

Supporting information

Organocatalytic dynamic kinetic resolution *via* conjugate addition: synthesis of chiral *trans*-2, 5-dialkylcyclohexanones.

Ganesh Pandey*^a, Priyanka Adate^a, Vedavati G. Puranik^b

^a *Dr. Ganesh Pandey, Division of Organic chemistry, National Chemical Laboratory, Pune-411 008 (India),
Fax: (+91) 202590-2628
E-mail: gp.pandey@ncl.res.in*

^b *Dr. Vedavati G. Puranik (Crystallographer), Centre for Material Characterization, National Chemical Laboratory
Pune-411 008 (India)*

General procedure for synthesis of enone starting from corresponding ketone¹: To a cold (-78°C) solution of ketone (2.0 mmol, 1.0 equiv.) in THF (20 mL) was added LiHMDS (5.0 mmol, 2.5equiv. 1.0 M in hexanes) dropwise over period of 10 min. After stirring for 30 min. at same temperature, TMSCl (5.0 mmol, 2.5 equiv.) was added drop wise over period of 5 min and reaction mixture was stirred for another 30 min, and then warmed to room temperature. Upon disappearance of the starting material (checked by TLC), the reaction mixture was poured in water (10 mL), and the biphasic reaction mixture was extracted with EtOAc (3 × 20 mL), and the combined organic layers were washed with brine (1 × 20 mL), and concentrated. The crude TMS enol ether was vacuum-dried to minimize the amount of (TMS)₂O present, as this was known to be detrimental for the desired reaction. IBX and MPO (4.0 equiv.) were dissolved in DMSO (0.4 M) in an equimolar ratio at room temperature. The IBX.MPO solution was added in one portion at ambient temperature to the crude TMS enol ether dissolved in a minimum of DMSO. Reaction mixture was stirred vigorously, and progress was monitored by means of thin-layer chromatography. Upon completion, the reaction mixture was diluted with aqueous NaHCO₃ (5%) and extracted with EtOAc (3 times). The combined organic phase was filtered through a pad of celite and washed with saturated aqueous NaHCO₃, water, and brine. After drying over anhy. NaSO₄, the solvent was removed in vacuum to yield the crude product, which was further purified further by means of column chromatography.

Ethyl 3-(8-oxo-1,4-dioxaspiro[4.5]dec-9-en-7-yl)propanoate 6: yellow solid, yield = 95%, M.P. = 55°C, IR (ν_{\max} cm⁻¹ CHCl₃): 2981, 3892, 1731, 1683, 1421, 1447, 1380, 1252, 1195, 1096, 1031, 949. ¹H NMR (400 MHz, CDCl₃) δ ppm: 1.26 (t, J = 7.1 Hz, 3 H), 1.75 (d, J = 6.3 Hz, 1 H), 2.00 - 2.08 (m, 1 H), 2.11 - 2.23 (m, 2 H), 2.38 - 2.46 (m, 2 H), 2.68 - 2.78 (m, 1 H), 3.94 - 4.18 (m, 6 H), 5.99 (d, J = 10.0 Hz, 1 H), 6.56 (dd, J = 10.2, 1.9 Hz, 1 H). ¹³C NMR (50 MHz, CDCl₃) δ ppm: 14.2, 24.7, 31.6, 38.6, 43.6, 60.4, 64.9, 65.2, 104.2, 130.2, 145.2, 173.3, 200.2. **m/z:** 409.14 (M + Na, 100), 387.2 (M+H, 25), 341(45), 249 (16), 241(22).

5-allylcyclopent-2-enone 7: colourless liquid, yield = 75%, IR (ν_{\max} cm⁻¹ CHCl₃): 3019, 2983, 1701, 1588, 1429, 1215, 1046, 755, 669. ¹H NMR (500 MHz, CDCl₃) δ ppm: 2.10 - 2.18 (m, 1 H), 2.37 - 2.45 (m, 2 H), 2.50 - 2.58 (m, 1 H), 2.79 - 2.87 (m, 1 H), 4.98 - 5.14 (m, 2 H), 5.74 (ddt, J = 17.0, 10.1, 6.9 Hz, 1 H), 6.10 - 6.24 (m, 1 H), 7.63 - 7.76 (m, 1 H). ¹³C NMR (126

MHz, CDCl₃) δ ppm: 34.8, 35.2, 43.9, 116.9, 133.7, 135.1, 163.8, 211.6. **m/z**: 145.46 (M + Na, 100), 123.16 (M+H, 25).

6-allylcyclohex-2-enone 8: pale yellow liquid, yield = 90%, **IR** (ν_{\max} cm⁻¹ CHCl₃): 2930, 2862, 1677, 1639, 1388, 1222, 912. **¹H NMR** (500 MHz, CDCl₃) δ ppm: 1.68 – 1.82 (m, 1H), 2.07 - 2.17 (m, 2 H), 2.31 - 2.41 (m, 3 H), 2.59 - 2.66 (m, 1 H), 5.02 - 5.09 (m, 2 H), 5.73 - 5.83 (m, 1 H), 6.00 (dt, J = 9.99, 1.72 Hz, 1 H), 6.91 - 6.98 (m, 1 H). **¹³C NMR** (50 MHz, CDCl₃) δ ppm: 25.2, 27.3, 33.6, 46.1, 116.7, 129.5, 136.1, 149.8, 200.9. **m/z**: 159.15 (M + Na, 100), 137.45 (M+H, 25).

7-allylcyclohept-2-enone 9: colourless liquid, yield = 87%, **IR** (ν_{\max} cm⁻¹ CHCl₃): 3017, 2931, 1705, 1454, 1216, 1048, 915, 755, 667. **¹H NMR** (400 MHz, CDCl₃) δ ppm 1.43 - 1.53 (m, 1 H), 1.65 - 1.75 (m, 1 H), 1.84 - 1.98 (m, 2 H), 2.05 - 2.19 (m, 1 H), 2.39 - 2.50 (m, 2 H), 2.52 - 2.61 (m, 1 H), 2.63 - 2.74 (m, 1 H), 4.97 - 5.09 (m, 2 H), 5.77 (ddt, J = 17.0, 10.1, 6.9, 6.9 Hz, 1 H), 5.99 - 6.07 (m, 1 H), 6.61 (ddd, J = 11.7, 6.6, 4.5 Hz, 1 H). **¹³C NMR** (101 MHz, CDCl₃) δ ppm: 25.2, 28.7, 29.8, 35.7, 51.6, 116.6, 132.7, 136.4, 146.0, 205.2. **m/z**: 183.16 (M + Na, 100), 151.49 (M + H, 51).

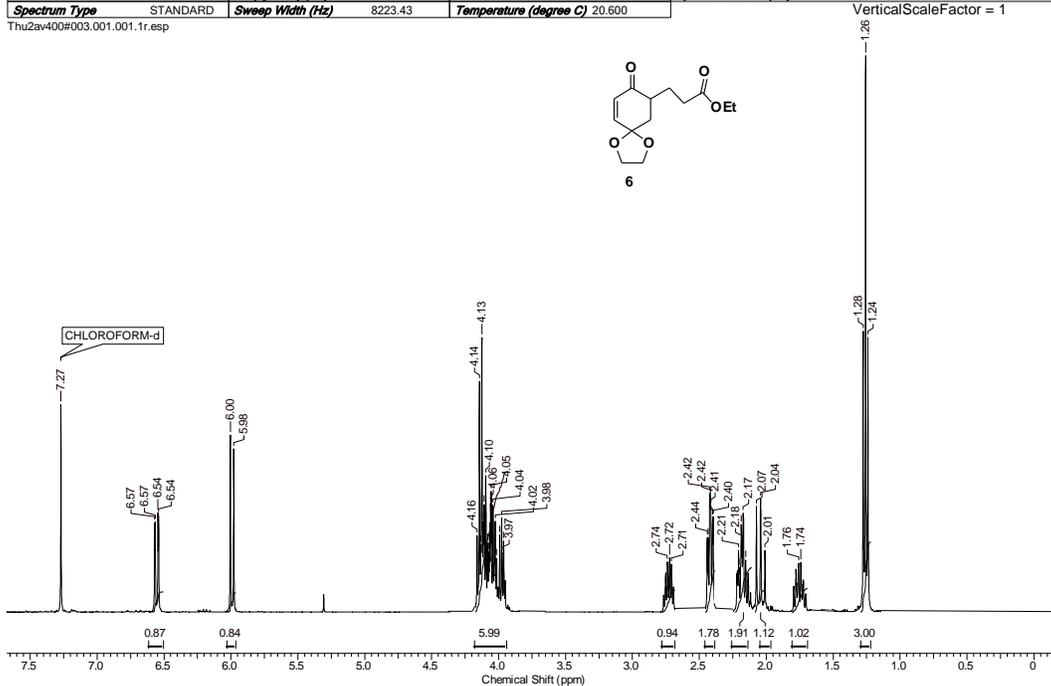
9-(((tert-butyldimethylsilyl)oxy)methyl)-1,4-dioxaspiro[4.5]dec-6-en-8-one 11: yield = 95%, colourless liquid, **IR** (ν_{\max} cm⁻¹ CHCl₃): 3583, 3444, 2957, 2930, 1683, 1216, 1141, 758. **¹H NMR** (400 MHz, CDCl₃) δ ppm: 0.05 (d, J = 2.0 Hz, 6 H), 0.87 (s, 9 H), 2.21 - 2.31 (m, 2 H), 2.73 - 2.82 (m, 1 H), 3.81 - 3.88 (m, 1 H), 3.91 - 4.00 (m, 2 H), 4.01 - 4.15 (m, 3 H), 5.99 (d, J = 10.0 Hz, 1 H), 6.60 (dd, J = 10.0, 1.7 Hz, 1 H). **¹³C NMR** (101 MHz, CDCl₃) δ ppm: 5.5, 18.2, 25.8, 35.5, 46.6, 61.4, 64.8, 65.1, 104.5, 130.5, 145.9, 198.8. **m/z**: 321.1((M + Na, 100), 310.3 (4), 283.1 (1).

Ethyl 3-(2-oxocyclohex-3-en-1-yl)propanoate 12: colourless liquid, **IR** (ν_{\max} cm⁻¹ CHCl₃): 2934, 1732, 1676, 1425, 1388, 1177, 1032. **¹H NMR** (500 MHz, CDCl₃) δ ppm: 1.25 (J = 7.2, 3 H), 1.67 - 1.81 (m, 2 H), 2.07 - 2.18 (m, 2 H), 2.31 - 2.44 (m, 5 H), 4.12 (q, J = 7.1 Hz, 2 H), 5.98 (dt, J = 10.1, 1.9 Hz, 1 H), 6.89 - 6.96 (m, 1 H). **¹³C NMR** (126 MHz, CDCl₃) δ ppm: 14.1, 24.7, 25.2, 28.1, 31.8, 45.7, 60.3, 129.4, 149.5, 173.5, 201.1. **m/z**: 219.15 (M + Na, 100), 197.56 (M + H).

^1H and ^{13}C spectra of new compounds

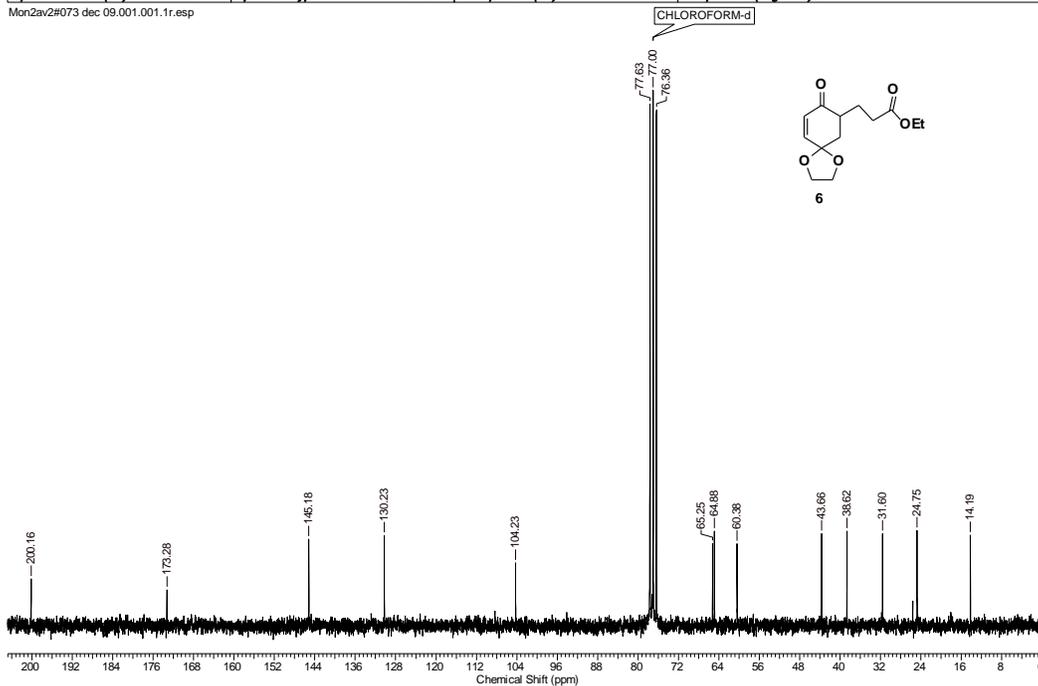
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H	Date	10 Dec 2009 16:38:32
Date Stamp	10 Dec 2009 16:38:32	File Name	\\172.16.2.18\mr_data\AV400\DEC_09\Thu2av400#003\1\pdata\1\1r		
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	287.00	SW(cyclical) (Hz)	8223.68	Solvent	DMSO-d6
Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43	Temperature (degree C)	20.600
				Spectrum Offset (Hz)	2465.3613

Thu2av400#003.001.001.1r.esp VerticalScaleFactor = 1

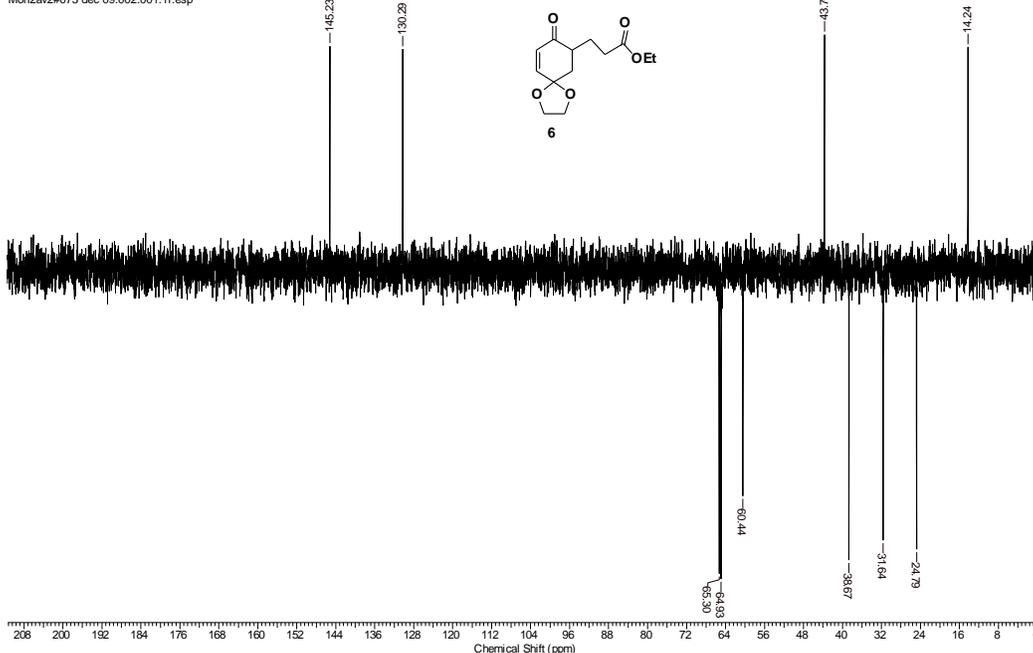


Acquisition Time (sec)	1.3664	Comment	Priyanka	Date	08 Dec 2009 05:09:28
Date Stamp	08 Dec 2009 05:09:28	File Name	E:\paper-1\DATA\substrate 1\Mon2av2#073 dec 09\1\pdata\1\1r		
Frequency (MHz)	50.32	Nucleus	13C	Number of Transients	1000
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	512.00	SW(cyclical) (Hz)	11990.41	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	5029.5049	Spectrum Type	STANDARD	Sweep Width (Hz)	11990.04
				Temperature (degree C)	27.000

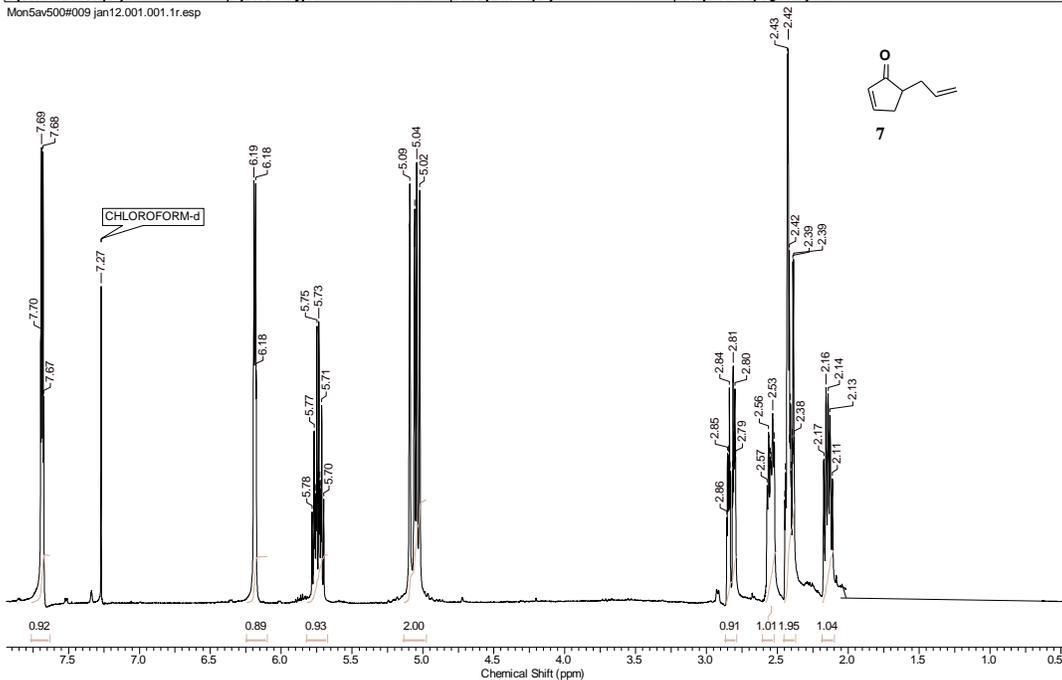
Mon2av2#073 dec 09.001.001.1r.esp VerticalScaleFactor = 1



Acquisition Time (sec)	1.3664	Comment	Priyanka	Date	08 Dec 2009 05:32:56
Date Stamp	08 Dec 2009 05:32:56	File Name	E:\paper-1\DATA\substrate 1\Mon2av2#073 dec 09\2\pdata\11r		
Frequency (MHz)	50.32	Nucleus	13C	Number of Transients	400
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	11990.41	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	5031.7993	Spectrum Type	DEPT135	Sweep Width (Hz)	11990.04
				Temperature (degree C)	27.000
Mon2av2#073 dec 09.002.001.1r.esp					

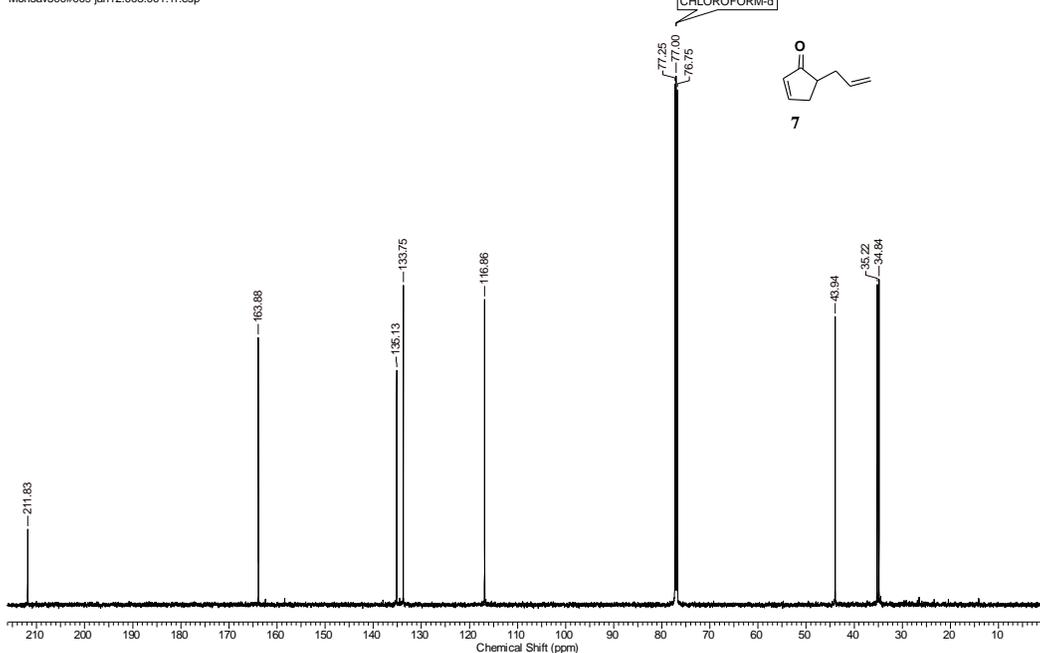


Acquisition Time (sec)	1.6384	Comment	1H Jagdish	Date	30 Jan 2012 11:27:12
Date Stamp	30 Jan 2012 11:27:12	File Name	E:\paper-1\DATA\allyl pentenone\Mon5av500#009 jan12\1\pdata\11r		
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	nmr	Points Count	32768
Receiver Gain	128.00	SW(cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3492.9702	Spectrum Type	STANDARD	Sweep Width (Hz)	9999.70
				Temperature (degree C)	22.100
Mon5av500#009 jan12.001.001.1r.esp					



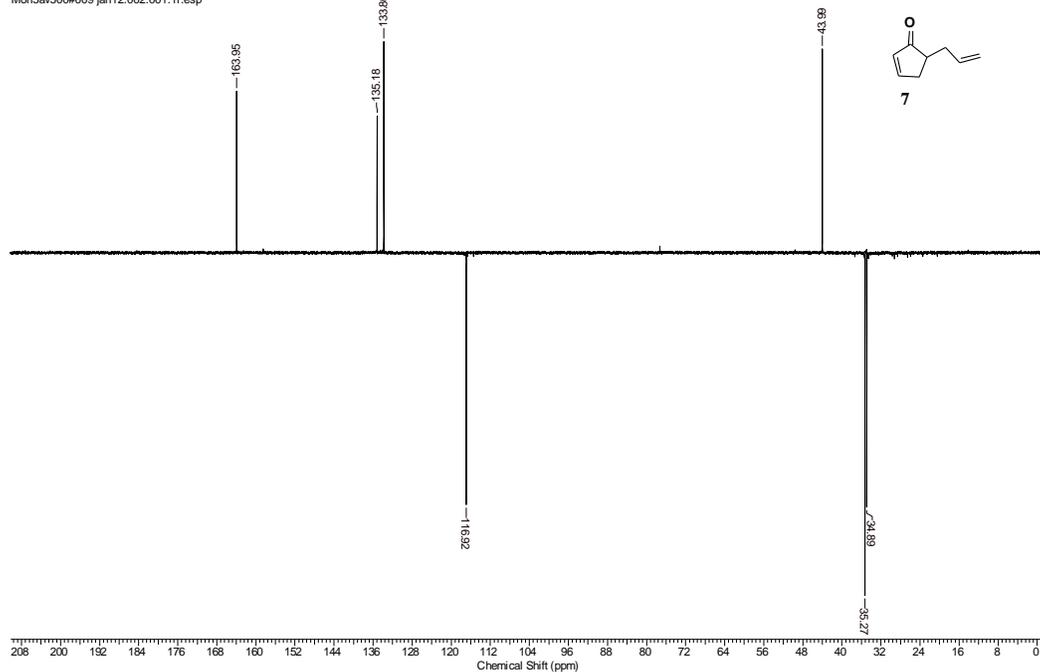
Acquisition Time (sec)	1.1010	Comment	13C	Date	30 Jan 2012 13:18:08
Date Stamp	30 Jan 2012 13:18:08	File Name	E:\paper-1\DATA\allyl pentenone\MonSav500#009 jan12\3\data1\11r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	920
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12569.3496	Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00
				Temperature (degree C)	23.100
				VerticalScaleFactor = 1	

MonSav500#009 jan12.003.001.1r.esp



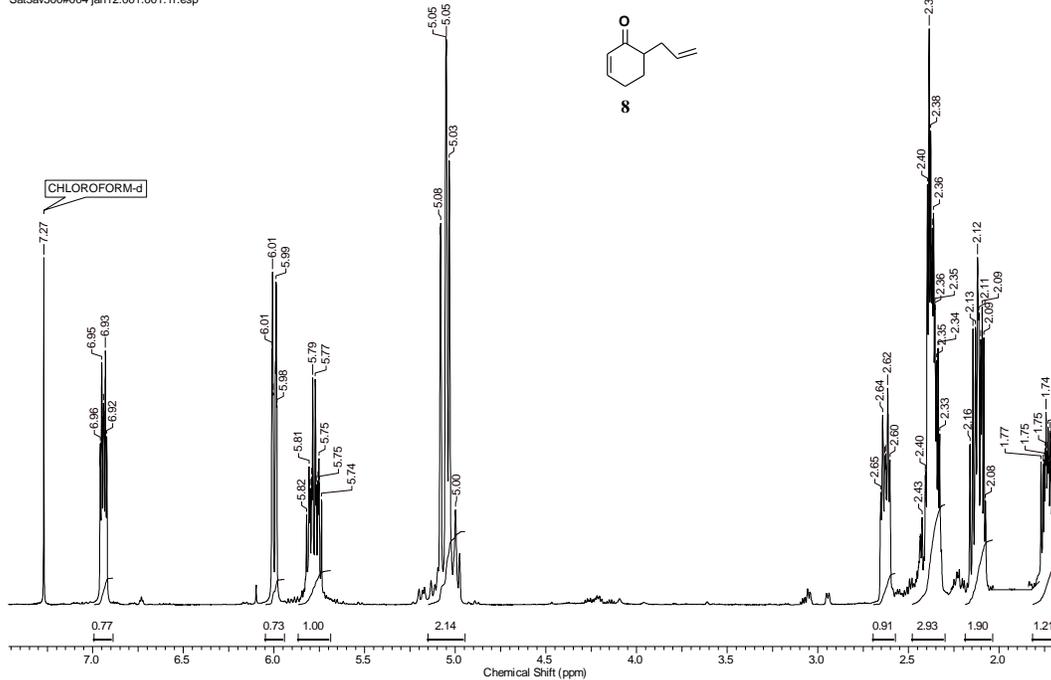
Acquisition Time (sec)	1.1010	Comment	DEPT135	Date	30 Jan 2012 12:33:20
Date Stamp	30 Jan 2012 12:33:20	File Name	E:\paper-1\DATA\allyl pentenone\MonSav500#009 jan12\2\data1\11r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	1200
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12575.7842	Spectrum Type	DEPT135	Sweep Width (Hz)	29761.00
				Temperature (degree C)	22.300
				VerticalScaleFactor = 1	

