPPORTING INFORMATION

An efficient and green procedure for synthesis of rhodanine derivatives by Aldol-thia-Michael protocol using aqueous diethylamine medium

Assem Barakat, [a,b,*] Abdullah M. Al-Majid,[a] Hany J. AL-Najjar,[a] Yahia N. Mabkhot,[a]

Hazem A. Ghabbour,[c] and Hoong-Kun Fun[c]

[a] *Department of Chemistry, Faculty of Science, King Saud University, P. O. Box 2455, Riyadh 11451, Saudi Arabia.*
[b] *Department of Chemistry, Faculty of Science, Alexandria University, P.O. Box 426, Ibrahimia- 21321 Alexandria, Egypt.*
[c] *Department of Pharmaceutical Chemistry, Faculty of Pharmacy, King Saud University, P. O. Box 2457, Riyadh 11451, Saudi Arabia.*

E-mail: ambarakat@ksu.edu.sa

Contents:

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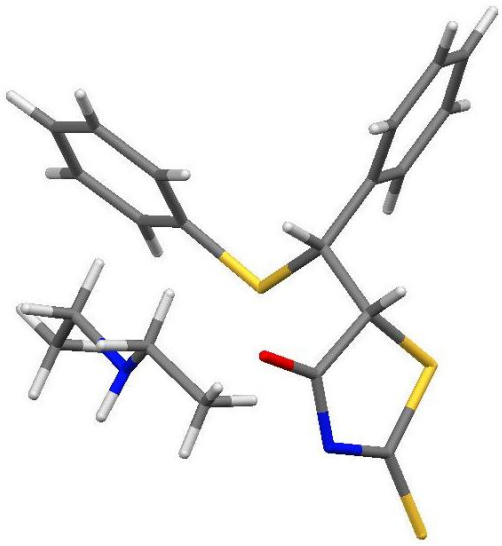

Figure 1. X-Ray structure of **4a**·$\mathbf{HNEt_2}$
(CCDC number 930797)

	Crystal data of **4a**·$\mathbf{HNEt_2}$
Empirical formula	$C_{20}H_{23}N_2OS_3$
Formula weight	403.58
Temperature	293(2) K
Wavelength (Cu *K*α radiation, λ)	1.54178 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 10.4111(3) Å α= 90.00° b = 11.3929(4) Å β= 90.00° c = 19.3963(6) Å γ= 90.00°
Volume	2162.23(12) $Å^3$
Z	4
Density (calculated)	1.240 kg/m^3
Absorption coefficient	3.214 mm^{-1}
F(000)	852
Crystal size	0.45 x 0.31 x 0.25 mm
Theta range for data collection	4.58 to 72.03°.
Index ranges	$-12\leq h\leq 10$, $-13\leq k\leq 13$, $-22\leq l\leq 23$
Reflections collected/ unique	14208/ 3541 [R(int) = 0.0358]
Completeness to theta = 72.03°	96.9 %
Absorption correction	multi-scan
Refinement	method Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0510, wR2 = 0.1266
R indices (all data)	R1 = 0.0452, wR2 = 0.1215
Largest diff. peak and hole	0.308 and -0.174 $e.Å^{-3}$

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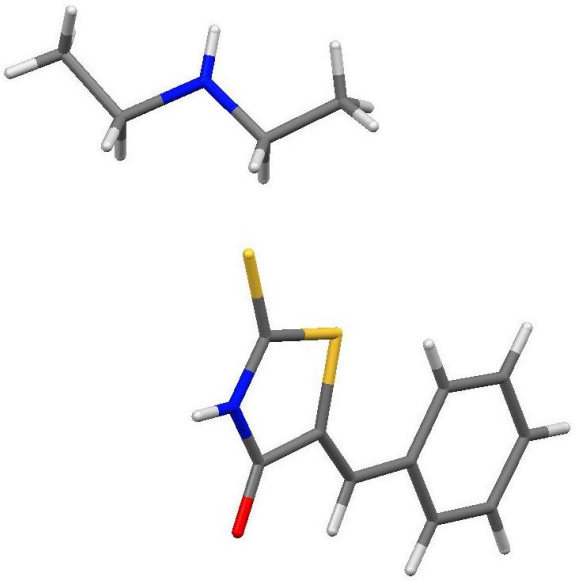

Figure 2. X-Ray structure of **3a**·**HNEt$_2$**
(CCDC number 931815)

	Crystal data of **3a**·**HNEt$_2$**
Empirical formula	$C1_4$ $H_{18}N_2OS_2$
Formula weight	294.42
Temperature	293(2) K
Wavelength (Cu *K*α radiation, λ)	1.54178 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 10.7960(3) Å α= 90.00° b = 13.0807(4) Å β= 126.696(2)° c = 14.6416(4) Å ɣ= 90.00°
Volume	1657.90(8) Å^3
Z	4
Density (calculated)	1.180 kg/m^3
Absorption coefficient	2.862 mm^{-1}
F(000)	624
Crystal size	0.49 x 0.43 x 0.29 mm
Theta range for data collection	4.16 to 69.73°.
Index ranges	-12≤h≤12, -14≤k≤15, -12≤l≤16
Reflections collected/ unique	10343 / 2247 [R(int) = 0.0388]
Completeness to theta = 69.73°	96.9 %
Absorption correction	multi-scan
Refinement	method Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0748, wR2 = 0.2214
R indices (all data)	R1 = 0.0666, wR2 = 0.2102
Largest diff. peak and hole	0.527 and -0.344 e.Å^{-3}

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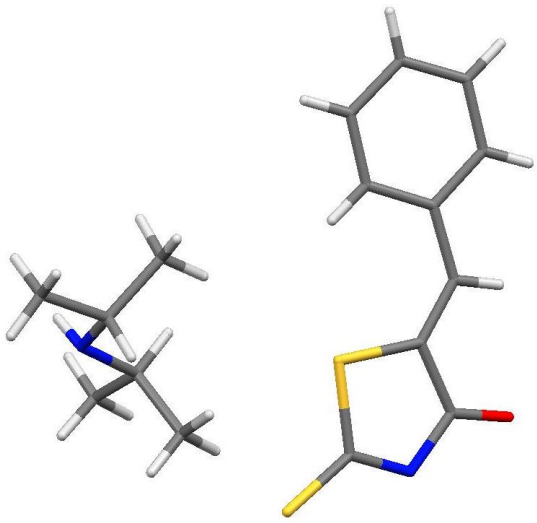

Figure 3. X-Ray structure of **3b**·HN^{i}**Pr**$_2$
(CCDC number 930934)

	Crystal data of **3b**·HN^{i}**Pr**$_2$
Empirical formula	$C_{16}H_{21}N_2OS_2$
Formula weight	321.47
Temperature	296(2) K
Wavelength (Cu *K*α radiation, λ)	1.54178 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 7.3038(2) Å α= 90.00° b = 13.6420(3)Å β= 99.589(2)° c = 17.9671(4) Å ɣ= 90.00°
Volume	1765.20(7) Å^3
Z	4
Density (calculated)	1.210 kg/m^3
Absorption coefficient	2.729 mm^{-1}
F(000)	684
Crystal size	0.34 x 0.28 x 0.26 mm
Theta range for data collection	4.09 to 69.84°.
Index ranges	-8≤h≤8, -15≤k≤16, -21≤l≤20
Reflections collected/ unique	12373 / 2771 [R(int) = 0.0406]
Completeness to theta = 69.84°	99.0 %
Absorption correction	multi-scan
Refinement	method Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0527, wR2 = 0.1294
R indices (all data)	R1 = 0.0450, wR2 = 0.1234
Largest diff. peak and hole	0.514 and -0.266 e.Å^{-3}

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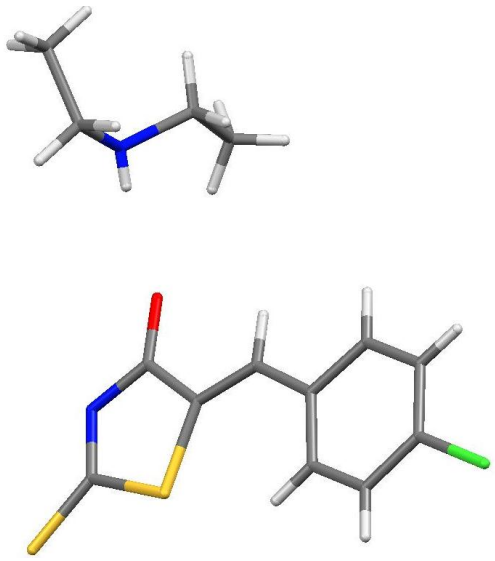
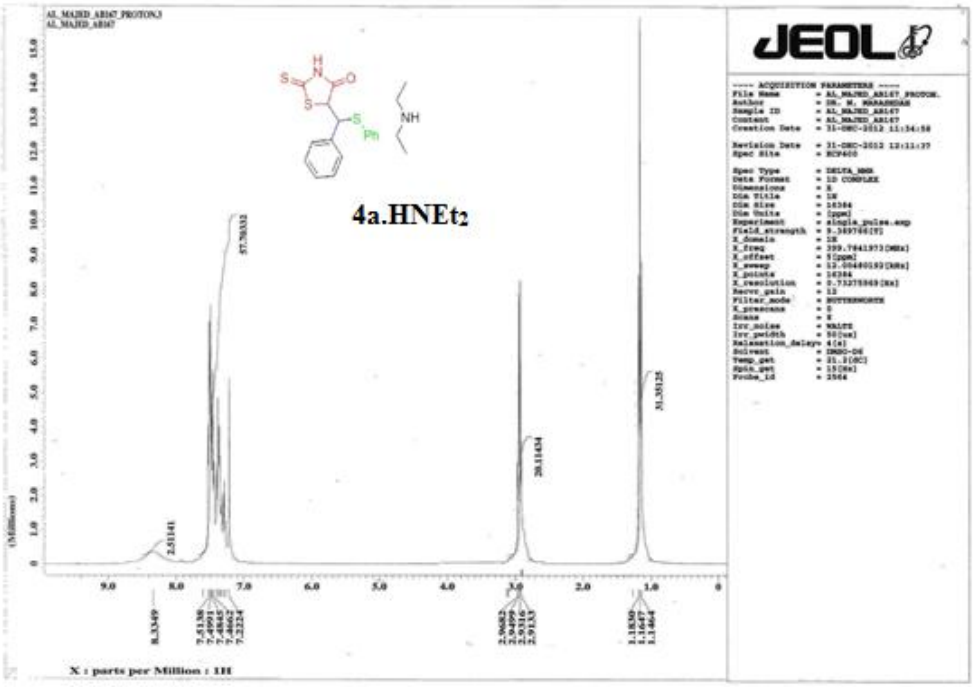


Figure 4. X-Ray structure of **3c**·**HNEt$_2$**
(CCDC number 930932)

