

Supplementary information

Mechanistic Investigation of *Anti*-Elimination in (*Z*)-1,2-bis(arylseleno)-1-alkenes and their Sulfur Analogs

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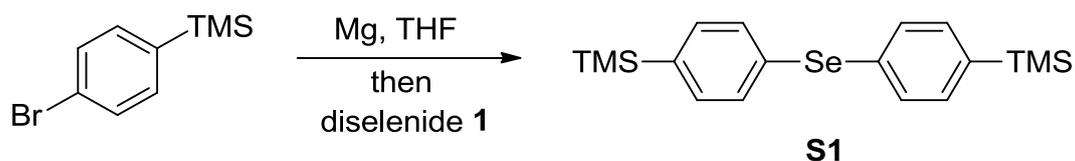
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Kagawa 769-2193, Japan

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Procedure for synthesis of bis(4-trimethylsilylphenyl)selenide (**S1**)



1-Bromo-4-trimethylsilylbenzene (195 μL , 1.0 mmol) was added to a suspension of Mg (36 mg, 1.5 mmol) and trace amount of I_2 in anhydrous tetrahydrofuran (6 mL) at room temperature, and the mixture was stirred at the same temperature for 2.5 h. Then, diselenide **1** (225 mg, 0.5 mmol) was added to the reaction mixture and vigorously stirred for 3 h at 60 $^\circ\text{C}$. The reaction was cooled and filtered through a celite pad. The filtrate was poured into cold a saturated aqueous solution of NH_4Cl (20 mL) and the mixture was extracted with EtOAc (20 mL \times 3). The organic layer was washed with brine (20 mL \times 2), dried over magnesium sulfate, and concentrated under vacuum. The residue was dissolved in ether (40 mL), treated with a solution of NaBH_4 (80 mg, 2.1 mmol) in methanol (2 mL), washed with 2N aqueous solution of KOH (20 mL). These treatment and washing were continued until the disappearance of the color of organic layer. The organic layer was dried over magnesium sulfate and concentrated under vacuum. The residue was purified by silica gel preparative thin layer chromatography (hexane) to give **S1** (146 mg, 77%).

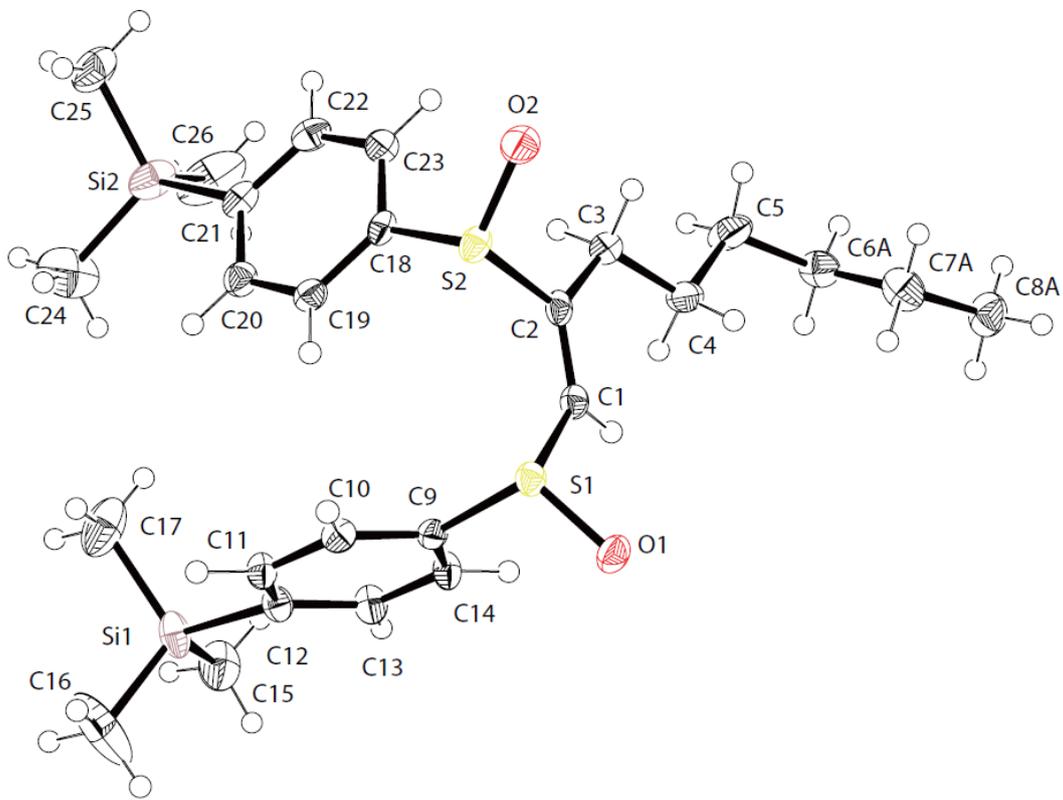
^1H NMR (400 MHz, CDCl_3) δ : 0.25 (18H, s, $\text{Si}(\text{CH}_3)_3$), 7.41 (4H, d, $J = 8.1$ Hz, Ar-H), 7.44 (4H, d, $J = 8.1$ Hz, Ar-H); ^{13}C -NMR (100 MHz, CDCl_3) δ : -1.2, 131.9, 132.2, 134.2, 139.5; MS (EI) m/z : 378 (M^+ , 100), 363 (91), 214 (9), 73 (52); HR-MS (EI) m/z : 378.0740 (Calcd for $\text{C}_{18}\text{H}_{27}\text{SeSi}_2$: 378.0738); *Anal.*: Found: C, 54.79; H, 6.40 (Calcd for $\text{C}_{18}\text{H}_{26}\text{OSeSi}_2$: C, 54.94; H, 6.66%).

Crystal data and structure refinement for compound 15

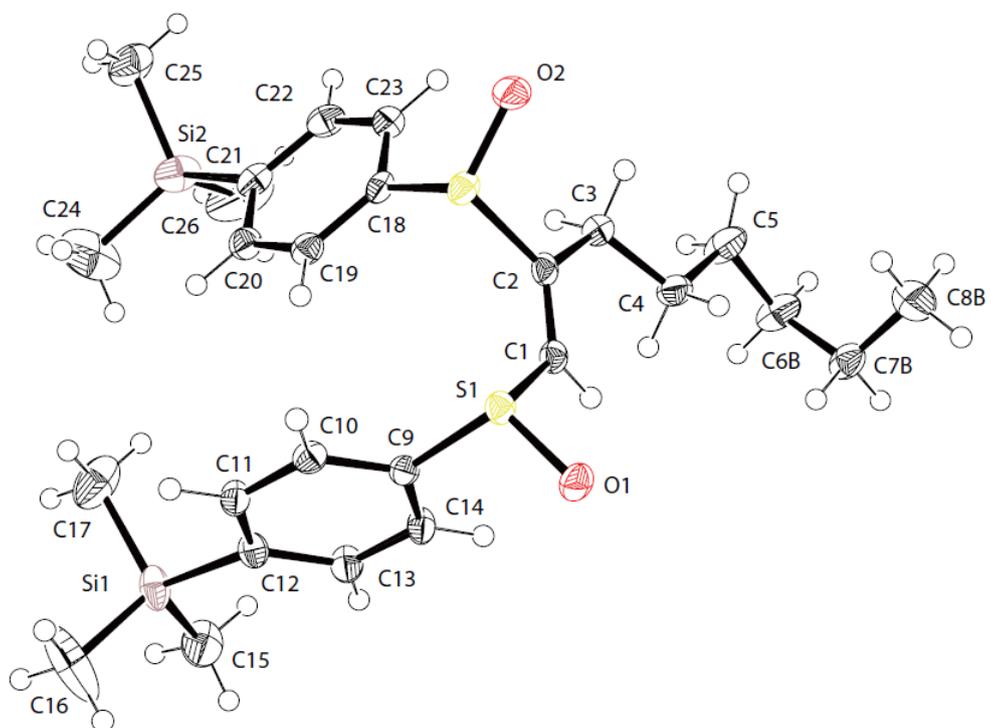
Empirical formula	C ₂₆ H ₄₀ O ₂ S ₂ Si ₂	
Formula weight	504.88	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 11.205(3) Å	a = 108.312(3)°.
	b = 11.346(3) Å	b = 90.218(3)°.
	c = 13.093(4) Å	g = 112.482(3)°.
Volume	1445.6(7) Å ³	
Z	2	
Density (calculated)	1.160 Mg/m ³	
Absorption coefficient	0.287 mm ⁻¹	
F(000)	544	
Crystal size	0.140 x 0.100 x 0.080 mm ³	
Theta range for data collection	1.655 to 26.811°.	
Index ranges	-13<=h<=14, -14<=k<=14, -16<=l<=16	
Reflections collected	14519	
Independent reflections	5515 [R(int) = 0.0315]	
Completeness to theta = 25.242°	98.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5515 / 0 / 325	
Goodness-of-fit on F ²	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0411, wR2 = 0.0986	
R indices (all data)	R1 = 0.0554, wR2 = 0.1064	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.859 and -0.529 e.Å ⁻³	