MonSav500#009 jan12.002.001.1r.esp



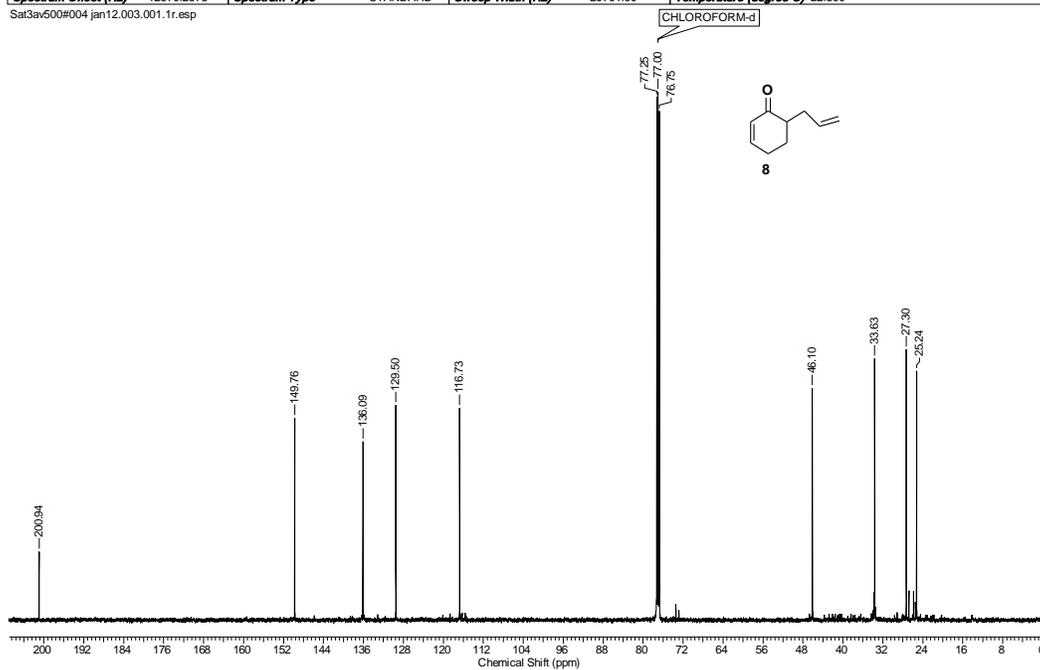
Acquisition Time (sec)	1.6384	Comment	1H priyanka	Date	21 Jan 2012 15:06:56
Date Stamp	21 Jan 2012 15:06:56	File Name	E:\paper-1\DATA\alilyl hexenone\Sat3av500#004 jan12\1\data\111r		
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	nmr	Points Count	32768
Receiver Gain	90.50	SW(cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3492.3599	Spectrum Type	STANDARD	Sweep Width (Hz)	9999.70
				Temperature (degree C)	21.000

Sat3av500#004 jan12.001.001.1r.esp



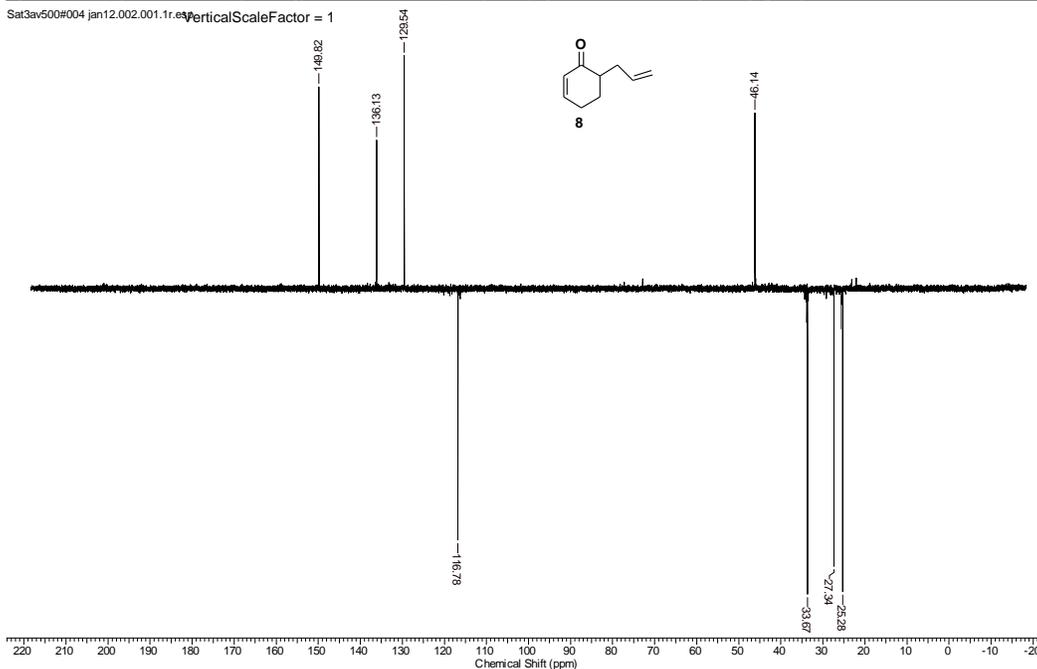
Acquisition Time (sec)	1.1010	Comment	13C	Date	21 Jan 2012 16:32:16
Date Stamp	21 Jan 2012 16:32:16	File Name	E:\paper-1\DATA\alilyl hexenone\Sat3av500#004 jan12\3\data\111r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	1206
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12570.2578	Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00
				Temperature (degree C)	22.800

Sat3av500#004 jan12.003.001.1r.esp



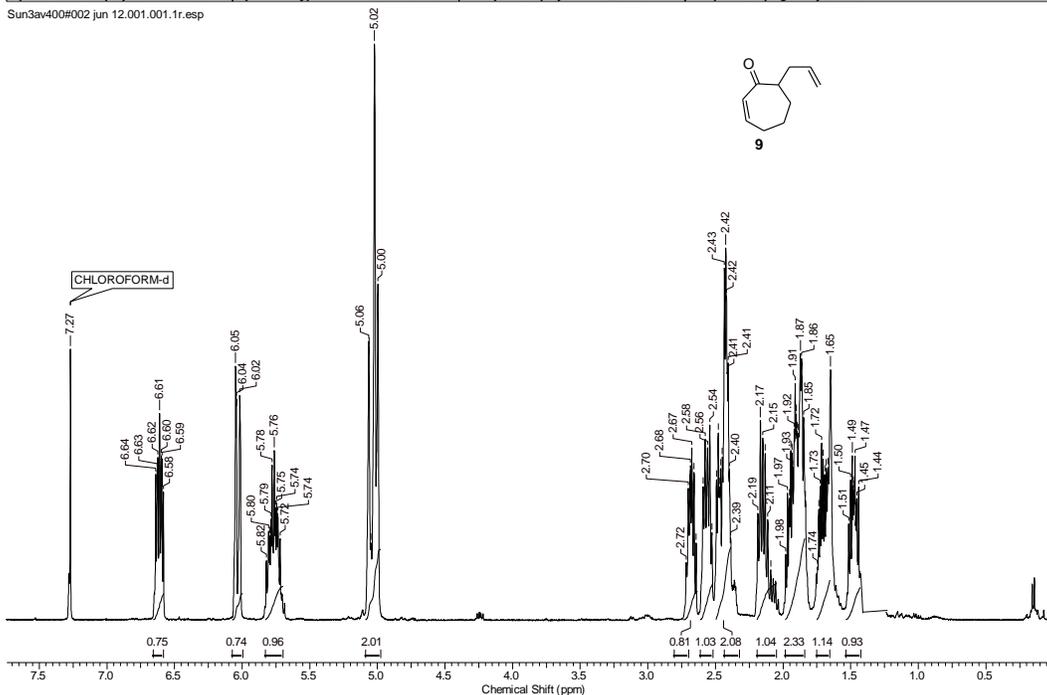
Acquisition Time (sec)	1.1010	Comment	DEPT135	Date	21 Jan 2012 15:30:24
Date Stamp	21 Jan 2012 15:30:24	File Name	E:\paper-1\DATA\allyl hexenone\Sat3av500#004 jan12\2\data1\11r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	427
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12575.7842	Spectrum Type	DEPT135	Sweep Width (Hz)	29761.00
				Temperature (degree C)	21.600

Sat3av500#004 jan12.002.001.1r.esp VerticalScaleFactor = 1



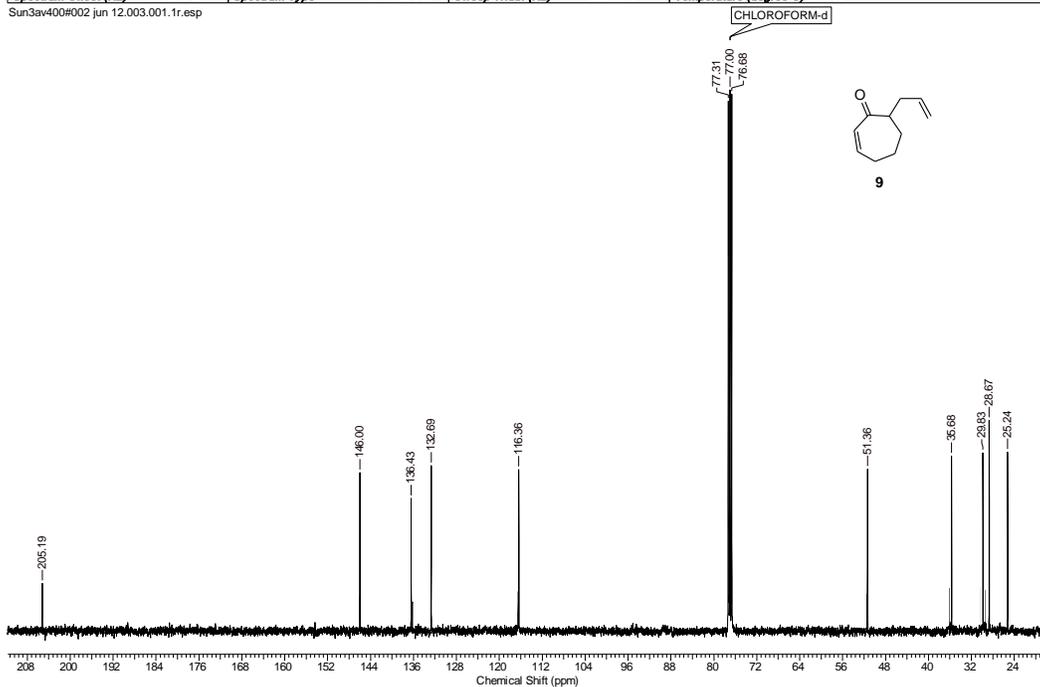
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H	Date	10 Jun 2012 09:36:08
Date Stamp	10 Jun 2012 09:36:08	File Name	E:\paper-1\DATA\allyl heptenone\Sun3av400#002 jun 12\1\data1\11r		
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	12
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	322.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.1101	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	24.400

Sun3av400#002 jun 12.001.001.1r.esp



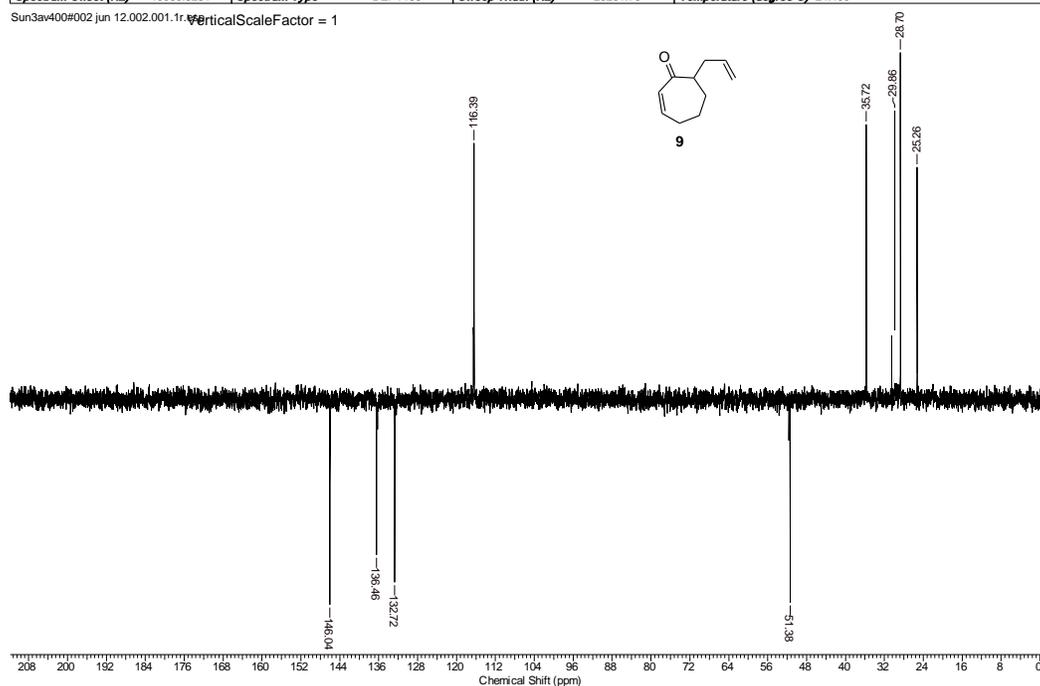
Acquisition Time (sec)	0.6488	Comment	13C	Date	10 Jun 2012 09:44:40
Date Stamp	10 Jun 2012 09:44:40	File Name	E:\paper-1\DATA\allyl heptenone\Sun3av400#002 jun 12\3\pdata1\11r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	569
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9555.5049	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	24.600

Sun3av400#002 jun 12.003.001.1r.esp



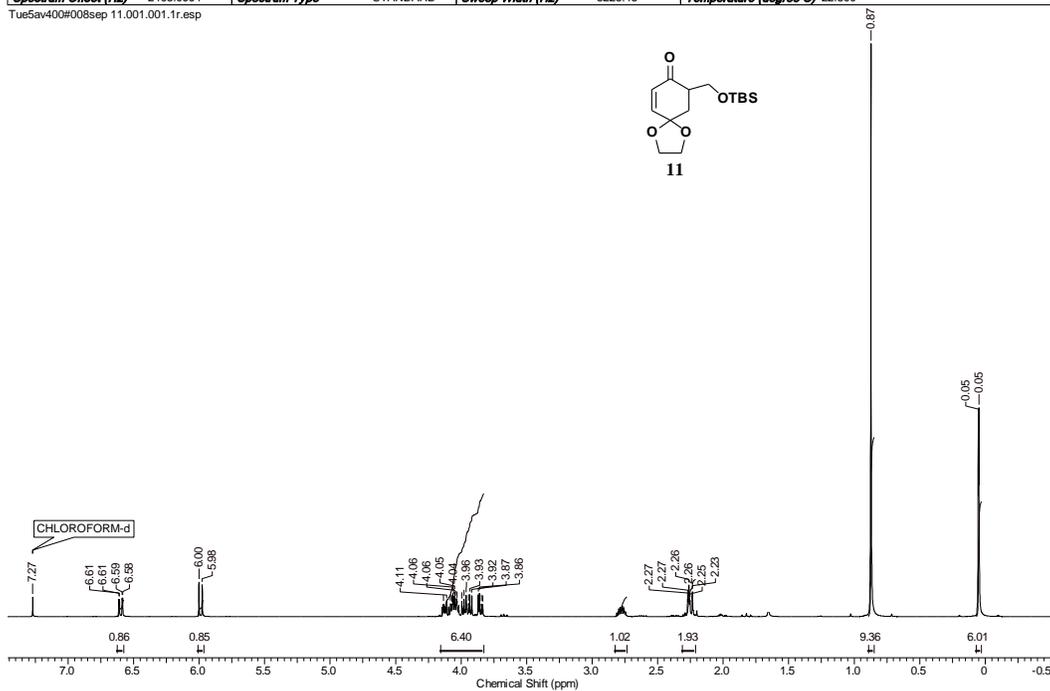
Acquisition Time (sec)	0.6488	Comment	DEPT	Date	10 Jun 2012 09:38:16
Date Stamp	10 Jun 2012 09:38:16	File Name	E:\paper-1\DATA\allyl heptenone\Sun3av400#002 jun 12\2\pdata1\11r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	152
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3281	Spectrum Type	DEPT135	Sweep Width (Hz)	25251.75
				Temperature (degree C)	24.400

Sun3av400#002 jun 12.002.001.1r.esp



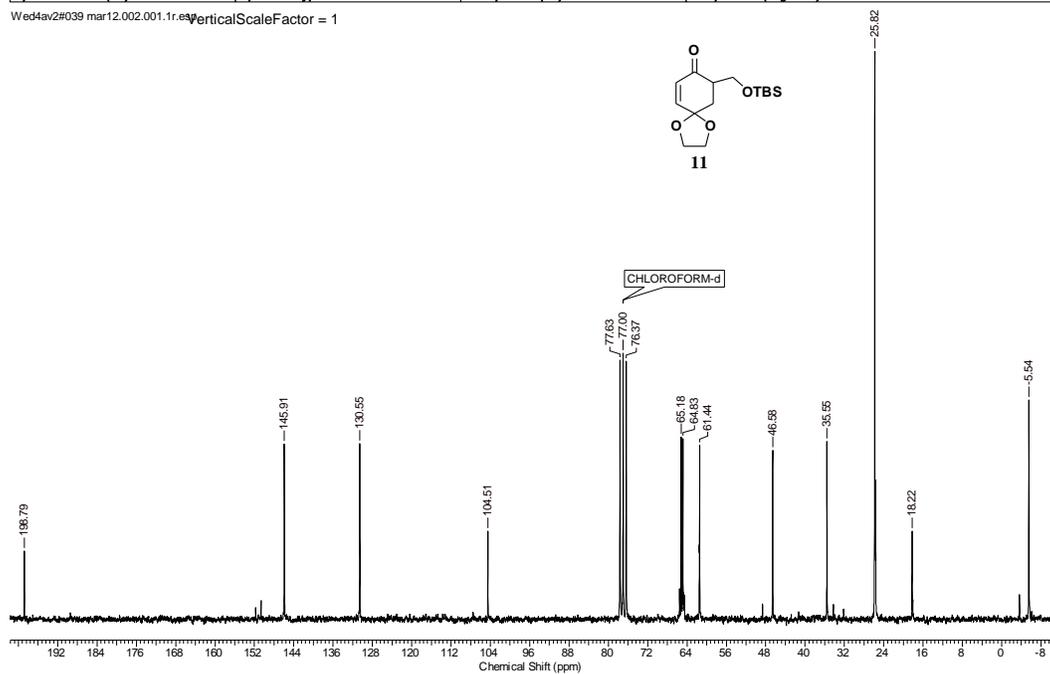
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H/ CDC13	Date	27 Sep 2011 15:13:12
Date Stamp	27 Sep 2011 15:13:12	File Name	E:\paper-1\DATA\tbs_enone\Tue5av400#008sep_11\11pdata\111r	Number of Transients	30
Frequency (MHz)	400.13	Nucleus	¹ H	Points Count	32768
Original Points Count	16384	Owner	Administrator	Pulse Sequence	zg30
Receiver Gain	144.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.0994	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	22.800

Tue5av400#008sep_11.001.001.1r.esp



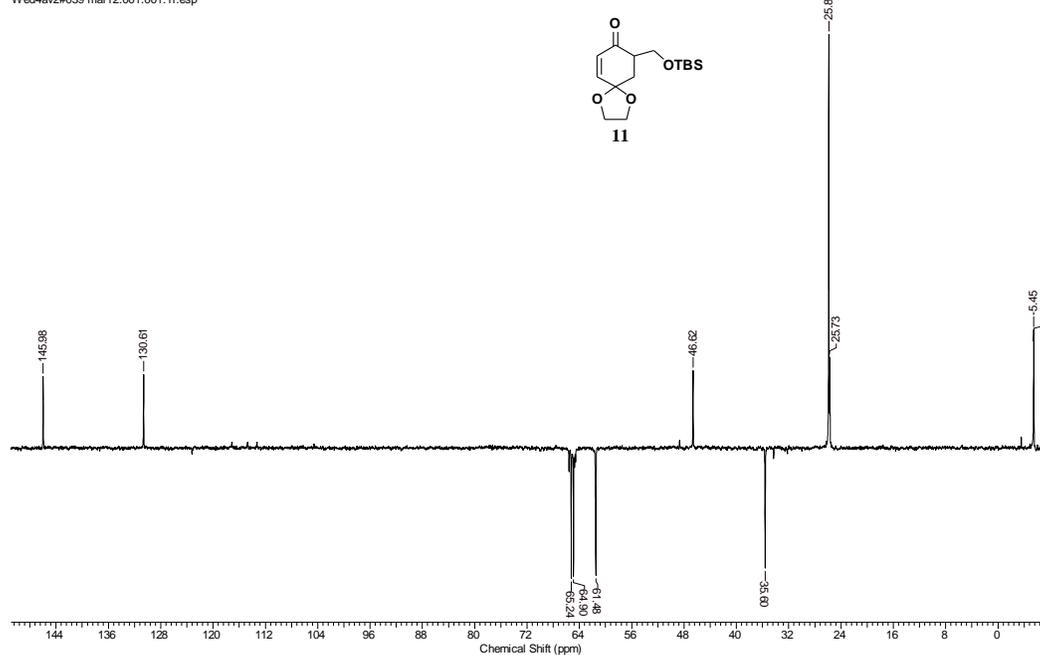
Acquisition Time (sec)	0.6832	Comment	Priyanka/10716	Date	22 Mar 2012 03:31:20
Date Stamp	22 Mar 2012 03:31:20	File Name	E:\paper-1\DATA\tbs_enone\Wed4av2#039_mar12\2\pdata\111r	Number of Transients	2400
Frequency (MHz)	50.32	Nucleus	¹³ C	Points Count	32768
Original Points Count	8192	Owner	Administrator	Pulse Sequence	zgpg30
Receiver Gain	2298.80	SW(cyclical) (Hz)	11990.41	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	5029.1387	Spectrum Type	STANDARD	Sweep Width (Hz)	11990.04
				Temperature (degree C)	27.000

Wed4av2#039_mar12.002.001.1r.esp VerticalScaleFactor = 1



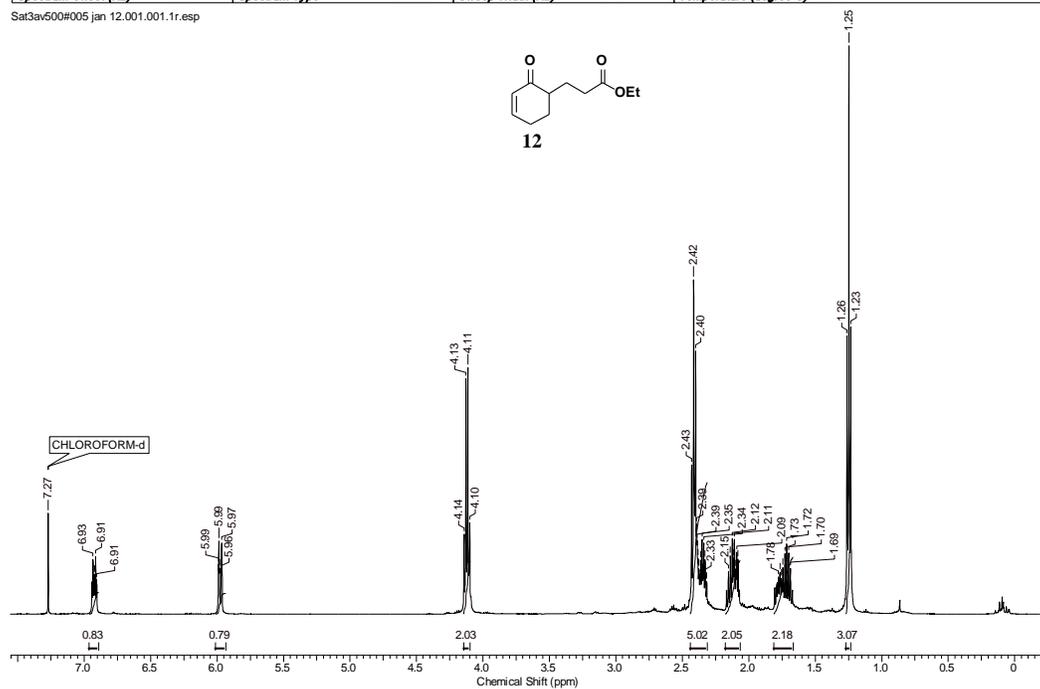
Acquisition Time (sec)	0.6832	Comment	Priyanka/10716	Date	22 Mar 2012 01:40:24
Date Stamp	22 Mar 2012 01:40:24	File Name	E:\paper-1\DATA\tlbs enone\Wed4av2#039 mar12\1\data\11r	Origin	av200
Frequency (MHz)	50.32	Nucleus	13C	Number of Transients	1800
Original Points Count	8192	Owner	Administrator	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	11990.41	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	5031.7993	Spectrum Type	DEPT135	Sweep Width (Hz)	11990.04
				Temperature (degree C)	27.000