	Crystal data of **3c**·**HNEt$_2$**
Empirical formula	$C1_4\ H_{16}\ ClN_2OS_2$
Formula weight	327.86
Temperature	296(2) K
Wavelength (Cu *K*α radiation, λ)	1.54178 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 7.3389(2) Å α= 90.00° b = 13.0121(3) Å β= 100.169(2)° c = 17.6769(4) Å γ= 90.00°
Volume	1661.53(7) Å^3
Z	4
Density (calculated)	1.311 kg/m^3
Absorption coefficient	4.357 mm^{-1}
F(000)	684
Crystal size	0.47 x 0.27 x 0.25 mm
Theta range for data collection	3.40 to 69.71°.
Index ranges	-8≤h≤8, -15≤k≤15, -21≤l≤21
Reflections collected/ unique	11035 / 2588 [R(int) = 0.0300]
Completeness to theta = 69.71°	98.6 %
Absorption correction	multi-scan
Refinement	method Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0518, wR2 = 0.1395
R indices (all data)	R1 = 0.0451, wR2 = 0.1341
Largest diff. peak and hole	0.450 and -0.220 e.Å^{-3}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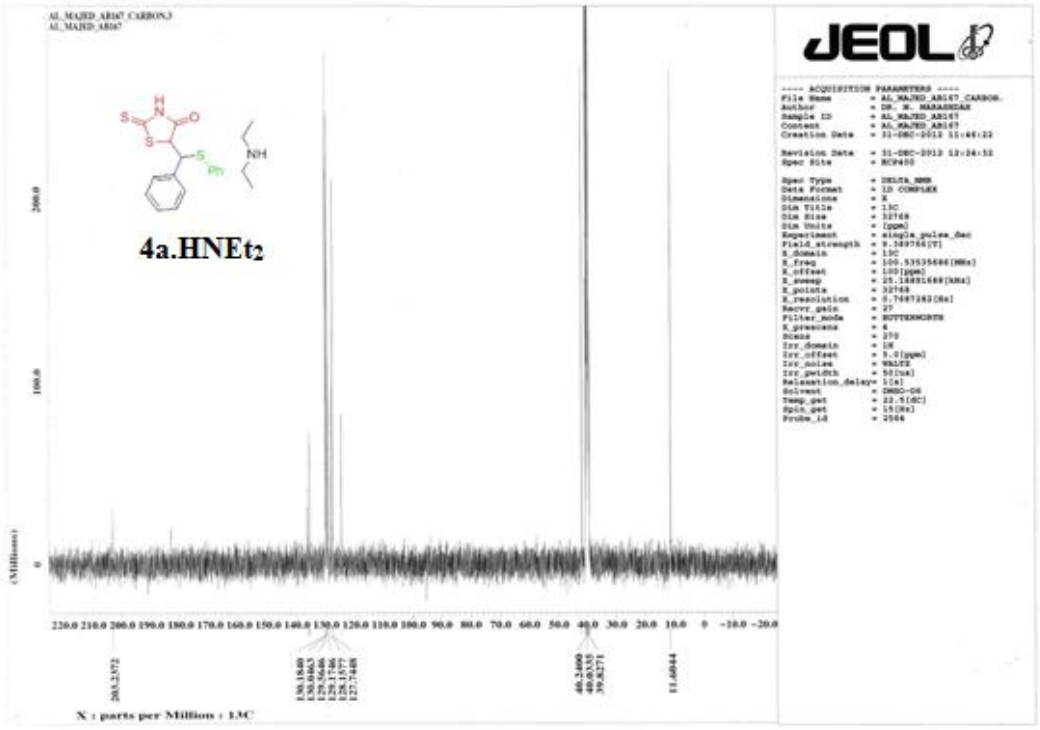
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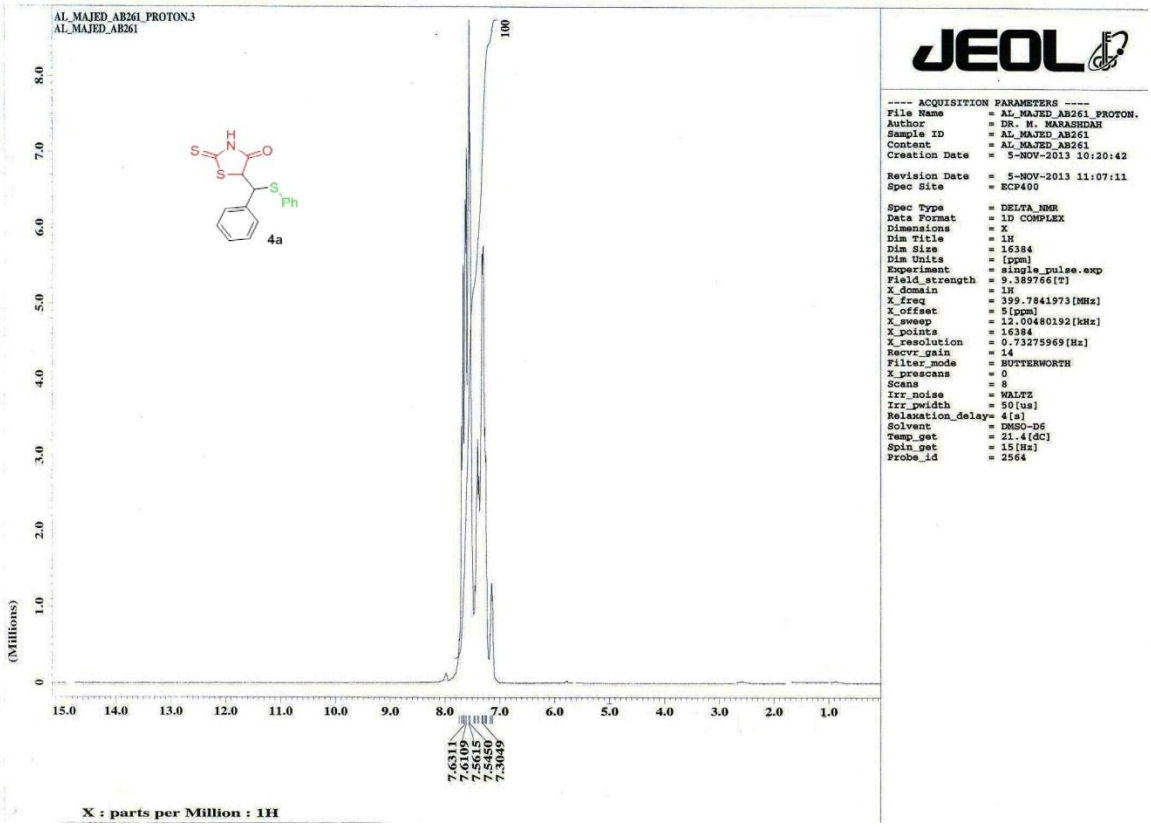
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7.6109
7.5615
7.5450
7.3049
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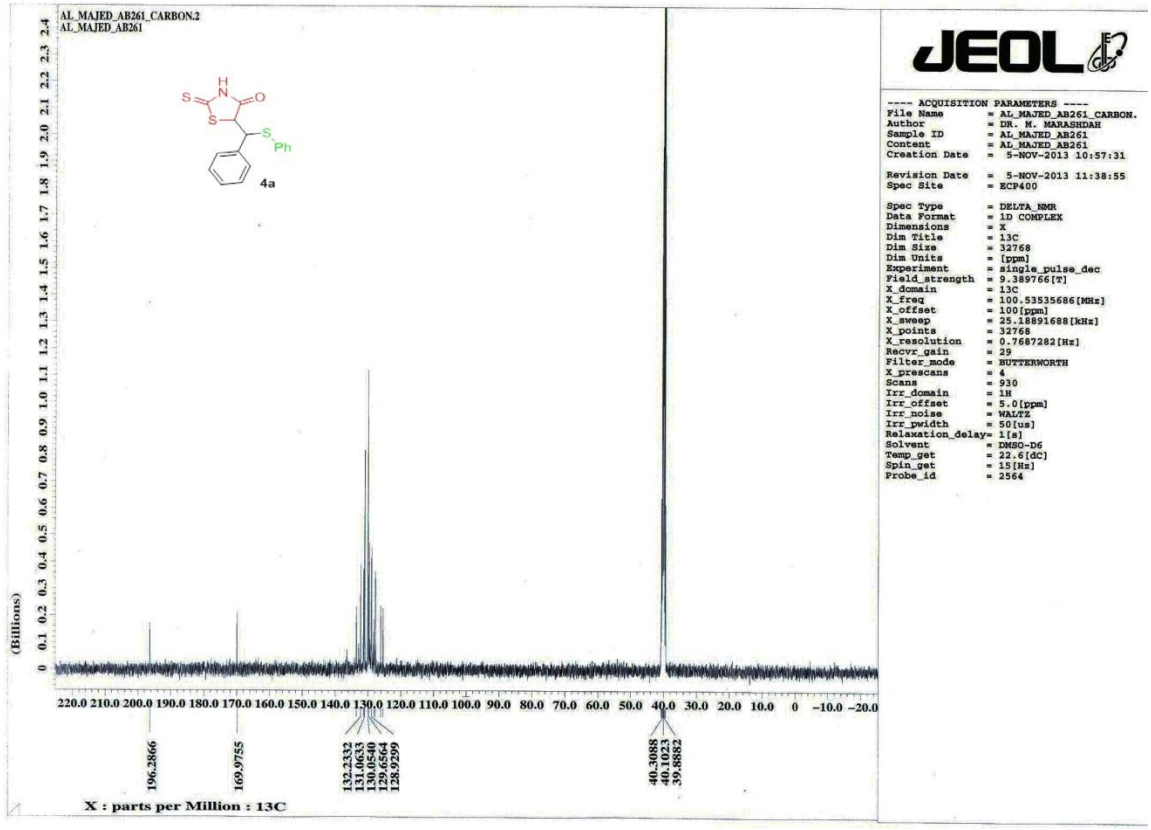