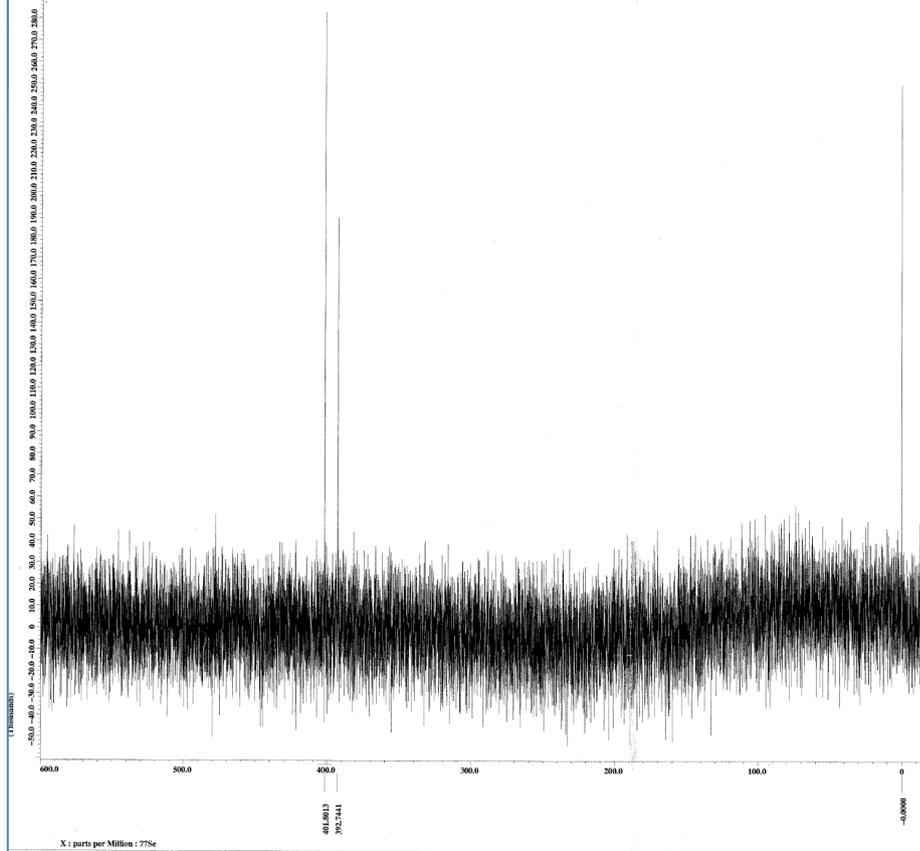
ORTEP Diagram of the compound 15

conformer A



conformer B

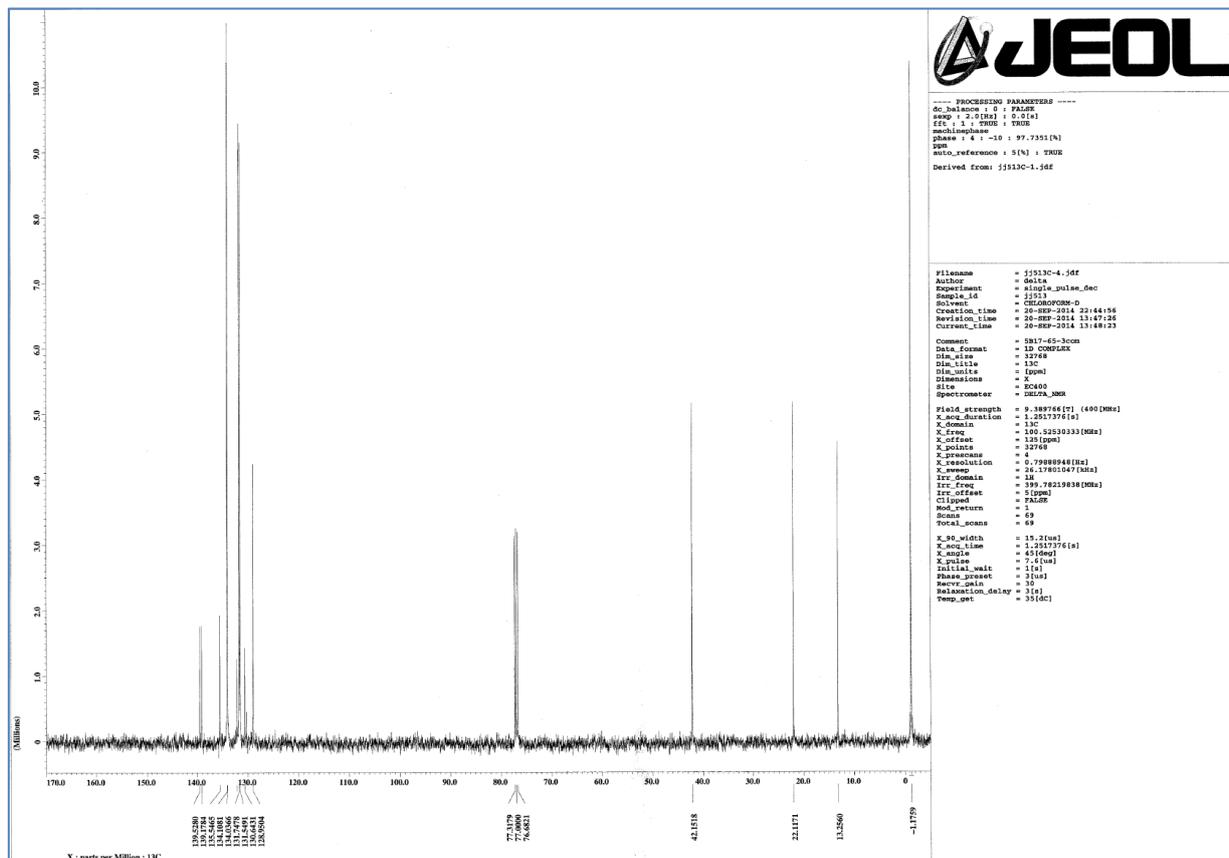
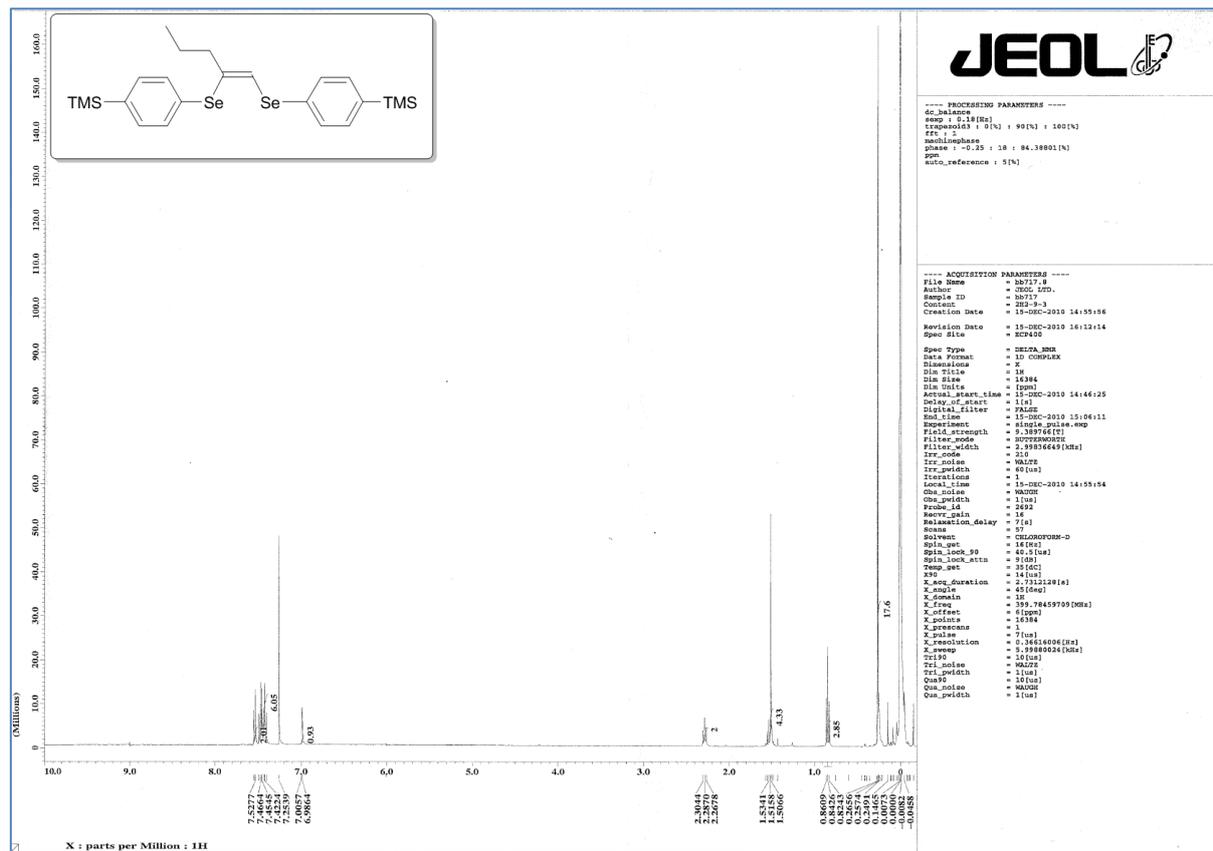




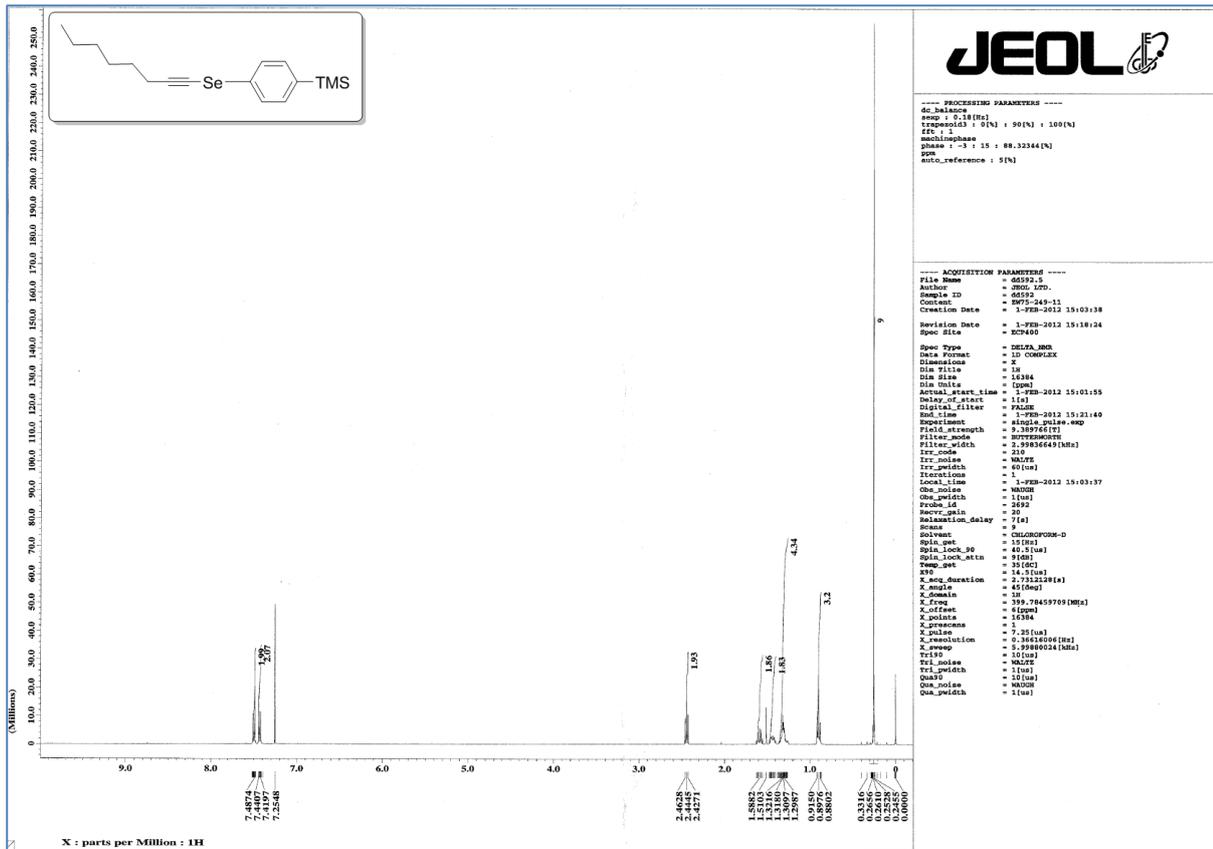
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fft : 1 : 77SE : 77SE
Nucleus1 : 13C
SOLVENT : CDCl3
Reference : 0 (ppm) : 0 (ppm)
Derived from: hhsa-1.j2f

Filename = hhsa-7.j2f
Author = Gelta
Experiment = single_pulse_2ec
Sample_ID = hah
Solvent = CDCl3
Creation_time = 10-APR-2011 21:26:35
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X_sweep = 66.1025641 (kHz)
X_resolution = 0.9781275 (Hz)
Int_freq = 100.6281205 (MHz)
Int_offset = 0 (ppm)
Clipped = 0 (Hz)
Mod_return = 1
Scans = 740
Total_scans = 740
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X_acq_time = 1.0231616 (s)
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X_pulse = 2.35333333 (us)
Initial_wait = 1 (s)
Phase_reset = 1 (us)
Revers_gain = 27
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Temp_get = 35 (C)

¹H and ¹³C NMR of 3c



¹H, ¹³C and ⁷⁷Se NMR of 4a

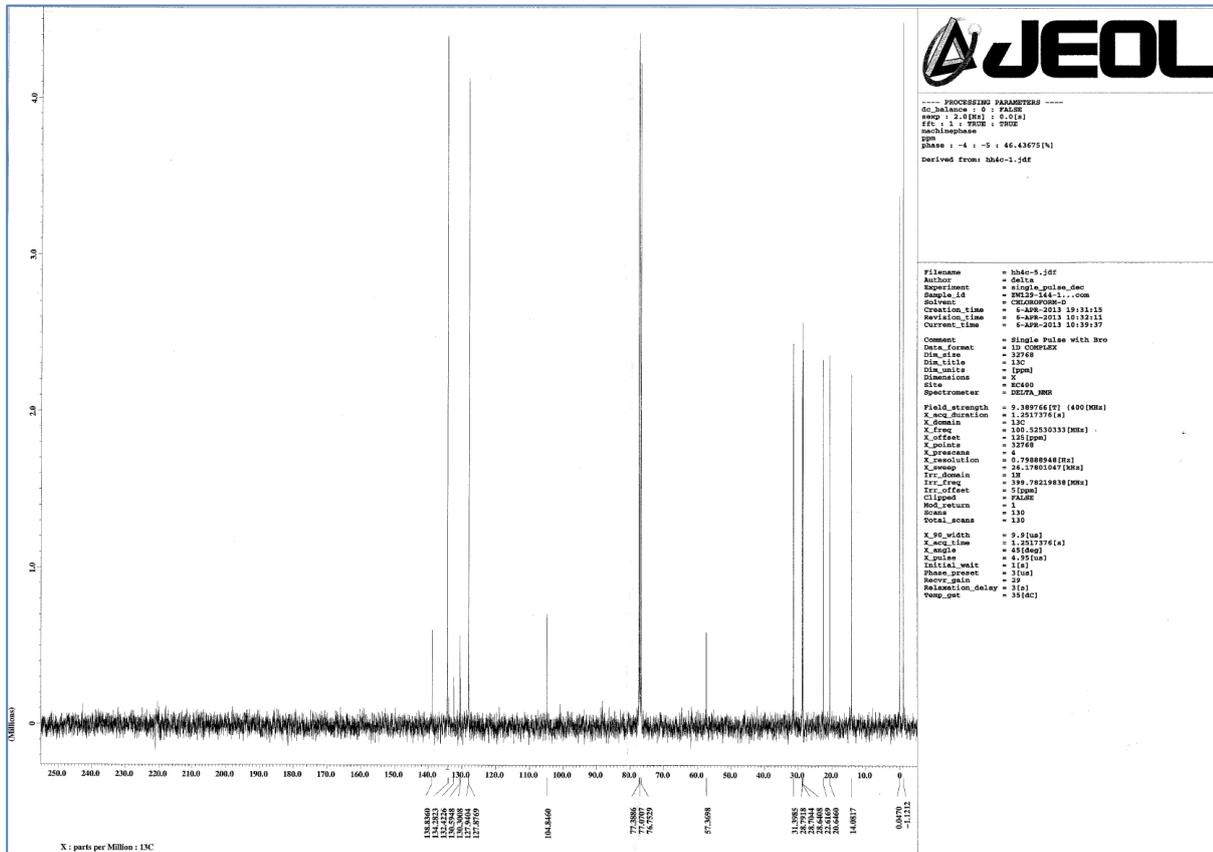


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Sample ID       = 46592
Sample Name     = 46592
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P1              = 3.15
P2              = 88.3244[Hz]
Auto Reference = 5[Hz]

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File Name      = 06592.9
Data Format    = JEOL STD
Sample ID     = 46592
Content       = 46592-249-11
Creation Date = 1-FEB-2012 15:03:18
Revision Date = 1-FEB-2012 15:18:24
Spec File    = ECF400

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Data Format  = 1D COMPOUND
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Dim Title   = 1H
Dim Units   = [ppm]
Dim Range   = 10.000
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Delay of Start = 1[sec]
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Filter Width = 2.9836648[MHz]
F2 Code     = 2D
F2 Name     = WALTZ
F2 Spin     = 60[Hz]
F2 Phase    = 1
F2 Pulse    = MUMU
F2 Program  = 1[sec]
F2 Wait     = 1[sec]
F2 Delay    = 20
F2 Recv     = 20
F2 Relax    = 7[sec]
F2 Delay    = 9
F2 Program  = CHLORFORM-D
F2 Spin     = 16[Hz]
F2 Lock    = 40.5[Hz]
F2 Lock Att = 9[dB]
F2 Temp     = 30[deg]
F2 X Acq Duration = 14.5[sec]
F2 X Sample = 2.73219[sec]
F2 X Domain = 40[sec]
F2 X Freq   = 399.7819799[MHz]
F2 X Offset = 4[ppm]
F2 X Phase  = 1
F2 X Program = 1
F2 X Pulse  = 7.20[sec]
F2 X Sweep  = 0.3661606[Hz]
F2 X Wait   = 2.9980014[sec]
F2 Y Spin   = 16[Hz]
F2 Y Lock  = WALTZ
F2 Y Pulse = 1[sec]
F2 Y Wait  = 1[sec]
F2 Y Delay = 20
F2 Y Recv  = 20
F2 Y Relax = 1[sec]
F2 Y Delay = 1[sec]
    
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```

----- PROCESSING PARAMETERS -----
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Acq Time        = 10:31:15
Acq File        = 46592
Sample ID       = 46592
Sample Name     = 46592
MachinePhase   = 88.3244[Hz]
P1              = 3.15
P2              = 88.3244[Hz]
Auto Reference = 5[Hz]
Derived from: hb4c-1.jdr

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Data Format    = 1D COMPOUND
Sample ID     = 46592
Content       = 46592-249-11
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Revision Date = 8-FEB-2012 10:39:37
Current Time  = 8-FEB-2012 10:39:37

Comment       = Single Pulse with Bro
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Dim Range    = 250.000
Dimension    = 1
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Spectrometer = JEOL NMR