Wed4av2#039 mar12.001.001.1r.esp

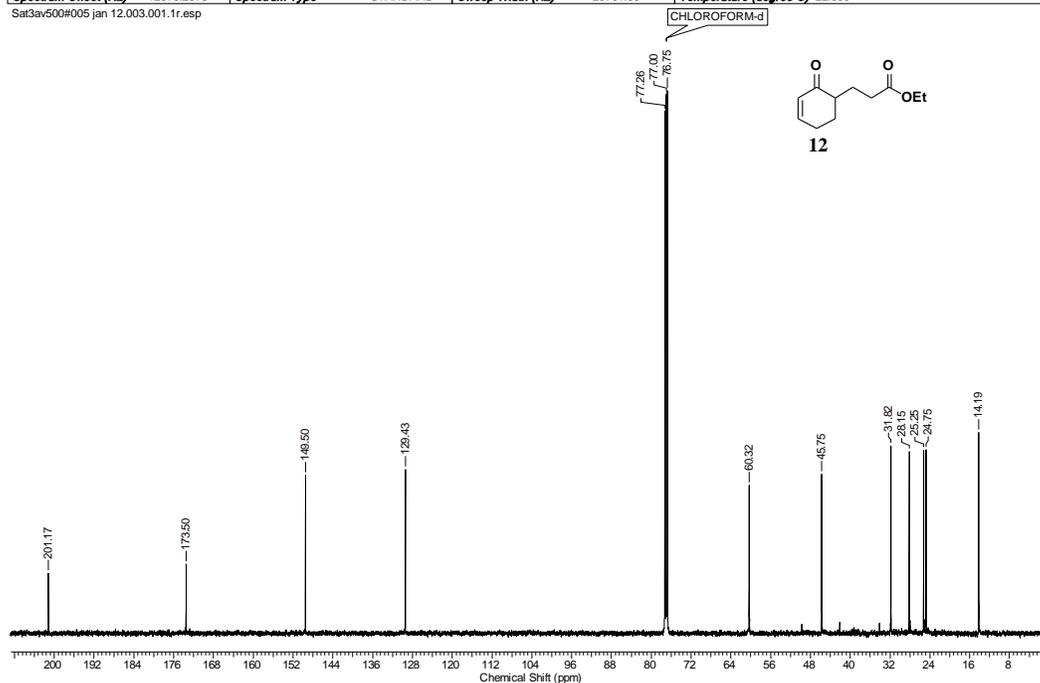


Acquisition Time (sec)	1.6384	Comment	1H priyanka	Date	21 Jan 2012 16:42:56
Date Stamp	21 Jan 2012 16:42:56	File Name	E:\paper-1\DATA\acrylate without ring\Sat3av500#005 jan 12\1\data\11r	Origin	spect
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	nmr	Points Count	32768
Receiver Gain	90.50	SW(cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3492.3599	Spectrum Type	STANDARD	Sweep Width (Hz)	9999.70
				Temperature (degree C)	21.700

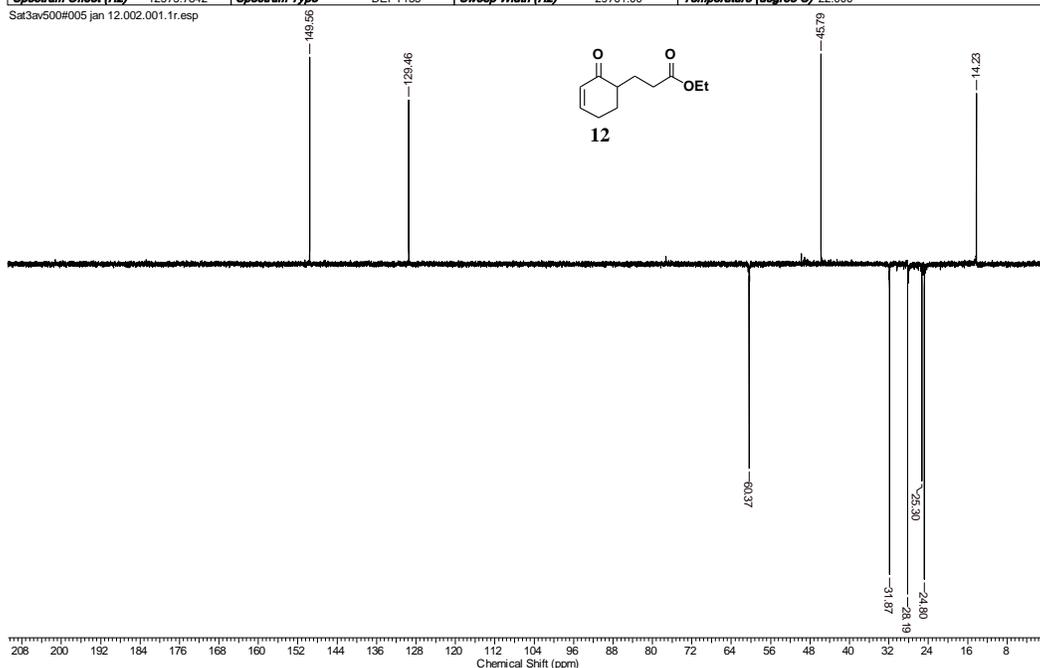
Sat3av500#005 jan 12.001.001.1r.esp



Acquisition Time (sec)	1.1010	Comment	13C	Date	21 Jan 2012 17:12:48
Date Stamp	21 Jan 2012 17:12:48	File Name	E:\paper-1\DATA\acrylate without ring\Sat3av500#005 jan 12\3\pdata\111r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	805
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12570.2578	Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00
				Temperature (degree C)	22.600
VerticalScaleFactor = 1					

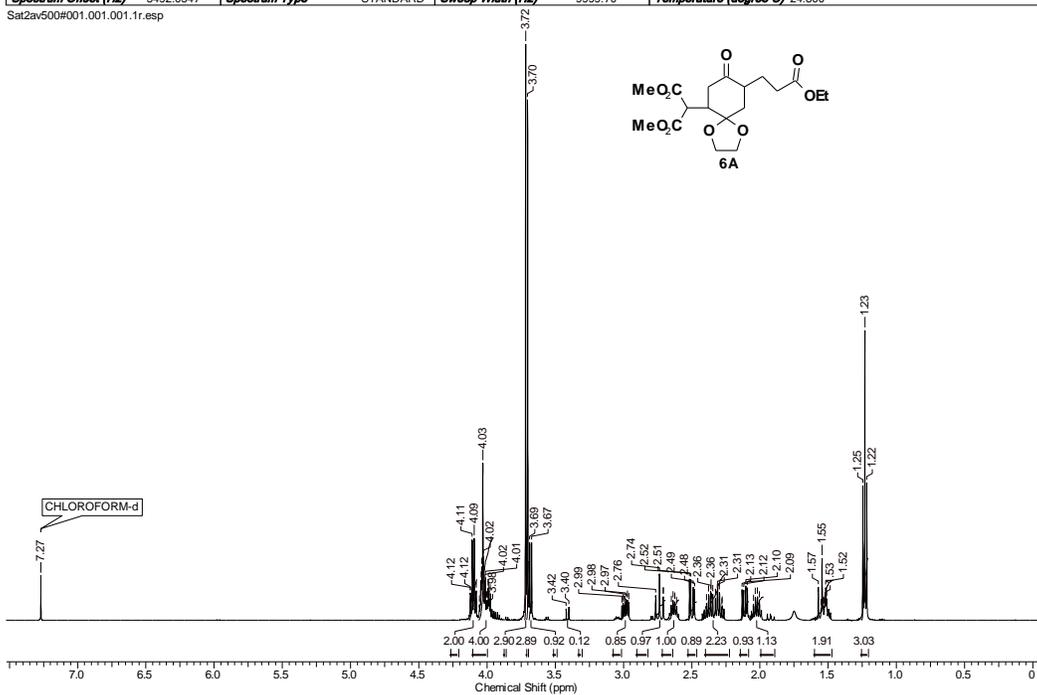


Acquisition Time (sec)	1.1010	Comment	DEPT135	Date	21 Jan 2012 17:10:40
Date Stamp	21 Jan 2012 17:10:40	File Name	E:\paper-1\DATA\acrylate without ring\Sat3av500#005 jan 12\2\pdata\111r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	547
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12575.7842	Spectrum Type	DEPT135	Sweep Width (Hz)	29761.00
				Temperature (degree C)	22.000
VerticalScaleFactor = 1					



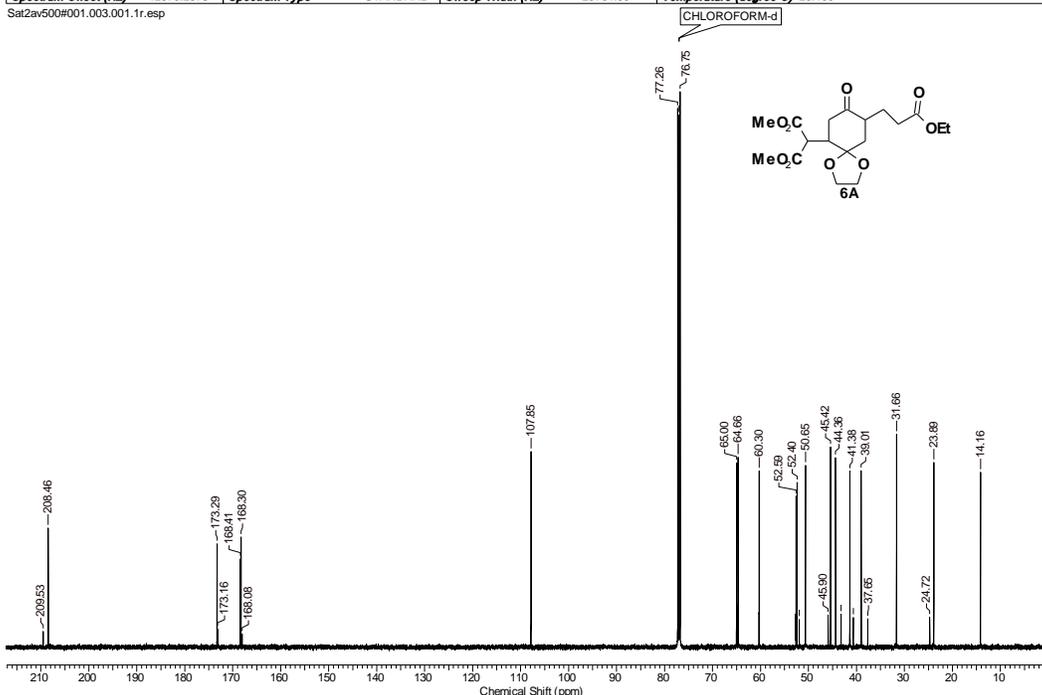
Acquisition Time (sec)	1.6384	Comment	1H Priyanka	Date	10 Sep 2011 11:04:00
Date Stamp	10 Sep 2011 11:04:00	File Name	D:\paper-1\DATA\1\Sat2av500#001\1\data1\1r		
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	nmr	Points Count	32768
Receiver Gain	90.50	SW(cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3492.0547	Spectrum Type	STANDARD	Sweep Width (Hz)	9999.70
				Temperature (degree C)	24.800

Sat2av500#001.001.001.1r.esp



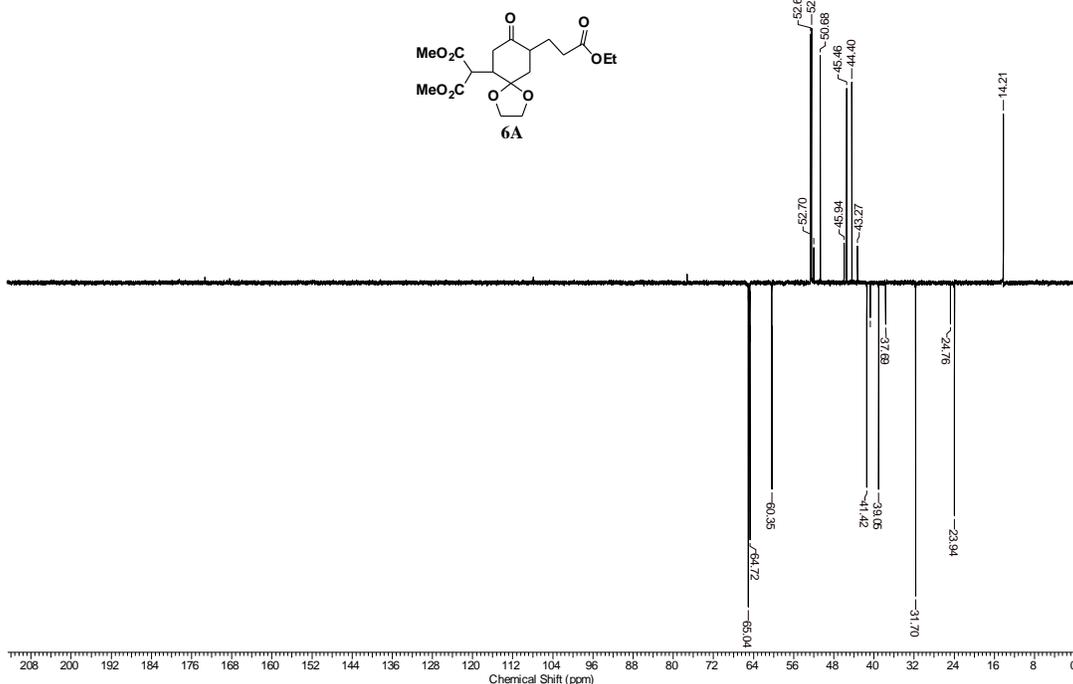
Acquisition Time (sec)	1.1010	Comment	13C	Date	10 Sep 2011 12:12:16
Date Stamp	10 Sep 2011 12:12:16	File Name	D:\paper-1\DATA\1\Sat2av500#001\3\data1\1r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	739
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12570.2578	Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00
				Temperature (degree C)	26.100

Sat2av500#001.003.001.1r.esp



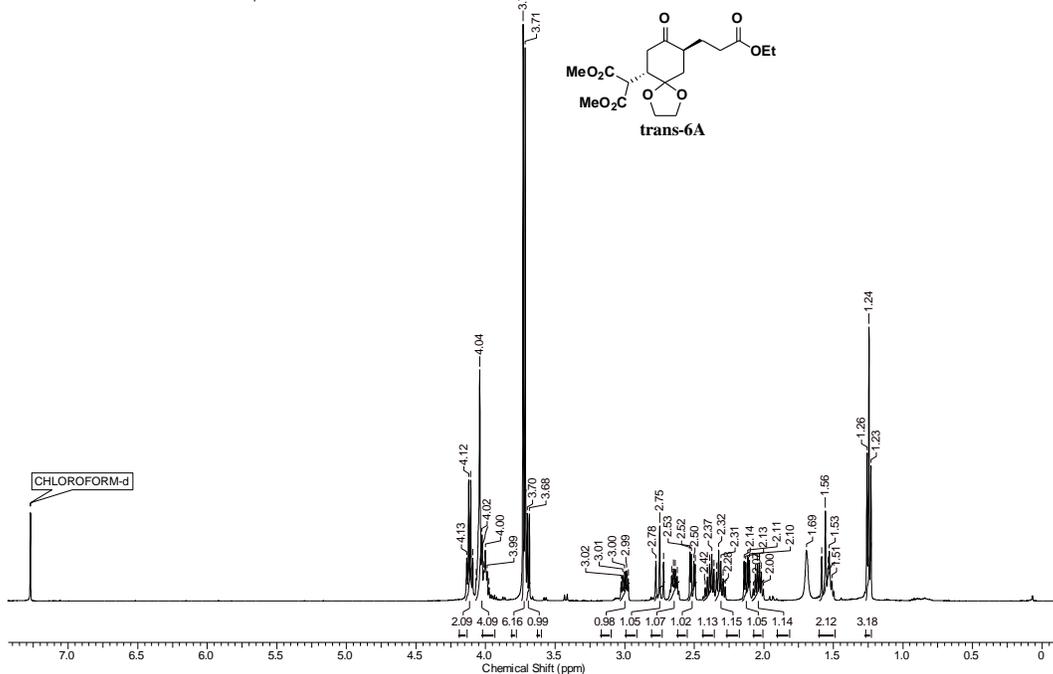
Acquisition Time (sec)	1.1010	Comment	DEPT135	Date	10 Sep 2011 11:33:52	
Date Stamp	10 Sep 2011 11:33:52	File Name	E:\paper-1\DATA\1\Sat2av500#001\2\pdata\1\1r			
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	531	
Original Points Count	32768	Owner	nmr	Points Count	32768	
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d	
Spectrum Offset (Hz)	12575.7842	Spectrum Type	DEPT135	Sweep Width (Hz)	29761.00	
					Temperature (degree C)	25.600
VerticalScaleFactor = 1						

Sat2av500#001.002.001.1r.esp



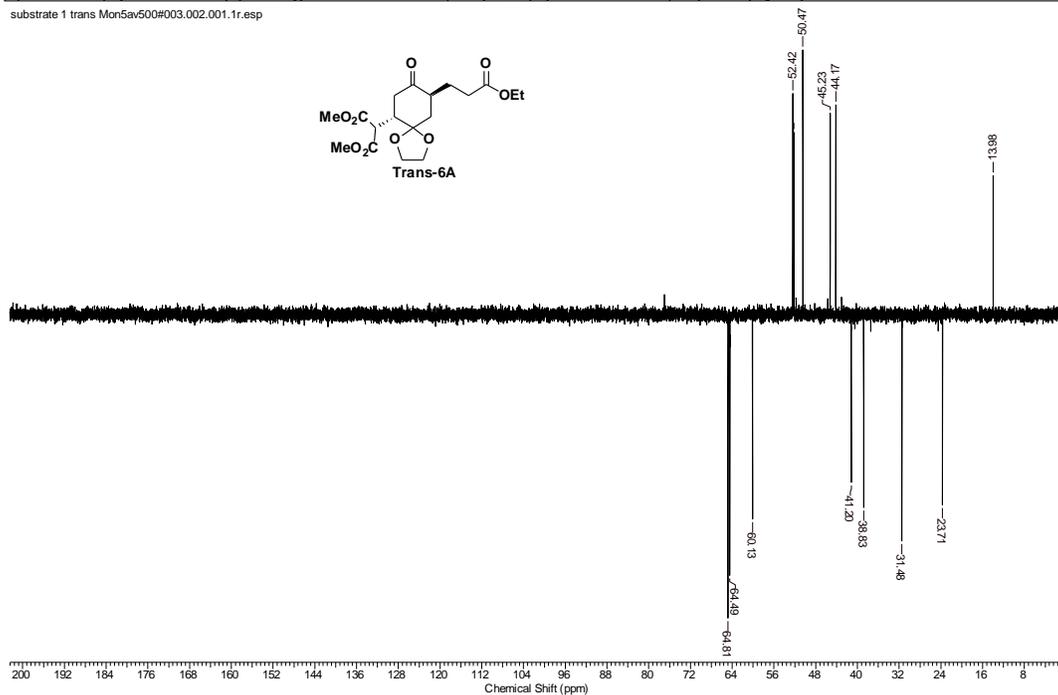
Acquisition Time (sec)	1.6384	Comment	Priyanka 1H	Date	25 Jun 2012 21:37:36	
Date Stamp	25 Jun 2012 21:37:36	File Name	E:\nmrdata\substrate 1 trans Mon5av500#003\1\pdata\1\1r			
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	46	
Original Points Count	16384	Owner	nmr	Points Count	32768	
Receiver Gain	203.00	SW(cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d	
Spectrum Offset (Hz)	3310.7805	Spectrum Type	STANDARD	Sweep Width (Hz)	9999.70	
					Temperature (degree C)	25.500
VerticalScaleFactor = 1						

substrate 1 trans Mon5av500#003.001.001.1r.esp

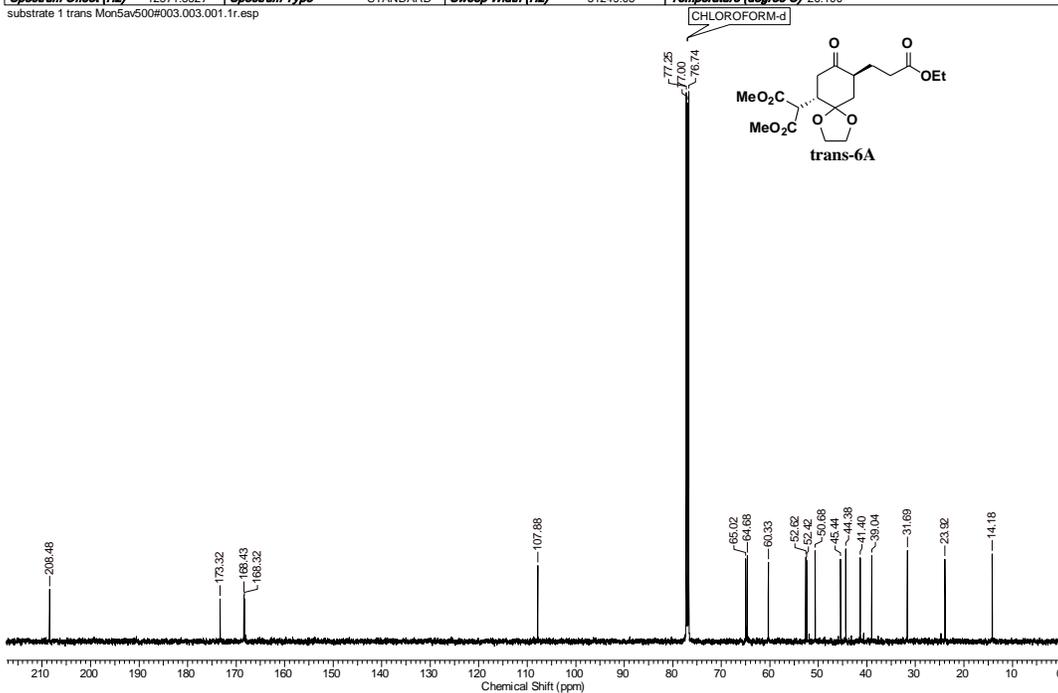


Acquisition Time (sec)	1.0486	Comment	DEPT135	Date	25 Jun 2012 21:41:52
Date Stamp	25 Jun 2012 21:41:52	File Name	E:\nmrdata\substrate 1 trans Mon5av500#003\2\data\111r		
Frequency (MHz)	125.76	Nucleus	¹³ C	Number of Transients	130
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	31250.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12545.8027	Spectrum Type	DEPT135	Sweep Width (Hz)	31249.05
				Temperature (degree C)	25.700

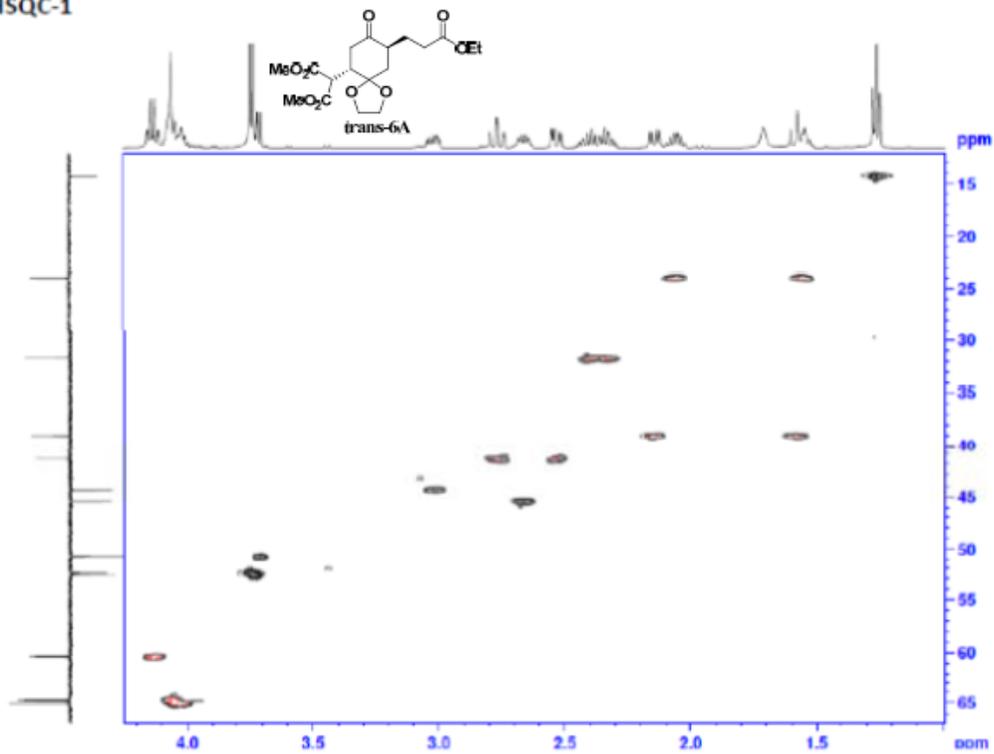
substrate 1 trans Mon5av500#003.002.001.1r.esp