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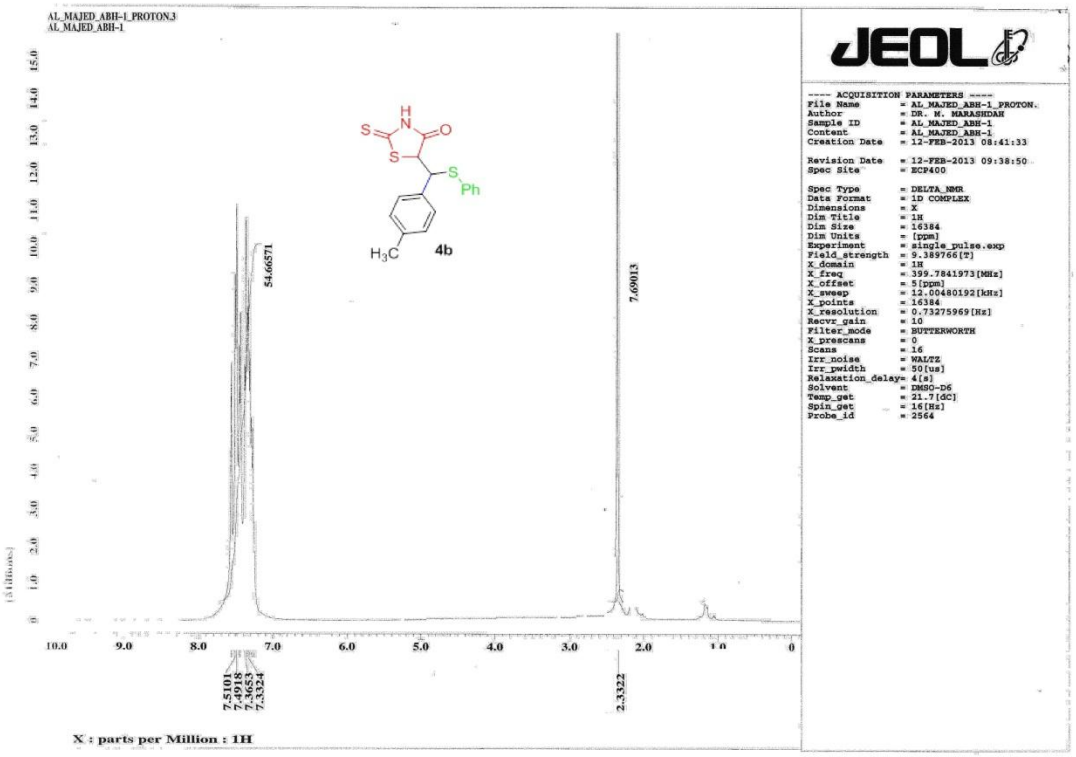
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JEOL
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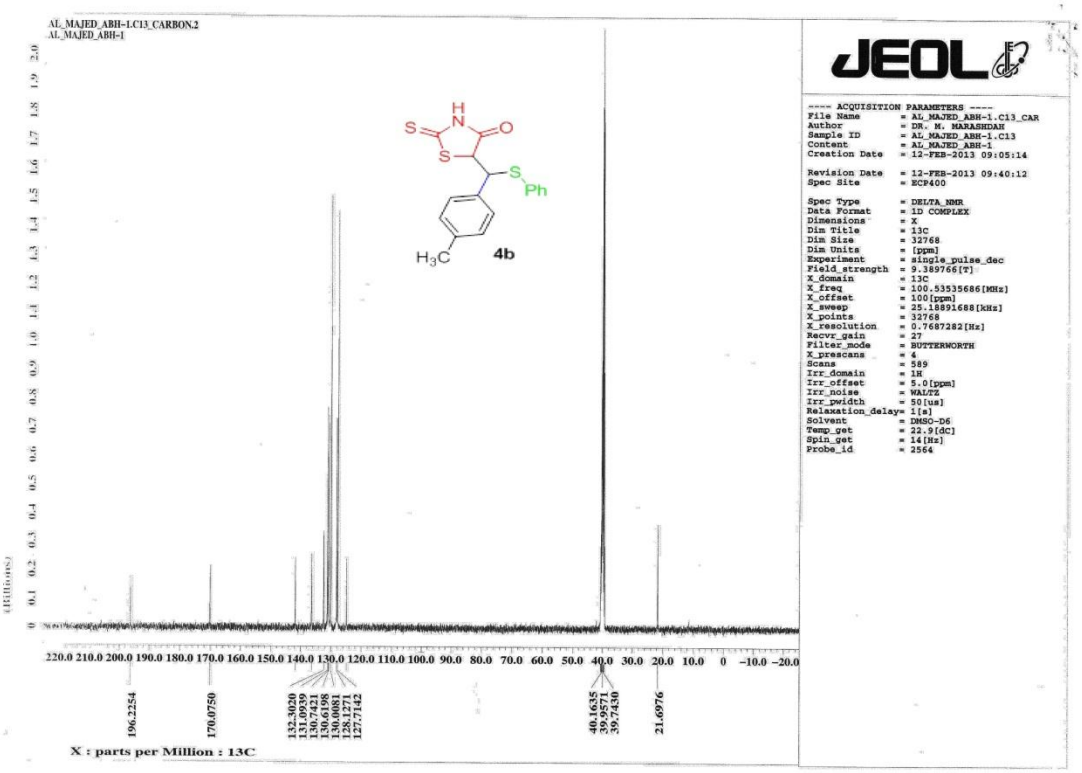
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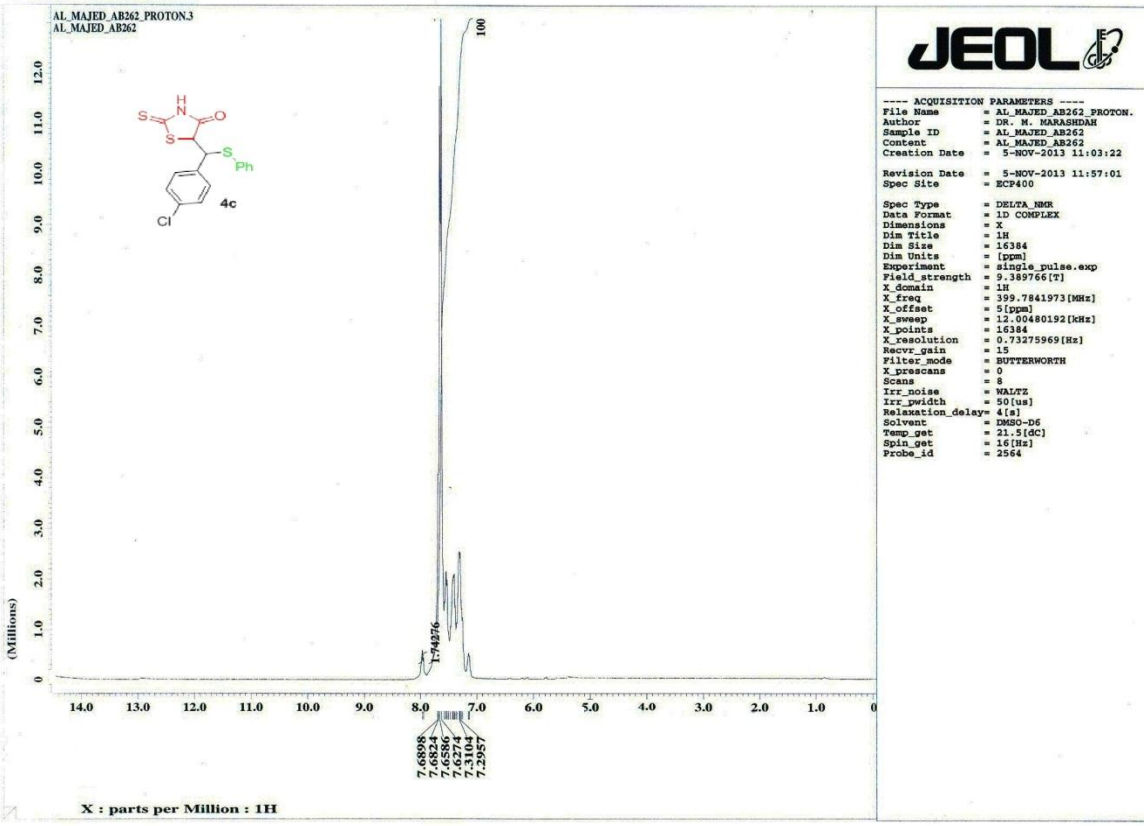
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AL_MAJED_AB262
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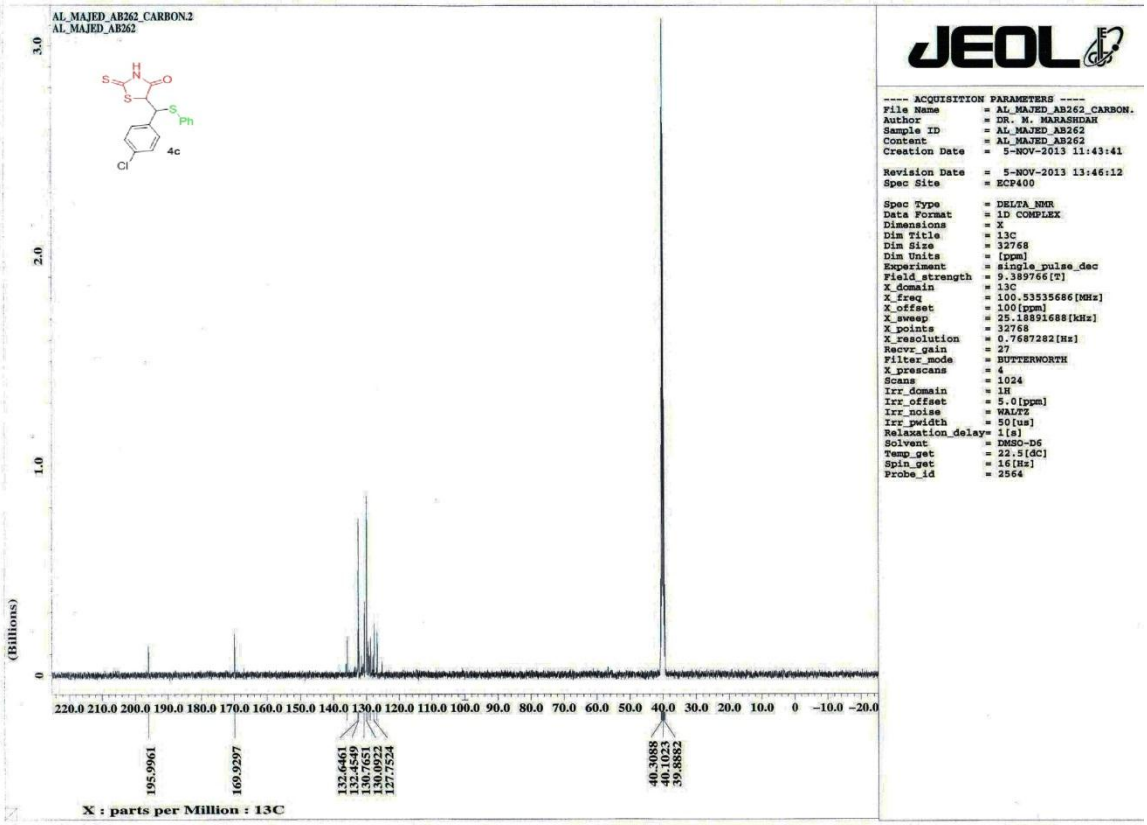
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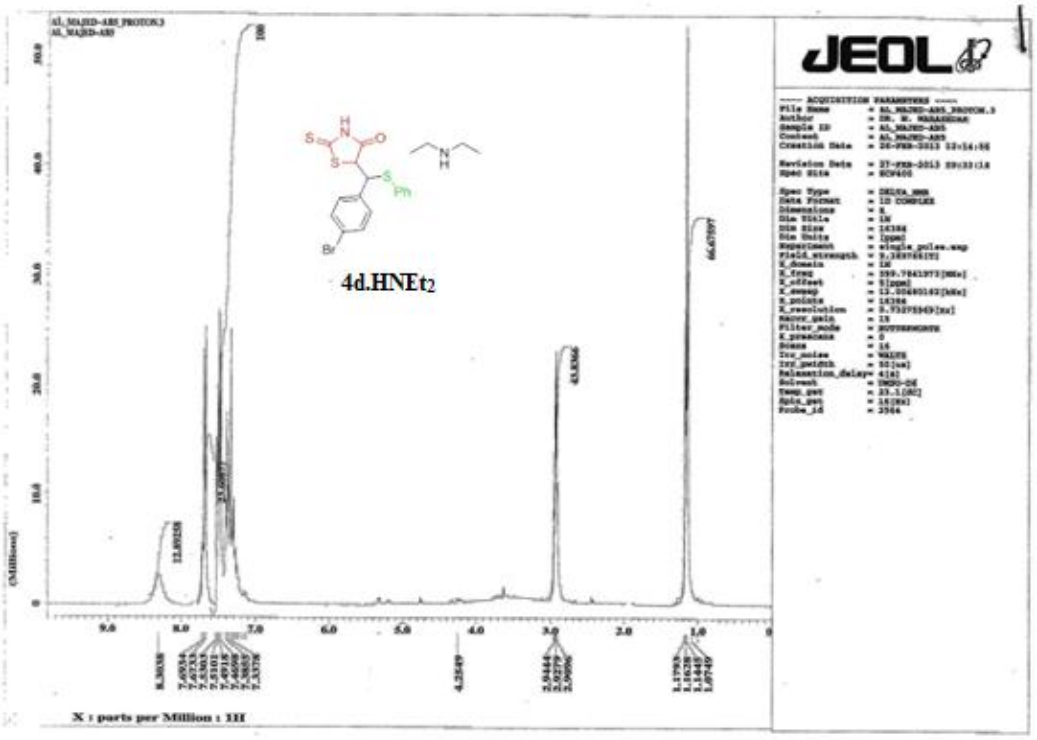
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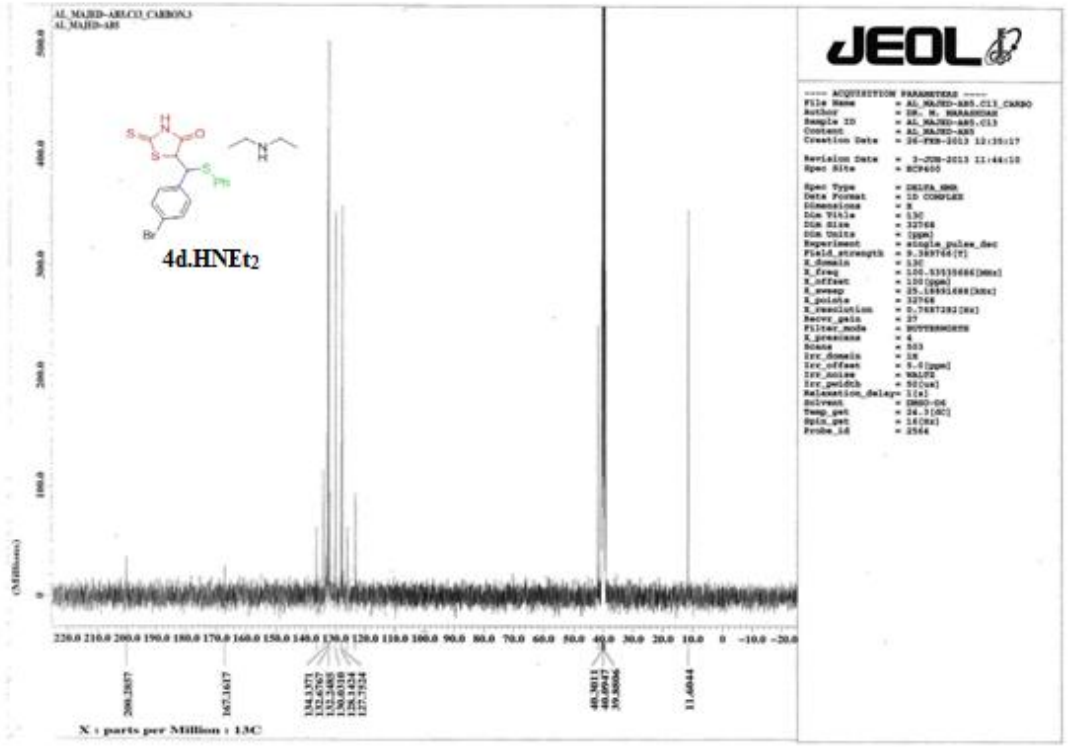
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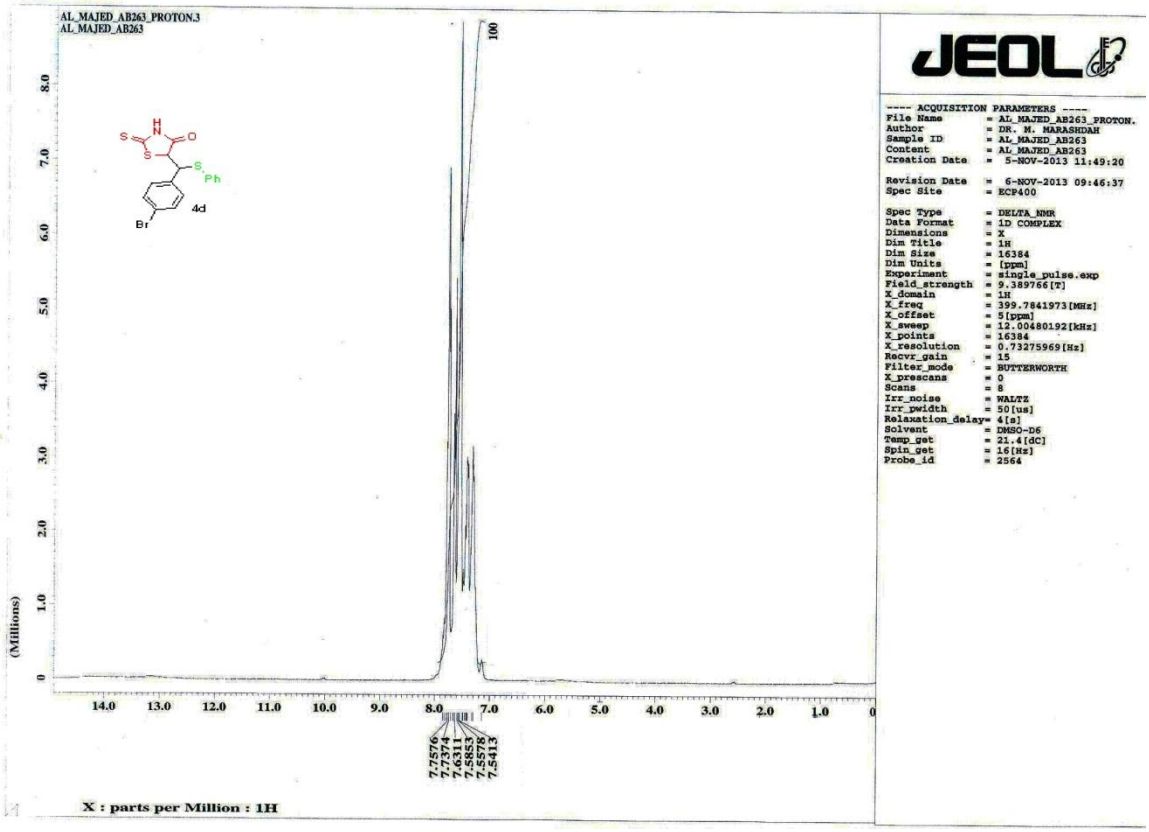
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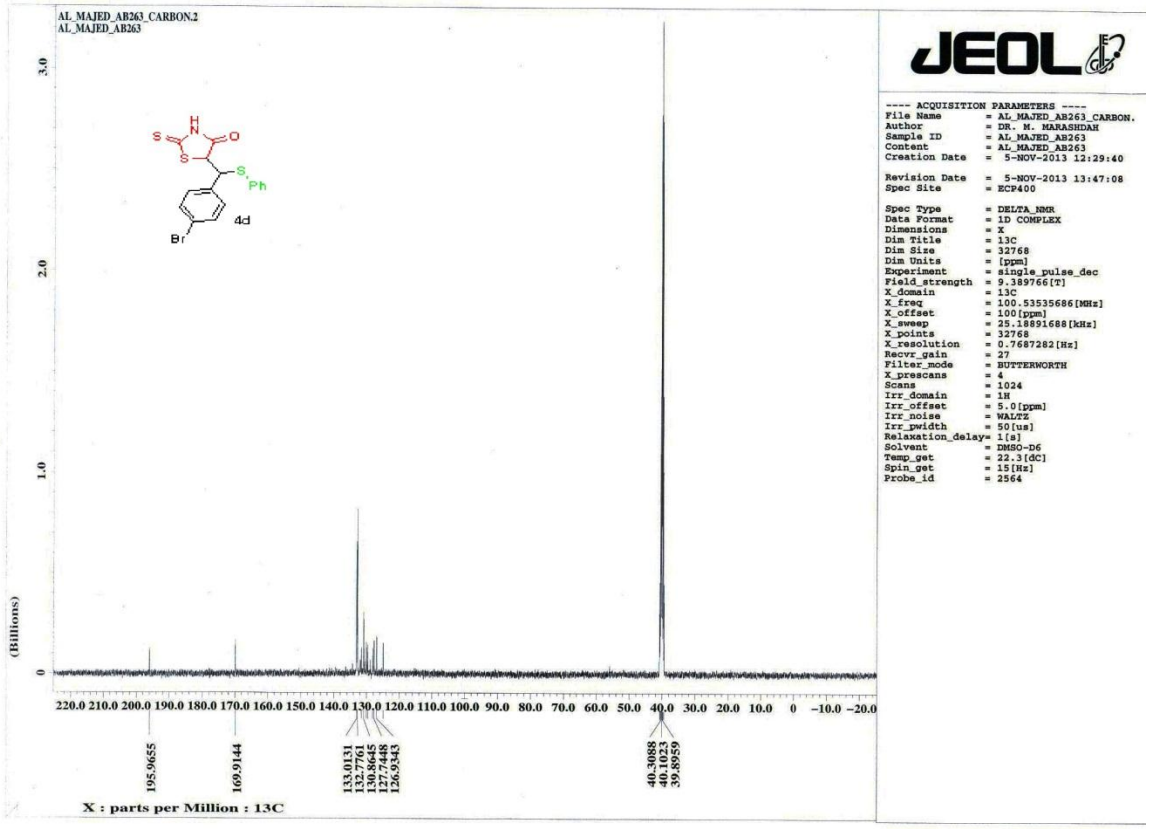
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Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 1024
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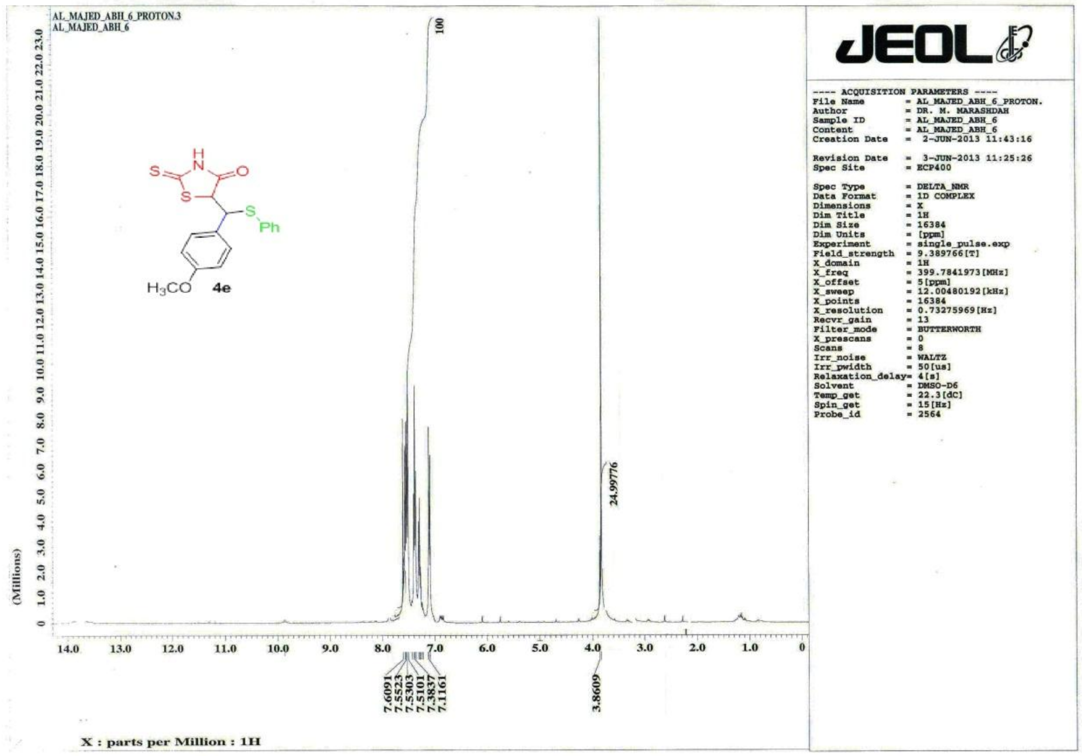
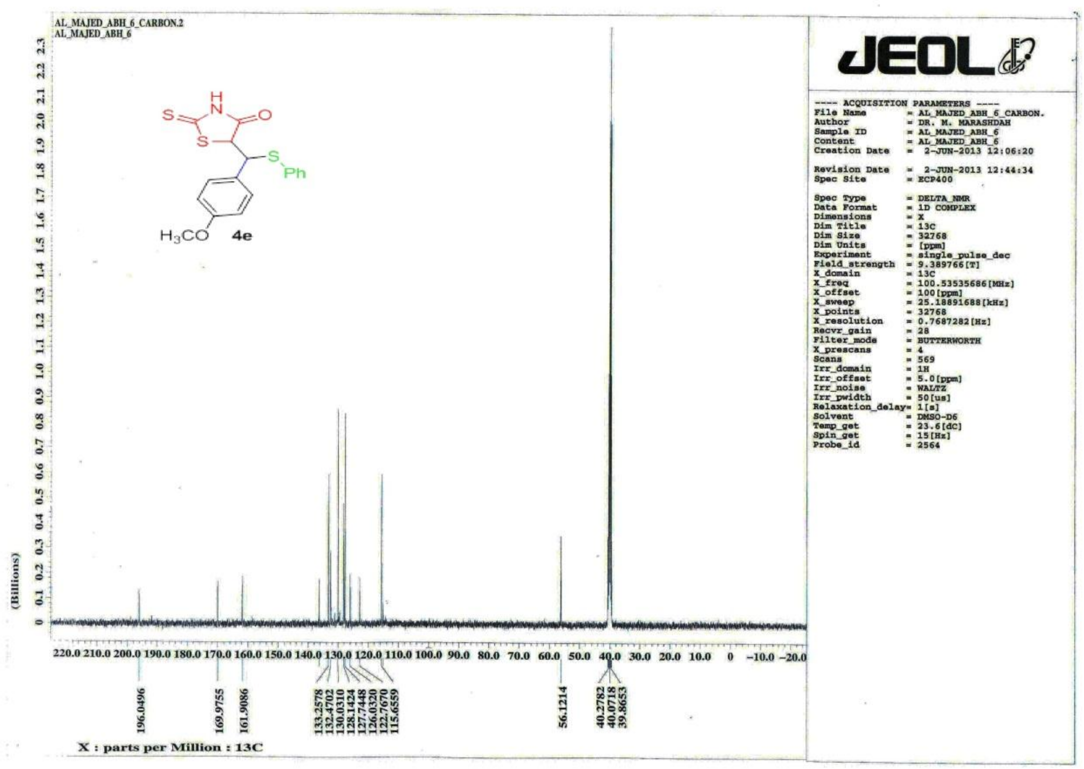
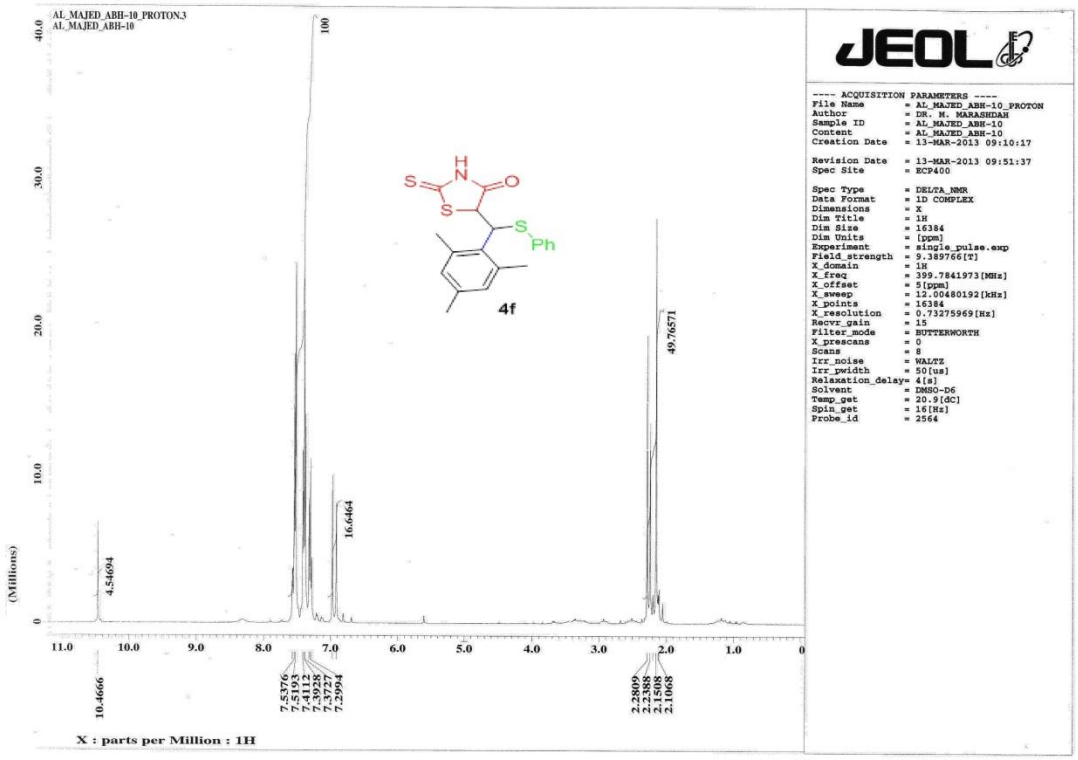
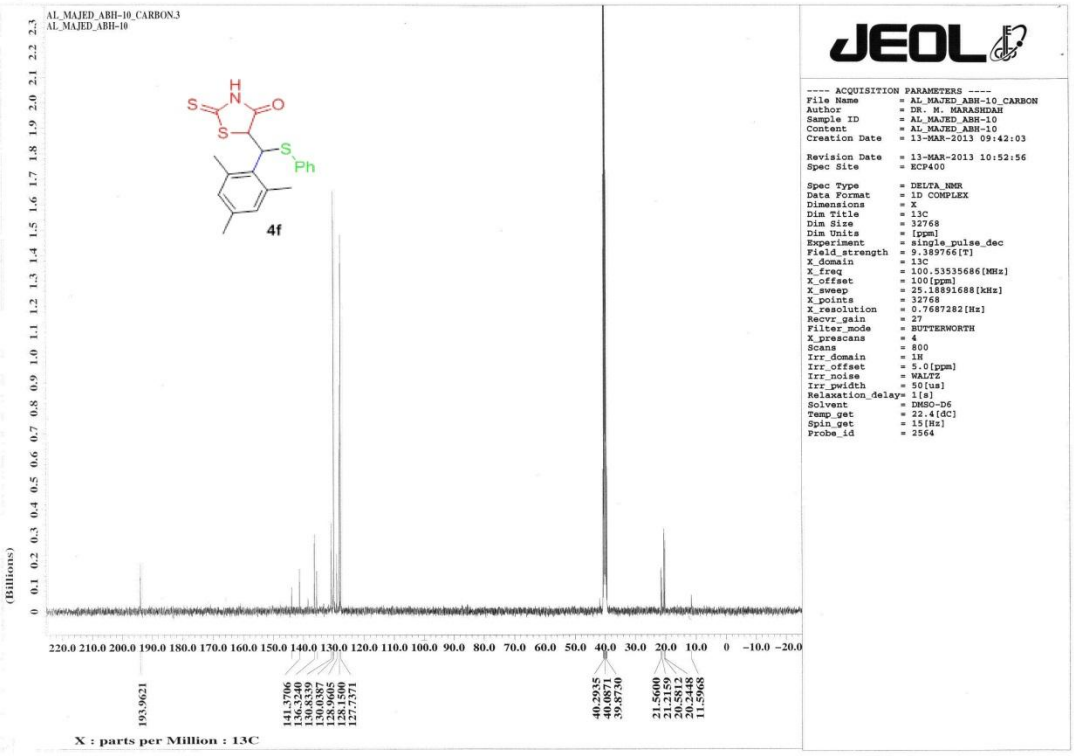
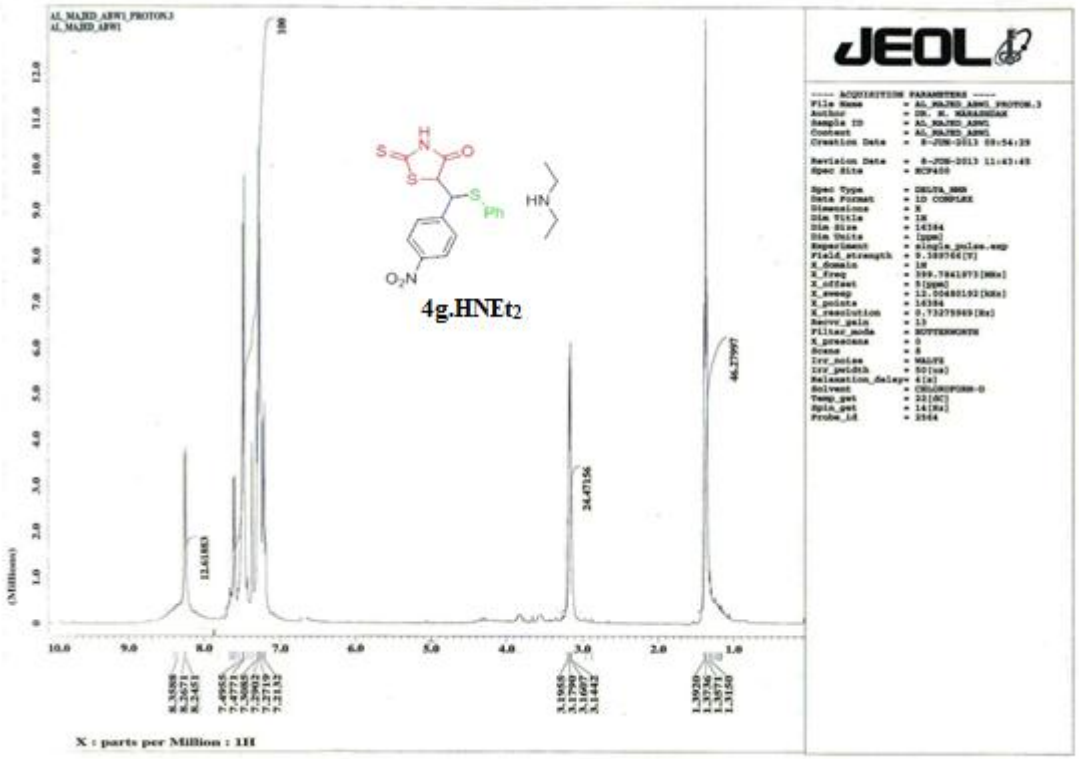
Spin_get = 15[Hz]
Probe_id = 2564