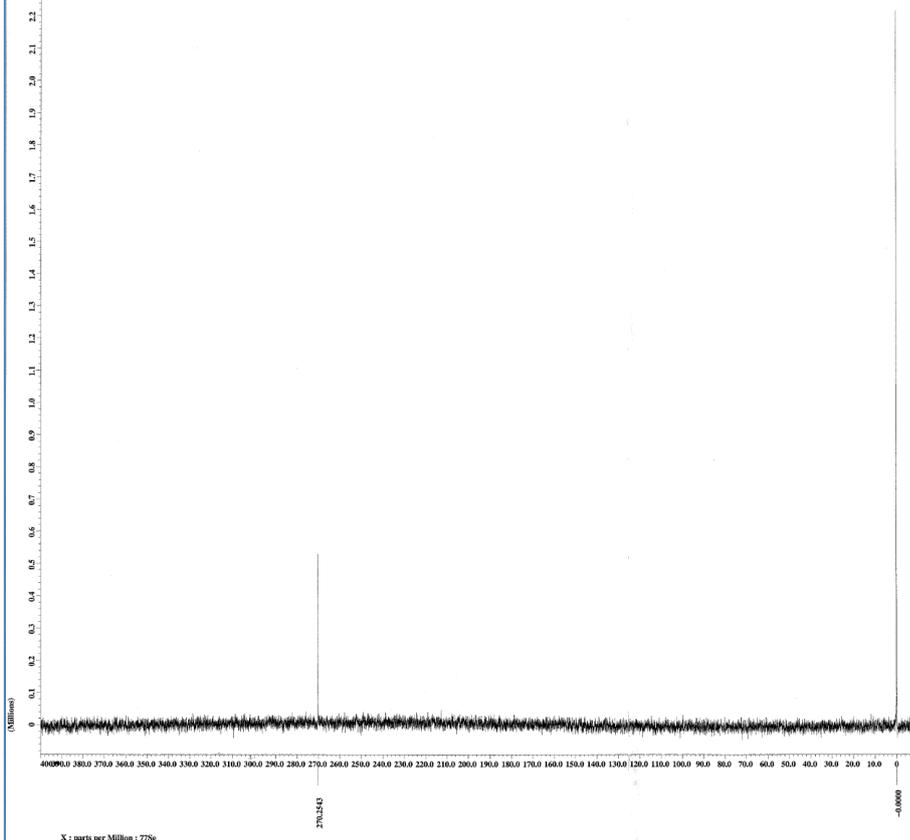
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X Freq        = 100.6263333[MHz]
X Offset      = 13[ppm]
X Phase       = 37[deg]
X Program     = 4
X Pulse       = 7.20[sec]
X Sweep       = 26.17801047[Hz]
X Wait        = 2.9980014[sec]
Y Spin        = 16[Hz]
Y Lock        = WALTZ
Y Pulse       = 1[sec]
Y Wait        = 1[sec]
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Y Recv        = 20
Y Relax       = 1[sec]
Y Delay       = 1[sec]
    
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----- PROCESSING PARAMETERS -----

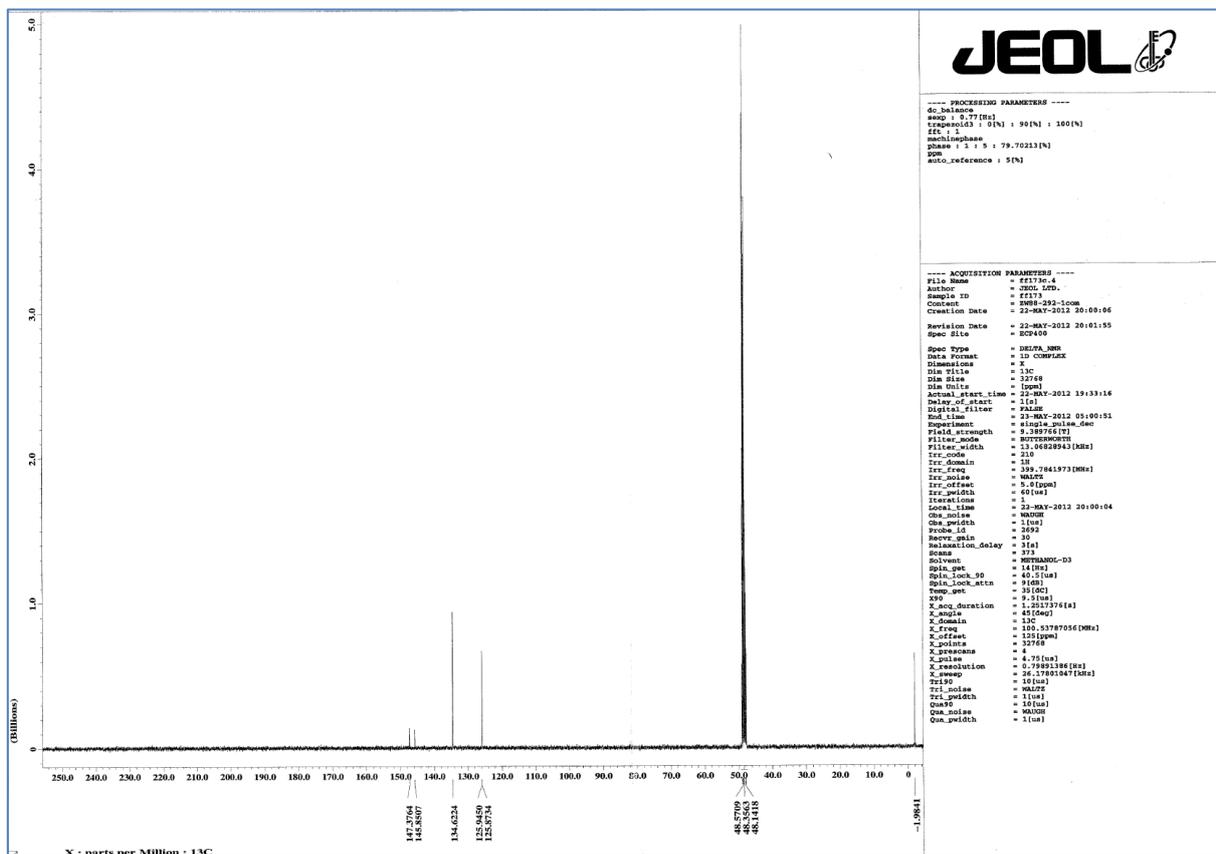
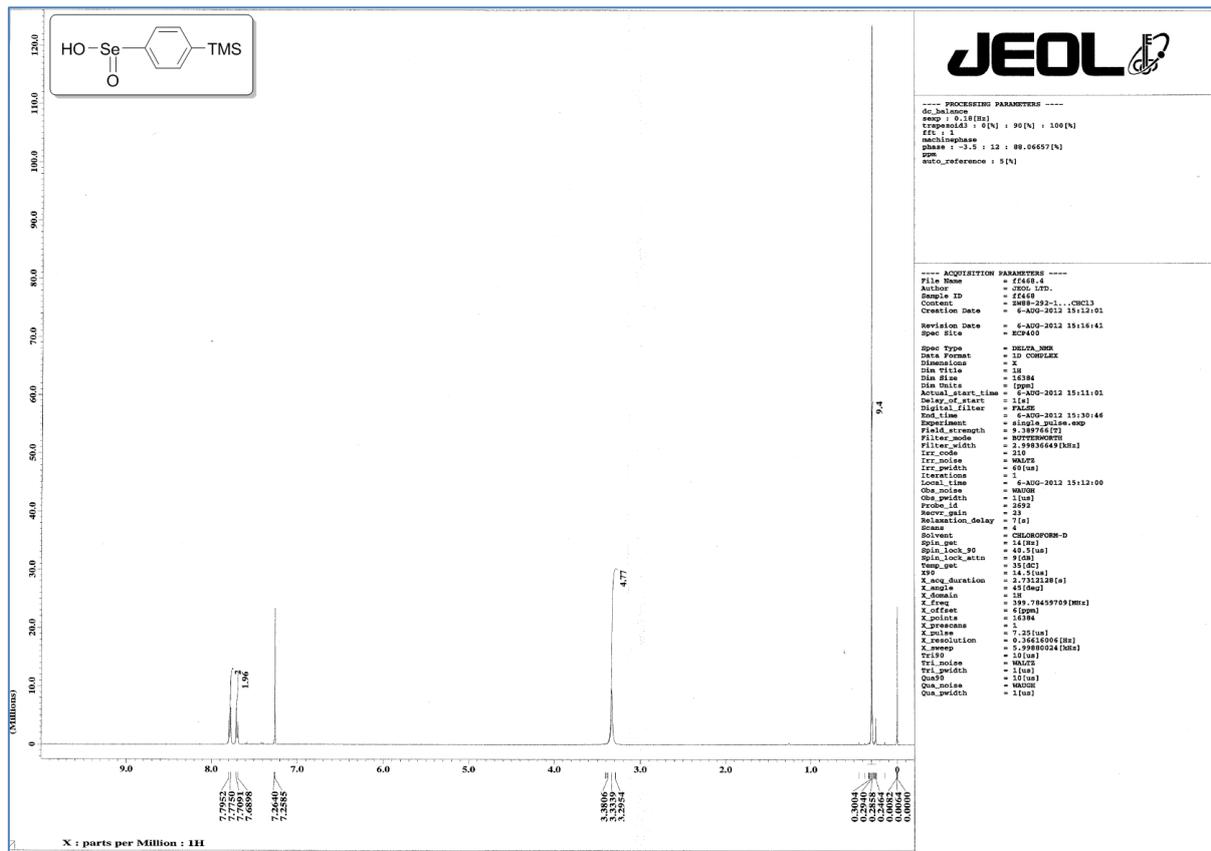
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exp : 3 ; (Hz) : 0.0141
fil : 1 ; FROM : FROM
machine : PALPS
REV
Derived from: hb4fe-3.jdf

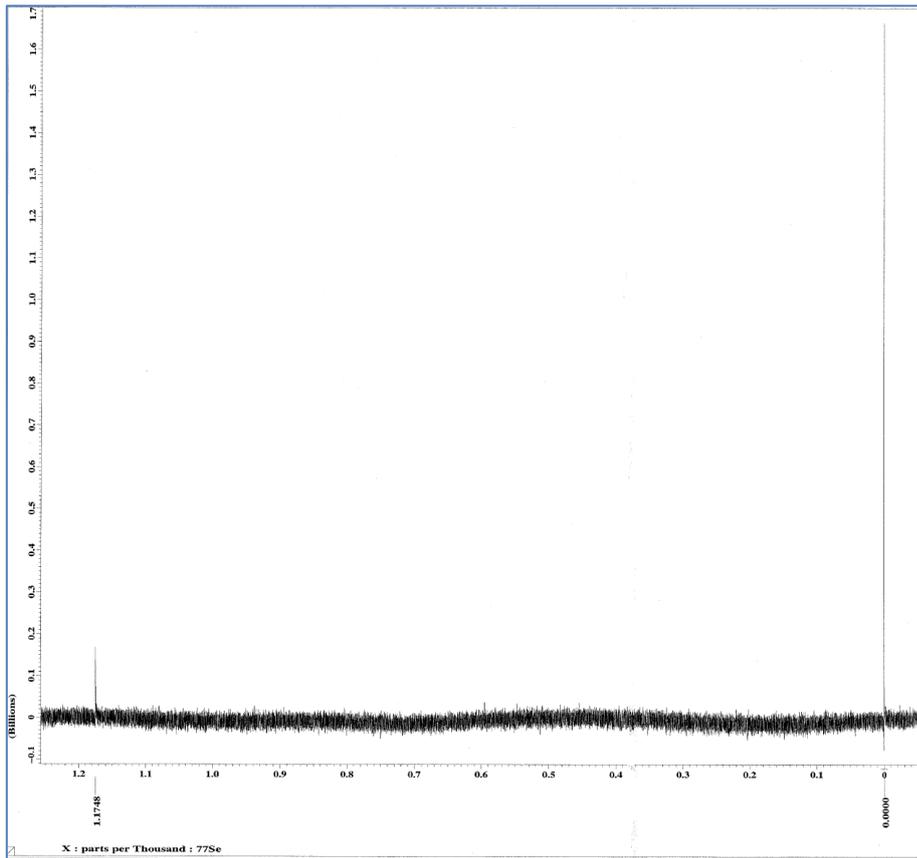
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Experiment = single_pulse_dec
Sample_id = 326
Solvent = CHLOROFORM-D
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Revision_time = 6-APR-2013 11:34:18
Current_time = 6-APR-2013 11:36:10
REV
Data_format = 1D_COMPLEX
Da_size = 65256
Da_min = 9794
Da_max = 10901
Dimensions = 2
File = 30440
Spectrometer = DELTA_300R
Field_strength = 9.389746171 (400 [MHz])
X_acq_duration = 1.3368844 [s]
X_domain = 7784
X_freq = 264442292 [MHz]
X_offset = 380 [ppm]
X_points = 65536
X_precomp = 4
X_resolution = 0.74797886 [Hz]
X_sweep = 45.01960784 [kHz]
X_resolution_min = 16
X_resolution_max = 45.01960784 [kHz]
Int_freq = 399.7819830 [MHz]
Int_offset = 5 [ppm]
Clipped = 3008
Mod_return = 1
Scans = 629
Total_scans = 629
X_90_width = 10 [us]
X_acq_time = 1.3368844 [s]
X_amplitude = 30 [deg]
X_pulse = 1.33333333 [us]
Initial_wait = 1 [s]
Phase_preset = 1 [um]
Recycle_gain = 20
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Temp_get = 35 [degC]