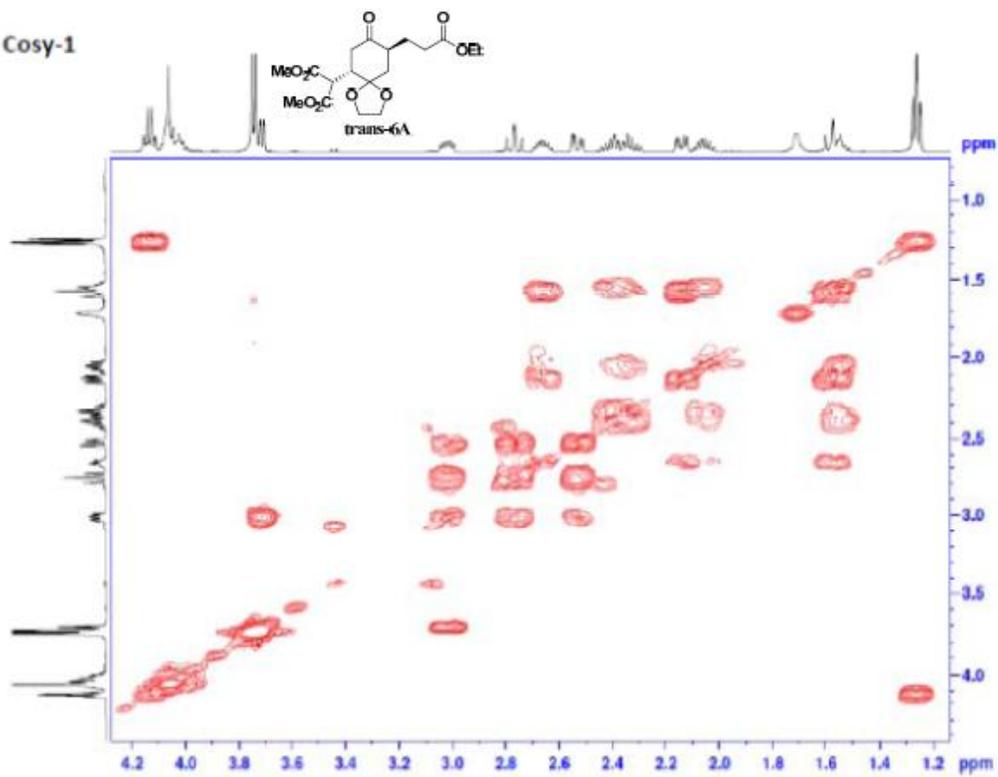
Acquisition Time (sec)	1.0486	Comment	13C	Date	25 Jun 2012 21:46:08
Date Stamp	25 Jun 2012 21:46:08	File Name	E:\nmrdata\substrate 1 trans Mon5av500#003\3\data\111r		
Frequency (MHz)	125.76	Nucleus	¹³ C	Number of Transients	367
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	575.00	SW(cyclical) (Hz)	31250.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12571.5527	Spectrum Type	STANDARD	Sweep Width (Hz)	31249.05
				Temperature (degree C)	26.100

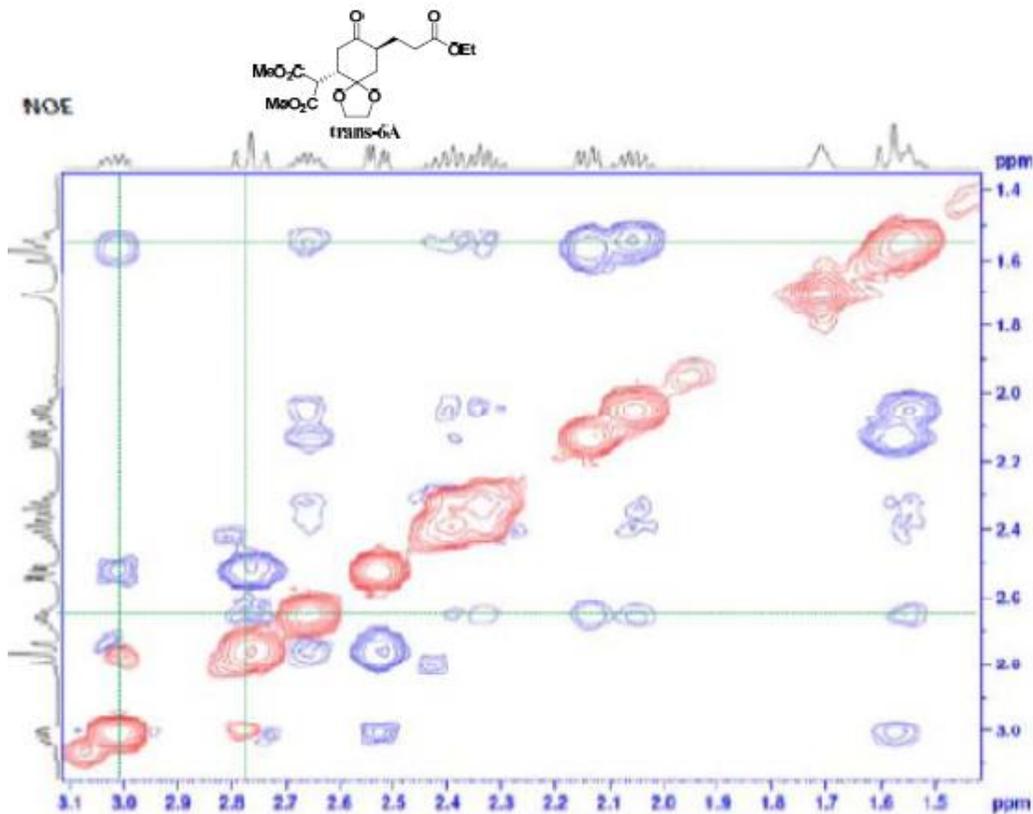


HSQC-1



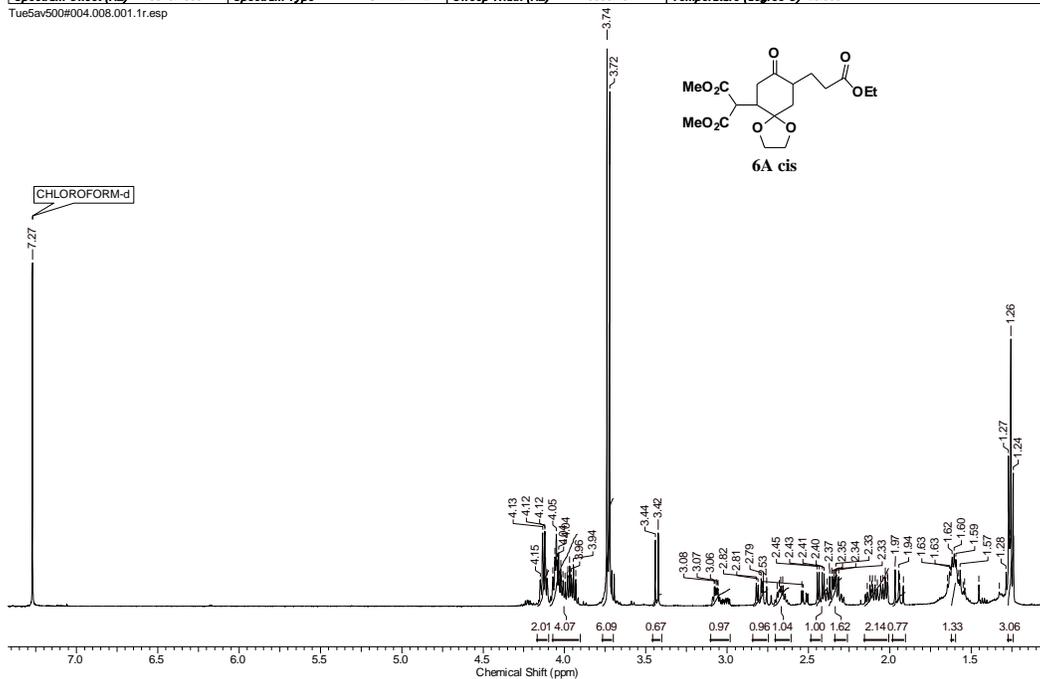
Cosy-1





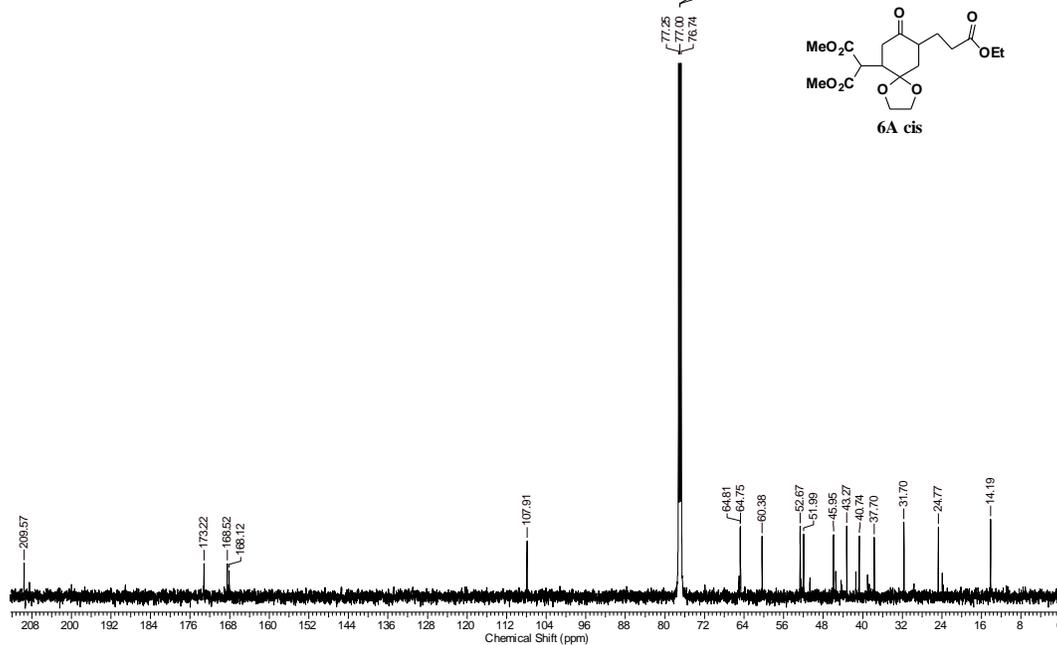
Acquisition Time (sec)	1.6384	Comment	1H	Date	29 Jun 2012 13:58:56
Date Stamp	29 Jun 2012 13:58:56	File Name	\\172.16.2.18\mr_data\AV_500\Jun_12_500Tue5av500#004i8\pddata\11r		
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	40
Original Points Count	16384	Owner	nmr	Points Count	32768
Receiver Gain	406.00	SW (cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3310.7805	Spectrum Type	STANDARD	Sweep Width (Hz)	9999.70
				Temperature (degree C)	26.500

Tue5av500#004.008.001.1r.esp



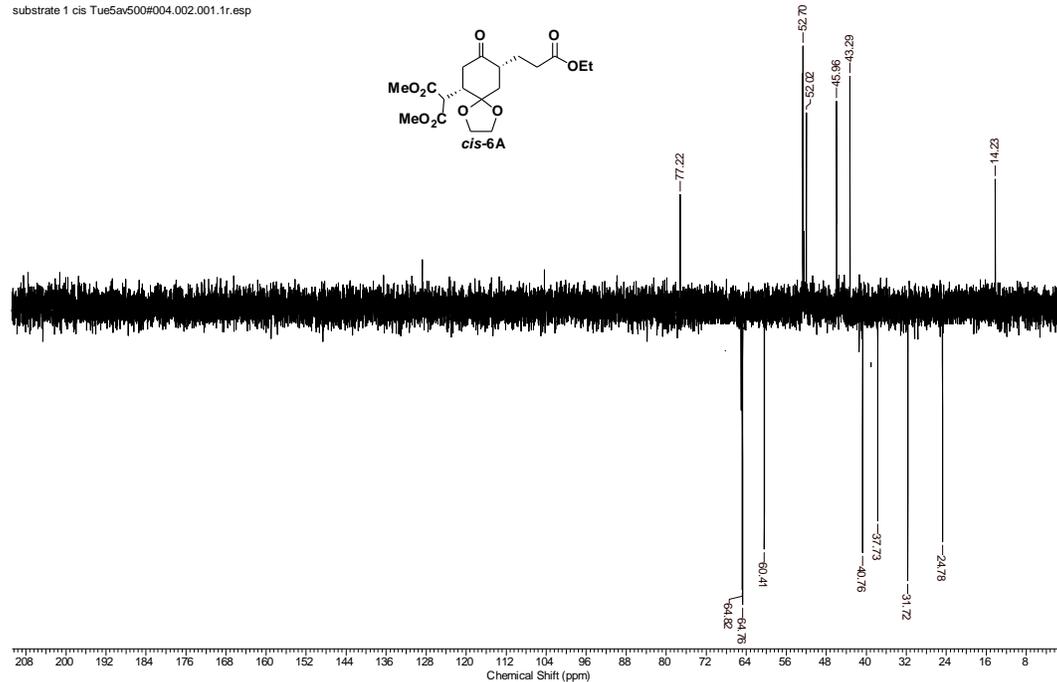
Acquisition Time (sec)	1.0486	Comment	13C	Date	26 Jun 2012 21:37:36
Date Stamp	26 Jun 2012 21:37:36	File Name	E:\nmrdata\substrate 1 cis Tue5av500#004\3\pdata\111r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	2201
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	575.00	SW(cyclical) (Hz)	31250.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12573.4600	Spectrum Type	STANDARD	Sweep Width (Hz)	31249.05
				Temperature (degree C)	26.300

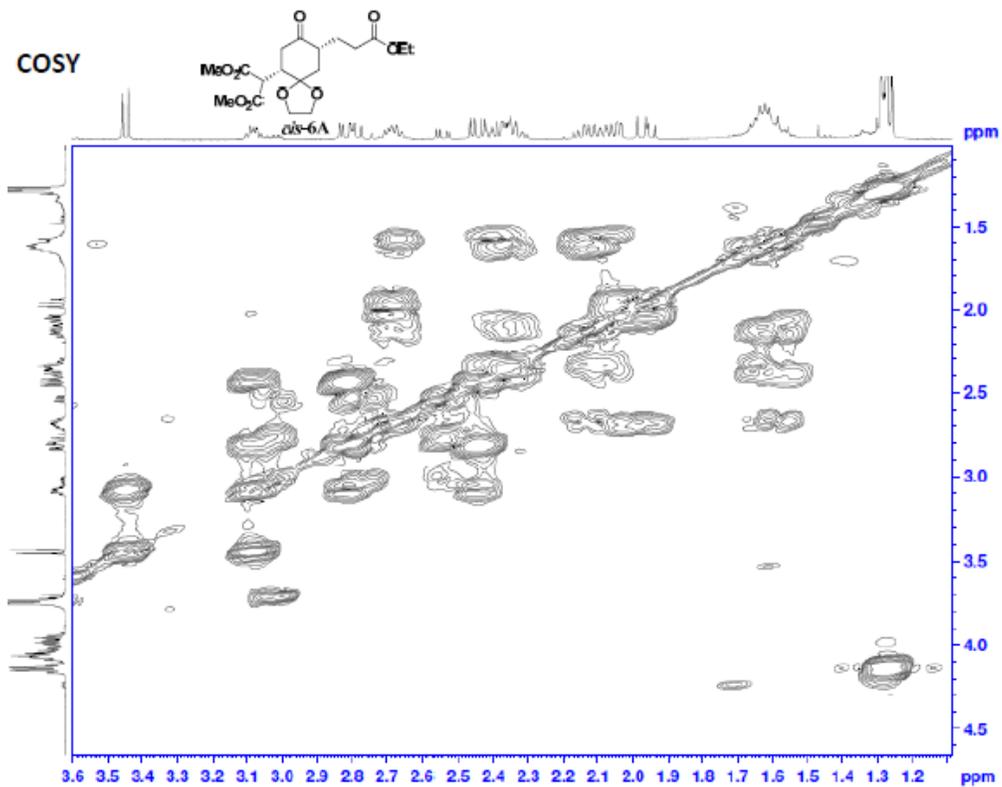
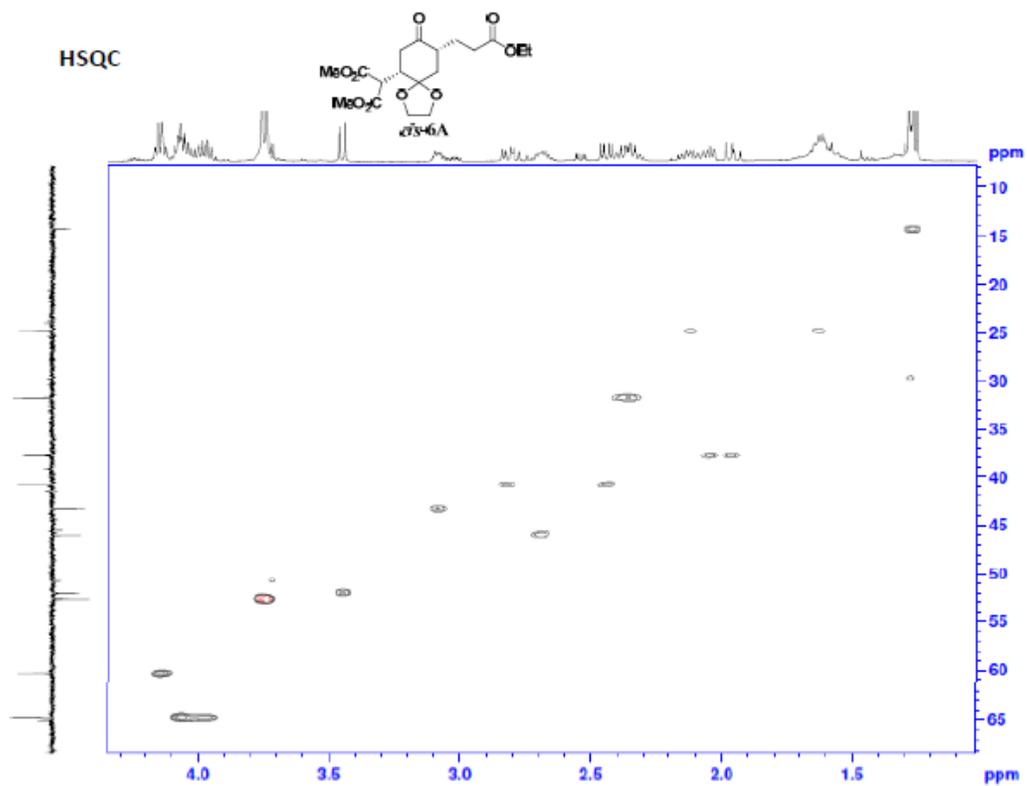
substrate 1 cis Tue5av500#004.003.001.1r.esp

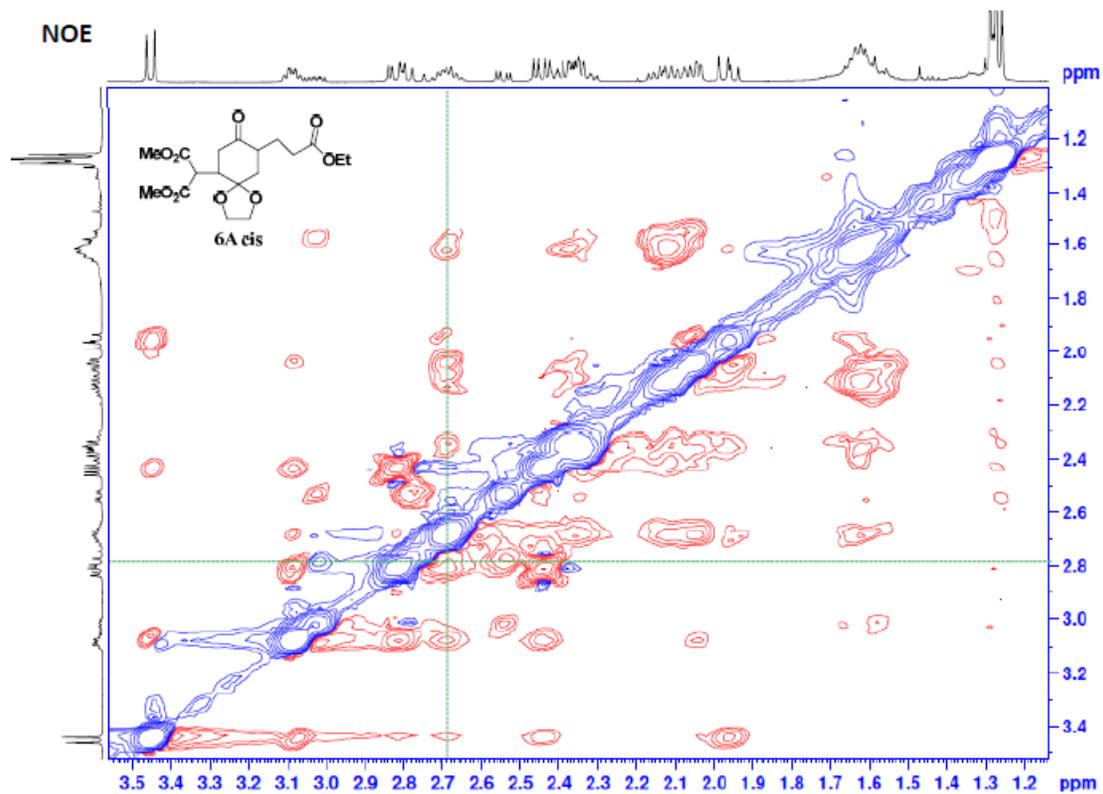


Acquisition Time (sec)	1.0486	Comment	DEPT135	Date	26 Jun 2012 18:59:44
Date Stamp	26 Jun 2012 18:59:44	File Name	E:\nmrdata\substrate 1 cis Tue5av500#004\2\pdata\111r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	1200
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	31250.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12575.7813	Spectrum Type	DEPT135	Sweep Width (Hz)	31249.05
				Temperature (degree C)	25.600

substrate 1 cis Tue5av500#004.002.001.1r.esp

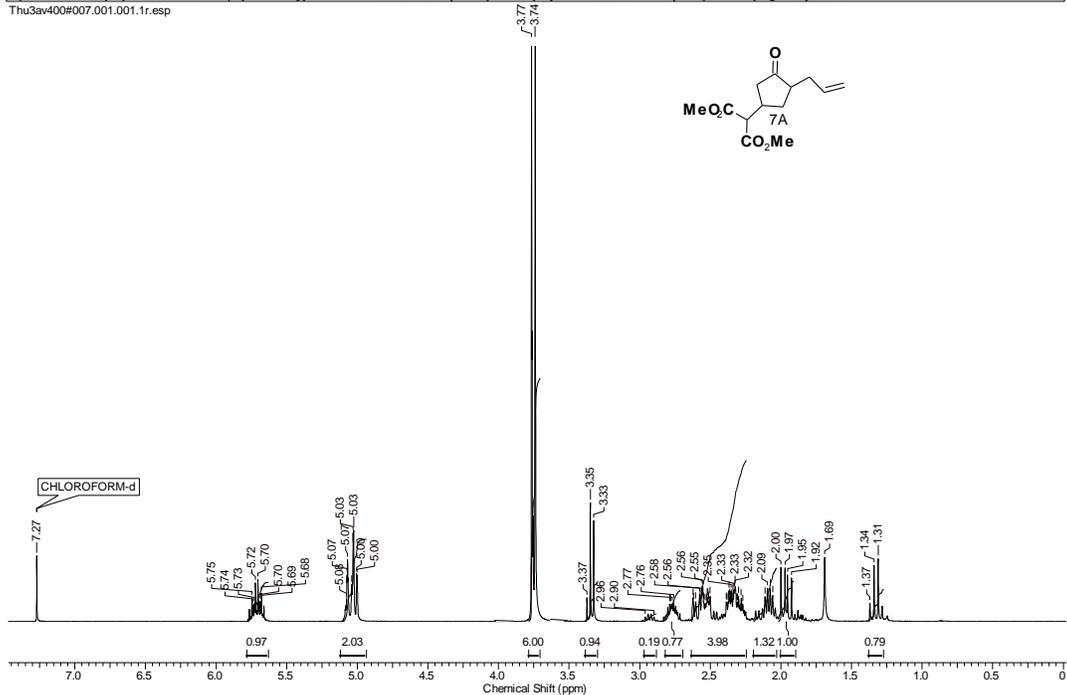






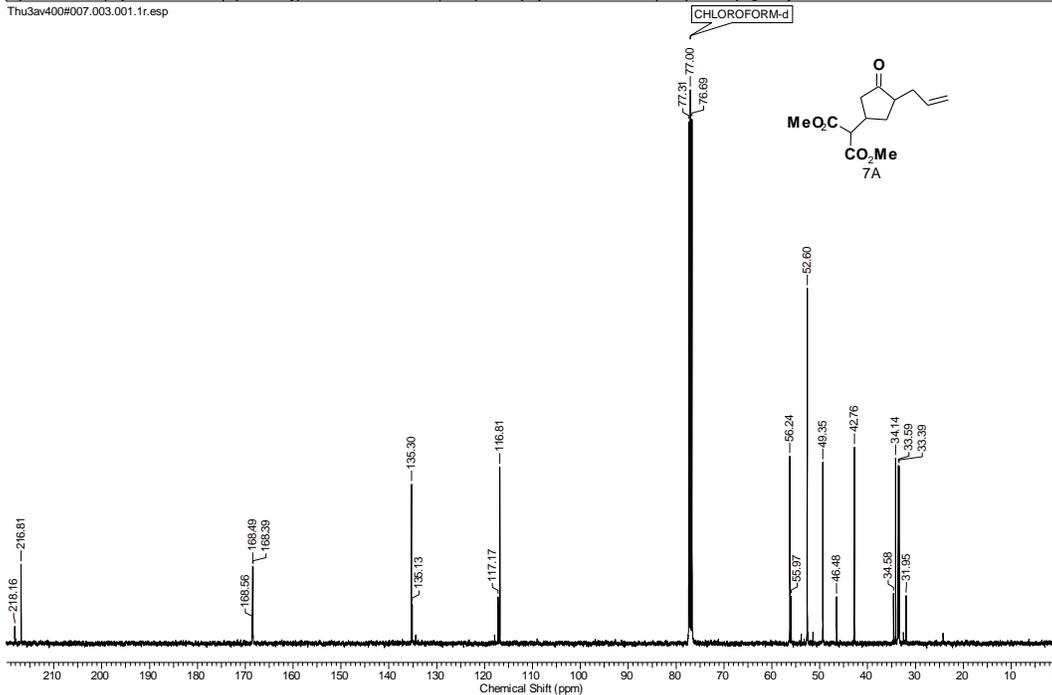
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H/CDCl3	Date	16 Jun 2011 10:14:32
Date Stamp	16 Jun 2011 10:14:32	File Name	D:\paper-1\DATA\12\Thu3av400#007\1\pdata1\11r	Origin	spect
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	161.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.1101	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	22.800