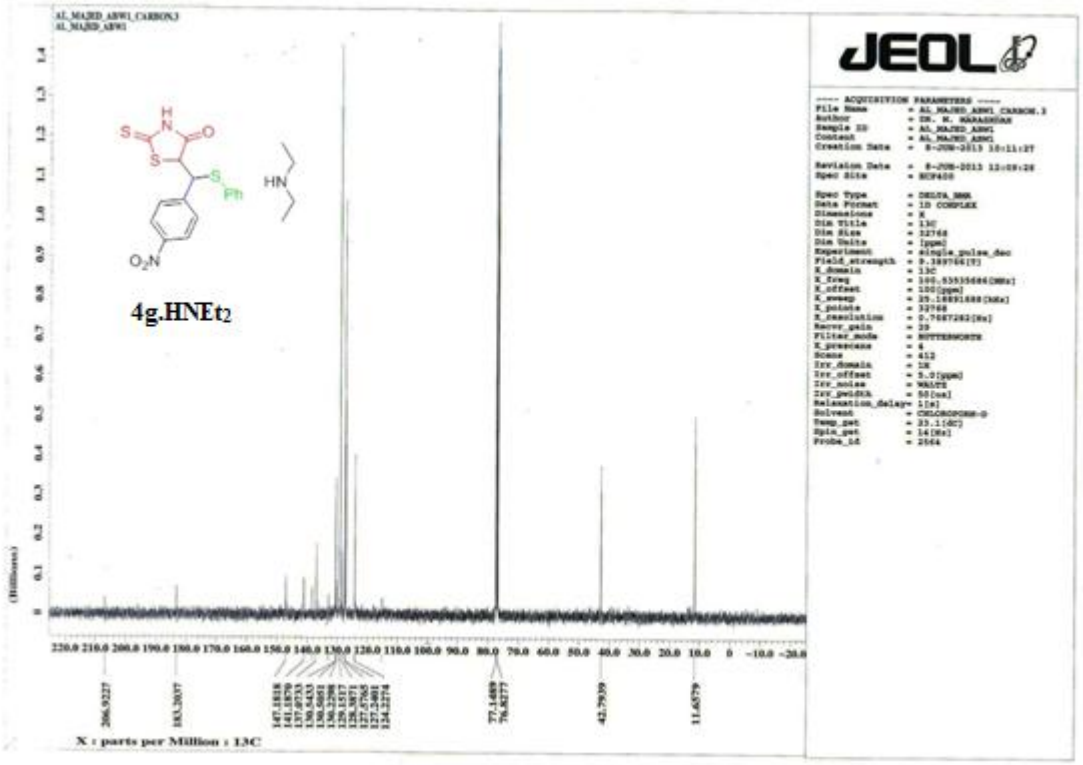

AL_MAJED_ABH_6_PROTON.3
AL_MAJED_ABH_6
H3CO 4e
S
N
H
O
Ph
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH_6_PROTON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH_6
Content = AL_MAJED_ABH_6
Creation Date = 2-JUN-2013 11:43:16
Revision Date = 3-JUN-2013 11:25:26
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 13
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 22.3[dC]
Spin_get = 15[Hz]
Probe_id = 2564
100
24.99776
7.6091
7.5523
7.5303
7.5101
7.3837
7.1161
3.8609
(Millions)
X : parts per Million : 1H

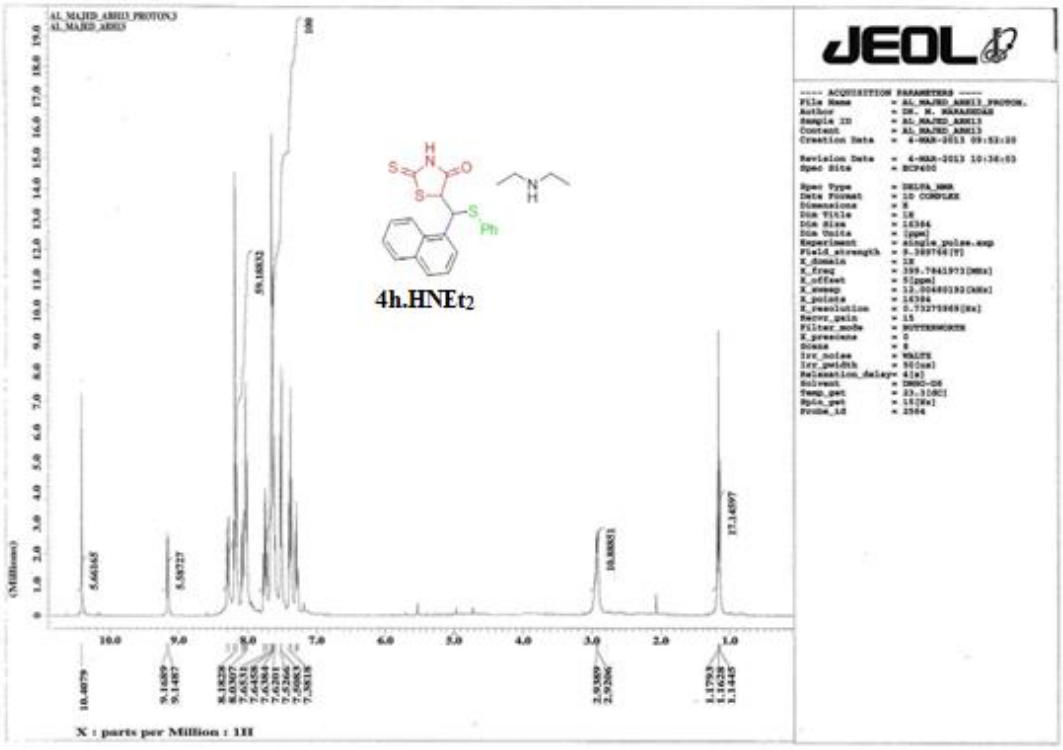

AL_MAJED_ABH_6_CARBON.2
AL_MAJED_ABH_6
H3CO 4e
S
N
H
O
Ph
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH_6_CARBON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH_6
Content = AL_MAJED_ABH_6
Creation Date = 2-JUN-2013 12:06:20
Revision Date = 2-JUN-2013 12:44:34
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 28
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 569
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 23.6[dC]
Spin_get = 15[Hz]
Probe_id = 2564
196.0496
169.9755
161.9086
133.2578
132.4702
130.0310
128.1424
127.7448
126.0320
122.7670
115.6559
56.1214
40.2782
40.0718
39.8653
(Billions)
X : parts per Million : 13C

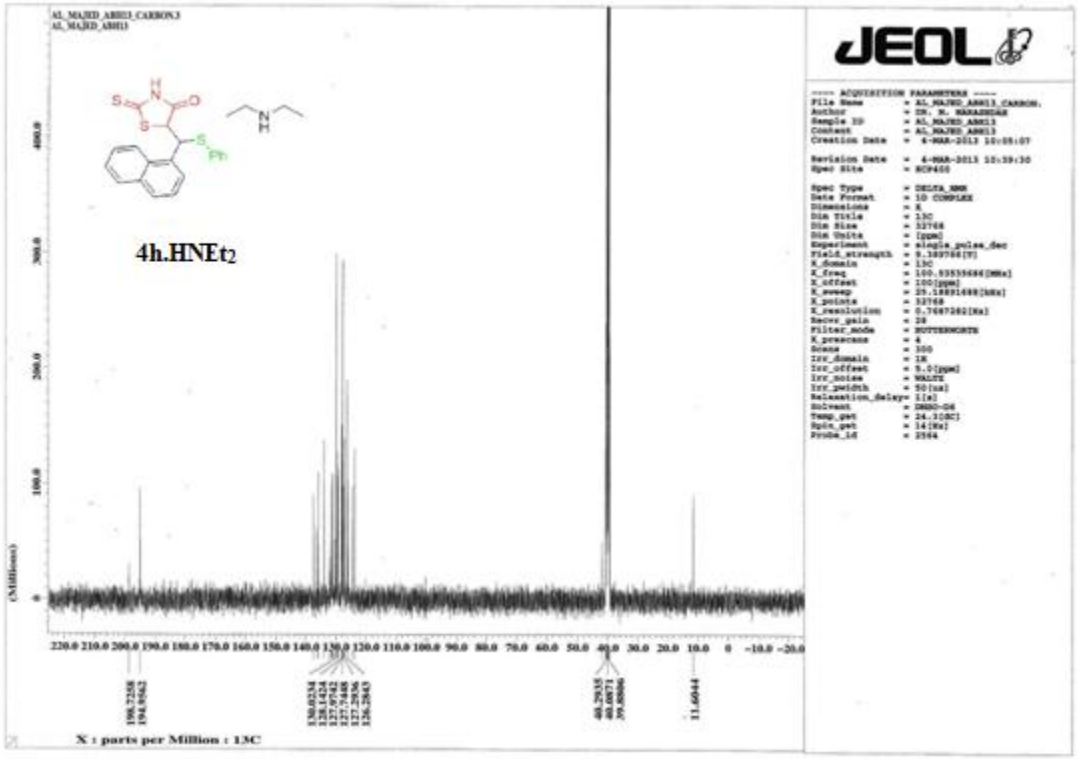

AL_MAJED_ABH-10_PROTON.3
AL_MAJED_ABH-10
4f
4.54694
16.6464
49.76571
10.4666
7.5376
7.5193
7.4112
7.3928
7.3777
7.2994
2.2809
2.2388
2.1508
2.1068
X : parts per Million : 1H
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH-10_PROTON
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH-10
Content = AL_MAJED_ABH-10
Creation Date = 13-MAR-2013 09:10:17
Revision Date = 13-MAR-2013 09:51:37
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 15
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 20.9[dC]
Spin_get = 16[Hz]
Probe_id = 2564