X: parts per Million : 778e

^1H , ^{13}C and ^{77}Se NMR of 5





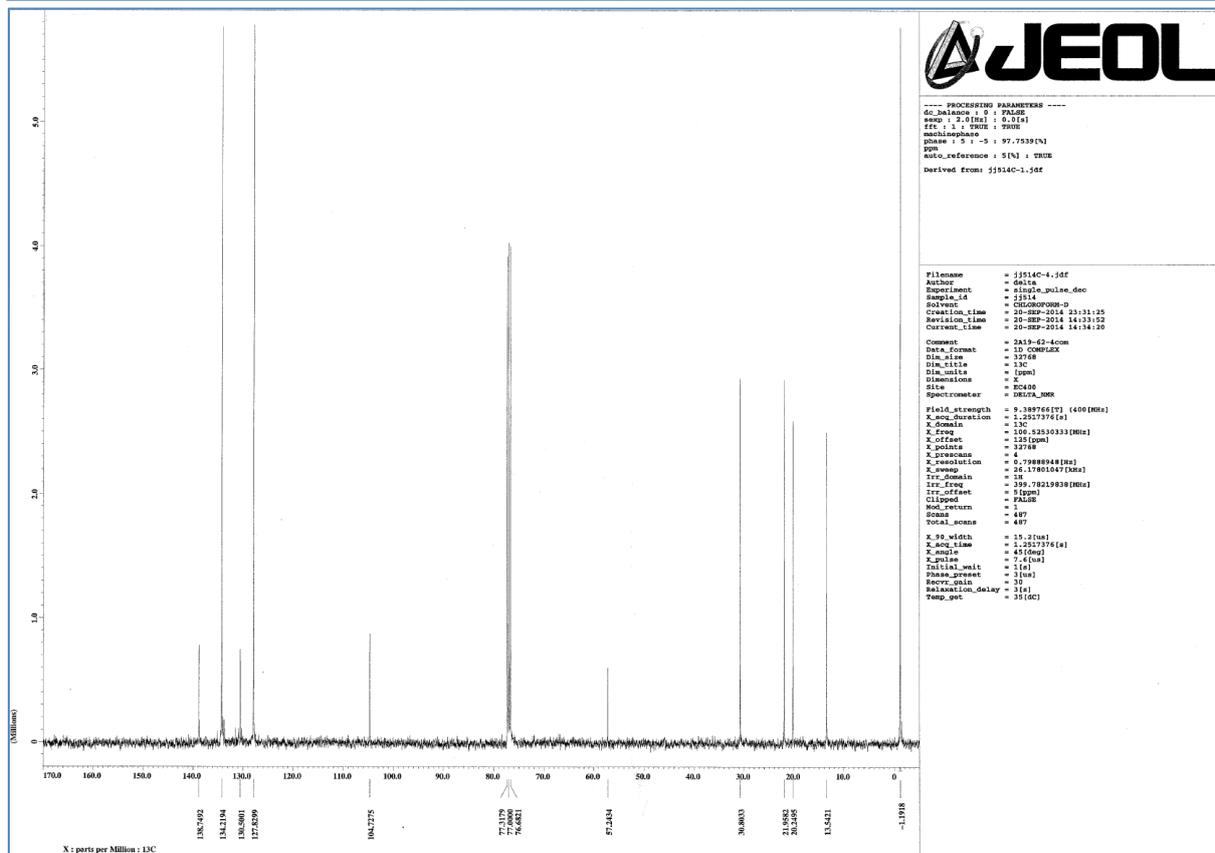
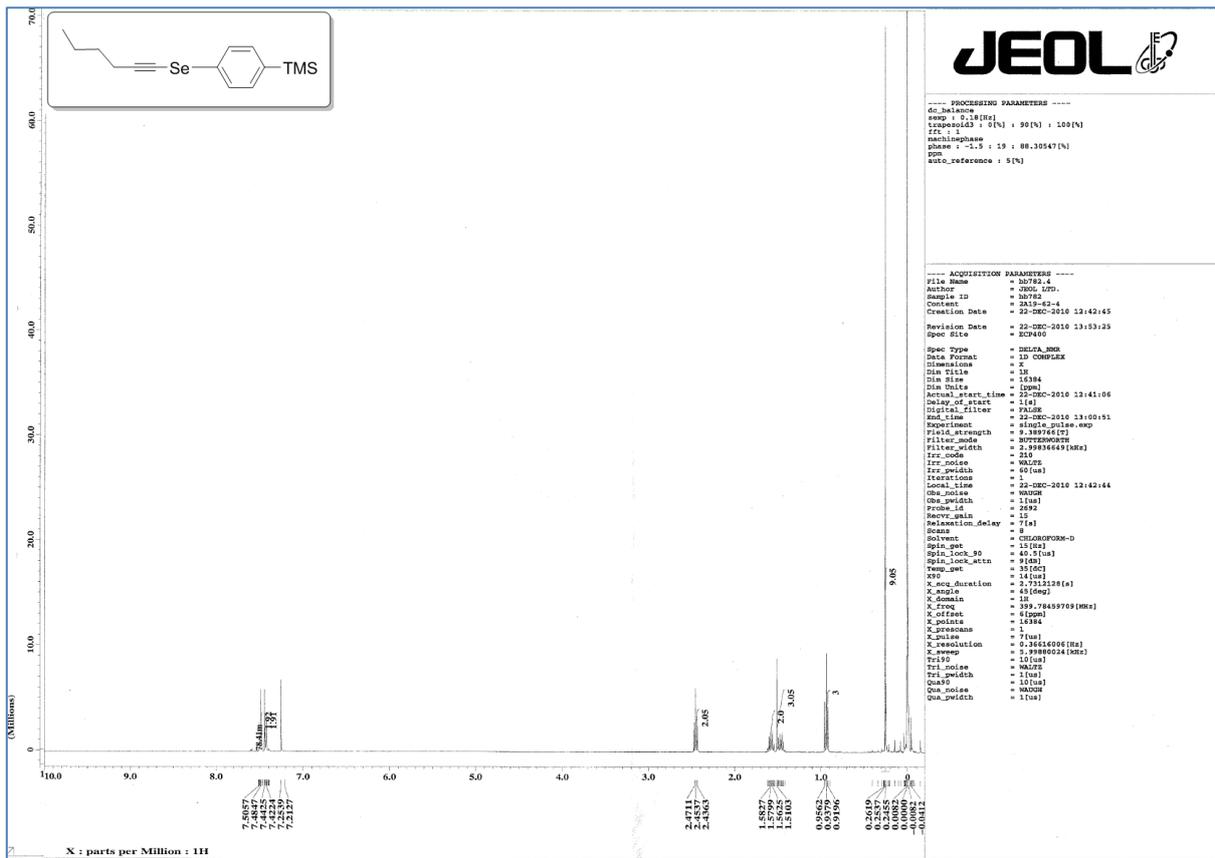
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Sample ID     = E7702
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Revision Date  = 24-NOV-2012 13:07:19
Spec Site    = SCV60