Thu3av400#007.001.001.1r.esp



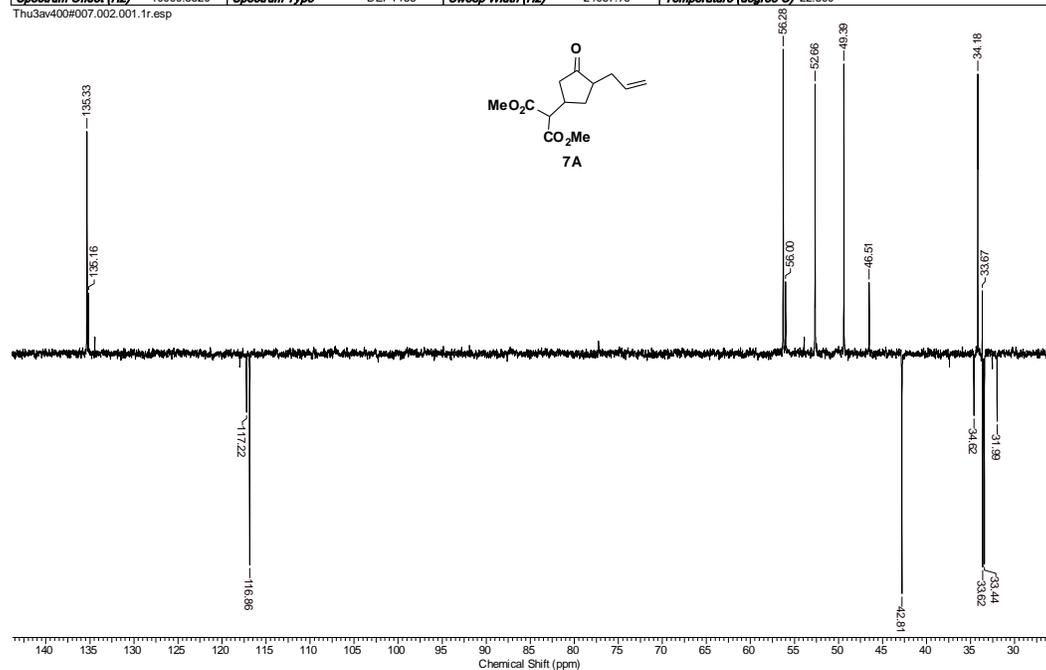
Acquisition Time (sec)	0.6488	Comment	13C	Date	16 Jun 2011 10:38:00
Date Stamp	16 Jun 2011 10:38:00	File Name		File Name	D:\paper-1\DATA\12\Thu3av400#007\3\pdata1\11r
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	1210
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	912.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9554.7334	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	23.100

Thu3av400#007.003.001.1r.esp



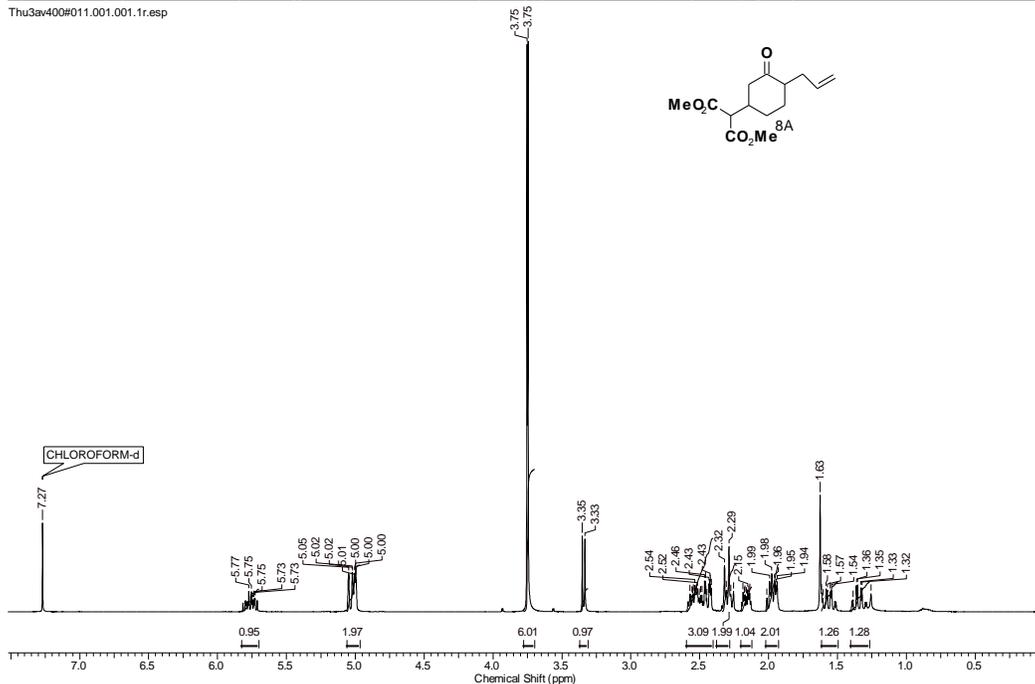
Acquisition Time (sec)	0.6816	Comment	Dept/CDCI3	Date	16 Jun 2011 10:18:48
Date Stamp	16 Jun 2011 10:18:48	File Name		File Name	E:\paper-1\DATA\12\Thu3av400#007\2\pdata1\11r
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	402
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	22.800

Thu3av400#007.002.001.1r.esp



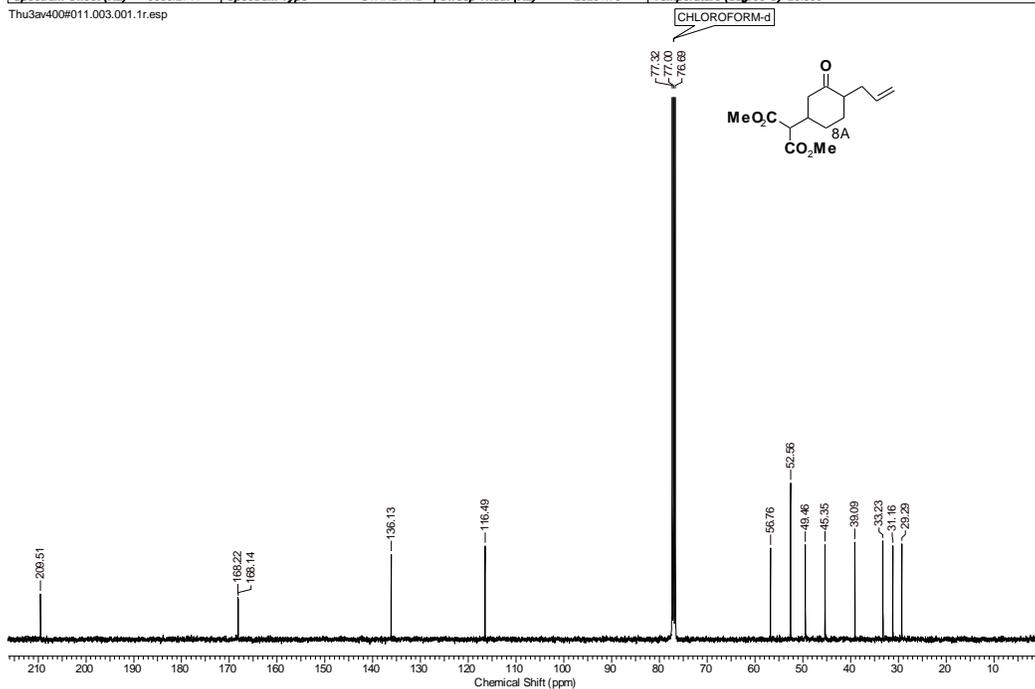
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H/CDCl3	Date	16 Jun 2011 12:09:44
Date Stamp	16 Jun 2011 12:09:44	File Name	D:\paper-1\DATA\9\Thu3av400#011\1\pdata111r	Number of Transients	64
Frequency (MHz)	400.13	Nucleus	1H	Points Count	32768
Original Points Count	16384	Owner	Administrator	Pulse Sequence	zg30
Receiver Gain	322.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.1101	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	22.500

Thu3av400#011.001.001.1r.esp



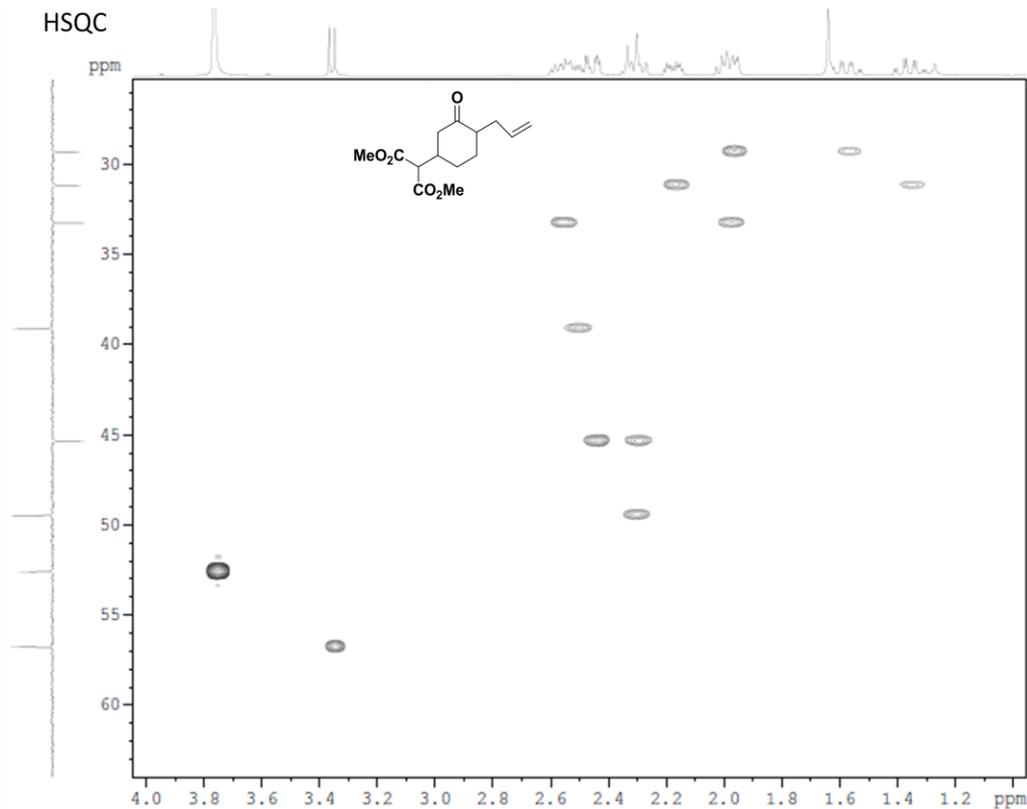
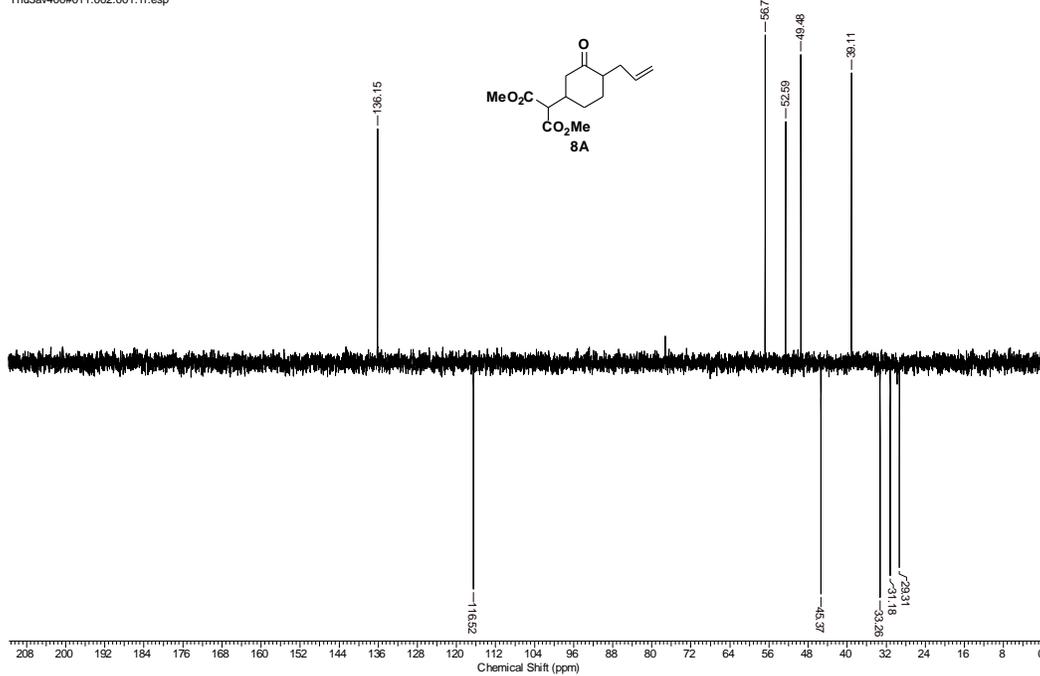
Acquisition Time (sec)	0.6488	Comment	13C	Date	16 Jun 2011 13:11:36
Date Stamp	16 Jun 2011 13:11:36	File Name	D:\paper-1\DATA\9\Thu3av400#011\3\pdata111r	Number of Transients	1104
Frequency (MHz)	100.61	Nucleus	13C	Points Count	32768
Original Points Count	16384	Owner	root	Pulse Sequence	zgpg30
Receiver Gain	912.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9556.2744	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	23.300

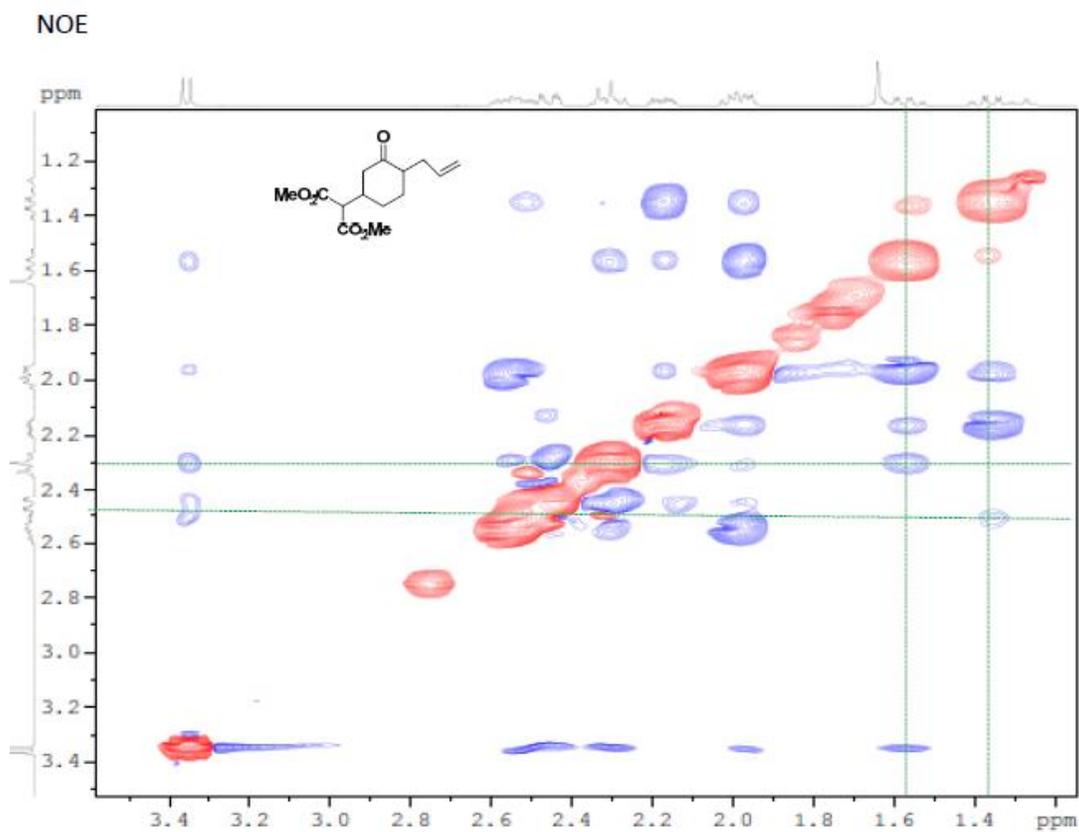
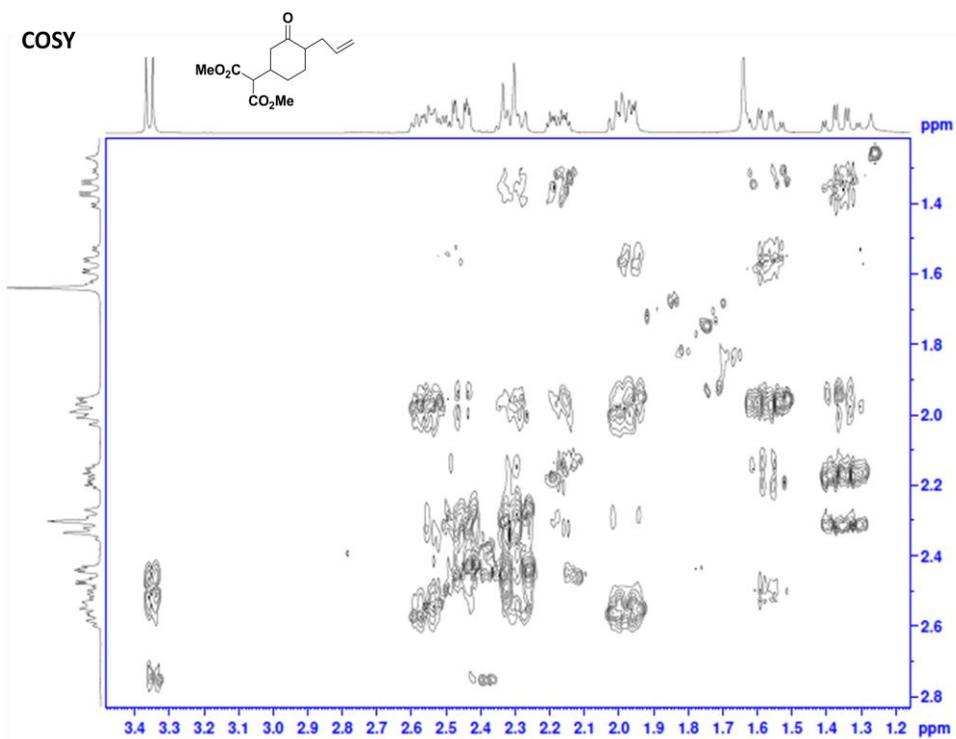
Thu3av400#011.003.001.1r.esp



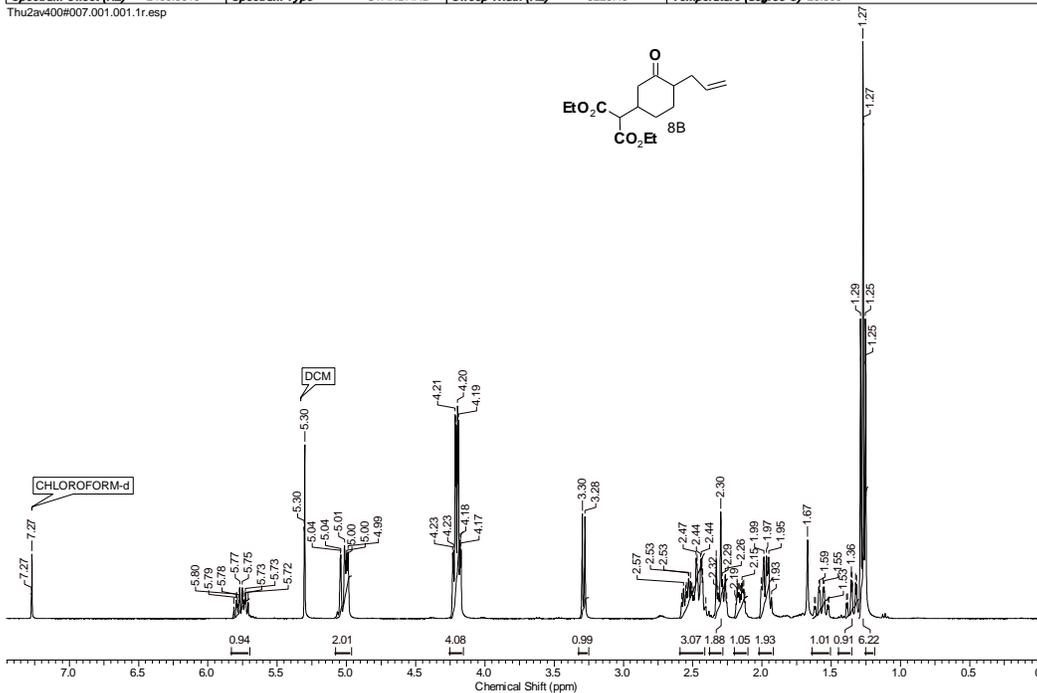
Acquisition Time (sec)	0.6816	Comment	Dept/CDCI3	Date	16 Jun 2011 12:16:08
Date Stamp	16 Jun 2011 12:16:08			File Name	E:\paper-1\DATA\9\Thu3av400#0112\data111r
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	250
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	22.600
					VerticalScaleFactor = 1

Thu3av400#011.002.001.1r.esp

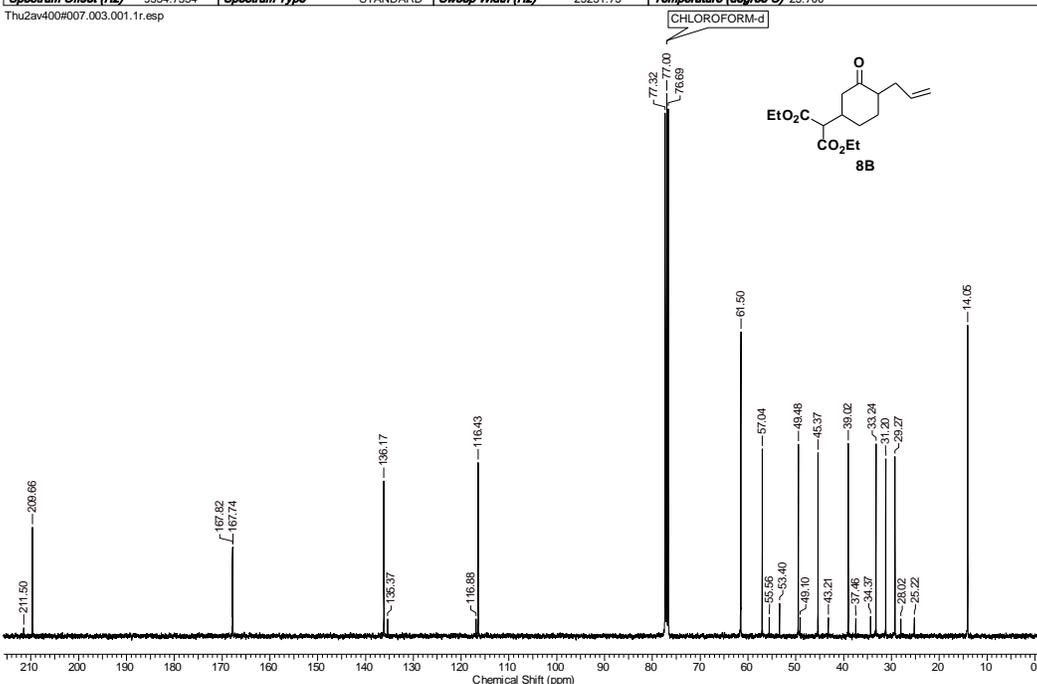




Acquisition Time (sec)	1.9923	Comment	Priyanka 1H/CDCL3	Date	11 Aug 2011 17:16:56
Date Stamp	11 Aug 2011 17:16:56	File Name	D:\paper-1\DATA\10\Thu2av400#007\1\pdata1\1\1r	Number of Transients	32
Frequency (MHz)	400.13	Nucleus	1H	Origin	spect
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	161.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.3613	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	23.300

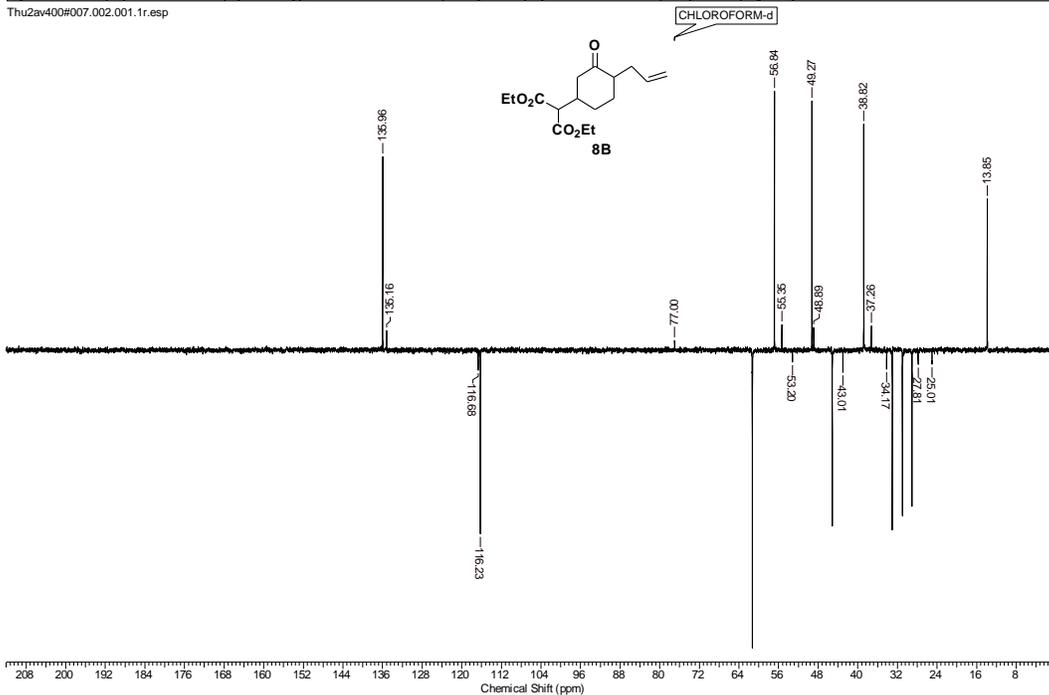


Acquisition Time (sec)	0.6488	Comment	13C	Date	11 Aug 2011 18:06:00
Date Stamp	11 Aug 2011 18:06:00	File Name	E:\paper-1\DATA\10\Thu2av400#007\3\pdata1\1\1r	Number of Transients	1570
Frequency (MHz)	100.61	Nucleus	13C	Origin	spect
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	912.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9554.7334	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	23.700