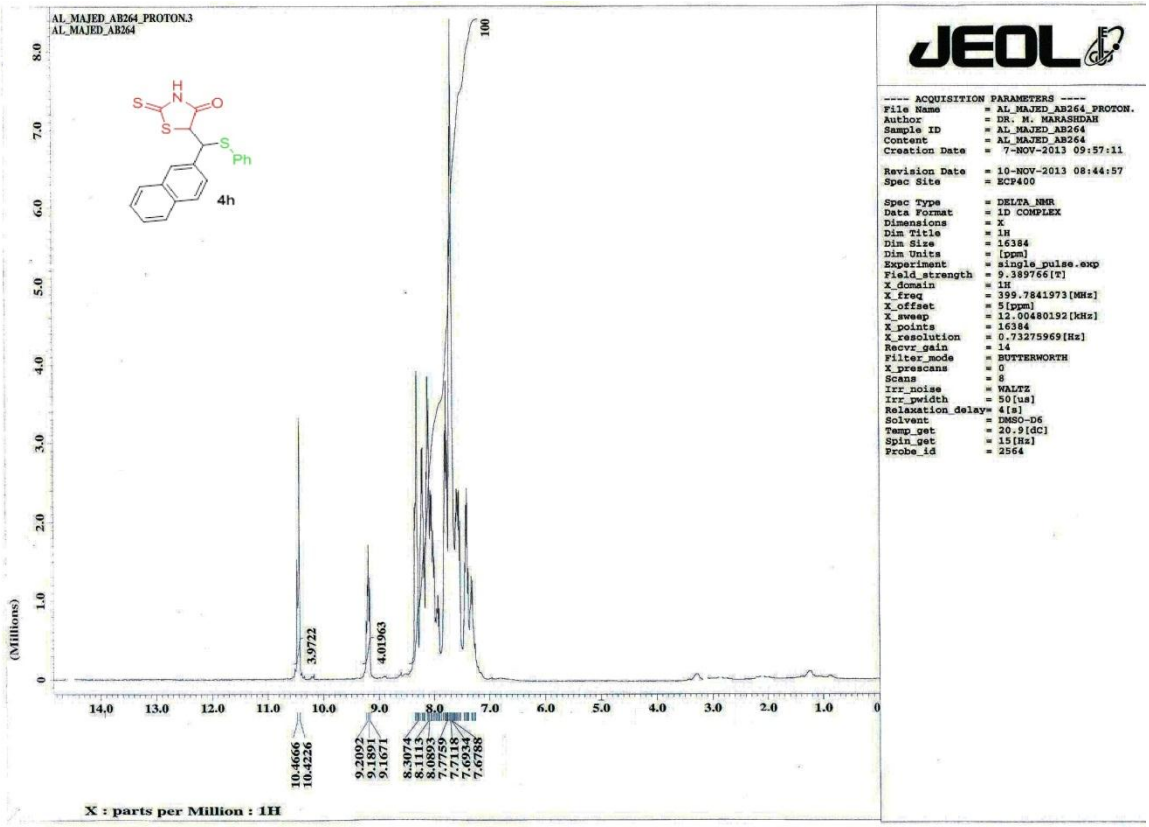

AL_MAJED_ABH-10_CARBON.3
AL_MAJED_ABH-10
4f
193.9621
141.3706
136.2340
130.8539
130.0387
128.9605
128.1600
125.7391
40.2935
40.0771
39.8730
21.5600
21.2159
20.5812
20.2448
11.5968
X : parts per Million : 13C
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH-10_CARBON
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH-10
Content = AL_MAJED_ABH-10
Creation Date = 13-MAR-2013 09:42:03
Revision Date = 13-MAR-2013 10:52:56
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 800
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 22.4[dC]
Spin_get = 15[Hz]
Probe_id = 2564

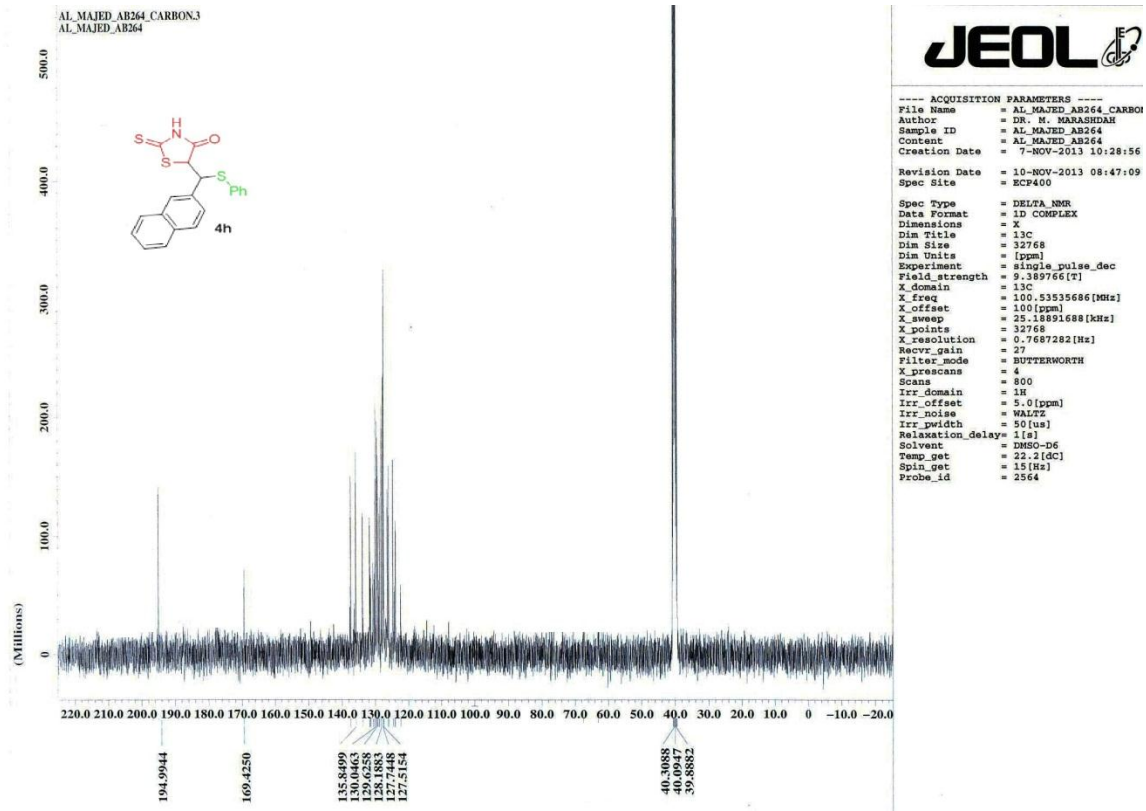

4g.HNEt2
X : parts per Million : 1H


4g.HNEt2
X : parts per Million : 13C


4h.HNEt2
X : parts per Million : 1H


4h.HNEt2
X : parts per Million : 13C


AL_MAJED_AB264_PROTON.3
AL_MAJED_AB264
4h
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_AB264_PROTON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_AB264
Content = AL_MAJED_AB264
Creation Date = 7-NOV-2013 09:57:11
Revision Date = 10-NOV-2013 08:44:57
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 14
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 20.9[dC]
Spin_get = 15[Hz]
Probe_id = 2564
3.9722
4.0196
10.4666
10.4226
9.2092
9.1891
9.1671
8.3074
8.1113
8.0893
7.7759
7.7118
7.6934
7.6788
X : parts per Million : 1H


AL_MAJED_AB264_CARBON.3
AL_MAJED_AB264
4h
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_AB264_CARBO
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_AB264
Content = AL_MAJED_AB264
Creation Date = 7-NOV-2013 10:28:56
Revision Date = 10-NOV-2013 08:47:09
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 800
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 22.2[dC]
Spin_get = 15[Hz]
Probe_id = 2564
194.9944
169.4250
135.8499
130.0463
129.4458
128.1883
127.7448
127.5154
40.3088
40.0947
39.8882

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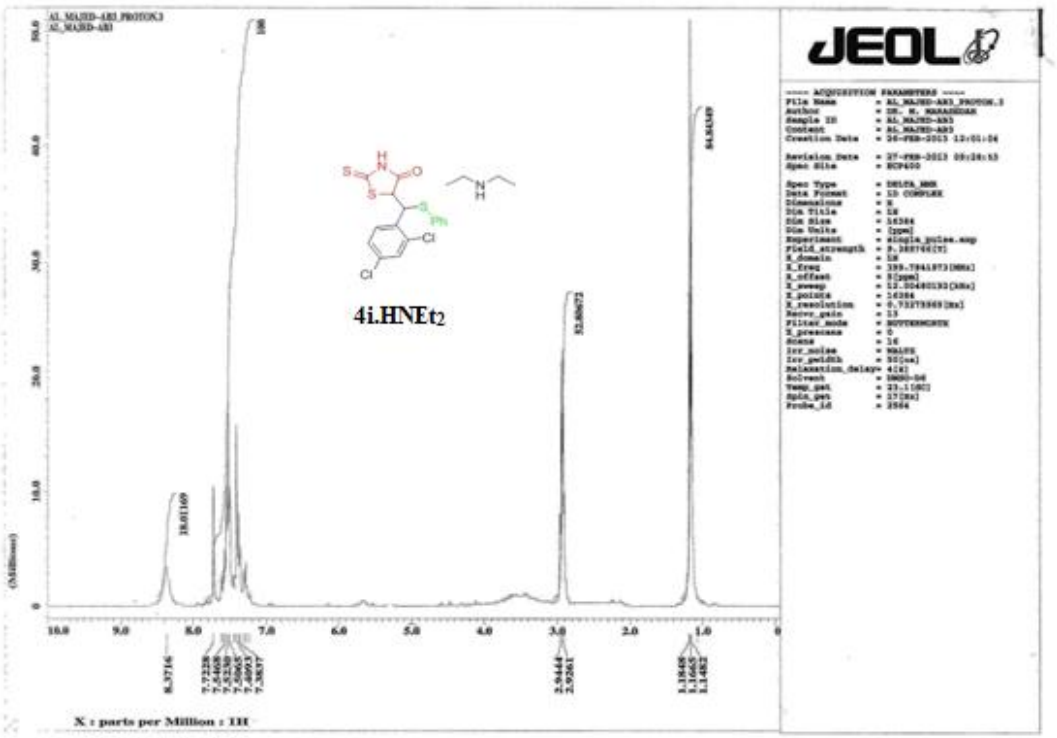
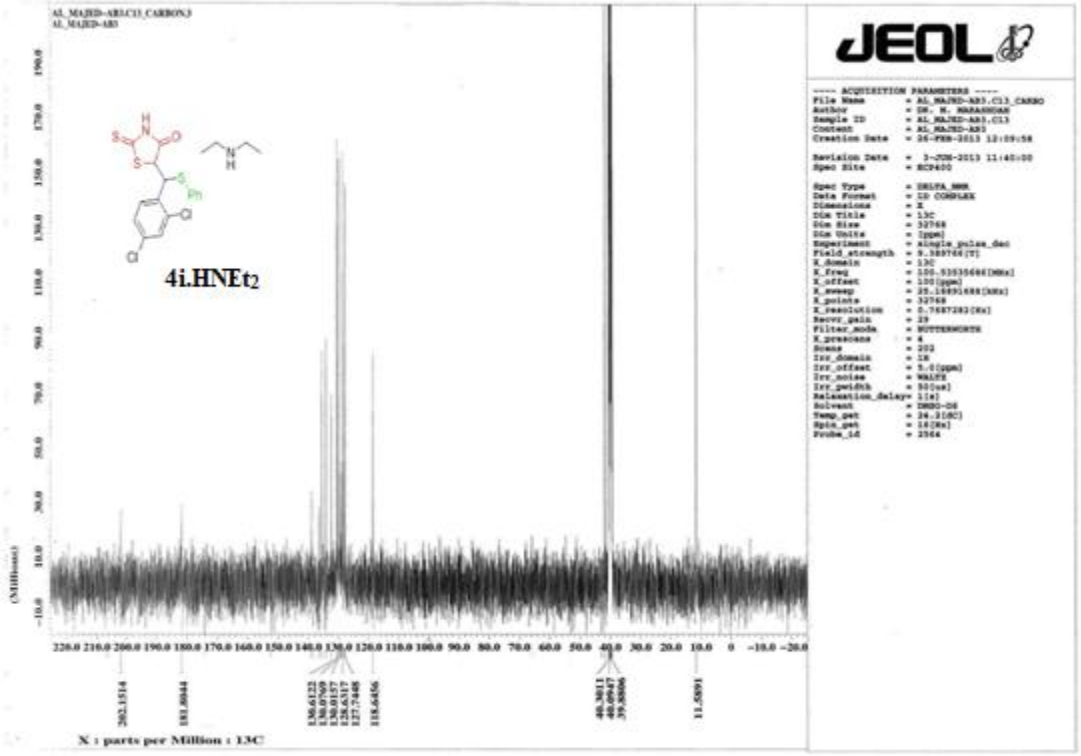
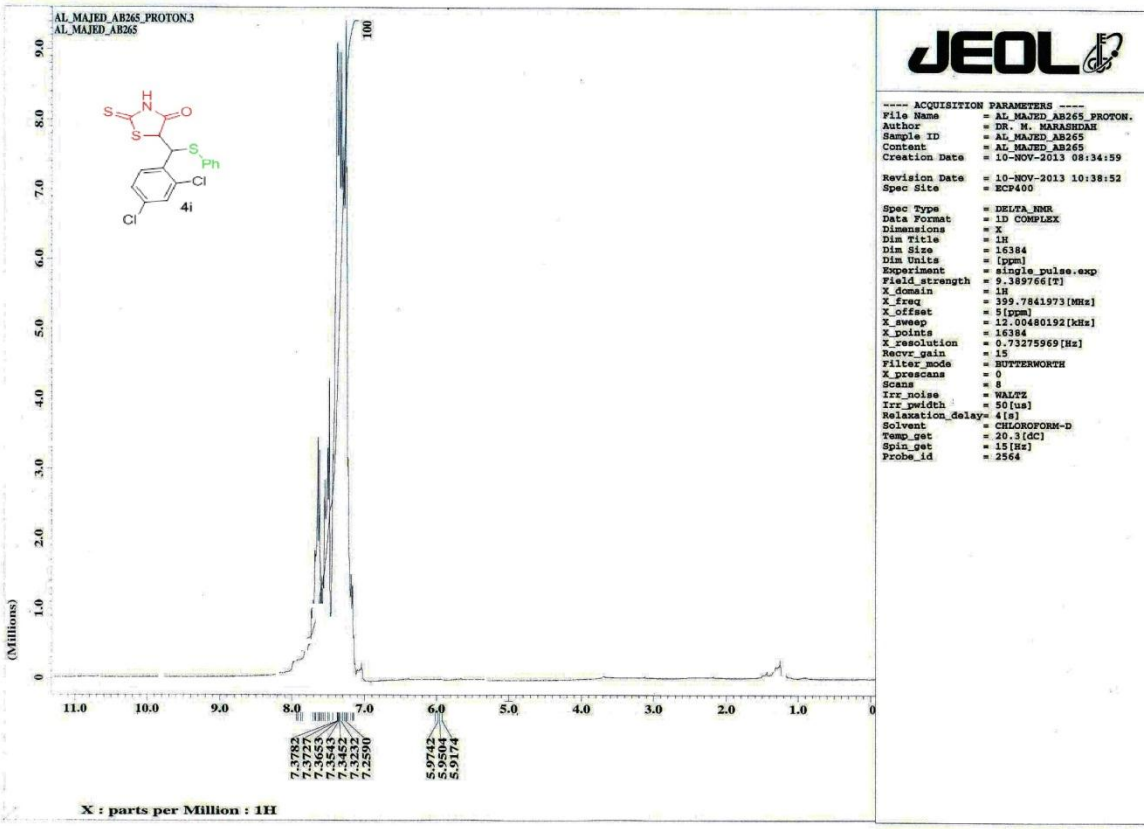
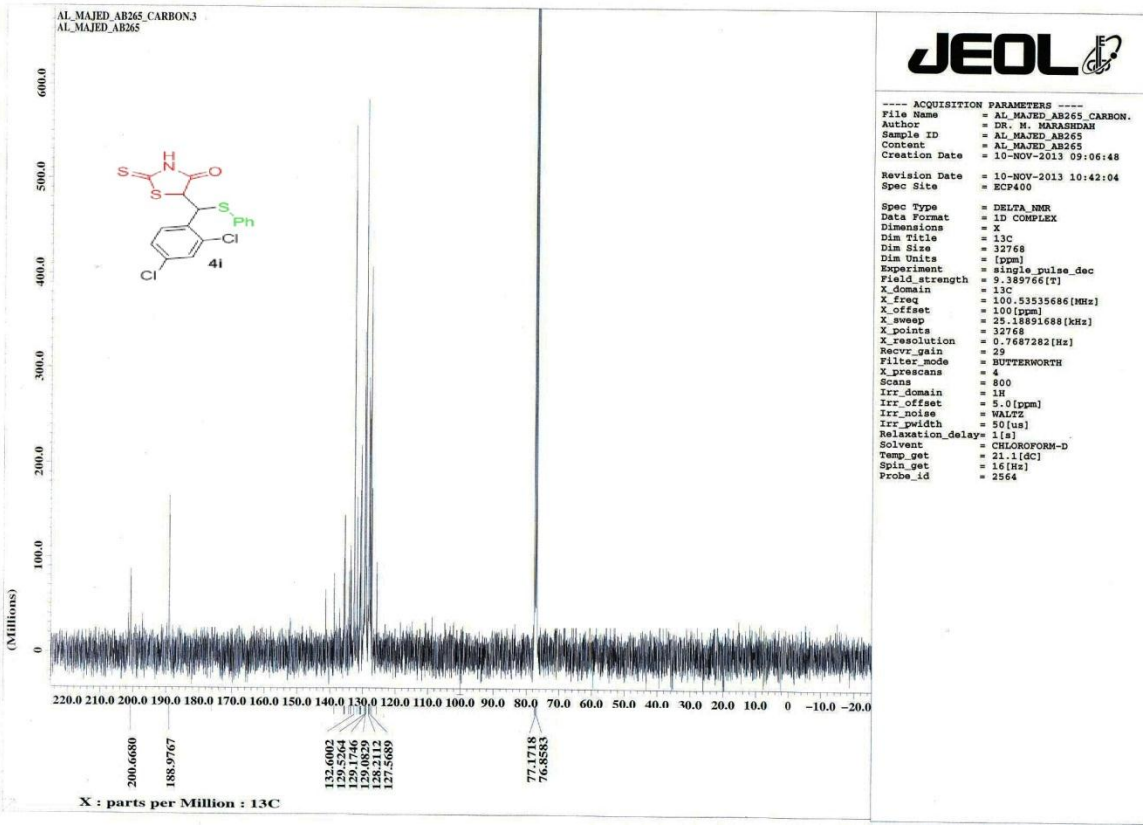
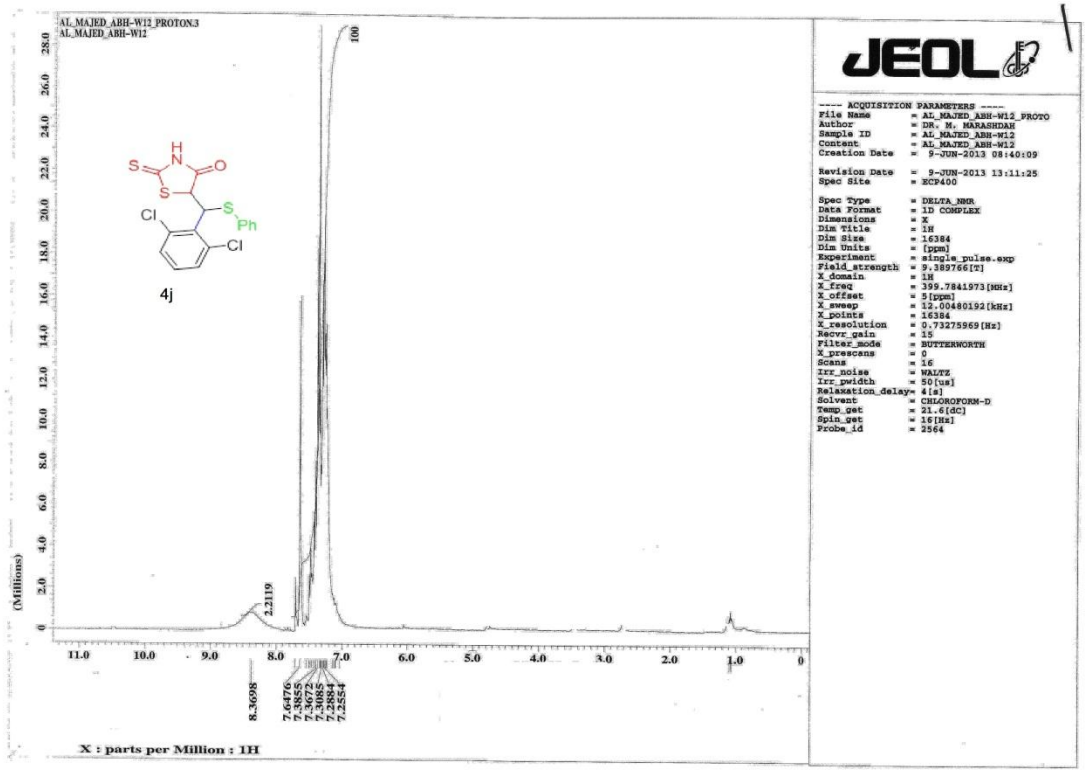
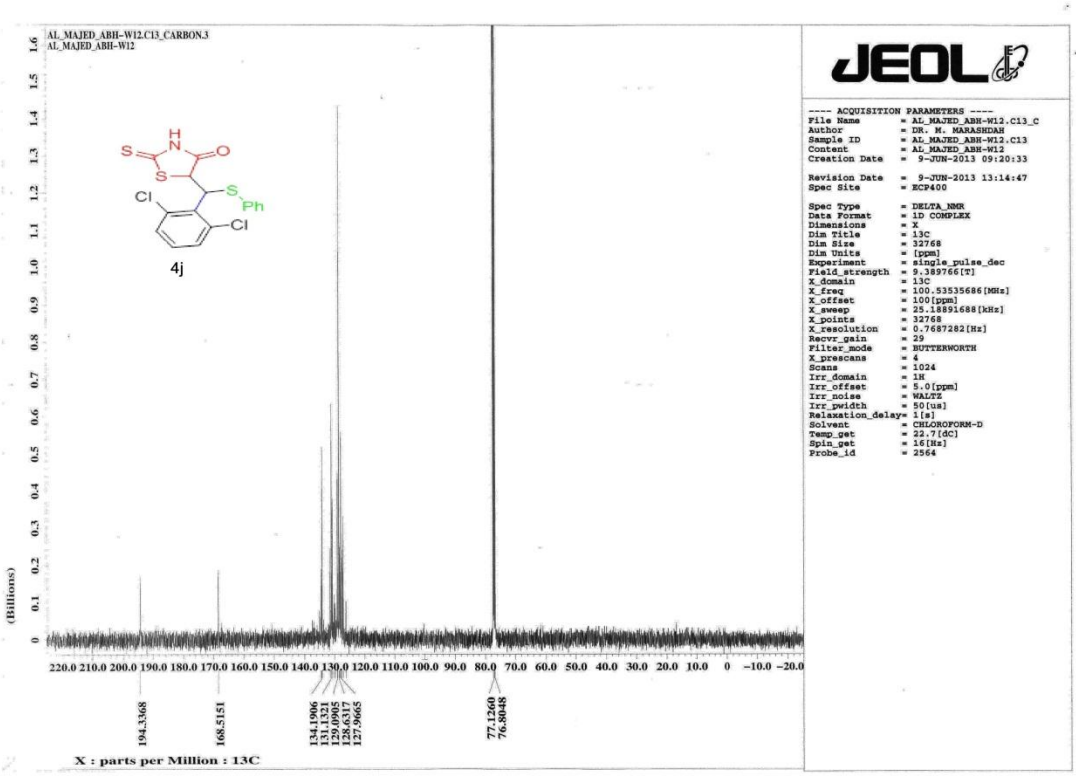