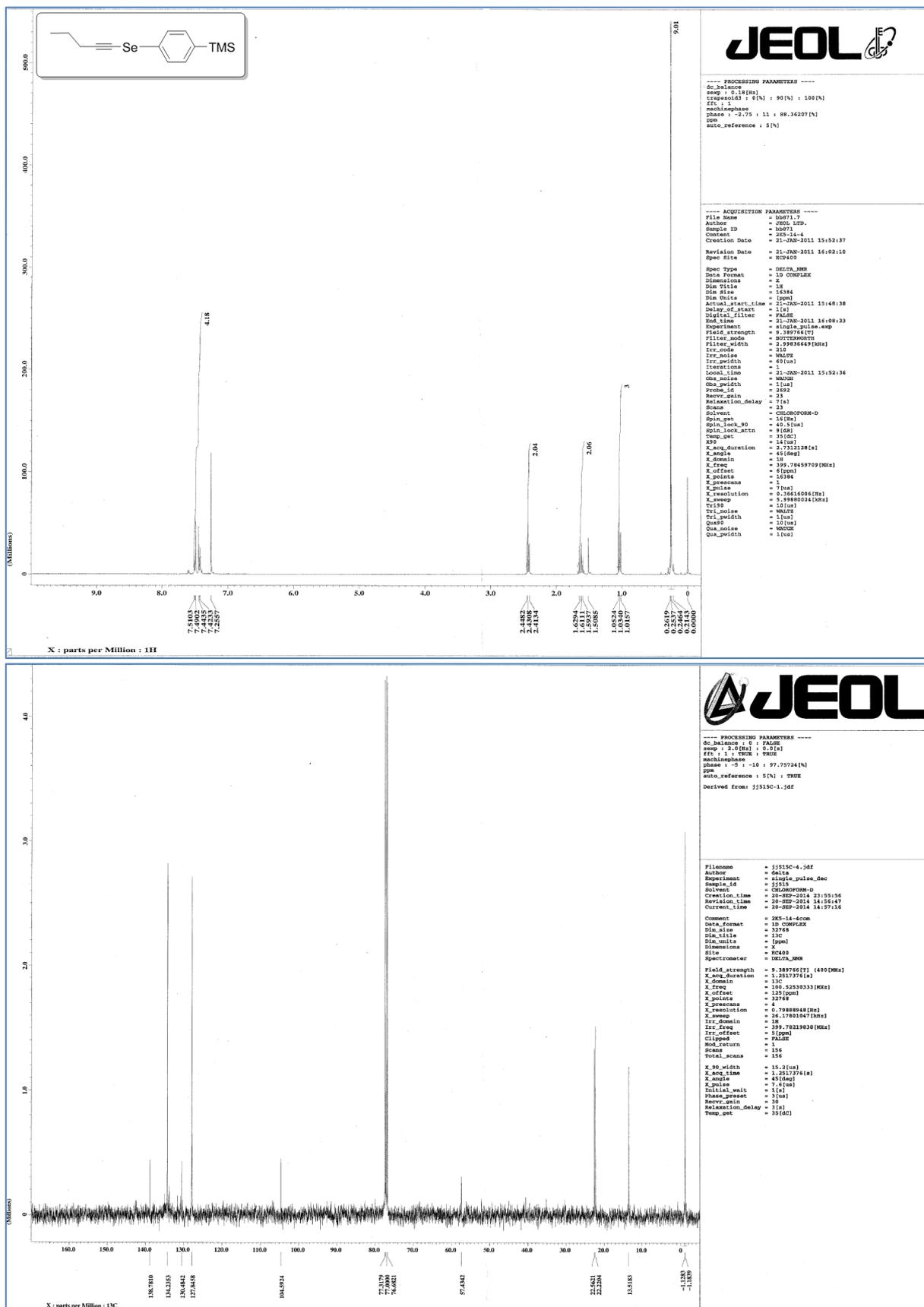
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Dir Units     = ppm
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Delay_of_start = 1(s)
Digital_Filter = FALSB
Exp_time      = 24-NOV-2012 19:07:48
Experiment    = single_pulse_2ec
Field_strength = 3.282746(T)
Filter_mode   = BUTTERWORTH
Filter_width  = 40.588748(Hz)
F1_code       = 210
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F1_freq       = 500.7941973(MHz)
F1_offset     = 0.00000
F1_resolution = 60(Hz)
F1_width      = 60(Hz)
F2_resolution = 1
Local_time   = 24-NOV-2012 13:48:24
Obs_noise    = WARDR
Obs_width    = 1(Hz)
Pulse_1d     = 2052
Recvr_gain   = 25
Relaxation_delay = 2(s)
Scales       = 801
Solvent      = CDCl3DMSO-D
Spin_get     = 16(Hz)
Spin_lock_90 = 40.5(Hz)
Spin_lock_atn = 9(Hz)
Temp_get     = 31(C)
XPD          = 10(Hz)
X_acq_duration = 30(Sec)
X_noise      = 77Se
X_offset     = 77Se
X_offset     = 600(ppm)
X_offset     = 65536
X_prescans   = 4
X_pulse      = 3.3333333(us)
X_resolution = 1.52596219(Hz)
X_sweep      = 100.0(Hz)
T1_rho       = 10(Hz)
T1_noise     = WARDR
T1_resolution = 1(Hz)
QNP5         = 10(Hz)
Obs_noise    = WARDR
Obs_width    = 1(Hz)

```

¹H and ¹³C NMR of 4b



¹H and ¹³C NMR of 4c



X : parts per Million : 1H

X : parts per Million : 13C

----- PROCESSING PARAMETERS -----

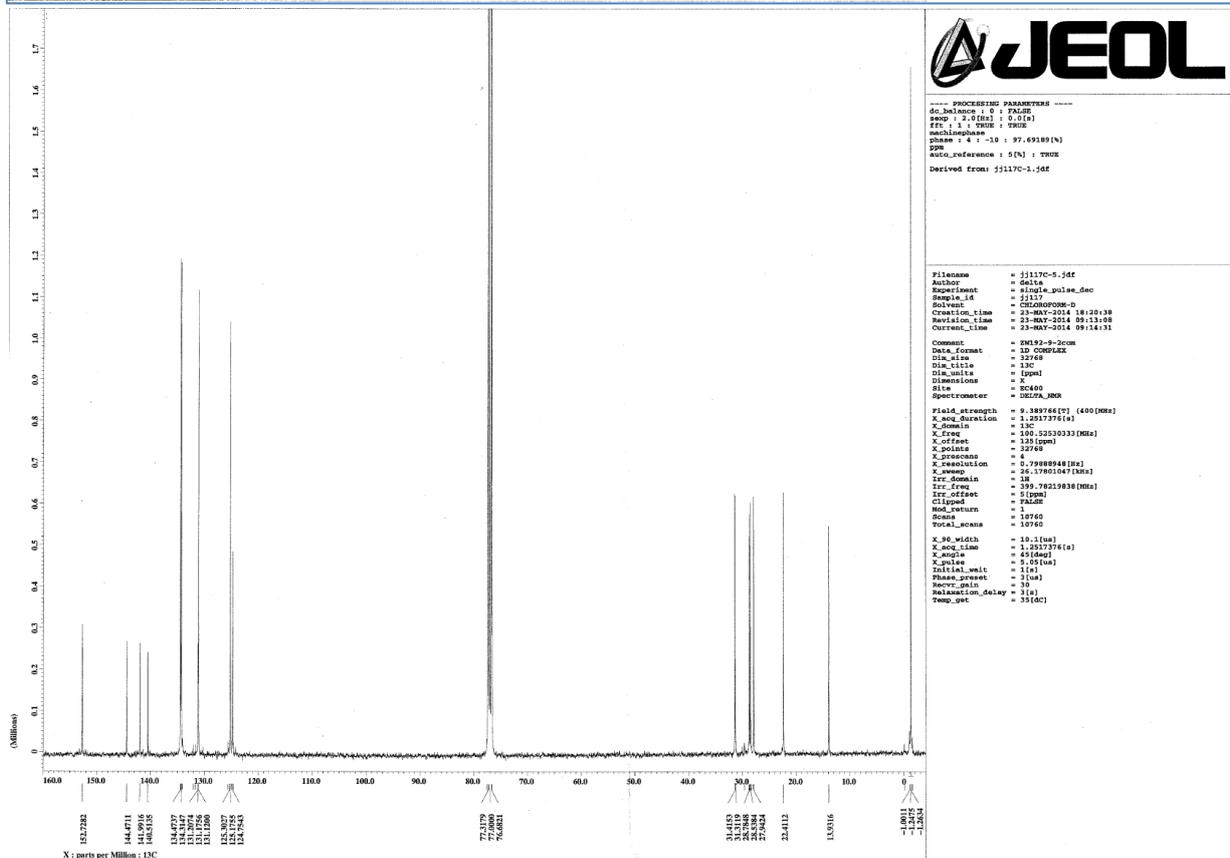
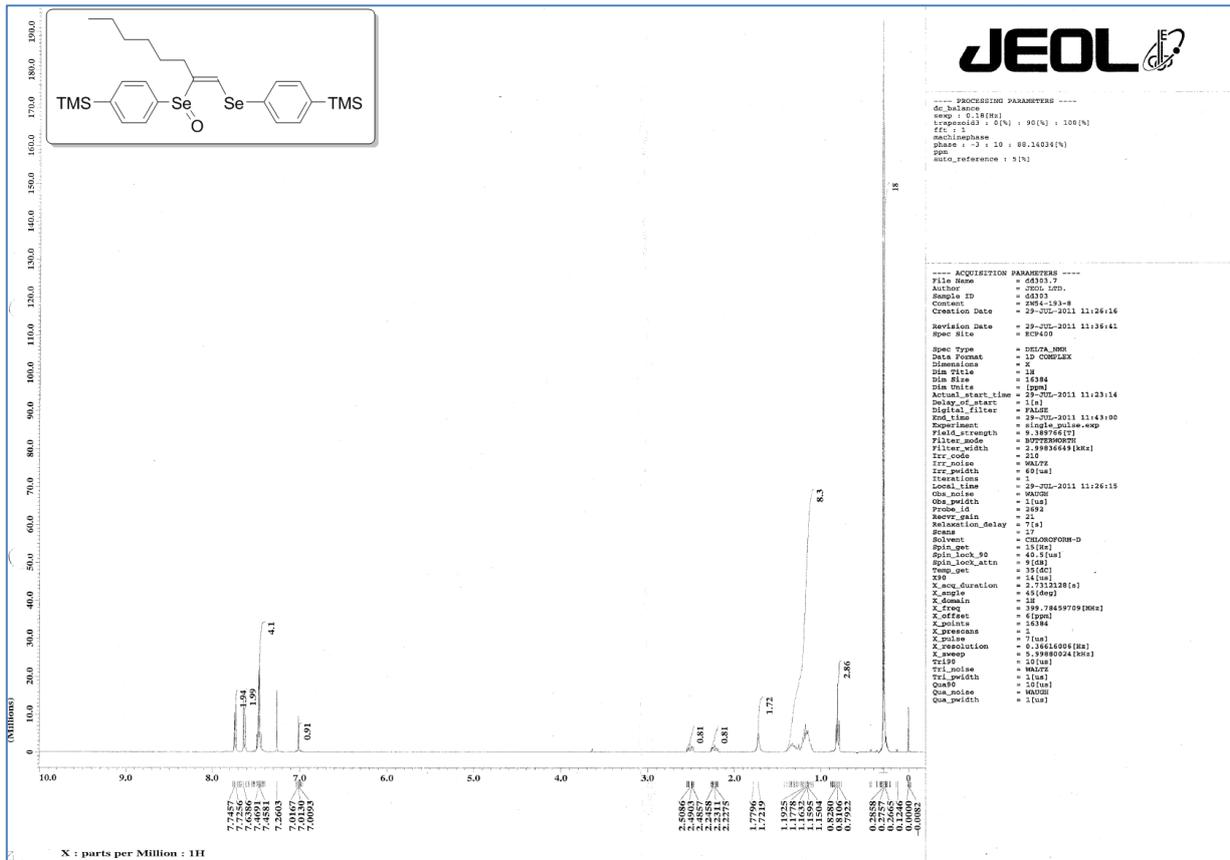
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 Date = 21-JAN-2011 15:55:56
 Revision = 16:02:10
 Site = RCP400

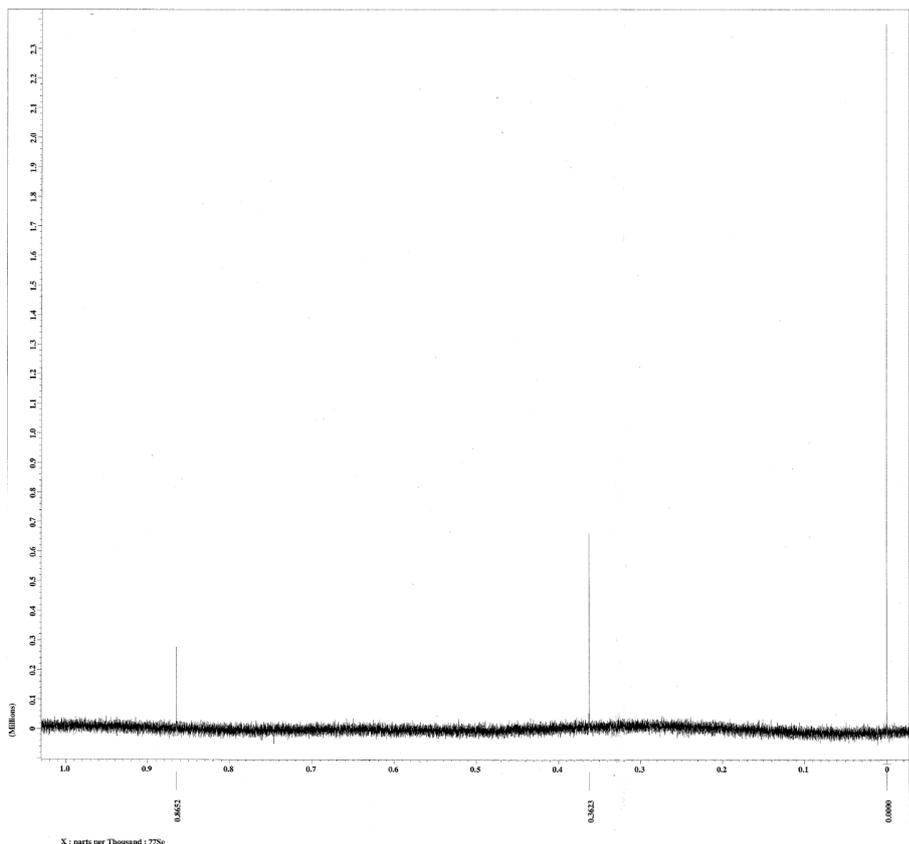
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 Filter Width = 2.99836649 [kHz]
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 Local Line = 1
 Obs Width = 1 [us]
 Phase = 0
 Recv Gain = 23
 Relaxation Delay = 7 [s]
 Scans = 23
 Solvent = CDCl3/FORM-D
 Spin Gas = 14 [Hz]
 Spin Lock 90 = 45 [us]
 Spin Lock Attn = 9 [dB]
 Temp Get = 30 [C]
 XFO = 2.32128 [s]
 X Acq Duration = 45 [sec]
 X Domain = 18
 X Freq = 399.7821938 [MHz]
 X Offset = 6 [Hz]
 X Pulse = 1684
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 X Pulse = 7 [us]