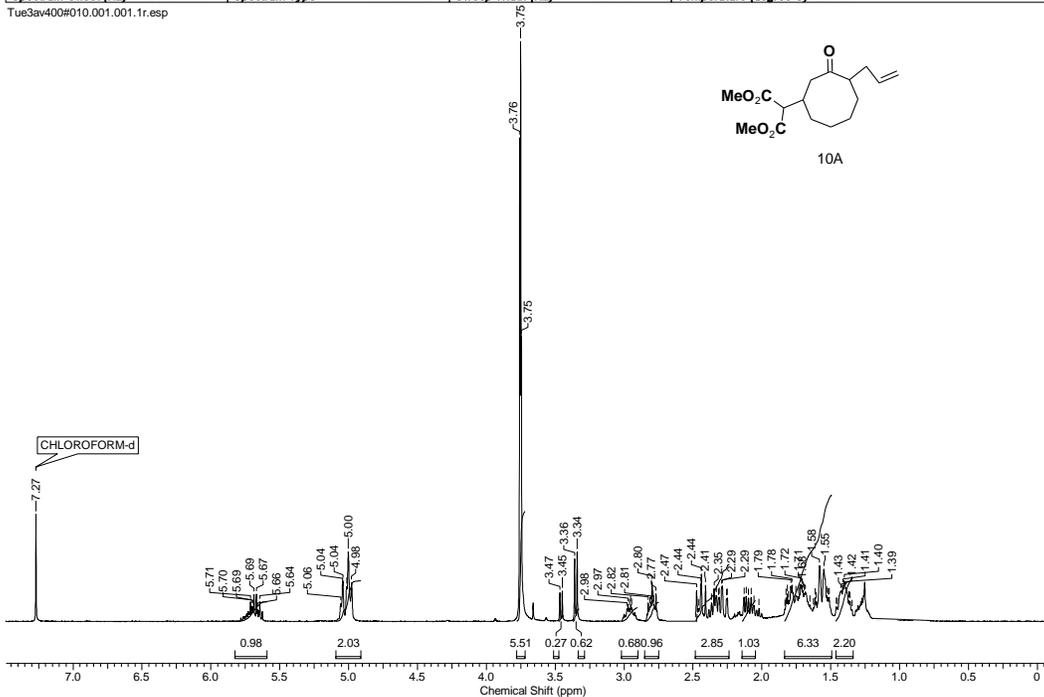
Acquisition Time (sec)	0.6816	Comment	Dept	Date	11 Aug 2011 17:19:04
Date Stamp	11 Aug 2011 17:19:04	File Name	E:\paper-1\DATA\110\Thu2av400#0072\pdata1\11r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	831
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10036.3682	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	23.400
VerticalScaleFactor = 1					

Thu2av400#007.002.001.1r.esp



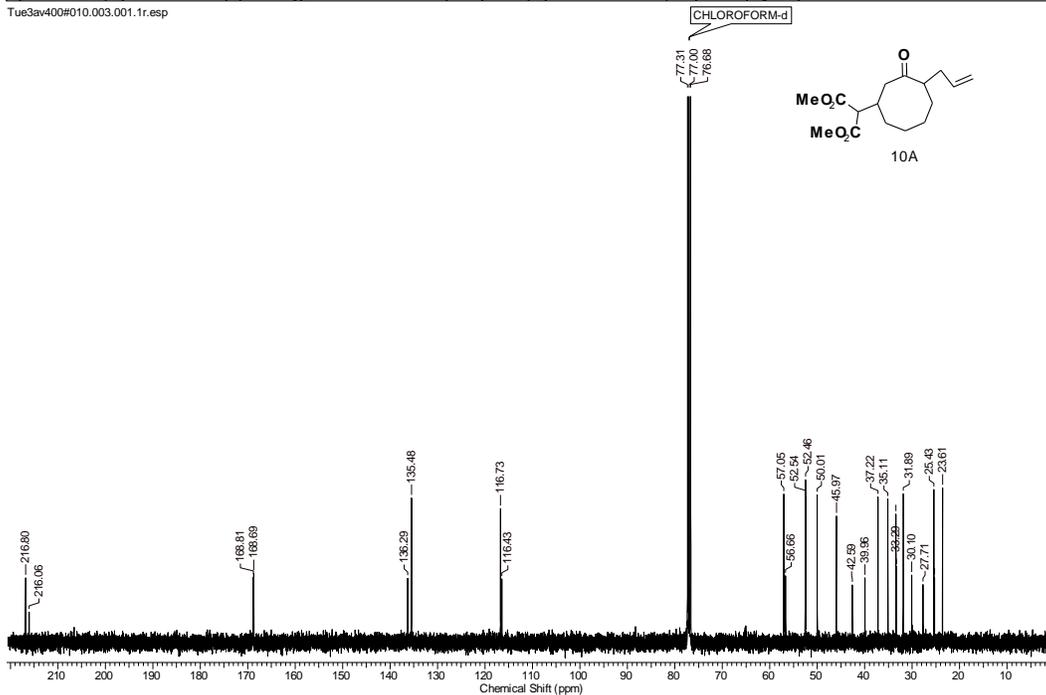
Acquisition Time (sec)	1.9923	Comment	Privanka 1H/CDCl3	Date	14 Jun 2011 14:24:08
Date Stamp	14 Jun 2011 14:24:08	File Name	D:\paper-1\DATA\14\Tue3av400#0101\pdata1\11r		
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	228.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.1101	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	22.400

Tue3av400#010.001.001.1r.esp



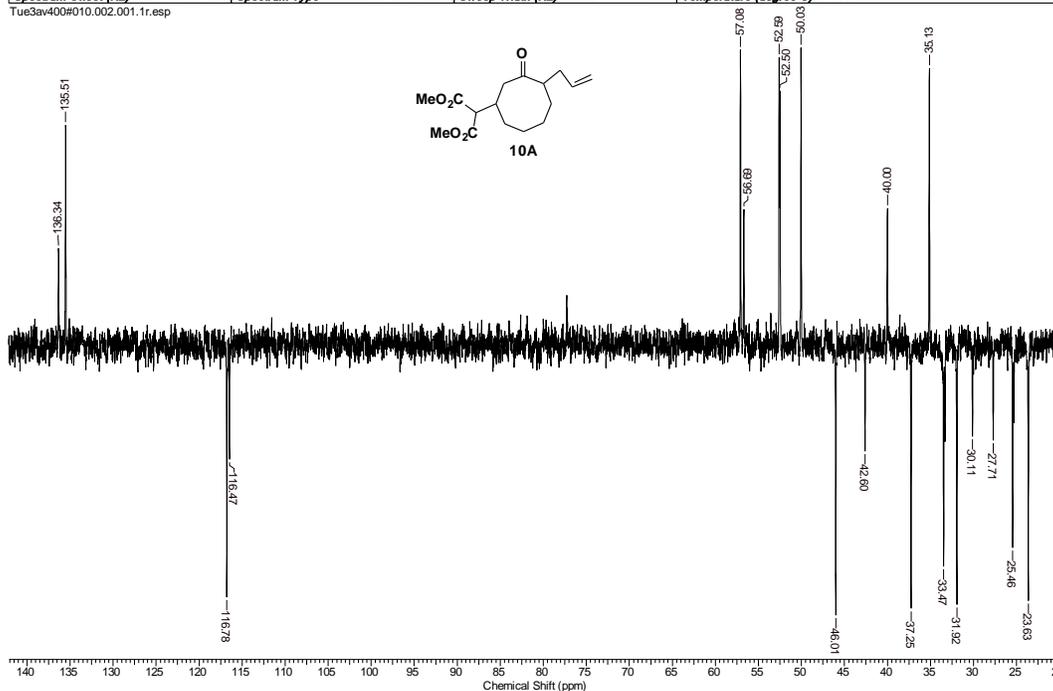
Acquisition Time (sec)	0.6488	Comment	Priyanka 13C	Date	14 Jun 2011 15:06:48
Date Stamp	14 Jun 2011 15:06:48	File Name	D:\paper-1\DATA\14\Tue3av400#010\3\data\11r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	1165
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9555.5039	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	22.600

Tue3av400#010.003.001.1r.esp



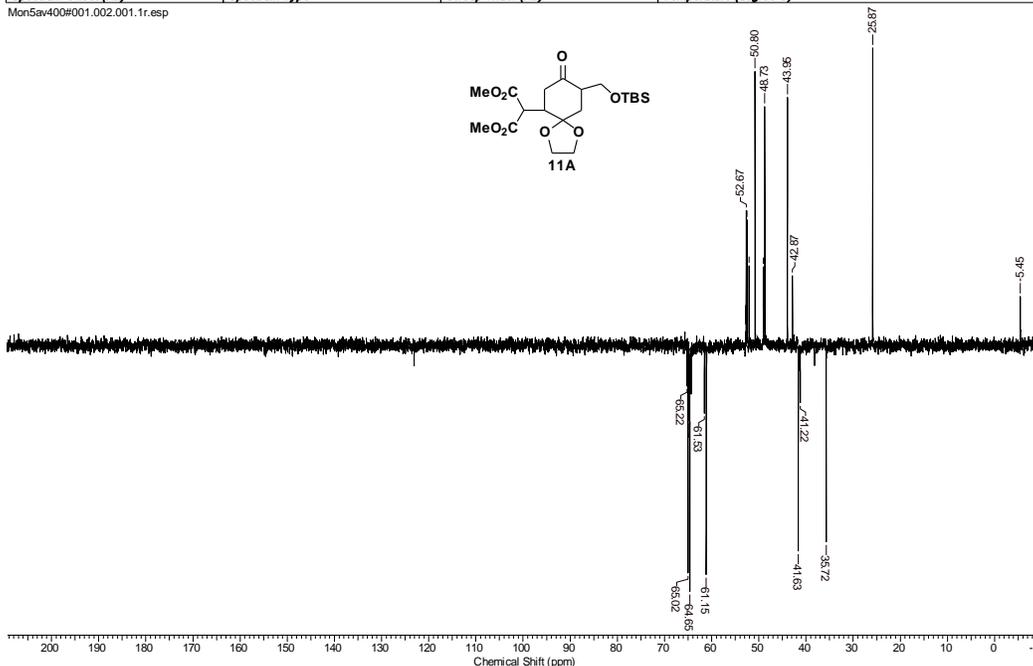
Acquisition Time (sec)	0.6816	Comment	Priyanka Dept/CDC13	Date	14 Jun 2011 14:34:48
Date Stamp	14 Jun 2011 14:34:48	File Name	E:\paper-1\DATA\14\Tue3av400#010\2\data\11r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	752
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	22.600

Tue3av400#010.002.001.1r.esp



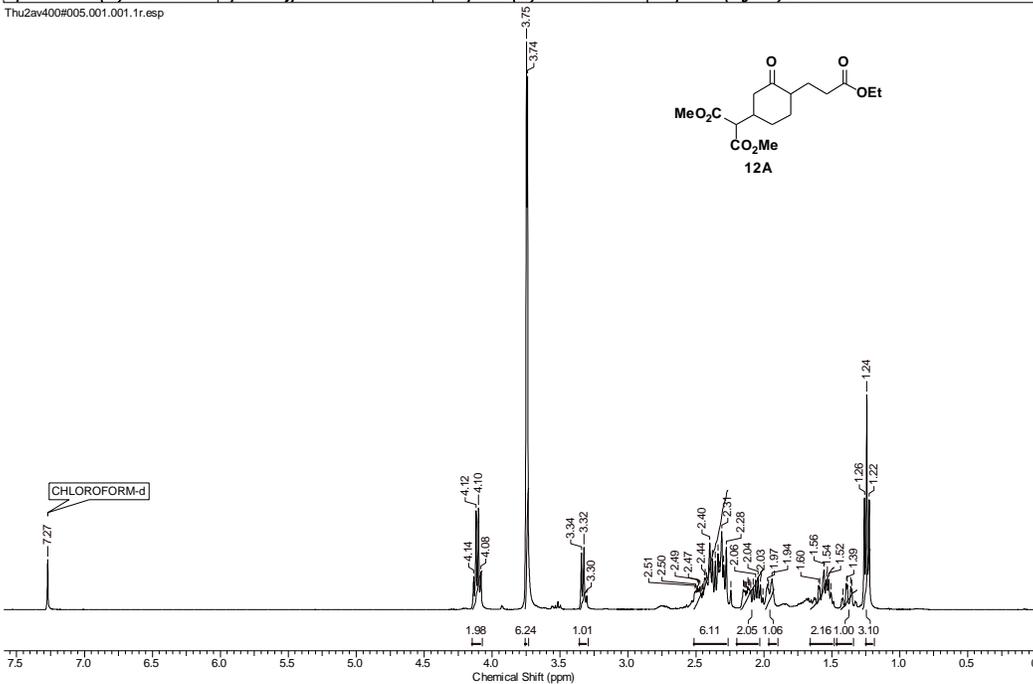
Acquisition Time (sec)	0.6816	Comment	Priyanka Dept	Date	30 May 2011 09:19:04
Date Stamp	30 May 2011 09:19:04	File Name	E:\paper-1\DATA\2\Mon5av400#0012\pdata111r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	1114
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Pulse Sequence	dept135
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Solvent	CHLOROFORM-d
				Sweep Width (Hz)	24037.73
				Temperature (degree C)	21.700

VerticalScaleFactor = 1
 Mon5av400#001.002.001.1r.esp



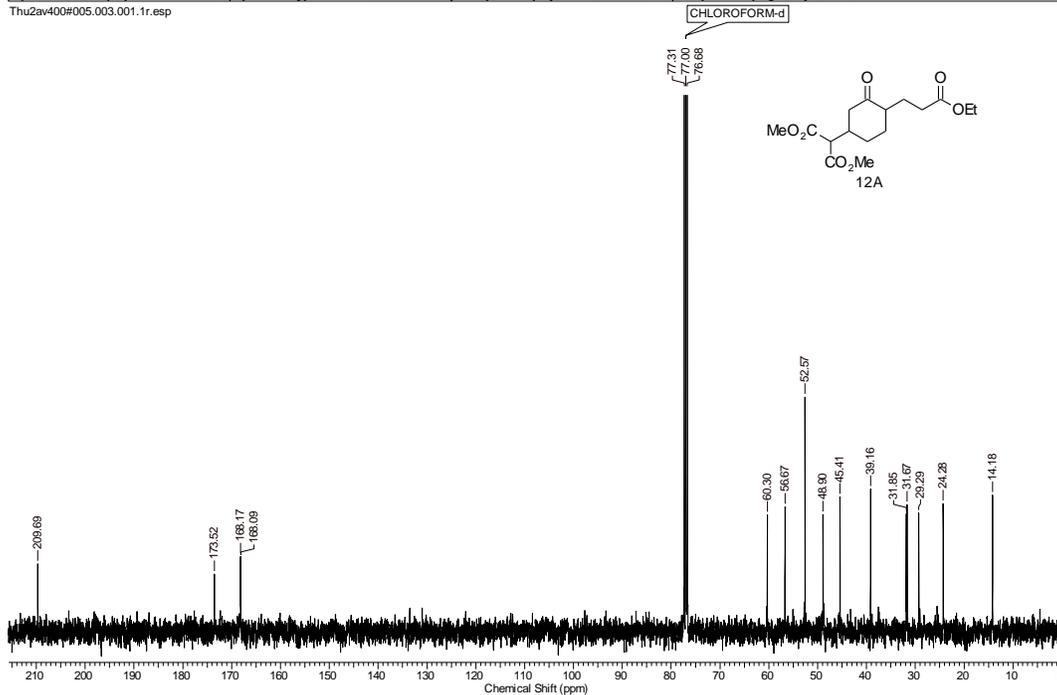
Acquisition Time (sec)	2.0447	Comment	Priyanka 1H	Date	12 May 2011 13:43:36
Date Stamp	12 May 2011 13:43:36	File Name	E:\paper-1\DATA\3\Thu2av400#005\1pdata111r	Origin	spect
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	144.00	SW(cyclical) (Hz)	8012.82	Pulse Sequence	zg30
Spectrum Offset (Hz)	2795.3604	Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
				Sweep Width (Hz)	8012.58
				Temperature (degree C)	20.000

VerticalScaleFactor = 1
 Thu2av400#005.001.001.1r.esp



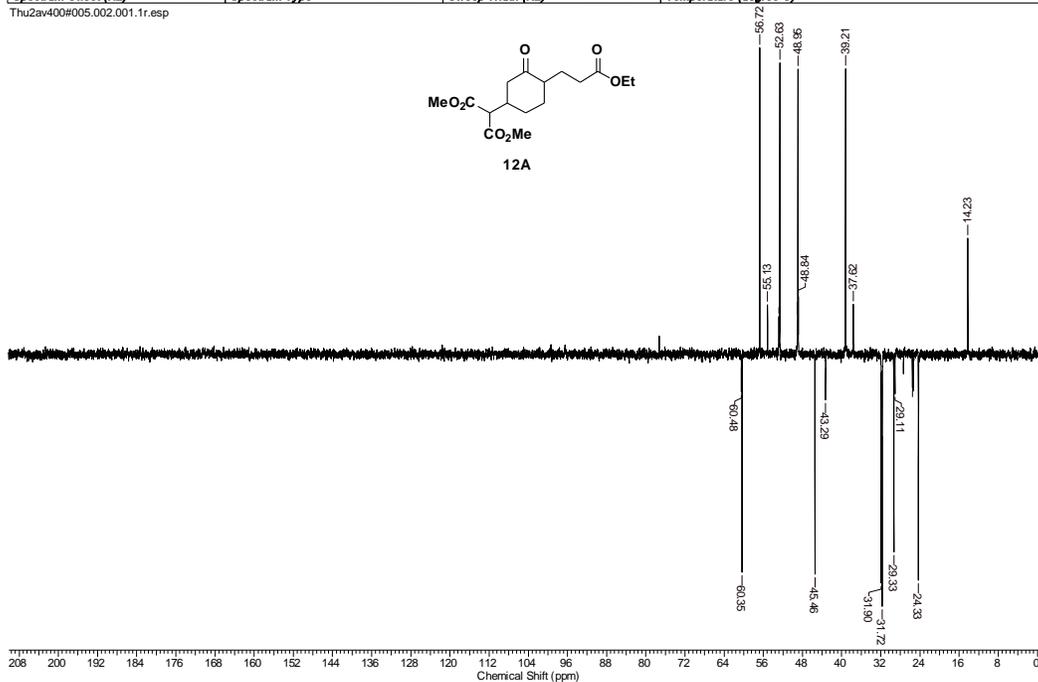
Acquisition Time (sec)	0.6816	Comment	Priyanka 13C	Date	12 May 2011 15:26:00
Date Stamp	12 May 2011 15:26:00	File Name	D:\paper-1\DATA\3\Thu2av400#005\3\data\111r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	195
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10055.4414	Spectrum Type	STANDARD	Sweep Width (Hz)	24037.73
				Temperature (degree C)	20.400

Thu2av400#005.003.001.1r.esp



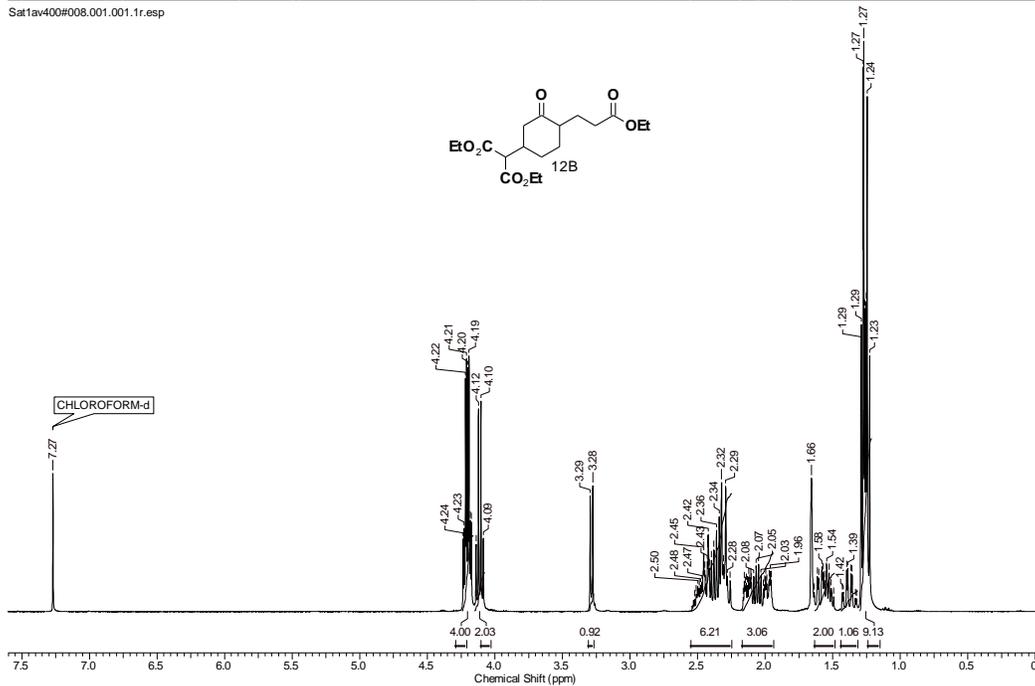
Acquisition Time (sec)	0.6816	Comment	Priyanka Dept	Date	12 May 2011 13:47:52
Date Stamp	12 May 2011 13:47:52	File Name	E:\paper-1\DATA\3\Thu2av400#005\2\data\111r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	697
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	20.100

Thu2av400#005.002.001.1r.esp



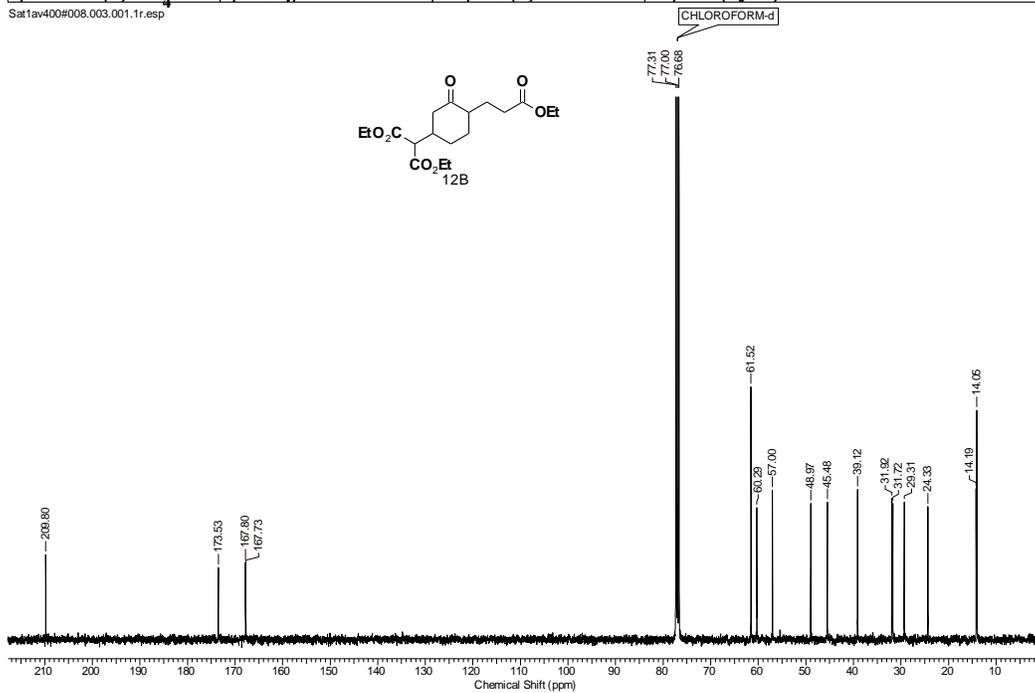
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H/CDCB	Date	02 Jul 2011 15:32:24
Date Stamp	02 Jul 2011 15:32:24	File Name	D:\paper-1\DATA\4\Sat1av400#008\1\pdata\1\1r	Number of Transients	32
Frequency (MHz)	400.13	Nucleus	1H	Origin	spect
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	181.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.3613	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	24.000

Sat1av400#008.001.001.1r.esp



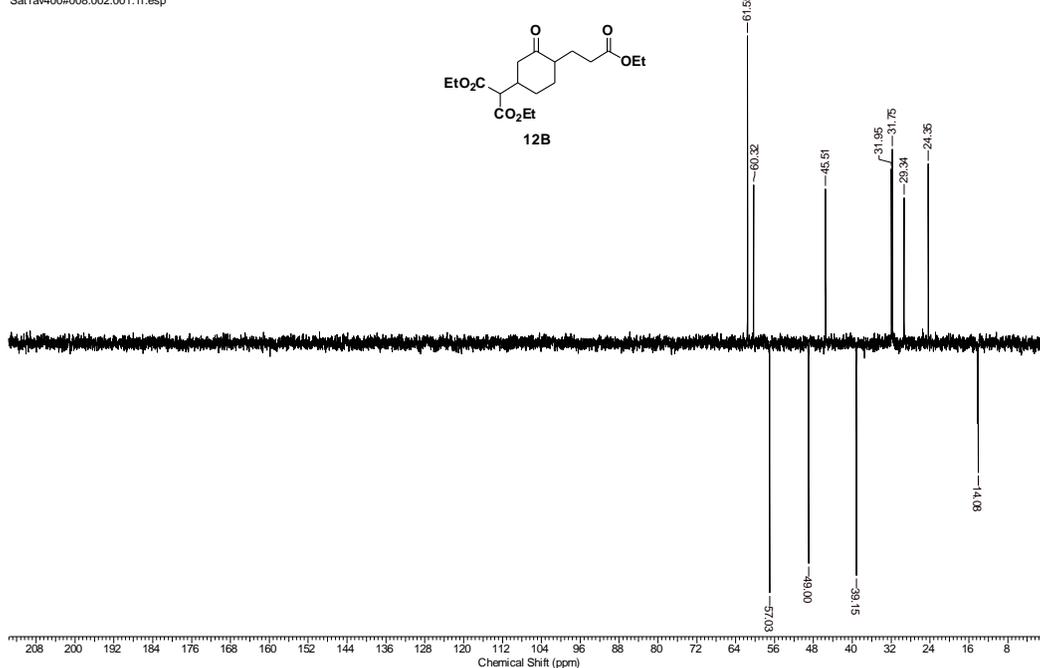
Acquisition Time (sec)	0.6488	Comment	13C	Date	02 Jul 2011 16:53:28
Date Stamp	02 Jul 2011 16:53:28	File Name	D:\paper-1\DATA\4\Sat1av400#008\3\pdata\1\1r	Number of Transients	826
Frequency (MHz)	100.61	Nucleus	13C	Origin	spect
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	912.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9555.5049	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	24.600