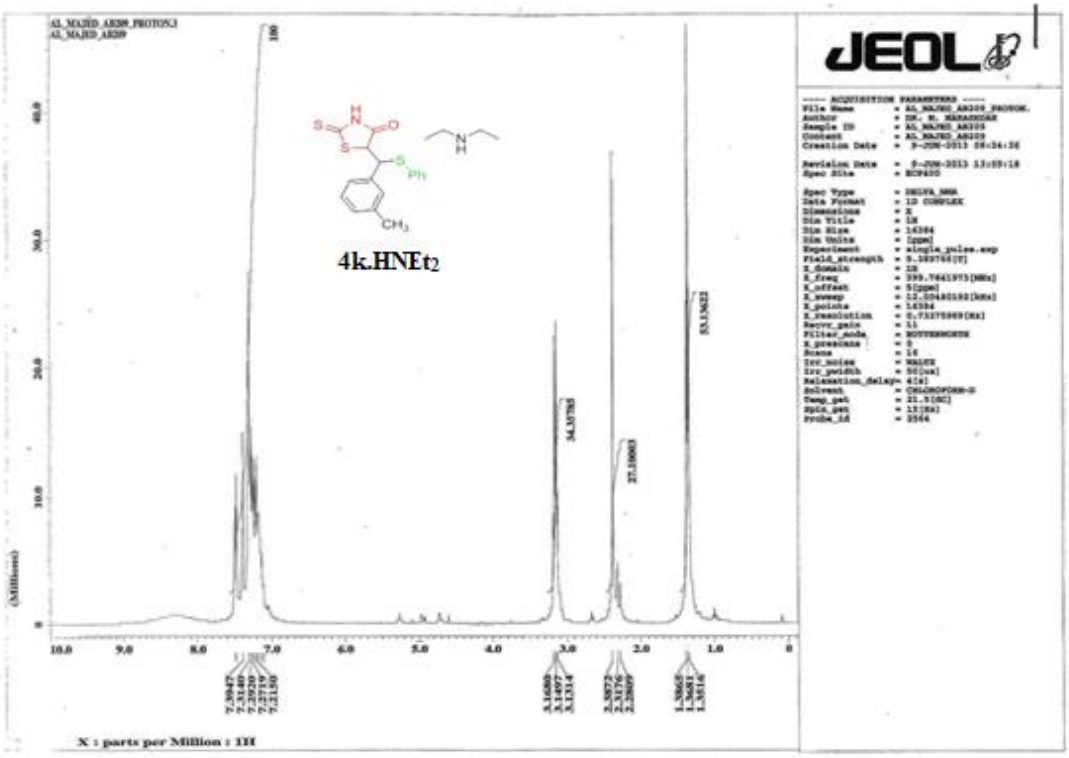


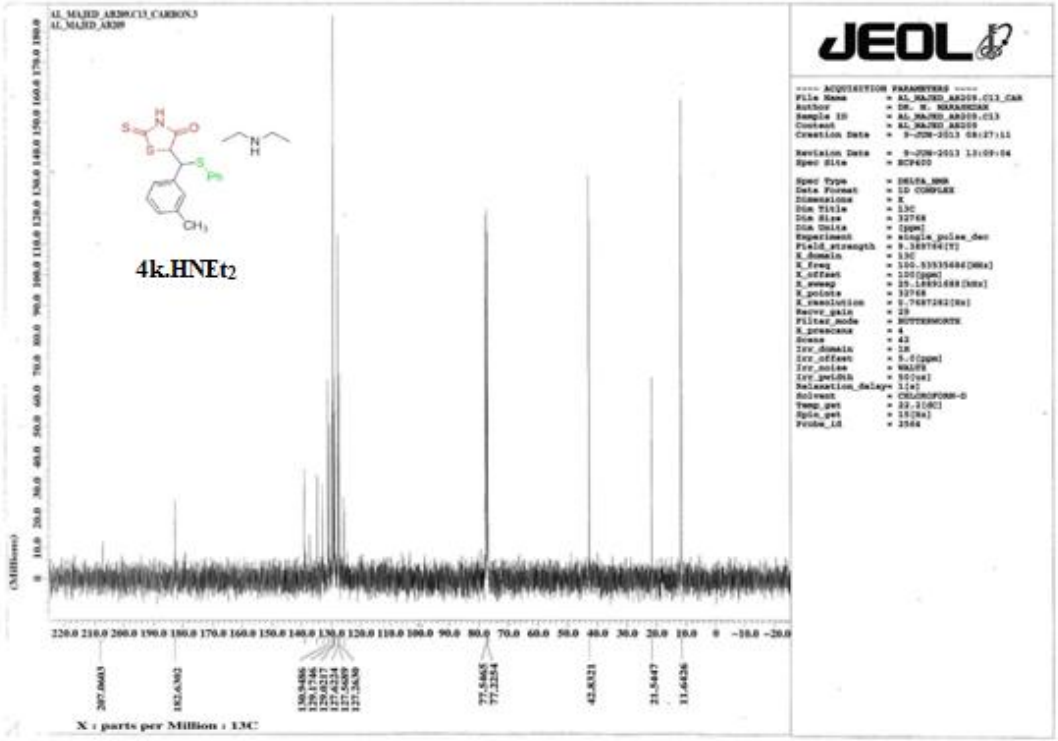

AL_MAJED_AB265_PROTON.3
AL_MAJED_AB265
4i
(Millions)
7.3782
7.3727
7.3653
7.3543
7.3452
7.3372
7.2590
5.9742
5.9504
5.9174
X : parts per Million : 1H
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_AB265_PROTON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_AB265
Content = AL_MAJED_AB265
Creation Date = 10-NOV-2013 08:34:59
Revision Date = 10-NOV-2013 10:38:52
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 15
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = CHLOROFORM-D
Temp_get = 20.3[dC]
Spin_get = 15[Hz]
Probe_id = 2564

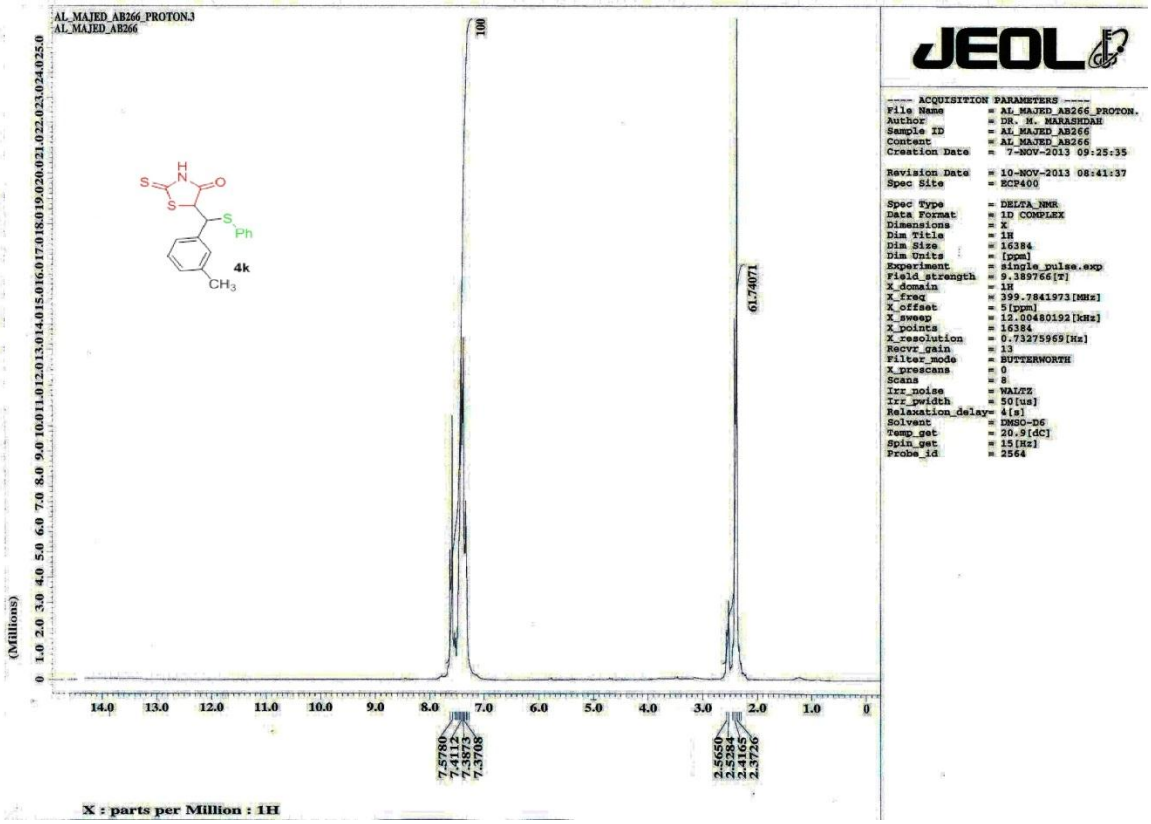

AL_MAJED_AB265_CARBON.3
AL_MAJED_AB265
4i
(Millions)
200.6680
188.9767
132.6002
129.5264
129.1746
129.0829
128.2112
127.5689
77.1718
76.8583
X : parts per Million : 13C
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_AB265_CARBON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_AB265
Content = AL_MAJED_AB265
Creation Date = 10-NOV-2013 09:06:48
Revision Date = 10-NOV-2013 10:42:04
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 29
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 800
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = CHLOROFORM-D
Temp_get = 21.1[dC]
Spin_get = 16[Hz]
Probe_id = 2564