 X Resolution = 0.3661606 [Hz]
 X Sweep = 2.99836649 [kHz]
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 T1 Noise = WALTZ
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 Qua Noise = WALTZ
 Qua Width = 1 [us]

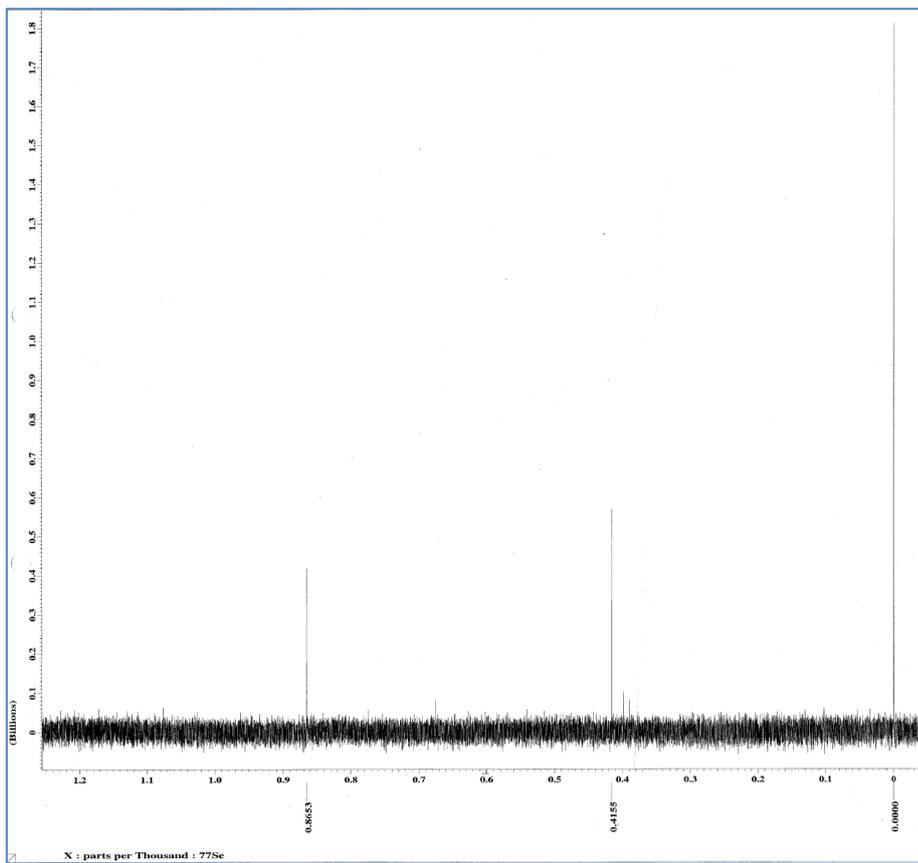
^1H , ^{13}C and ^{77}Se NMR of 6





----- PROCESSING PARAMETERS -----
 Acquisition : 0 : F4G5
 Date_ : 2-01-2013 : 0:01
 Exp : 1 : WWS : WWS
 MachinePhase :
 SW :
 Phase : 80 : -40 : 97.4259(N)
 Derived from: h1828e-1.jdf

Filename : h1828e-1.jdf
 Author :
 Experiment : single_pulse_2e
 Sample_ID : h1828
 Solvent : CHLOROFORM-D
 Creation_Time : 12-09-2013 19:57:00
 Revision_Time : 12-09-2013 10:47:05
 Current_Time : 12-09-2013 10:47:05
 Comment : 4C10-50-2...Se
 Data_Format : 13 COMPACT
 Dia_size : 5039
 Dia_title : 778e
 Dia_units : [ppm]
 Dimensions : X
 Site : MCA00
 Spectrometer : JEOL-NOX
 Field_strength : 9.39766(2) (400MHz)
 X_acq_duration : 0.8126464(s)
 X_domain : 778e
 X_freq : 96.2644292(MHz)
 X_offset : 501.000
 X_prescans : 4
 X_resolution : 1.3554975(Hz)
 X_sweep : 80.6451612(KHz)
 Ir_Scan : 25
 Ir_freq : 399.7821983(MHz)
 Ir_offset : 0.000
 clipped : TRUE
 Mod_pulses : 1
 Scans : 961
 Total_scans : 961
 X_xf_width : 10(Hz)
 X_acq_time : 0.8126464(s)
 X_angle : 30.000
 X_gain : 1.3333333(us)
 Initial_wait : 1(s)
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 Recv_gain : 25
 Relaxation_delay : 21(s)
 Temp_set : 35(OC)



X : parts per Thousand : 77Se



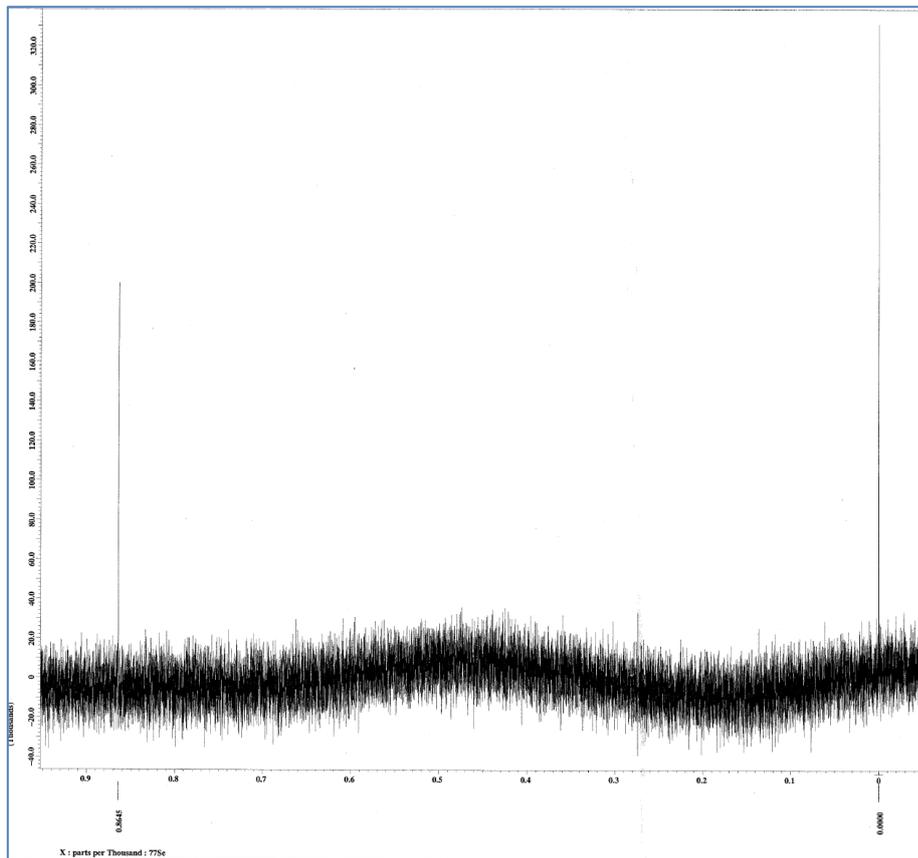
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 fit : 1
 machingphase
 ppm
 reference : -1.529 [ppm] : 0 [ppm]

----- ACQUISITION PARAMETERS -----
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 Author = JEOL LTD.
 Sample ID = 442456-13..._86-COM
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 Spec Type = INSLA_NMR
 Date Format = DD MONTH
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 Dim Title = 77Se
 Dim Size = 65536
 Dim Units = [ppm]
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 Delay_of_start = 1181
 Digital_filter = FALSO