Sat1av400#008.003.001.1r.esp



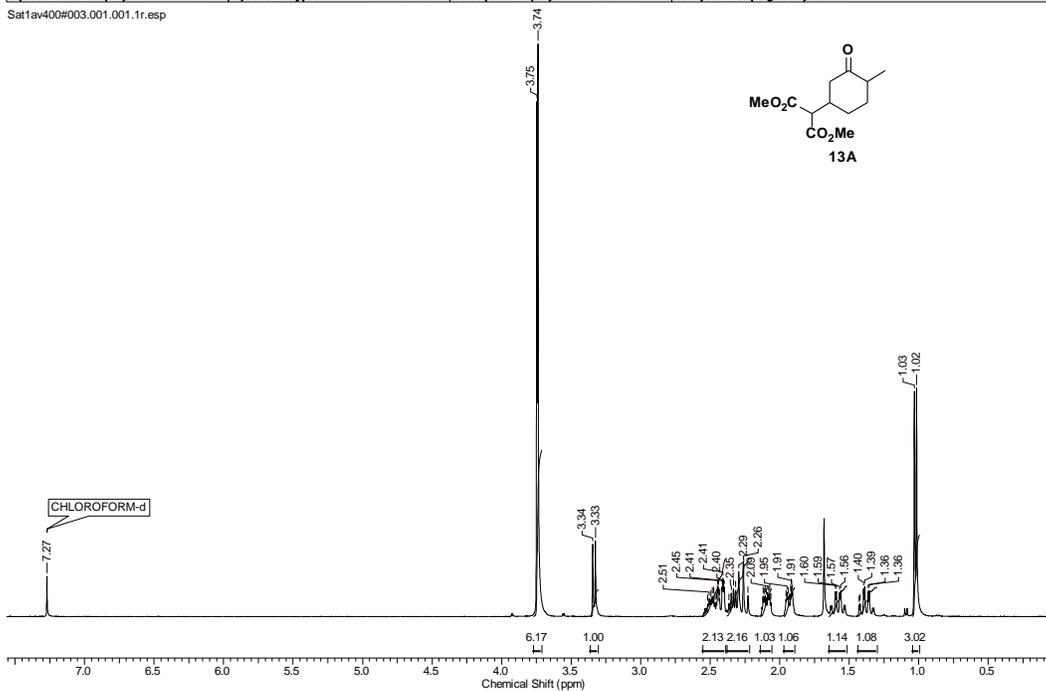
Acquisition Time (sec)	0.6816	Comment	Dept/CDCI3	Date	02 Jul 2011 15:45:12
Date Stamp	02 Jul 2011 15:45:12	File Name	E:\paper-1\DATA\1\Sat1av400#008\2\data\111r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	1200
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	24.300
VerticalScaleFactor = 1					

Sat1av400#008.002.001.1r.esp



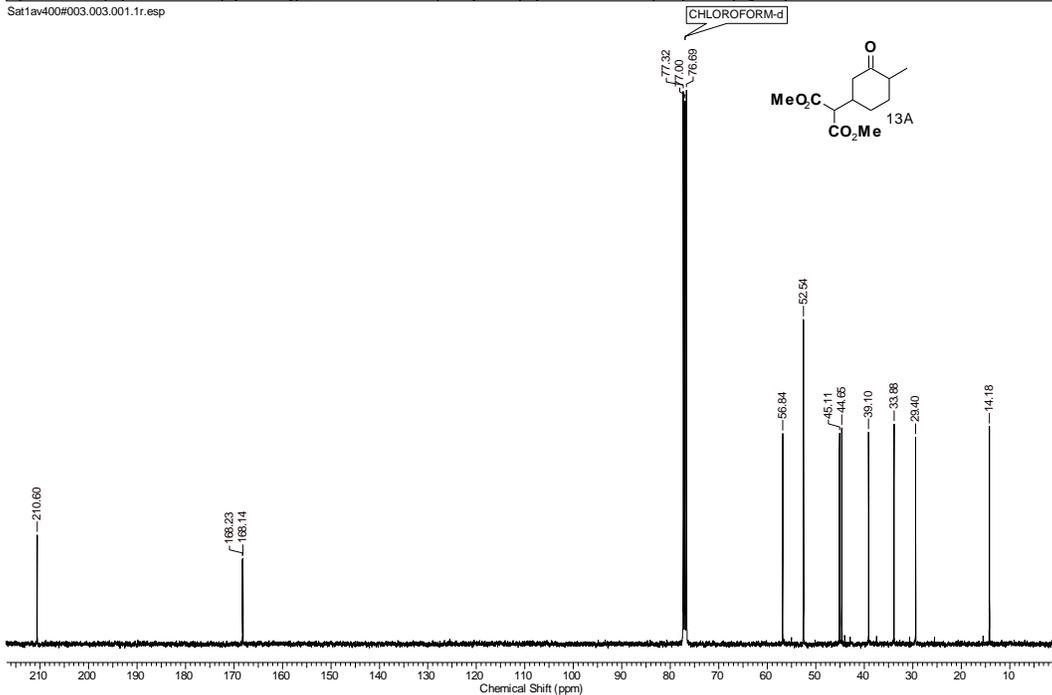
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H/ CDCI3	Date	02 Jul 2011 09:06:16
Date Stamp	02 Jul 2011 09:06:16	File Name	E:\paper-1\DATA\6\Sat1av400#003\1\data\111r		
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	181.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.1101	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	25.000
VerticalScaleFactor = 1					

Sat1av400#003.001.001.1r.esp



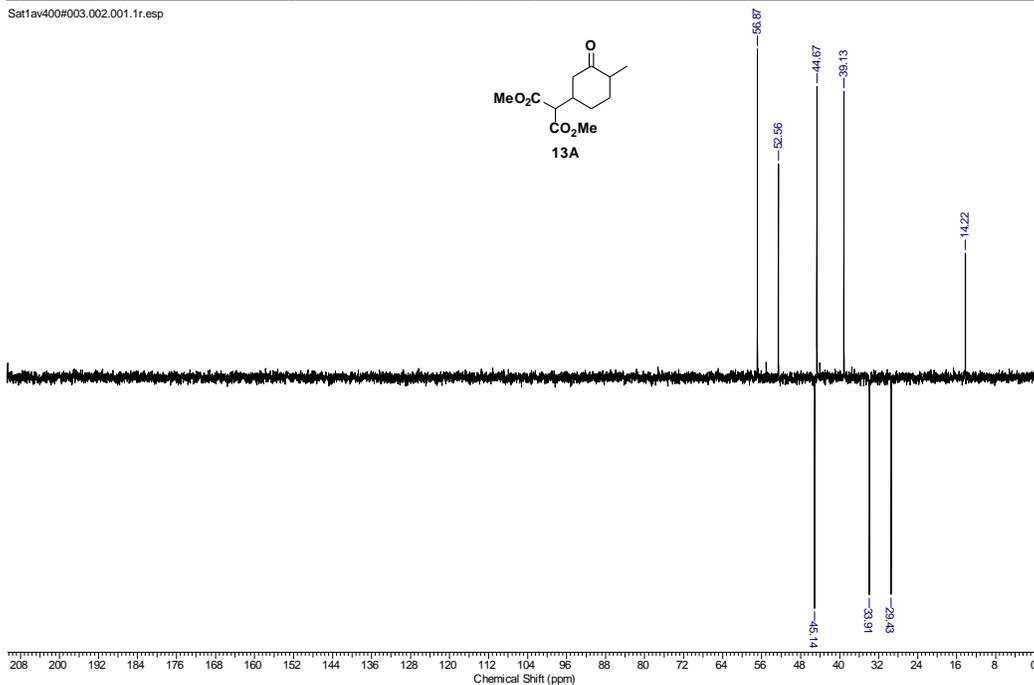
Acquisition Time (sec)	0.6488	Comment	13C	Date	02 Jul 2011 10:03:52
Date Stamp	02 Jul 2011 10:03:52	File Name	D:\paper-1\DATA\6\Sat1av400#003\3\data111r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	1436
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	912.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9555.5049	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	25.000

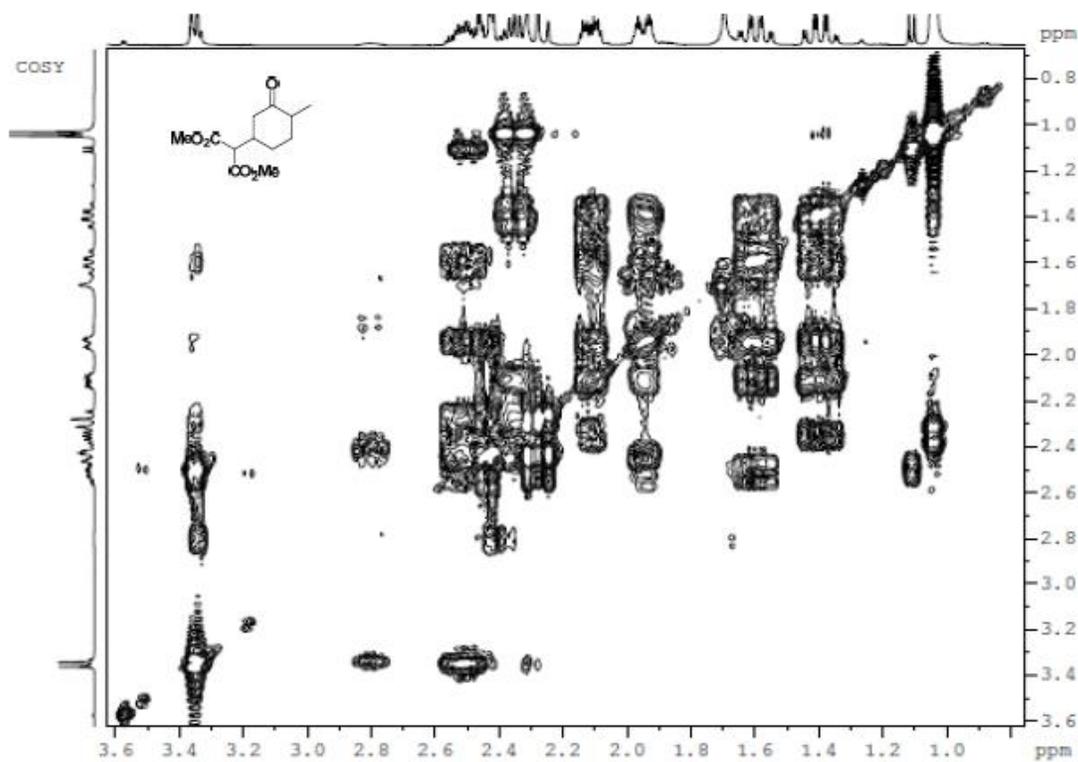
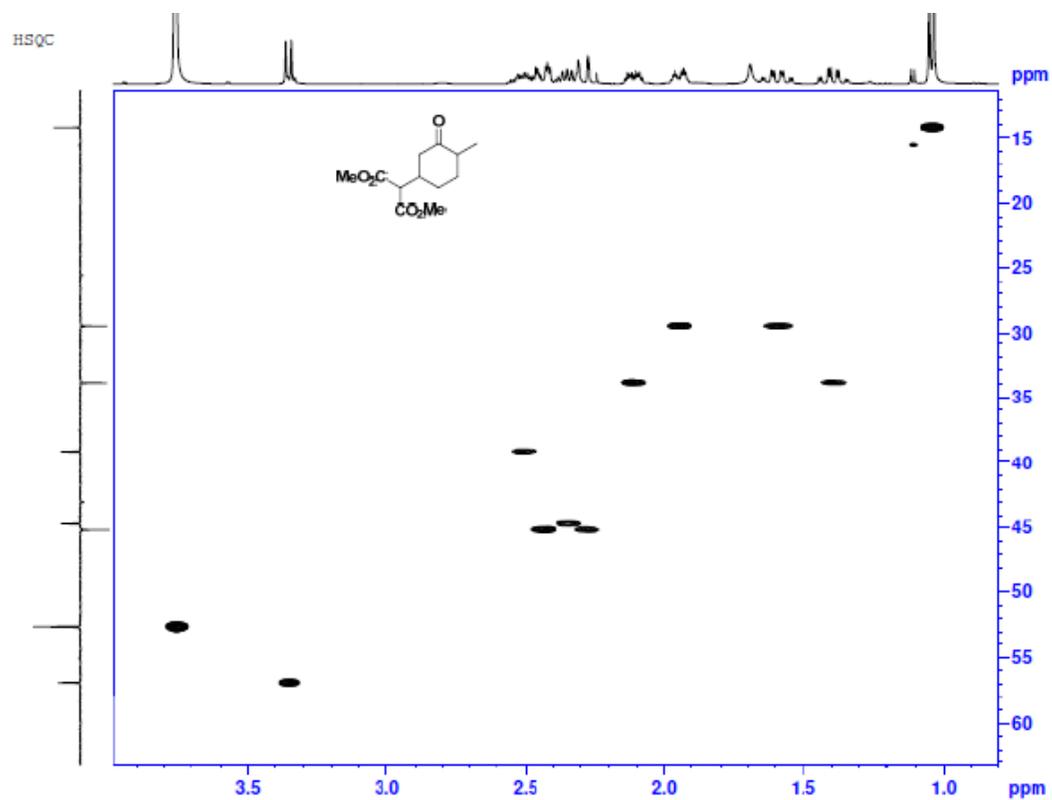
Sat1av400#003.003.001.1r.esp

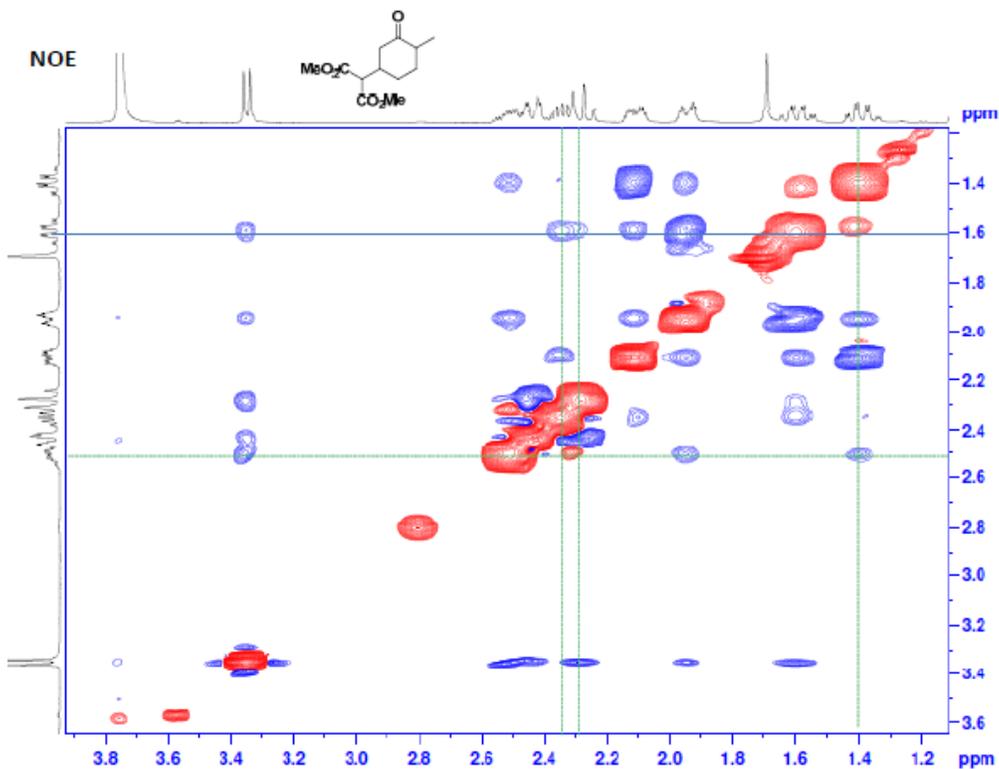


Acquisition Time (sec)	0.6816	Comment	Dept/CDC13	Date	02 Jul 2011 09:16:56
Date Stamp	02 Jul 2011 09:16:56	File Name	E:\paper-1\DATA\6\Sat1av400#003\2\data111r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	239
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	25.000

Sat1av400#003.002.001.1r.esp

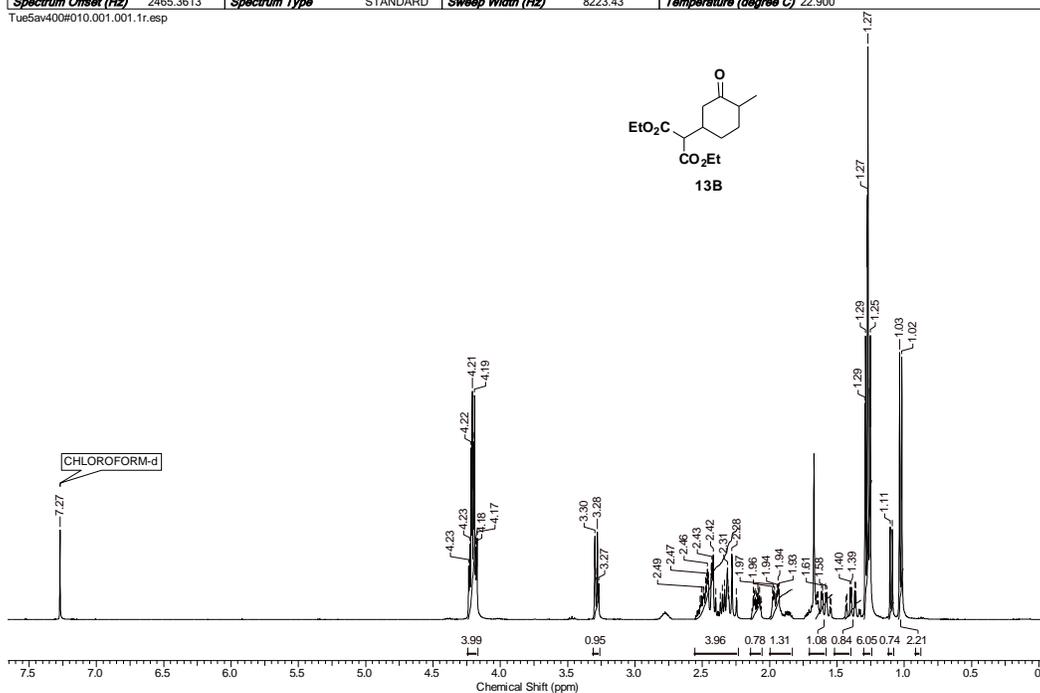




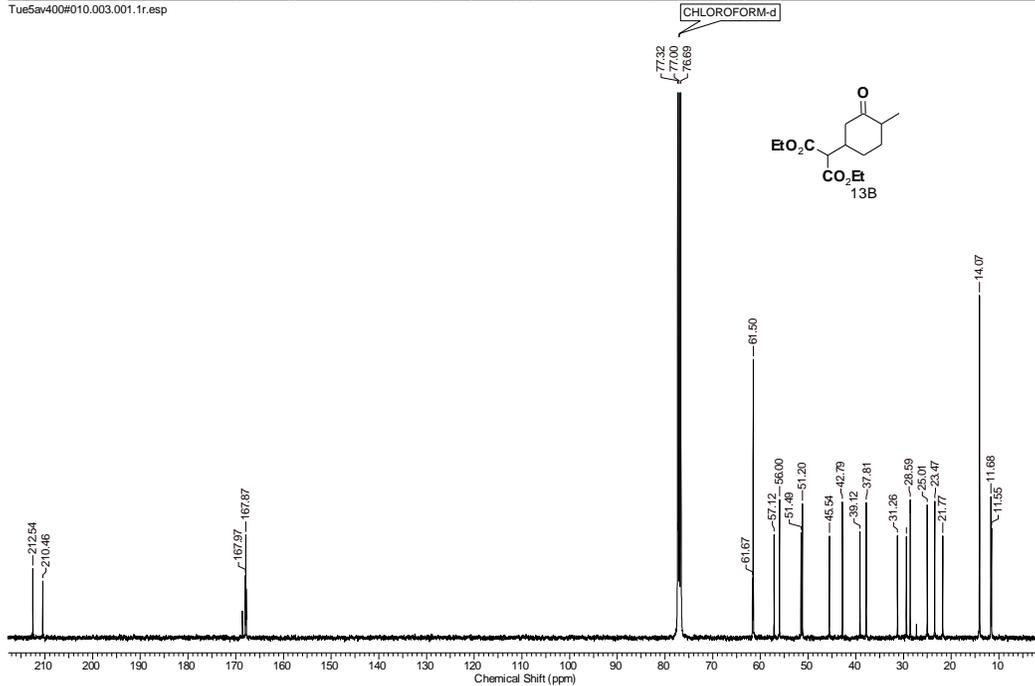


Acquisition Time (sec)	1.9923	Comment	Priyanka 1H	Date	25 Aug 2011 14:49:44
Date Stamp	25 Aug 2011 14:49:44	File Name	E:\paper-1\DATA\7\TueSav400#010\1\data\111r		
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	203.00	SW(cyclical) (Hz)	8223.68	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	2465.3613	Spectrum Type	STANDARD	Sweep Width (Hz)	8223.43
				Temperature (degree C)	22.900

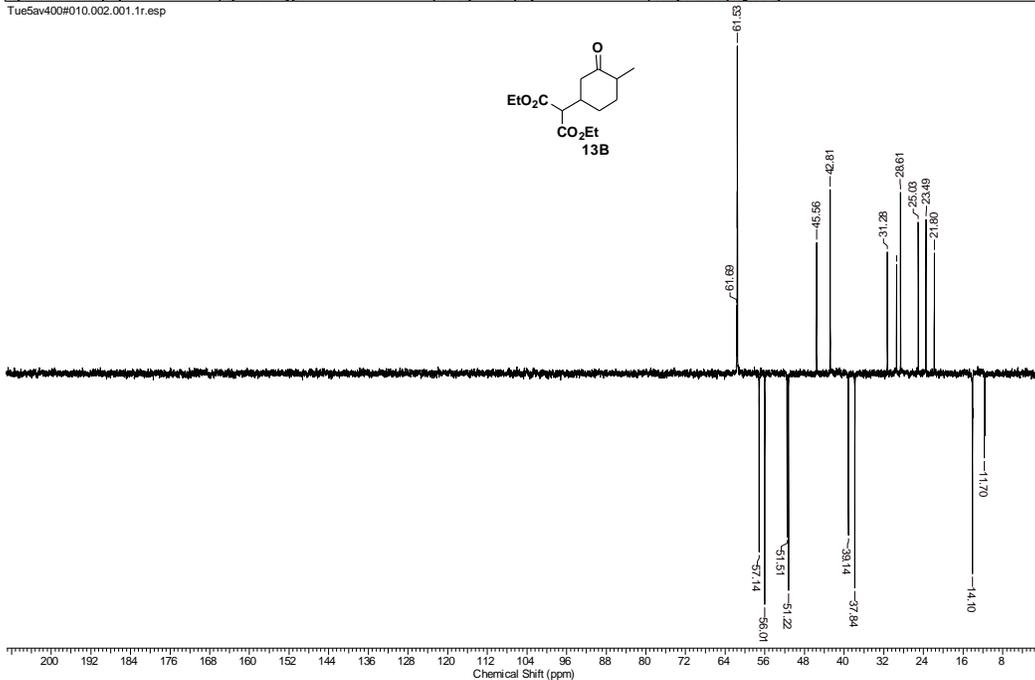
TueSav400#010.001.1f.esp
 VerticalScaleFactor = 1



Acquisition Time (sec)	0.6488	Comment	13C	Date	31 Aug 2011 08:53:28
Date Stamp	31 Aug 2011 08:53:28	File Name	D:\paper-1\DATA\7\TueSav400#010\3\pdata\11r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	13074
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	912.00	SW(cyclical) (Hz)	25252.53	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	9556.2744	Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75
				Temperature (degree C)	24.300

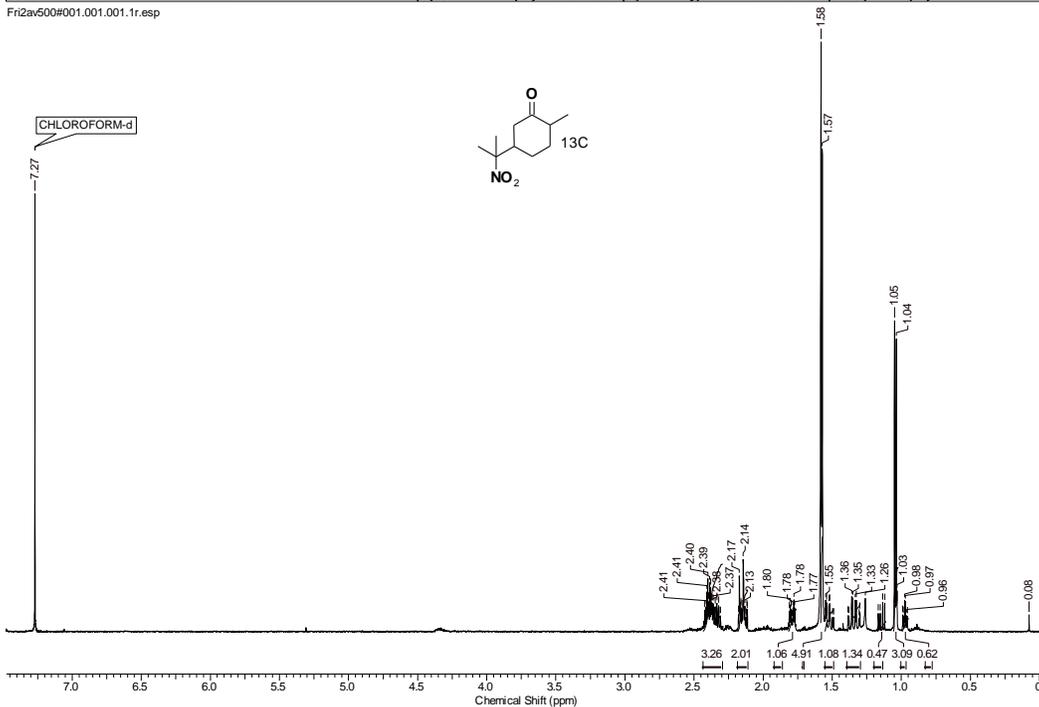


Acquisition Time (sec)	0.6816	Comment	DEPT	Date	30 Aug 2011 23:08:56
Date Stamp	30 Aug 2011 23:08:56	File Name	E:\paper-1\DATA\7\TueSav400#010\2\pdata\11r		
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	4000
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	10060.3320	Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73
				Temperature (degree C)	24.100