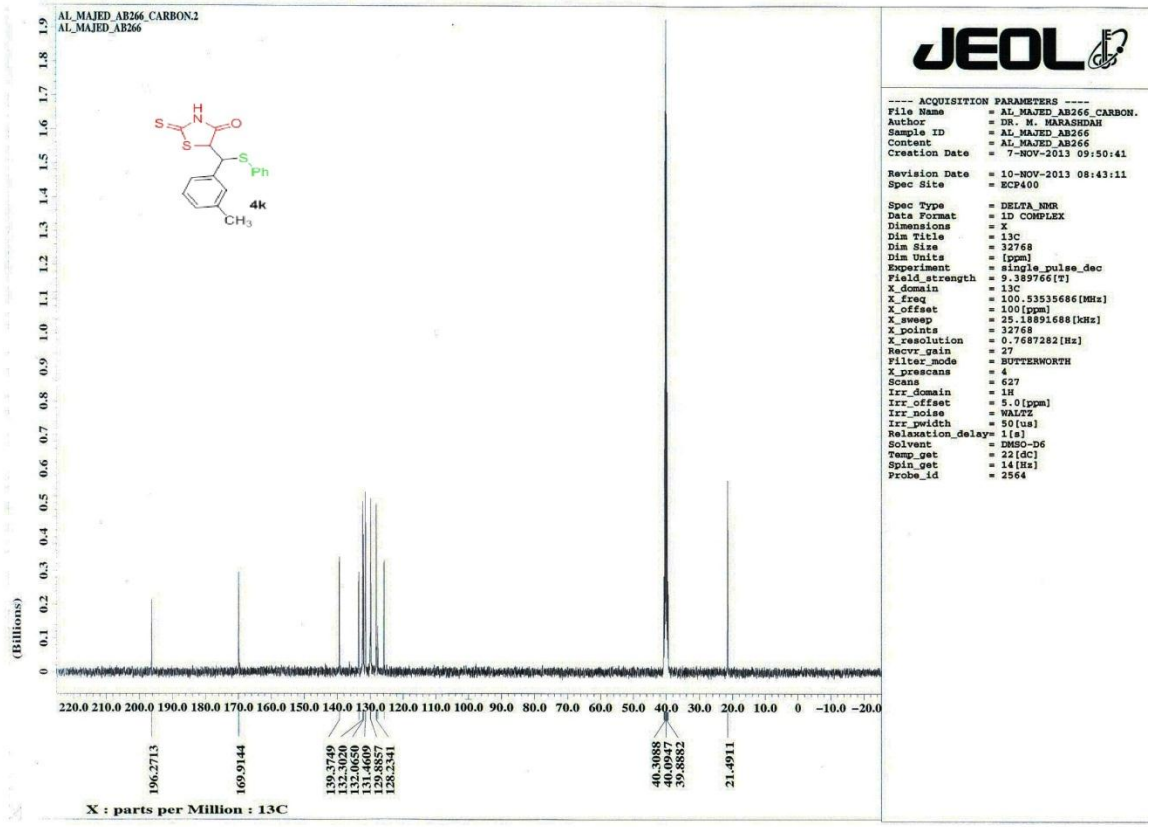

AL_MAJED_ABH-W12_PROTON.3
AL_MAJED_ABH-W12
4j
(Millions)
2.2119
8.3698
7.6476
7.3855
7.3672
7.3085
7.2584
7.2524
X : parts per Million : 1H
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH-W12_PROTO
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH-W12
Content = AL_MAJED_ABH-W12
Creation Date = 9-JUN-2013 08:40:09
Revision Date = 9-JUN-2013 13:11:25
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 15
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 16
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = CHLOROFORM-D
Temp_get = 21.6[dC]
Spin_get = 16[Hz]
Probe_id = 2564

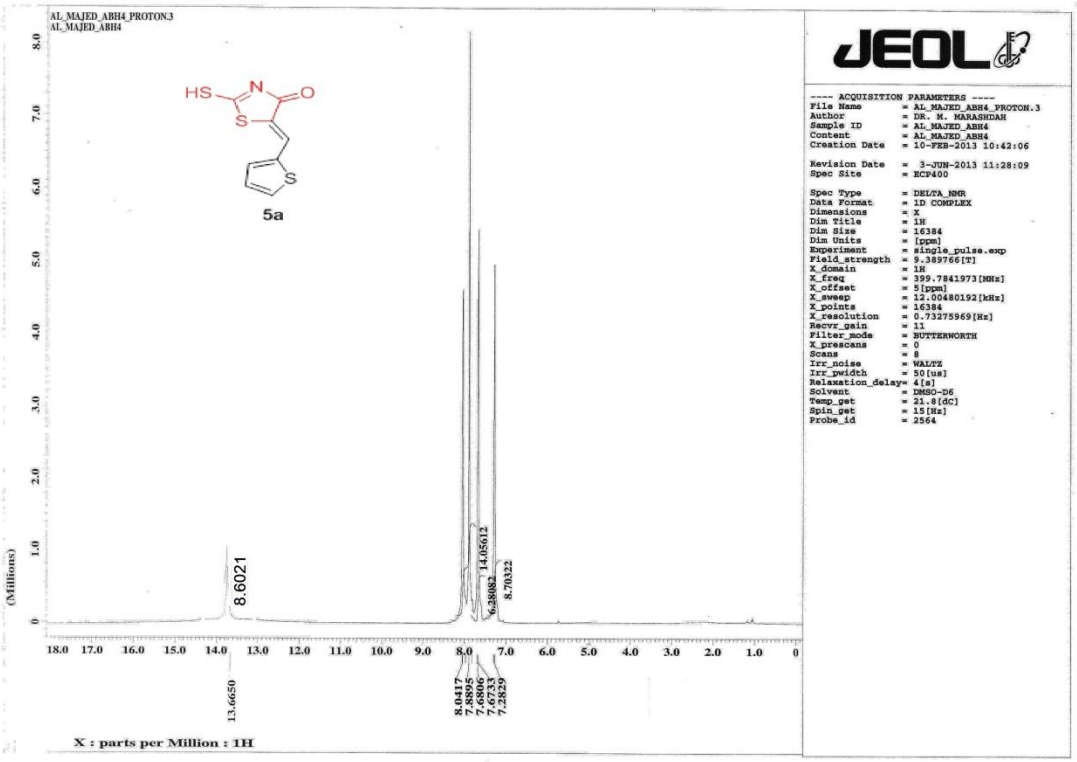

AL_MAJED_ABH-W12.C13_CARBON.3
AL_MAJED_ABH-W12
4j
(Billions)
194.3368
168.5151
134.1906
133.1321
129.0905
126.6317
127.9665
77.1260
76.8048
X : parts per Million : 13C
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH-W12.C13_C
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH-W12.C13
Content = AL_MAJED_ABH-W12
Creation Date = 9-JUN-2013 09:20:33
Revision Date = 9-JUN-2013 13:14:47
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 29
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 1024
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = CHLOROFORM-D
Temp_get = 22.7[dC]
Spin_get = 16[Hz]
Probe_id = 2564

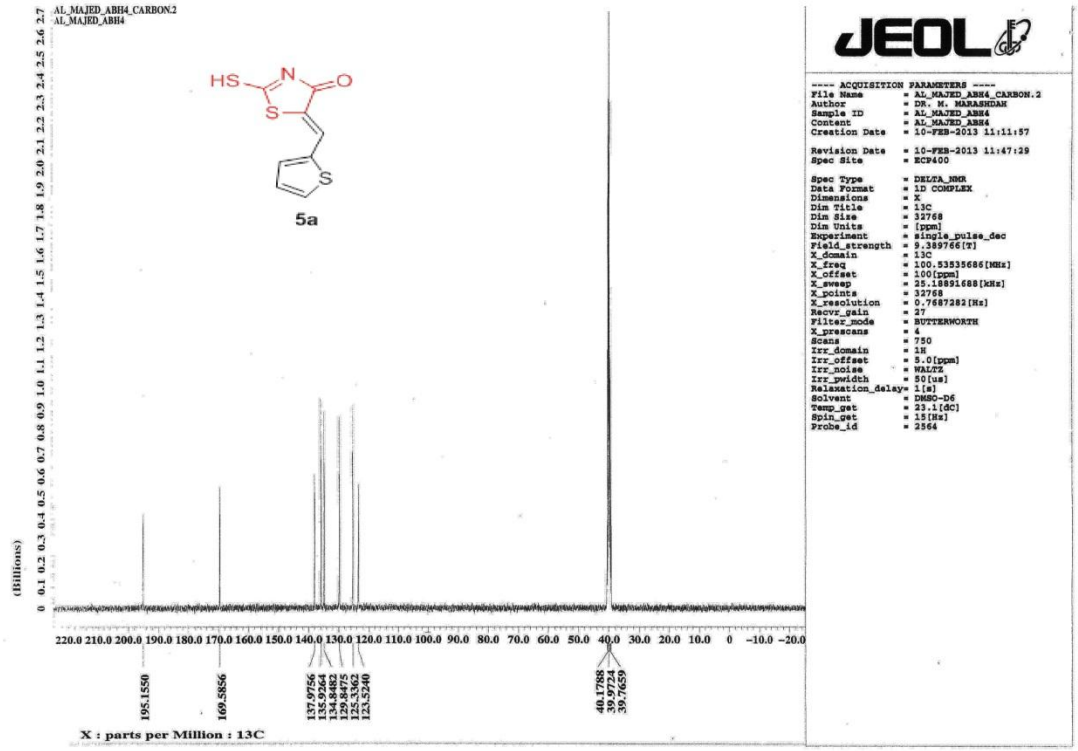

4k.HNEt2
X : parts per Million : 1H

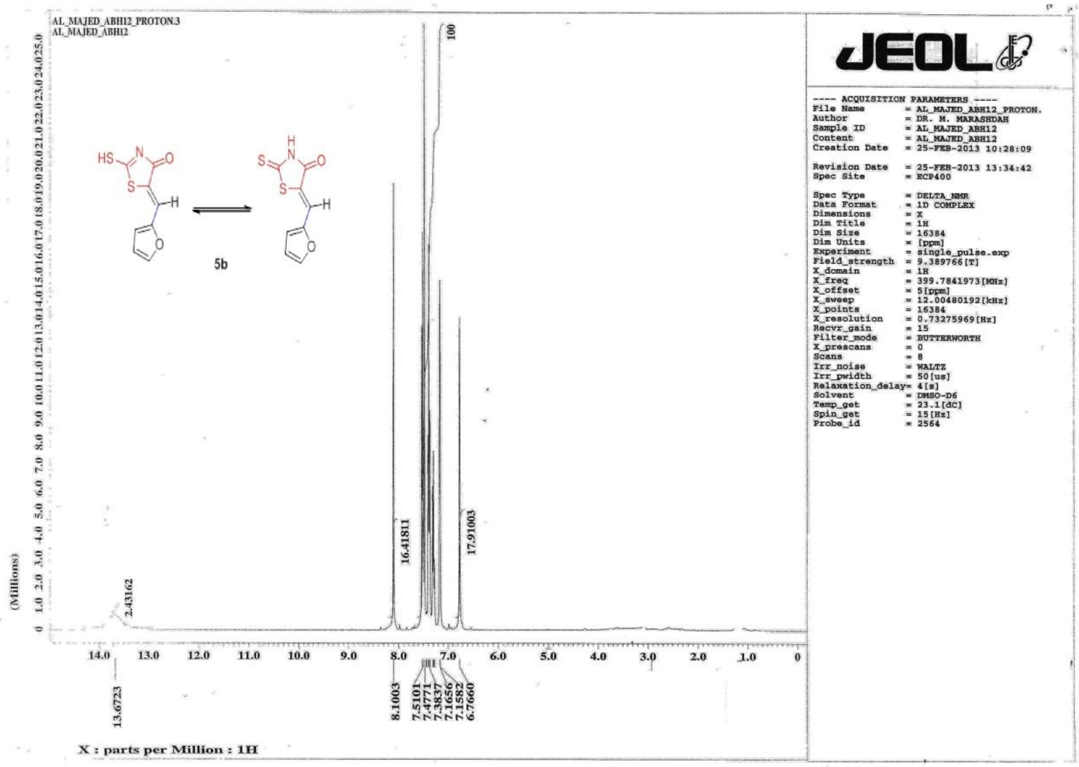

4k.HNEt2
X : parts per Million : 13C

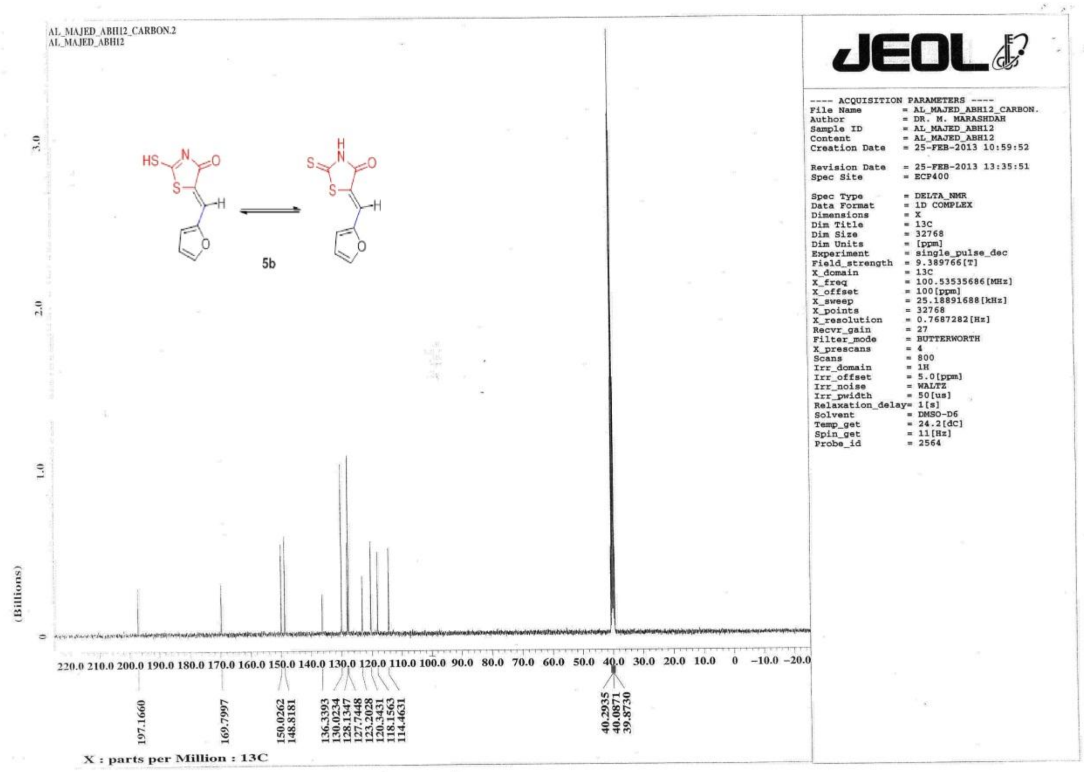

AL_MAJED_AB266_PROTON.3
AL_MAJED_AB266
4k
61.74071
7.5780
7.4112
7.3873
7.3708
2.5650
2.5284
2.4165
2.3726
X : parts per Million : 1H
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_AB266_PROTON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_AB266
Content = AL_MAJED_AB266
Creation Date = 7-NOV-2013 09:25:35
Revision Date = 10-NOV-2013 08:41:37
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 13
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 20.9[dC]
Spin_get = 15[Hz]
Probe_id = 2564