 End_time = 30-OCT-2012 08:07:09
 Experiment = slmcp_gmsa_6ac
 Field_strength = 11.7473579 [T]
 Filter_mode = HERTZBURG
 Filter_width = 62.0021671 [kHz]
 Irf_freq = 154
 Irf_solmn = 18
 Irf_freq = 500.16241602 [MHz]
 Irf_solnt = WALTZ
 Irf_offset = 5.9 [ppm]
 Irf_swidth = 45 [us]
 Iterations = 0
 Local_time = 30-OCT-2012 08:56:59
 Obs_noise = WANDR
 Obs_swidth = 11081
 Probe_id = 2692
 Recv_gain = 23
 Relaxation_delay = 2161
 scans = 2600
 Solvent = CHLOROFORM-D
 Spin_get = 13 [us]
 Spin_lock_90 = 40 [us]
 Spin_lock_attn = 30 [dB]
 Temp_get = 35 [C]
 TSP = 10 [us]
 X_ang_duration = 0.324888 [s]
 X_ang = 30 [deg]
 X_solmn = 77Se
 X_freq = 95.44814551 [MHz]
 X_offset = 650 [ppm]
 X_points = 65536
 X_pvsolmn = 4
 X_pulse = 3.3333333 [us]
 X_resolution = 1.5073774 [Hz]
 X_sweep = 125.0 [kHz]
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 Qus9_noise = WANDR
 Qus9_swidth = 1 [us]

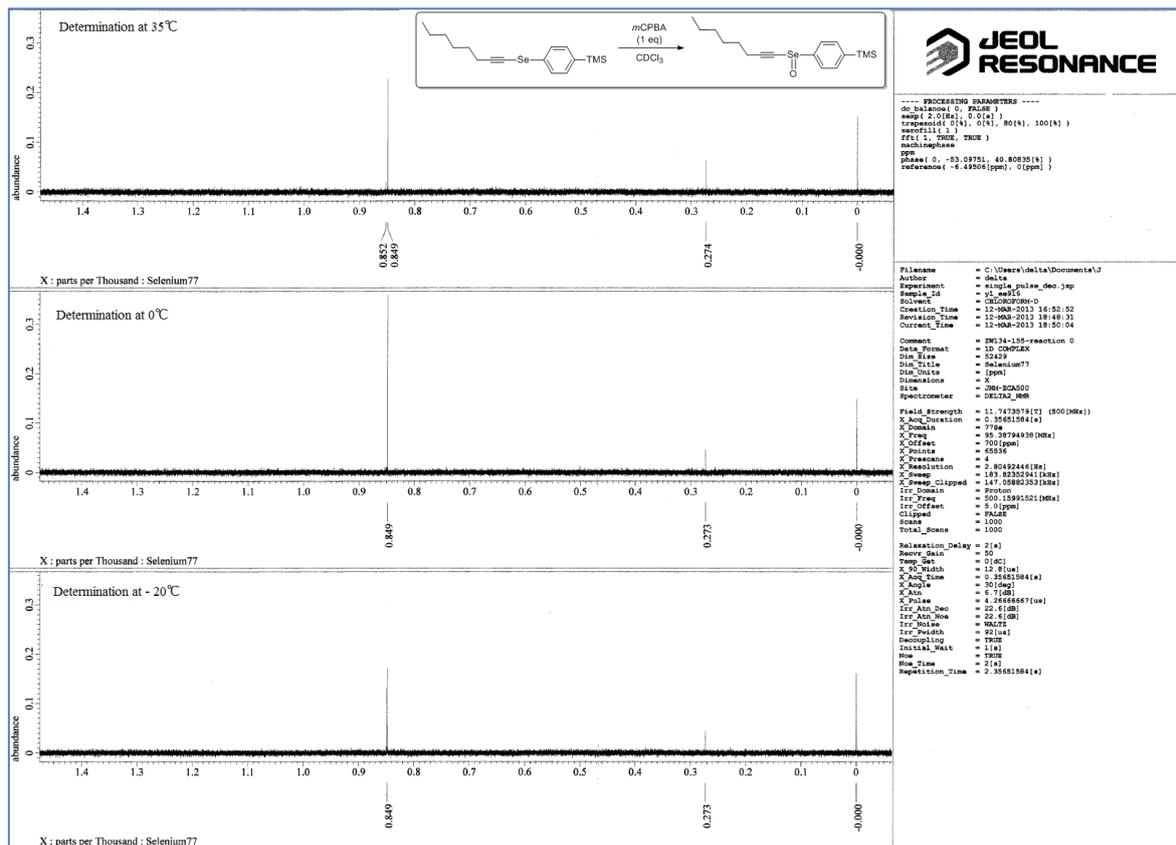


----- PROCESSING PARAMETERS -----
dc_balance : 0 : FALSE
freq : 3 : 770.0 : 0.0100
f1 : 1 : 770.0 : 0.0100
machinename :
Phase : 23 : -40 : 95.21633 [N]
PPM :
ppm_reference : 0 [N] : 7700
reference : 0.001 [ppm] : 0 [ppm]
Derived from : j52839e-2.jdf

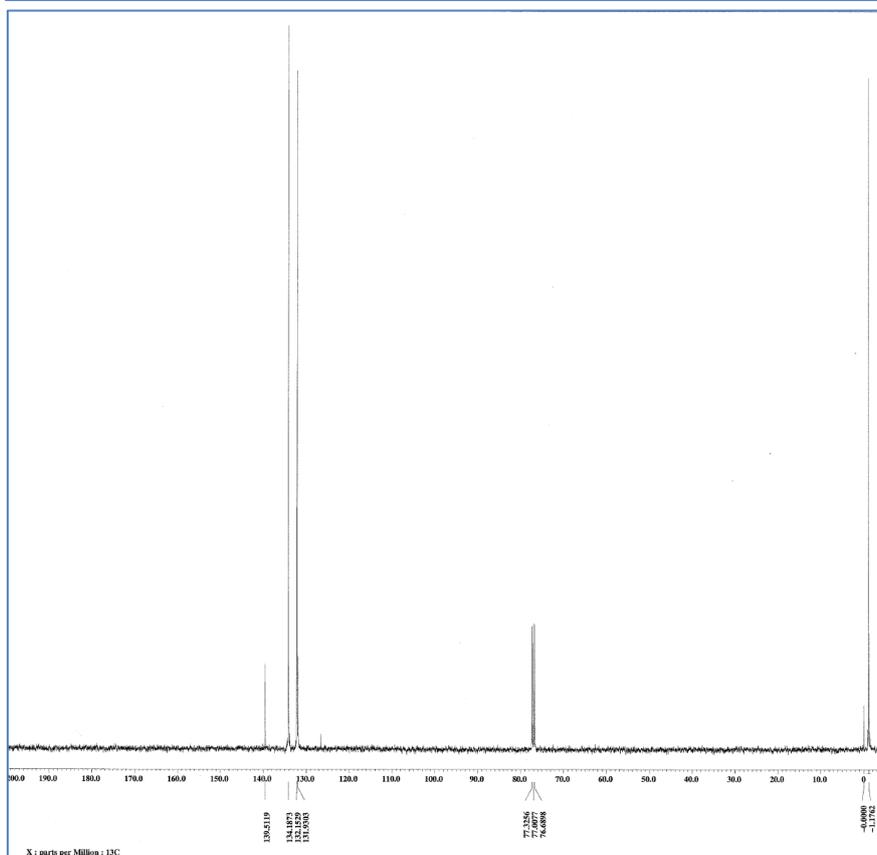
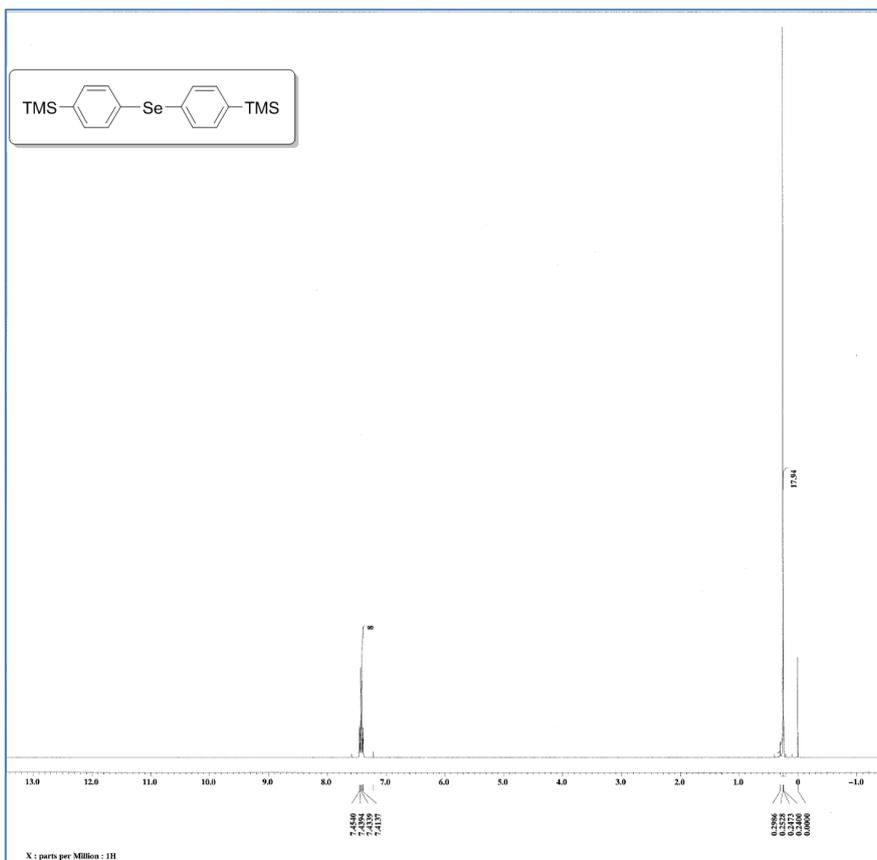
Filename : j52839e-14.jdf
Author : delta
Experiment : single_pulse_sec
Sample_id : j5283
Solvent : CDCl3
Creation_time : 28-JUN-2014 02:31:49
Revision_time : 27-JUN-2014 17:24:23
Current_time : 27-JUN-2014 17:24:44
Comment : SWH5-34-1...se
Data_format : 3D COMPLEX
Dia_size : 5536
Dia_unit : 770
Dia_units : [ppm]
Dimension : 2
Site : EC40
Spectrometer : MSL500-MR
Field_strength : 4.389766 [T] (400 [MHz])
X_acq_duration : 0.8585216 [s]
X_domain : 770
X_freq : 76.2644229 [MHz]
X_offset : 450 [ppm]
X_points : 6556
X_precision : 4
X_resolution : 3.14479306 [Hz]
X_sampling : 76.3388766 [Hz]
F1_domain : 10
F1_freq : 399.7821938 [MHz]
F1_offset : 0 [ppm]
Clipped : FALSE
Mag_return : 1
Scans : 540
Total_scans : 540
X_90_width : 10 [us]
X_acq_time : 0.8585216 [s]
X_angle : 90 [deg]
X_pulse : 3.3333333 [us]
Initial_wait : 1 [s]