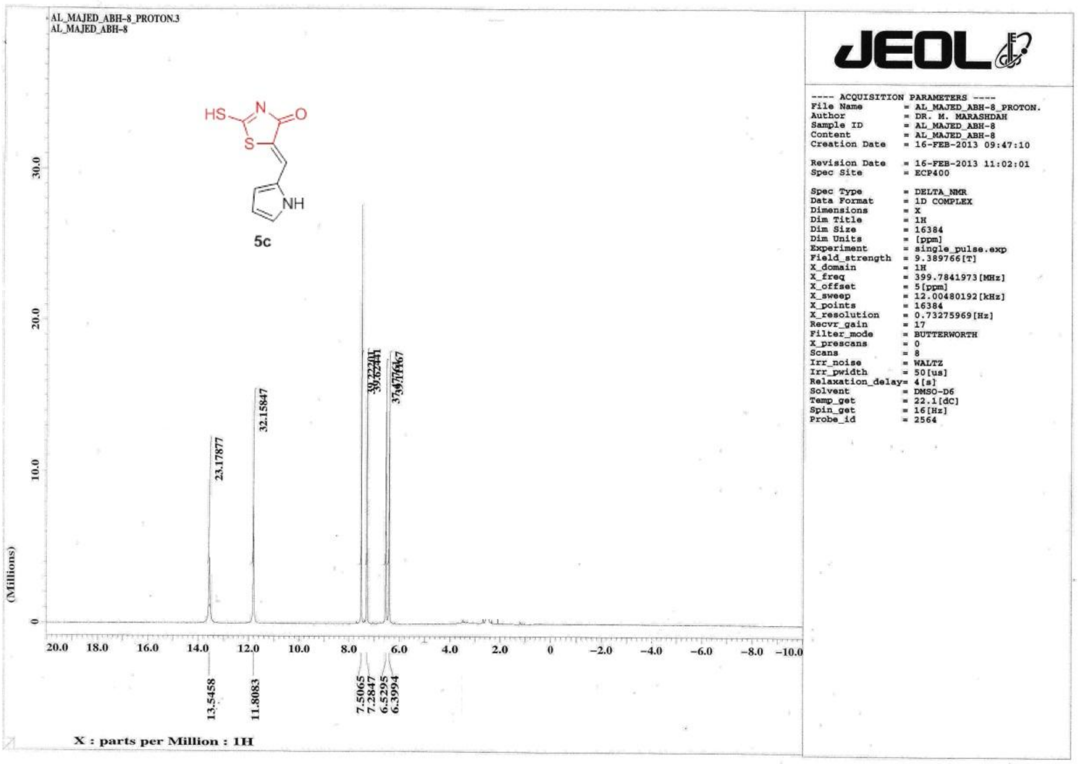

AL_MAJED_AB266_CARBON.2
AL_MAJED_AB266
4k
196.2713
169.9144
139.3749
132.3029
132.0650
131.4609
129.8857
128.2341
40.3088
40.0947
39.8882
21.4911
X : parts per Million : 13C
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_AB266_CARBON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_AB266
Content = AL_MAJED_AB266
Creation Date = 7-NOV-2013 09:50:41
Revision Date = 10-NOV-2013 08:43:11
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 627
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 22[dC]
Spin_get = 14[Hz]
Probe_id = 2564

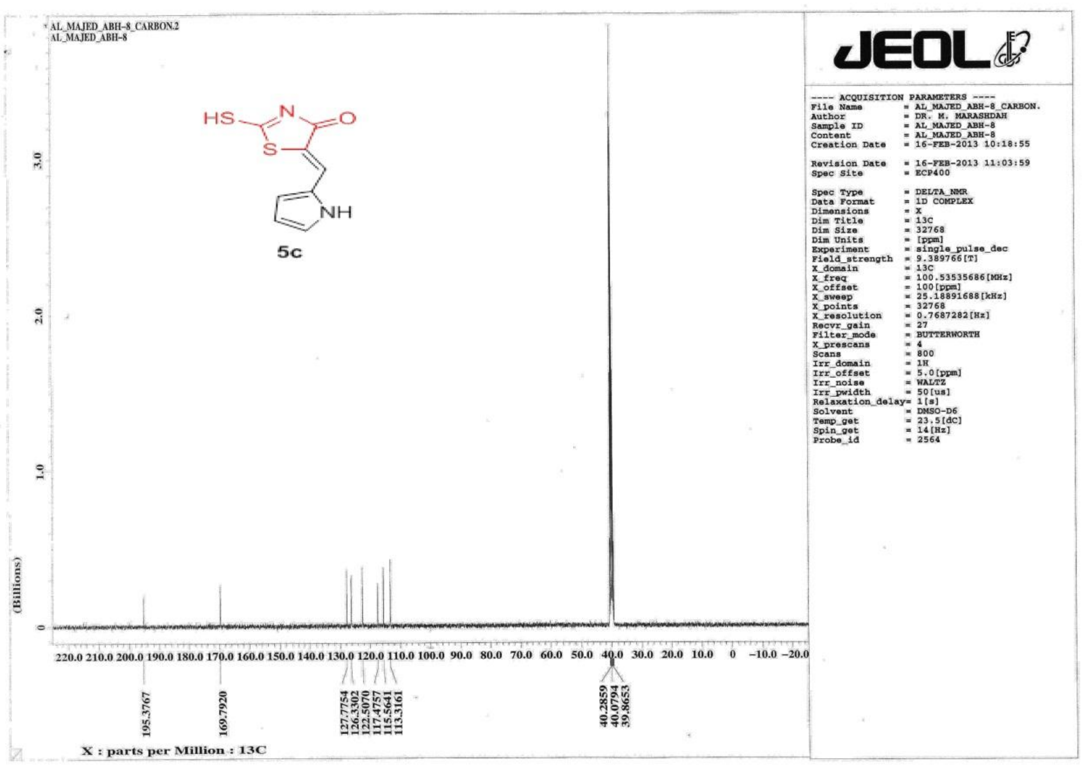

AL_MAJED_ABH4_PROTON.3
AL_MAJED_ABH4
HS
N
O
S
S
5a
8.6021
14.05612
6.38082
8.70322
13.6650
8.0417
7.8895
7.6806
7.5753
7.2829
X : parts per Million : 1H
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH4_PROTON.3
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH4
Content = AL_MAJED_ABH4
Creation Date = 10-FEB-2013 10:42:06
Revision Date = 3-JUN-2013 11:28:09
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 11
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 21.8[dC]
Spin_get = 15[Hz]
Probe_id = 2564

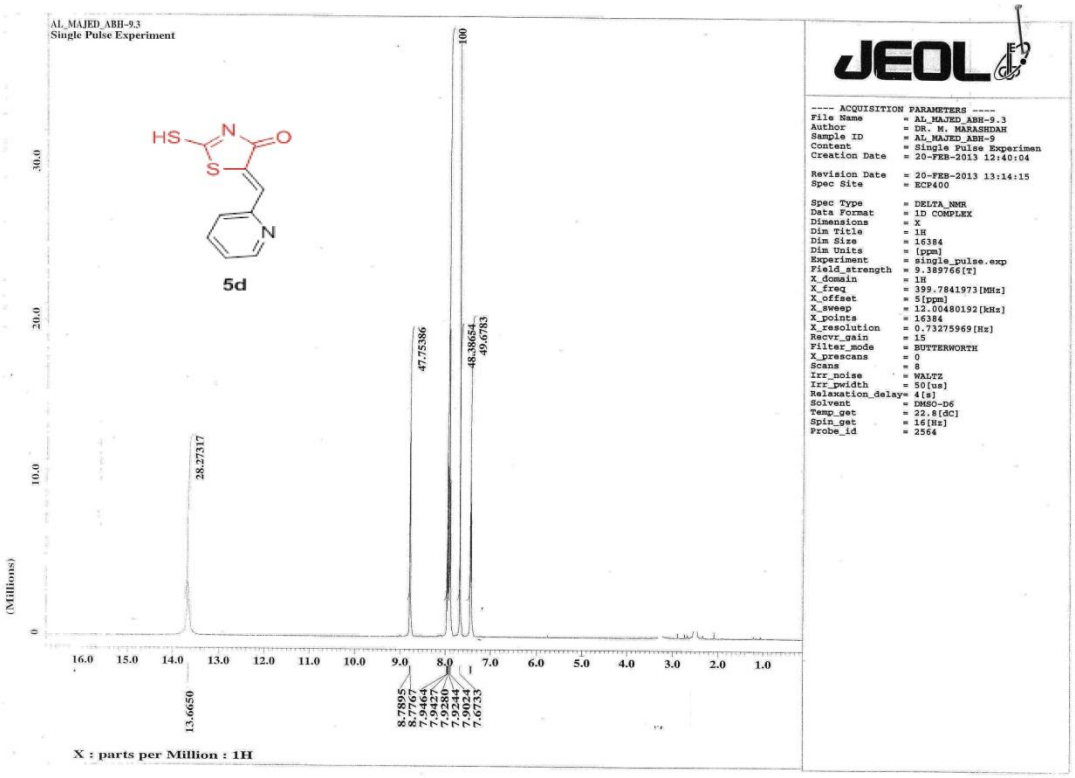

AL_MAJED_ABH4_CARBON.2
AL_MAJED_ABH4
HS
N
O
S
S
5a
195.1550
169.5856
137.9756
135.2064
134.8482
129.8475
125.3362
123.5240
40.1788
39.9724
39.7659
X : parts per Million : 13C
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH4_CARBON.2
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH4
Content = AL_MAJED_ABH4
Creation Date = 10-FEB-2013 11:11:57
Revision Date = 10-FEB-2013 11:47:29
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 750
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 23.1[dC]
Spin_get = 15[Hz]
Probe_id = 2564

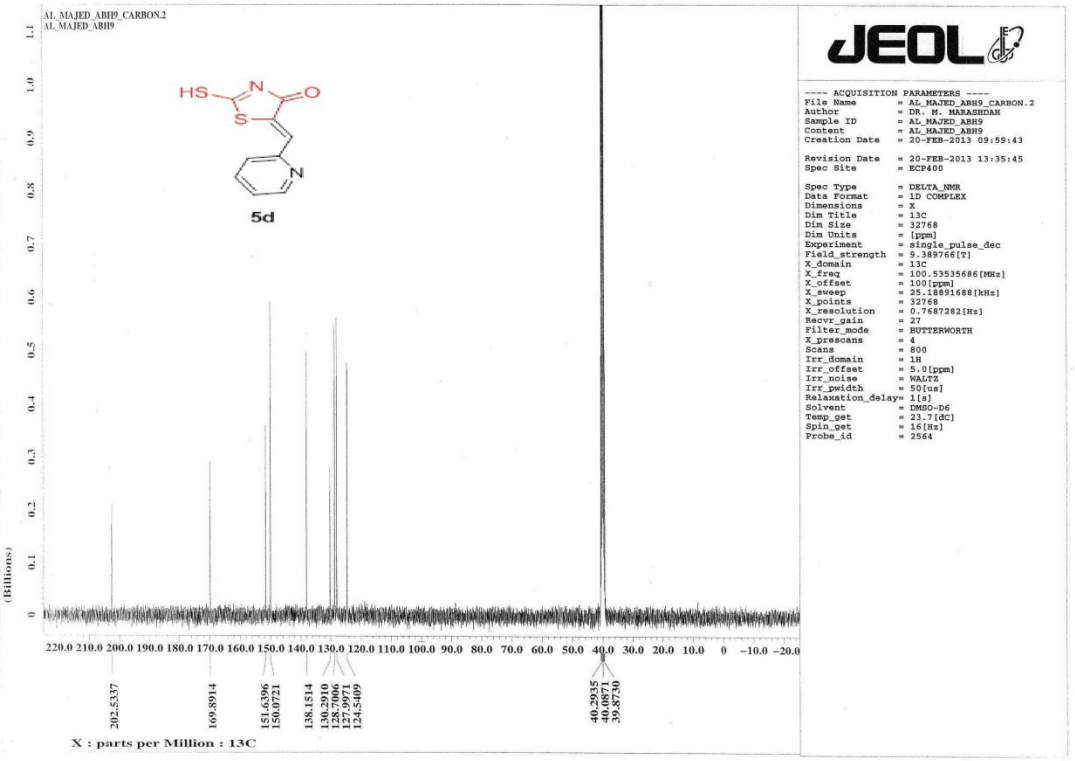

AL_MAJED_ABH12_PROTON.3
AL_MAJED_ABH12
5b
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH12_PROTON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH12
Content = AL_MAJED_ABH12
Creation Date = 25-FEB-2013 10:28:09
Revision Date = 25-FEB-2013 13:34:42
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 15
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 23.1[dC]
Spin_get = 15[Hz]
Probe_id = 2564
X : parts per Million : 1H


AL_MAJED_ABH12_CARBON.2
AL_MAJED_ABH12
5b
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH12_CARBON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH12
Content = AL_MAJED_ABH12
Creation Date = 25-FEB-2013 10:59:52
Revision Date = 25-FEB-2013 13:35:51
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 800
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 24.2[dC]
Spin_get = 11[Hz]
Probe_id = 2564
X : parts per Million : 13C


AL_MAJED_ABH-8_PROTON.3
AL_MAJED_ABH-8
HS
N
O
S
NH
5c
23.17877
32.15847
13.5458
11.8083
7.5065
7.2847
6.5295
6.3994
(Millions)
X : parts per Million : 1H
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH-8_PROTON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH-8
Content = AL_MAJED_ABH-8
Creation Date = 16-FEB-2013 09:47:10
Revision Date = 16-FEB-2013 11:02:01
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 17
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 22.1[dC]
Spin_get = 16[Hz]
Probe_id = 2564


AL_MAJED_ABH-8_CARBON.2
AL_MAJED_ABH-8
HS
N
O
S
NH
5c
(Billions)
195.3767
169.7920
127.7754
126.3302
122.5070
117.4757
115.5641
113.3161
40.2859
40.0794
39.8653
X : parts per Million : 13C
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH-8_CARBON.
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH-8
Content = AL_MAJED_ABH-8
Creation Date = 16-FEB-2013 10:18:55
Revision Date = 16-FEB-2013 11:03:59
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 800
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 23.5[dC]
Spin_get = 14[Hz]
Probe_id = 2564


AL_MAJED_ABH-9.3
Single Pulse Experiment
5d
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH-9.3
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH-9
Content = Single Pulse Experiman
Creation Date = 20-FEB-2013 12:40:04
Revision Date = 20-FEB-2013 13:14:15
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 16384
Dim Units = [ppm]
Experiment = single_pulse.exp
Field_strength = 9.389766[T]
X_domain = 1H
X_freq = 399.7841973[MHz]
X_offset = 5[ppm]
X_sweep = 12.00480192[kHz]
X_points = 16384
X_resolution = 0.73275969[Hz]
Recvr_gain = 15
Filter_mode = BUTTERWORTH
X_prescans = 0
Scans = 8
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 4[s]
Solvent = DMSO-D6
Temp_get = 22.8[dC]
Spin_get = 16[Hz]
Probe_id = 2564
100
47.75386
48.38654
49.6783
28.27317
(Millions)
13.6650
8.7895
8.7767
7.9464
7.9427
7.9324
7.9244
7.9024
7.6733
X : parts per Million : 1H


AL_MAJED_ABH9_CARBON.2
AL_MAJED_ABH9
5d
JEOL
---- ACQUISITION PARAMETERS ----
File Name = AL_MAJED_ABH9_CARBON.2
Author = DR. M. MARASHDAH
Sample ID = AL_MAJED_ABH9
Content = AL_MAJED_ABH9
Creation Date = 20-FEB-2013 09:59:43
Revision Date = 20-FEB-2013 13:35:45
Spec Site = ECP400
Spec Type = DELTA_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 32768
Dim Units = [ppm]
Experiment = single_pulse_dec
Field_strength = 9.389766[T]
X_domain = 13C
X_freq = 100.53535686[MHz]
X_offset = 100[ppm]
X_sweep = 25.18891688[kHz]
X_points = 32768
X_resolution = 0.7687282[Hz]
Recvr_gain = 27
Filter_mode = BUTTERWORTH
X_prescans = 4
Scans = 800
Irr_domain = 1H
Irr_offset = 5.0[ppm]
Irr_noise = WALTZ
Irr_pwidth = 50[us]
Relaxation_delay= 1[s]
Solvent = DMSO-D6
Temp_get = 23.7[dC]
Spin_get = 16[Hz]
Probe_id = 2564
(Billions)
202.5337
169.8914
151.6396
150.0721
138.1514
130.2910
125.7906
125.9971
124.5409
40.2935
40.0871
39.8730
X : parts per Million : 13C