Phase_preset : 1 [us]
Recvr_gain : 20
Relaxation_delay : 1 [s]
Temp_set : 30 [C]

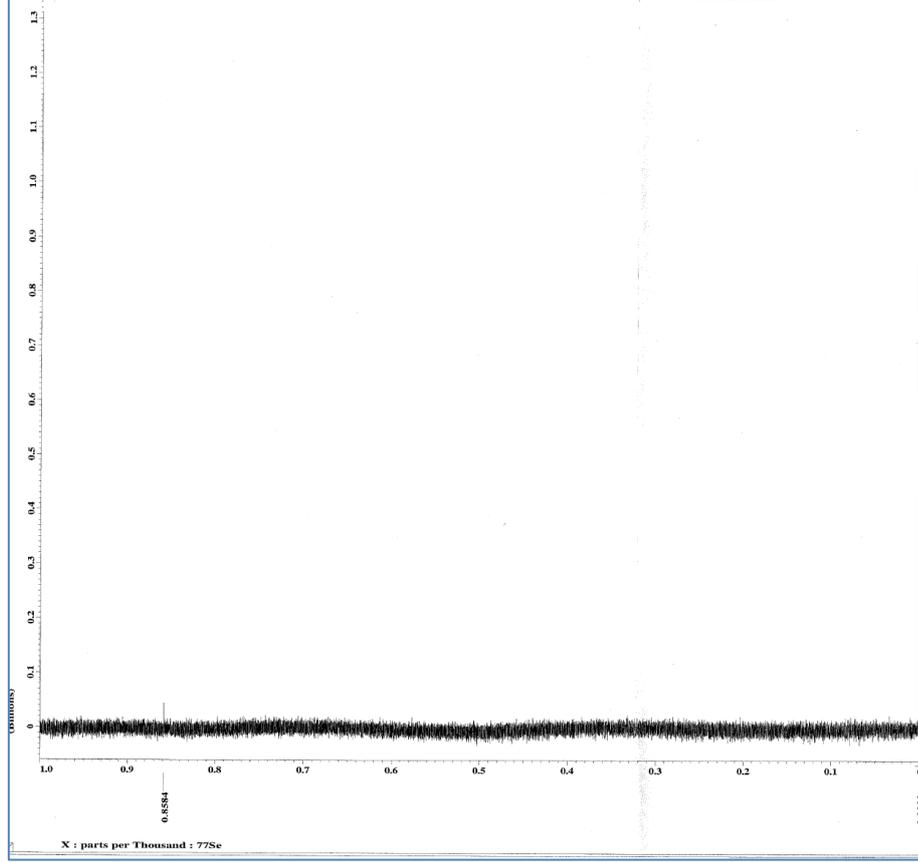


⁷⁷Se NMR of reaction mixture of 8a



^1H and ^{13}C NMR of S1

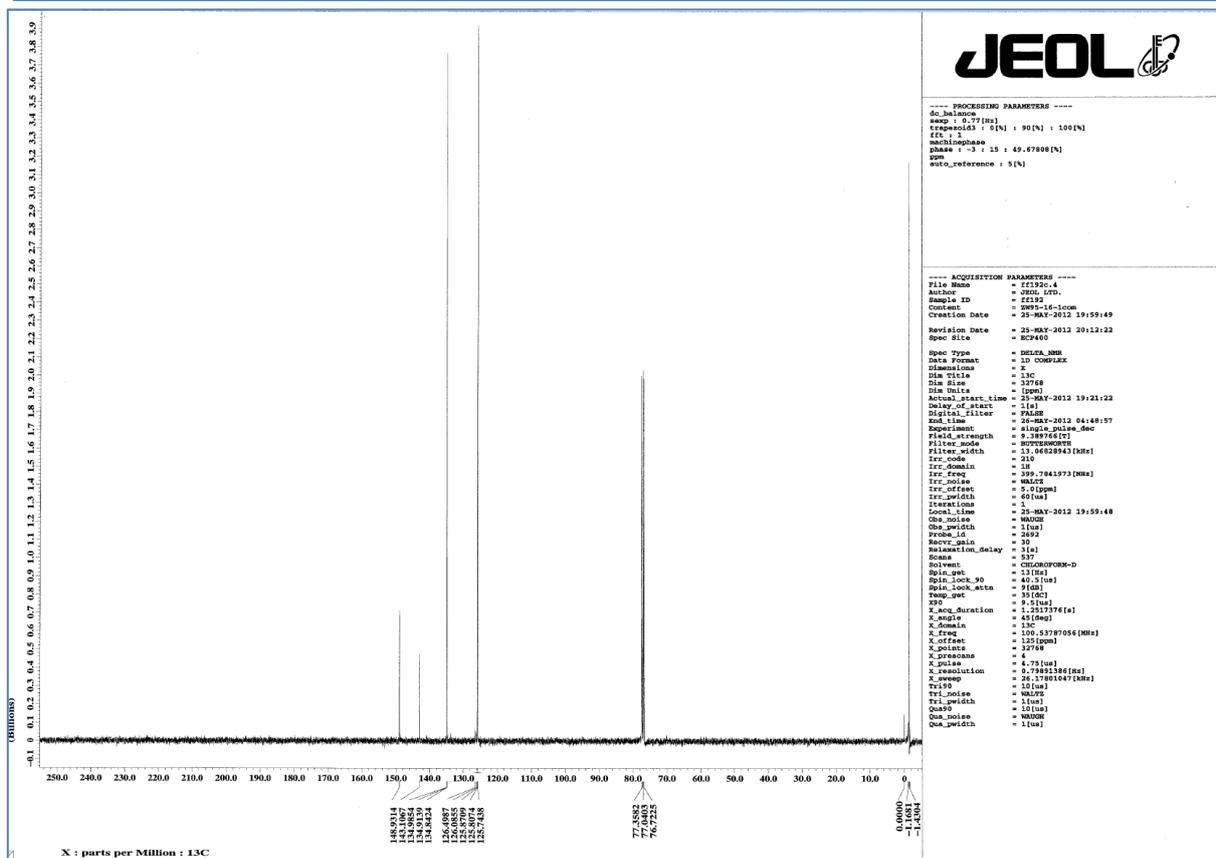
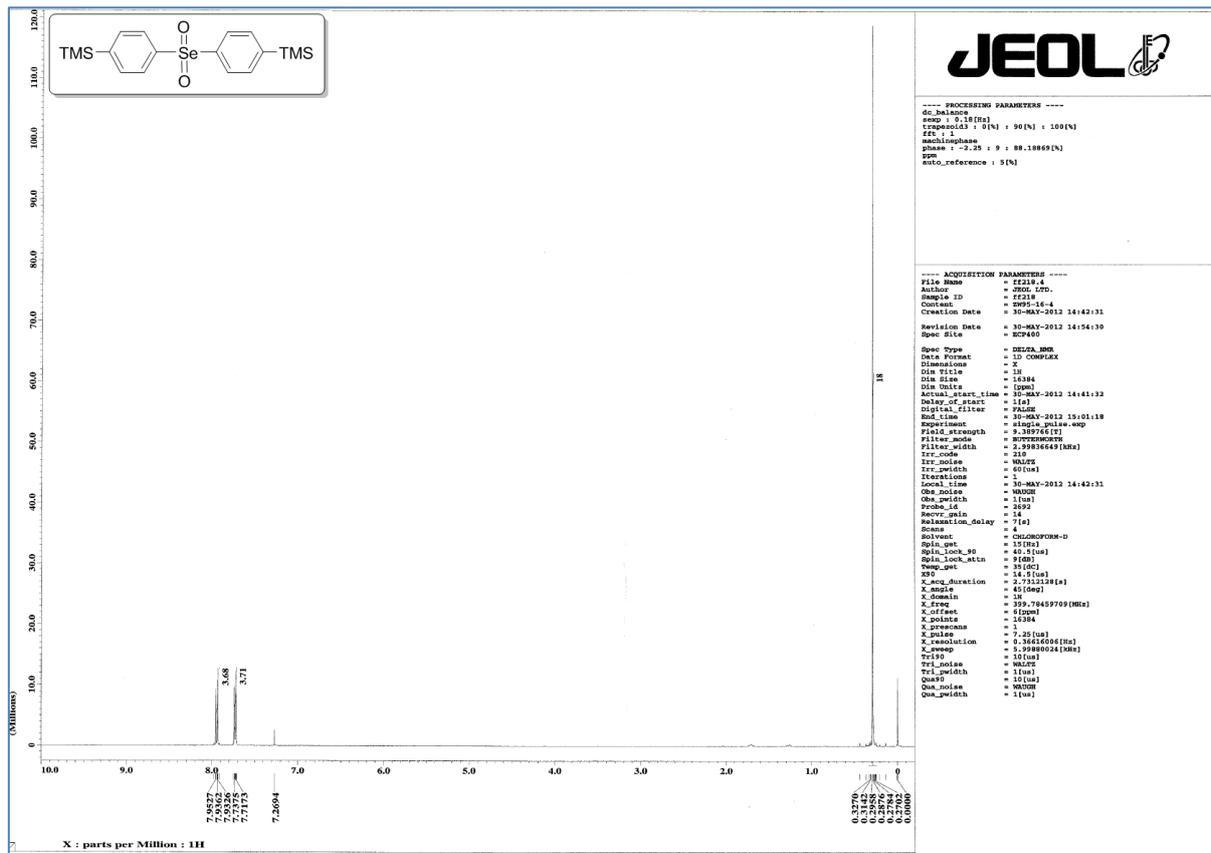




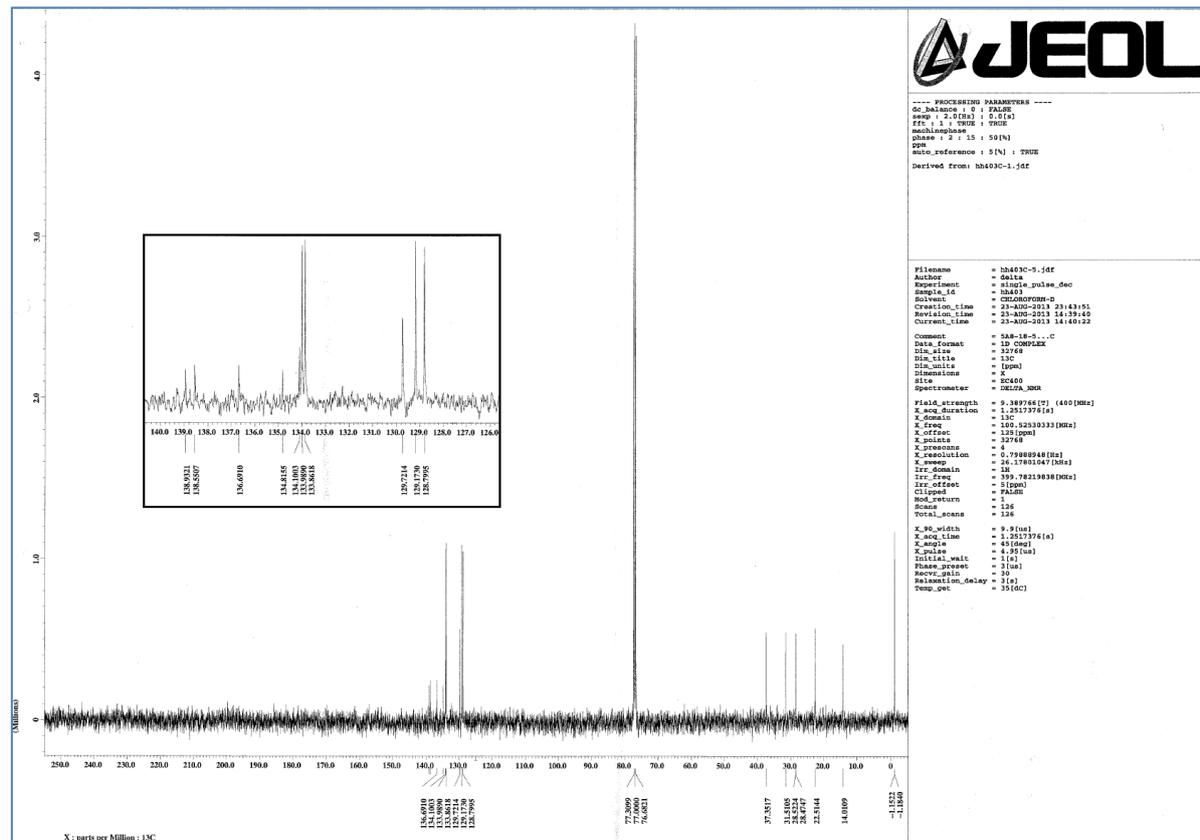
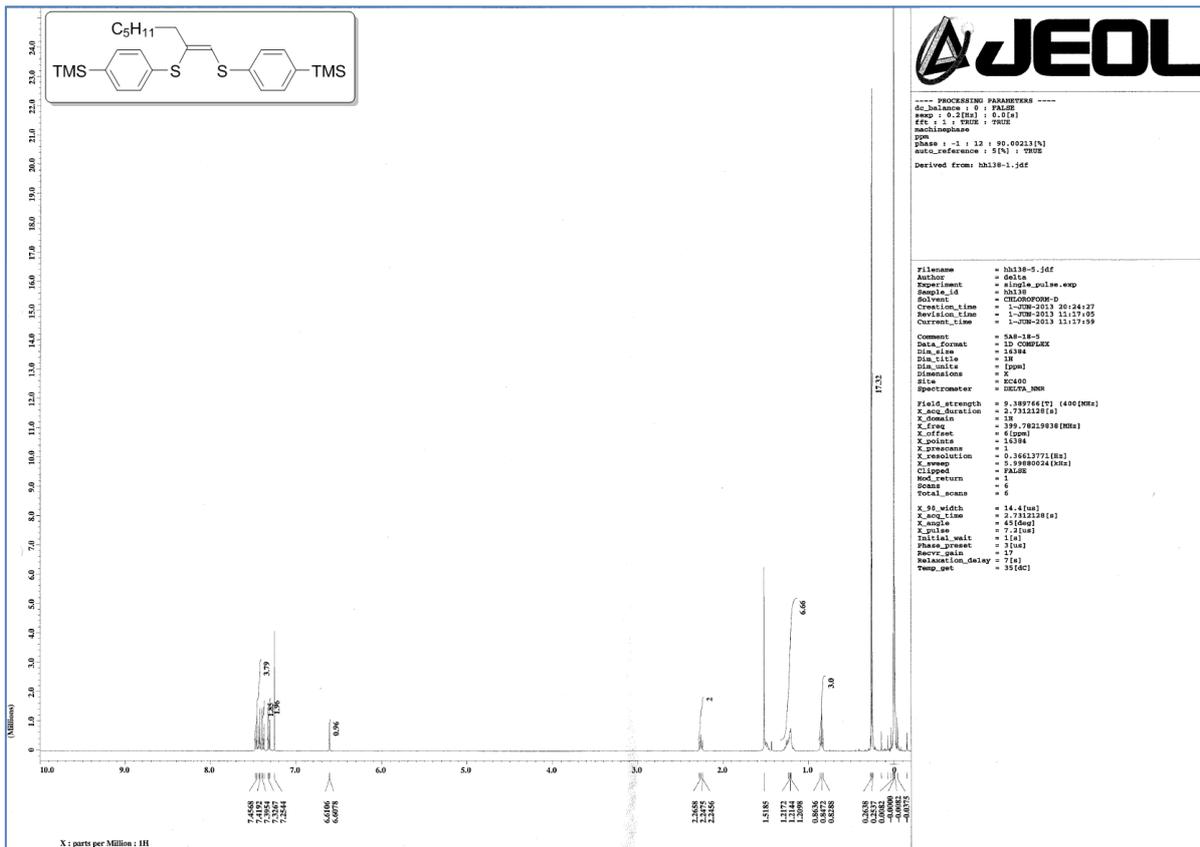
----- PROCESSING PARAMETERS -----
dc_bkspcra
smp1 : 0.77[Hz]
tprpsol03 : 0[Hz] : 90[Hz] : 100[Hz]
f1c : 1
mchlinep04wa
Phase : 0 : 0 : 95.89991[Hz]
ppm
reference : -1.649[ppm] : 0[ppm]

----- ACQUISITION PARAMETERS -----
File Name = f2644a-10
Author = JEOL CRT
Sample ID = f2644
Content = 2MS3-218-4...Se
Creation Date = 7-NOV-2012 16:26:08
Revision Date = 8-NOV-2012 02:40:00
Spec Site = RCP410
Spec Type = DELTA_NMR
Data Format = ID COMPLEX
Dimensions = X
Dir file = 77se
Dir file = 65536
Dir units = [ppm]
Actual_start_time = 7-NOV-2012 15:31:17
End_time = 7-NOV-2012 11:26:25
Digital_filter = PALSI
Inp_of_start = 1[Hz]
Experiment = single_pulse_6ec
Field_strength = 9.18716[Hz]
Filter_mode = BUTTERWORTH
Filter_width = 49.338749[Hz]
Irr_code = 210
Irr_domain = 18
Irr_freq = 399.7641973[MHz]
Irr_noise = WARM
Irr_offset = 5.0[ppm]
Irr_width = 60[Hz]
Iterations = 1
Lock_time = 7-NOV-2012 16:26:07
Obs_noise = WARM
Obs_width = 1[Hz]
Pulse_id = 2092
Recvr_gain = 23
Relaxation_delay = 21[us]
Scans = 1233
Solvent = CDCl3/FORM-D
Spin_get = 13[Hz]
Spin_lock_90 = 40.5[us]
Spin_lock_attn = 91[us]
Temp_get = 38[Hz]
X0 = 10[us]
X_acq_duration = 0.65316[us]
X_angle = 30[deg]
X_domain = 77se
X_freq = 76.29019704[MHz]
X_offset = 600[ppm]
X_points = 65536
X_pulse = 4
X_pulse = 3.3333333[us]
X_resolution = 1.3190218[Hz]
X_sweep = 100.0[MHz]
Z190 = 10[us]
Z1_pulse = WARM
Z1_width = 1[Hz]
Z190 = 15[us]
Z190_noise = WARM
Z190_width = 1[us]

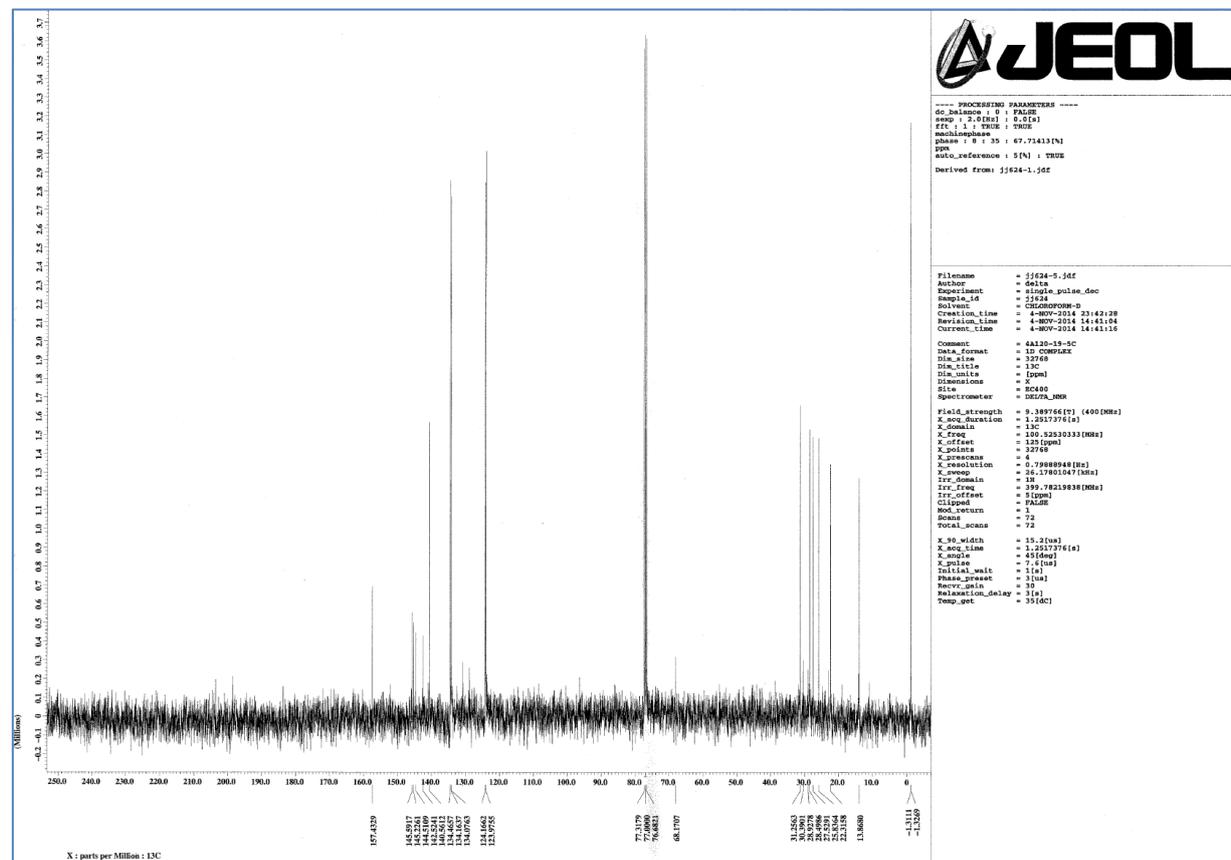
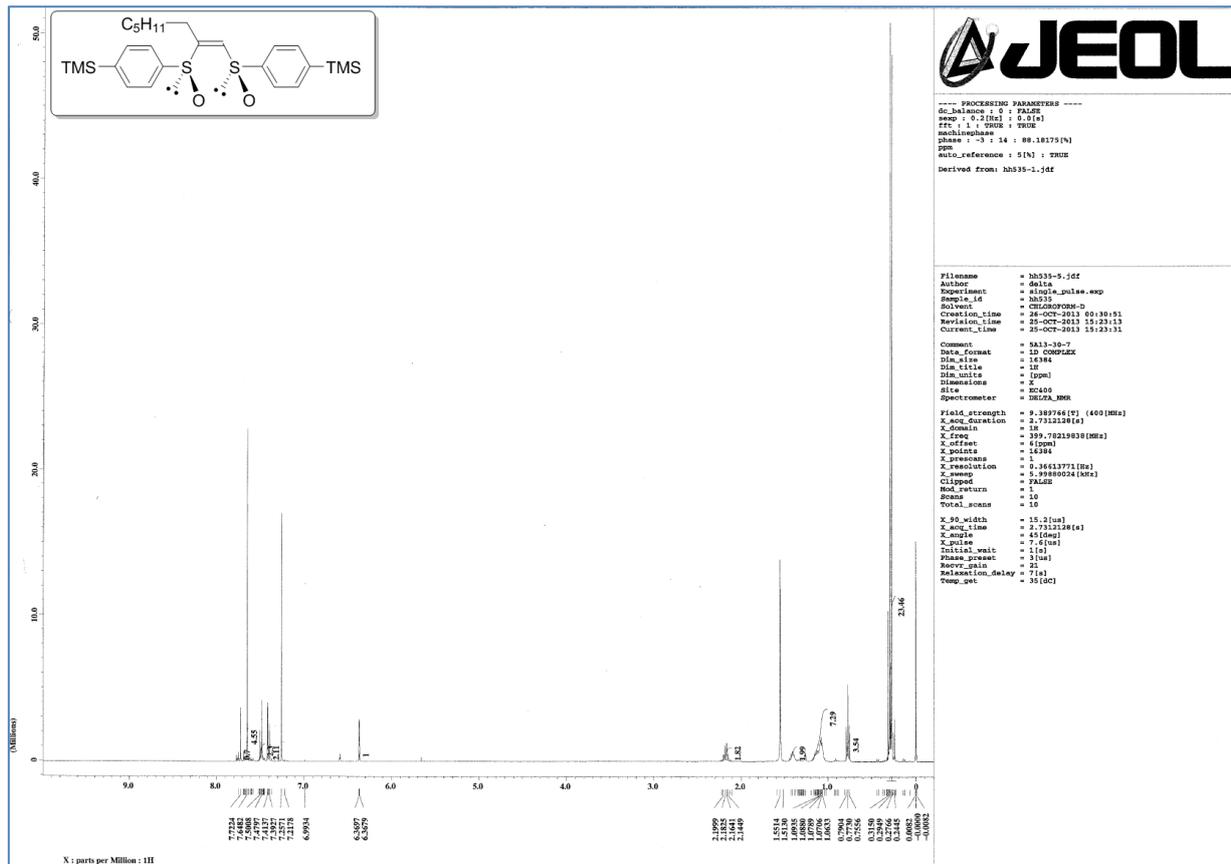
^1H , ^{13}C and ^{77}Se NMR of 10



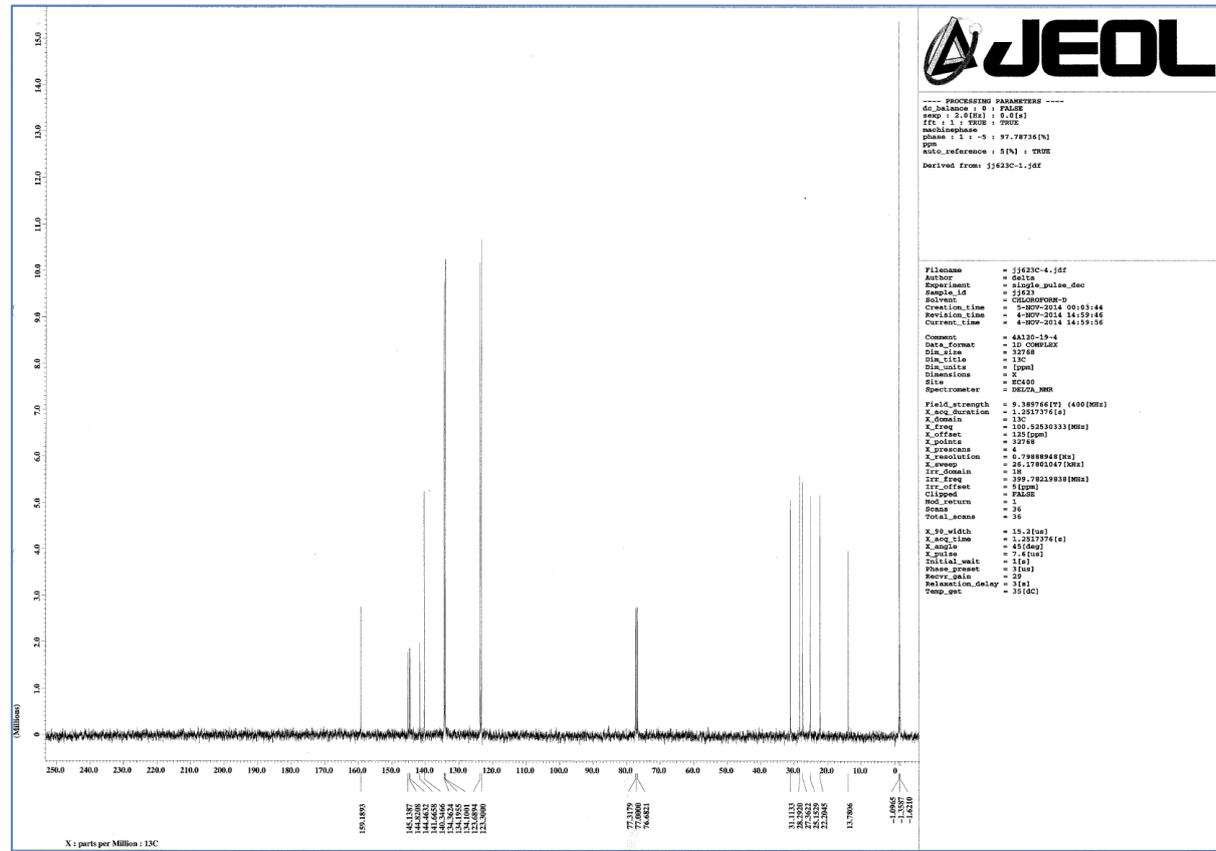
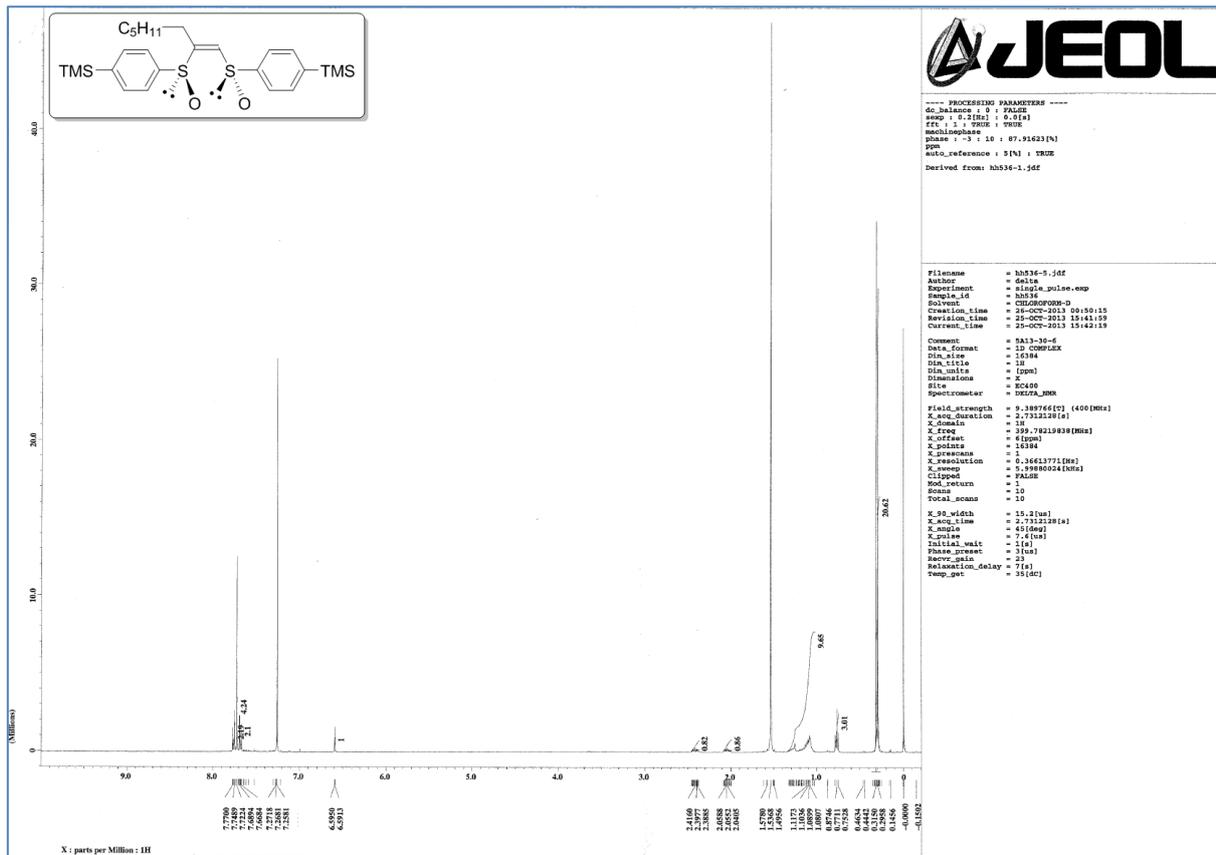
¹H and ¹³C NMR of 14



^1H and ^{13}C NMR of 15



¹H and ¹³C NMR of 15'



¹H and ¹³C NMR of 17