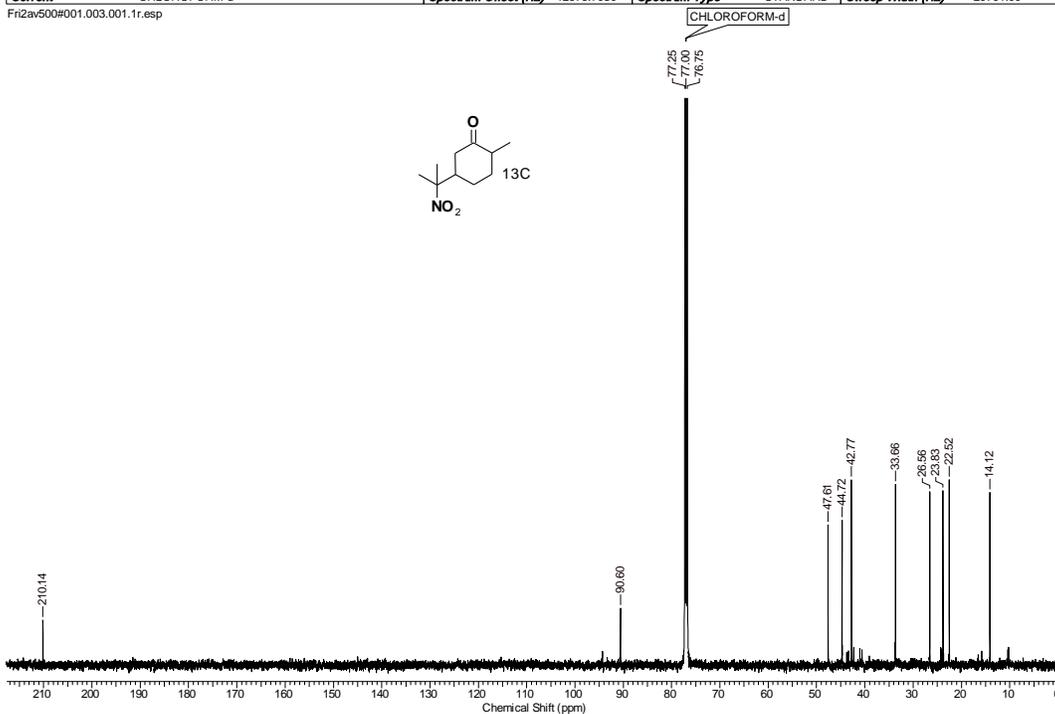
Acquisition Time (sec)	1.6384	Comment	1H Priyanka	Date	12 Aug 2011 11:25:20	Frequency (MHz)	500.13
Date Stamp	12 Aug 2011 11:25:20	File Name	D:\paper-1\DATA\8\Fri2av500#001\1\data1\11r	Origin	spect	Original Points Count	16384
Nucleus	1H	Number of Transients	64	Receiver Gain	912.00	SW(cyclical) (Hz)	10000.00
Points Count	32768	Pulse Sequence	zg30	Spectrum Offset (Hz)	3492.9702	Spectrum Type	STANDARD
Solvent	CHLOROFORM-d					Sweep Width (Hz)	9999.70

Fri2av500#001.001.001.1r.esp



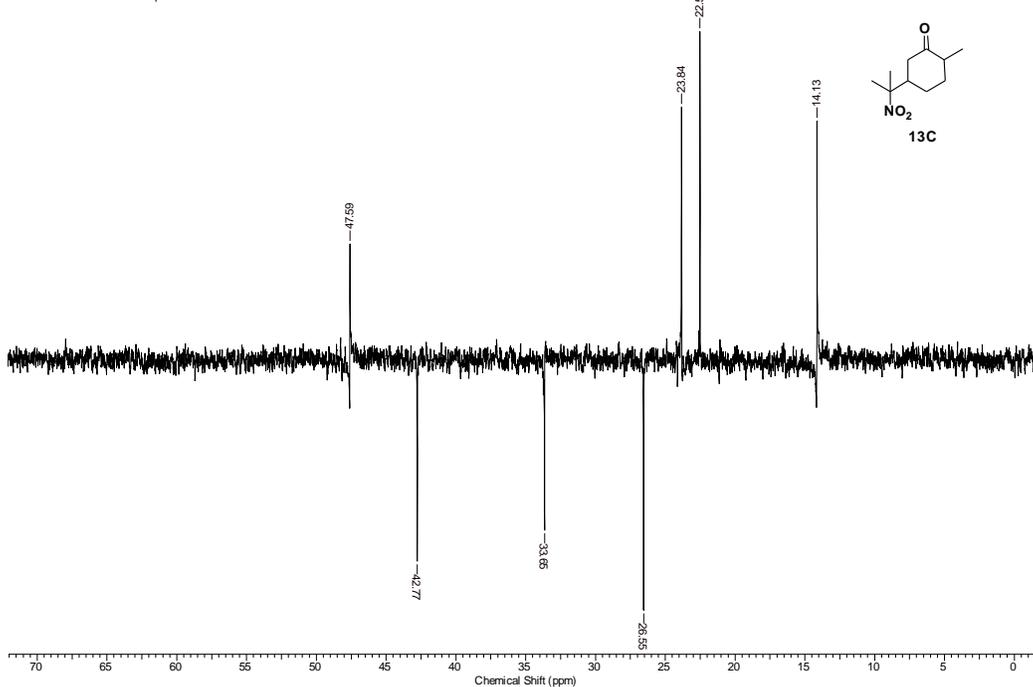
Acquisition Time (sec)	1.1010	Comment	13C	Date	12 Aug 2011 14:30:56	Frequency (MHz)	125.76
Date Stamp	12 Aug 2011 14:30:56	File Name	D:\paper-1\DATA\8\Fri2av500#001\3\data1\11r	Origin	spect	Original Points Count	32768
Nucleus	13C	Number of Transients	2390	Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90
Points Count	32768	Pulse Sequence	zgpg	Spectrum Offset (Hz)	12575.7080	Spectrum Type	STANDARD
Solvent	CHLOROFORM-d					Sweep Width (Hz)	29761.00

Fri2av500#001.003.001.1r.esp



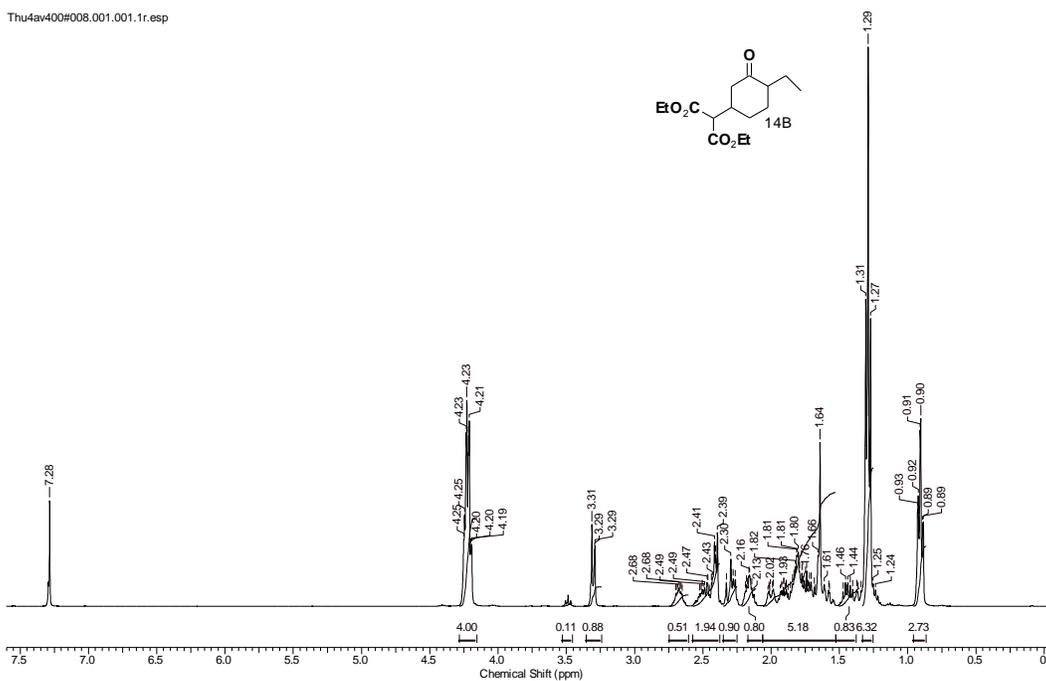
Acquisition Time (sec)	1.1010	Comment	DEPT135	Date	12 Aug 2011 11:29:36	Frequency (MHz)	125.76
Date Stamp	12 Aug 2011 11:29:36	File Name	E:\paper-1\DATA\8\Fr2av500#001\2\data111r	Origin	spect	Original Points Count	32768
Nucleus	13C	Number of Transients	1200	Points Count	32768	SW(cyclical) (Hz)	29761.90
Points Count	32768	Pulse Sequence	dept135	Receiver Gain	2050.00	VerticalScaleFactor	= 1
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12575.7842	Spectrum Type	DEPT135	Sweep Width (Hz)	29761.00

Fr2av500#001.002.001.1r.esp



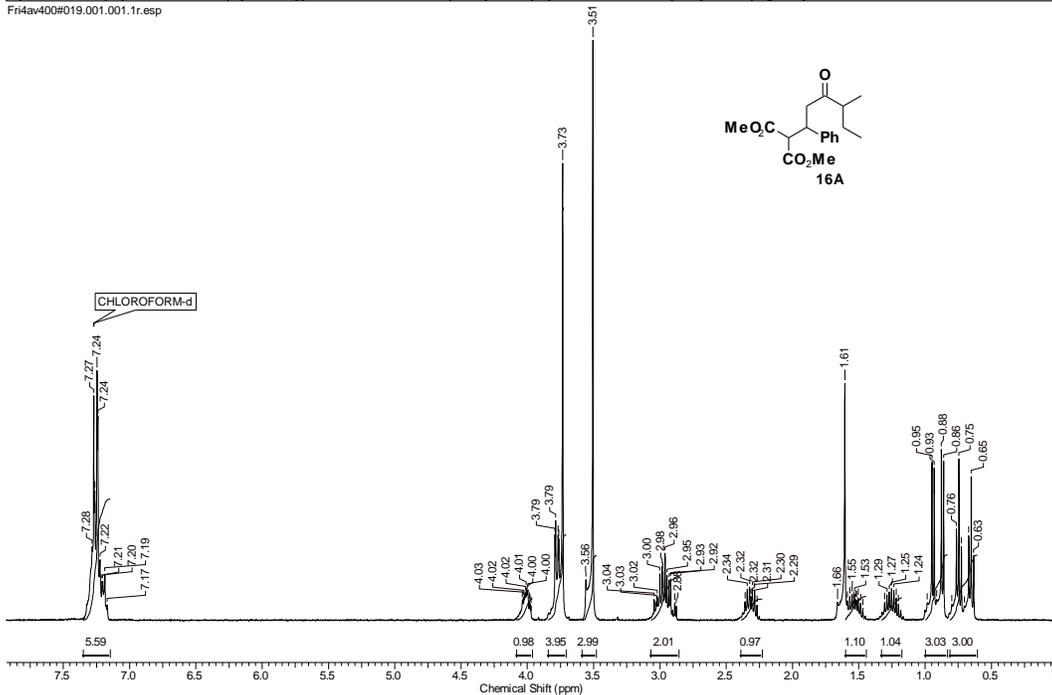
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H	Date	30 Aug 2011 20:05:28
Date Stamp	30 Aug 2011 20:05:28	File Name	D:\paper-1\DATA\11\Thu4av400#008\1\data111r	Origin	spect
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	287.00	SW(cyclical) (Hz)	8223.68	Pulse Sequence	zg30
Spectrum Offset (Hz)	2470.9644	Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
				Sweep Width (Hz)	8223.43
				Temperature (degree C)	23.500

Thu4av400#008.001.001.1r.esp



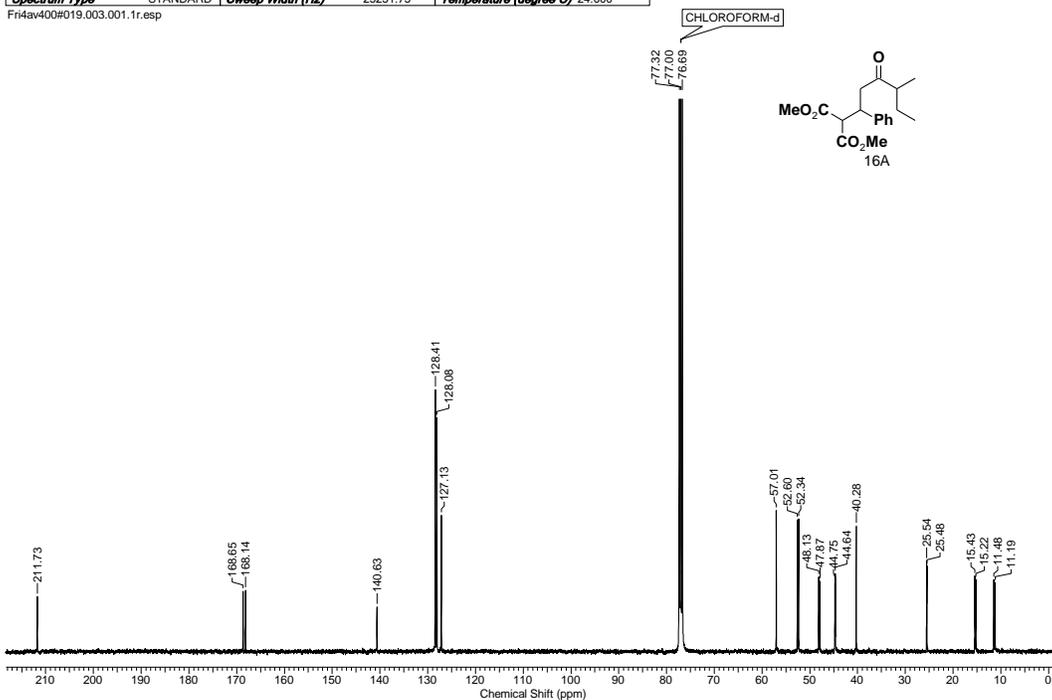
Acquisition Time (sec)	1.9923	Comment	Priyanka 1H/CDCL3	Date	26 Aug 2011 19:59:04
Date Stamp	26 Aug 2011 19:59:04	File Name	D:\paper-1\DATA\15\Fri4av400#019\1\data\111r	Origin	spect
Frequency (MHz)	400.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	Administrator	Points Count	32768
Receiver Gain	256.00	SW(cyclical) (Hz)	8223.68	Pulse Sequence	zg30
Spectrum Offset (Hz)	2465.3613	Spectrum Type	STANDARD	Solvent	CHLOROFORM-d
				Sweep Width (Hz)	8223.43
				Temperature (degree C)	23.400

Fri4av400#019.001.001.1r.esp



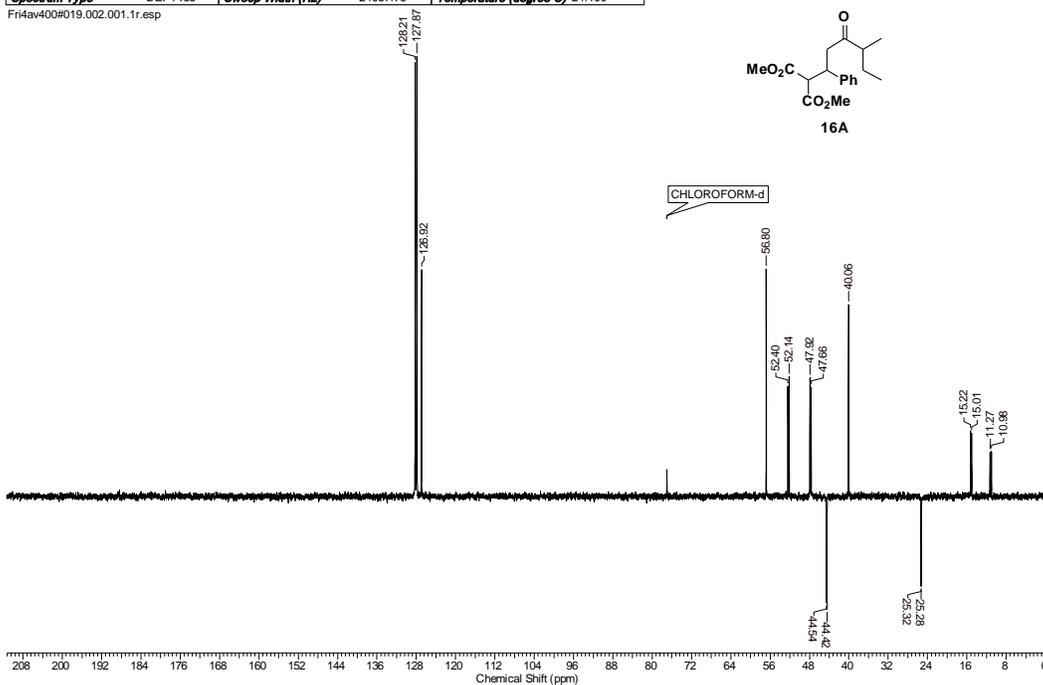
Acquisition Time (sec)	0.6488	Comment	13C	Date	27 Aug 2011 08:42:48
Date Stamp	27 Aug 2011 08:42:48	File Name	D:\paper-1\DATA\15\Fri4av400#019\3\data\111r	Origin	spect
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	12790
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	912.00	SW(cyclical) (Hz)	25252.53	Pulse Sequence	zgpg30
Spectrum Type	STANDARD	Sweep Width (Hz)	25251.75	Solvent	DMSO-d6
				Spectrum Offset (Hz)	9556.2744
				Temperature (degree C)	24.600

Fri4av400#019.003.001.1r.esp



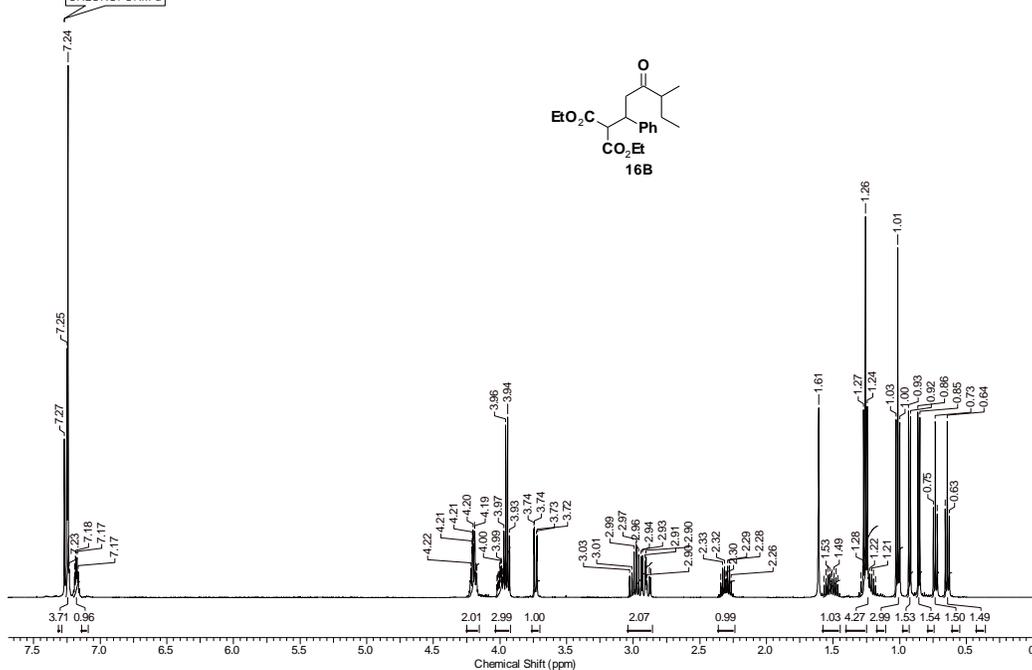
Acquisition Time (sec)	0.6816	Comment	Dept	Date	26 Aug 2011 23:04:40
Date Stamp	26 Aug 2011 23:04:40	File Name			E:\paper-1\DATA\15\Fri4av400#019\2\pdata\1\1r
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	4000
Original Points Count	16384	Owner	root	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24038.46	Solvent	DMSO-d6
Spectrum Type	DEPT135	Sweep Width (Hz)	24037.73	Temperature (degree C)	24.100
				Spectrum Offset (Hz)	10037.1016 VerticalScaleFactor = 1

Fri4av400#019.002.001.1r.esp



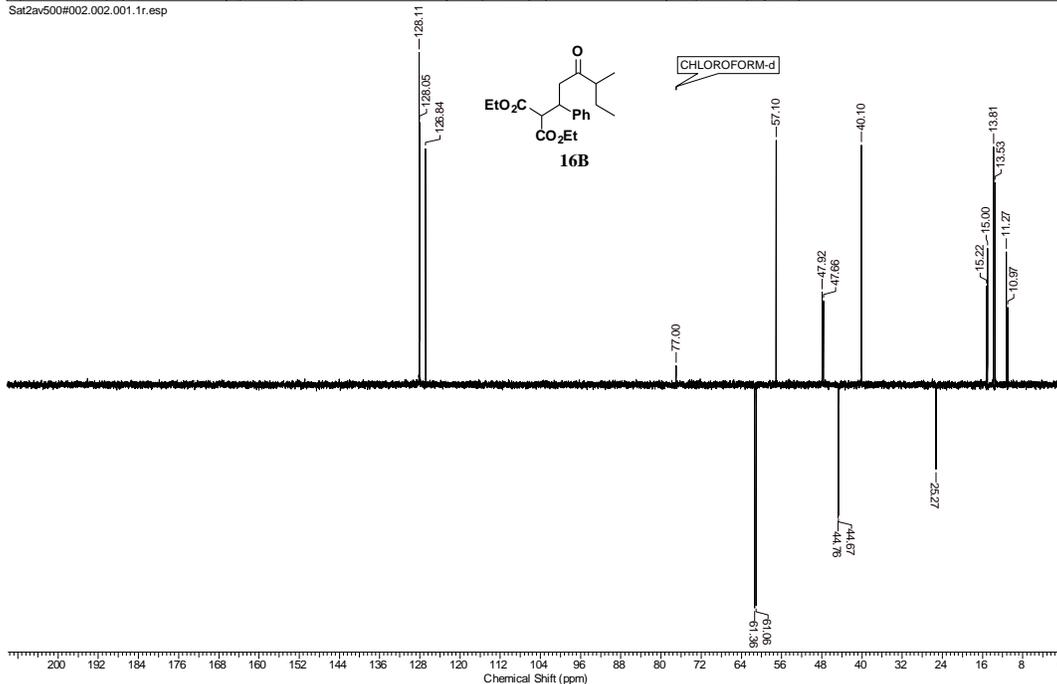
Acquisition Time (sec)	1.6384	Comment	1H Priyanka	Date	10 Sep 2011 12:27:12
Date Stamp	10 Sep 2011 12:27:12	File Name			D:\paper-1\DATA\16\Sat2av500#002\1\pdata\1\1r
Frequency (MHz)	500.13	Nucleus	1H	Number of Transients	64
Original Points Count	16384	Owner	nmr	Points Count	32768
Receiver Gain	203.00	SW(cyclical) (Hz)	10000.00	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	3491.7498	Spectrum Type	STANDARD	Sweep Width (Hz)	9999.70
				Temperature (degree C)	25.000

Sat2av500#002.001.001.1r.esp



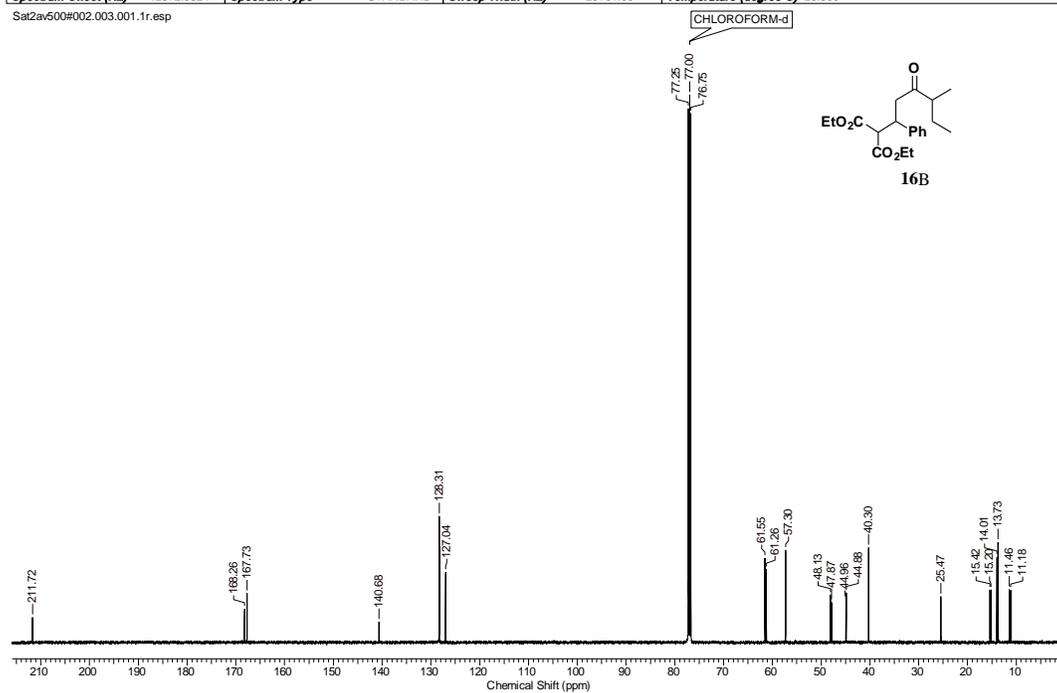
Acquisition Time (sec)	1.1010	Comment	DEPT135	Date	10 Sep 2011 12:37:52
Date Stamp	10 Sep 2011 12:37:52	File Name	E:\paper-1\DATA\16\Sat2av500#002\2\pdata1\11r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	1200
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12547.5518	Spectrum Type	DEPT135	Sweep Width (Hz)	29761.00
				Temperature (degree C)	25.200
VerticalScaleFactor = 1					

Sat2av500#002.002.001.1r.esp



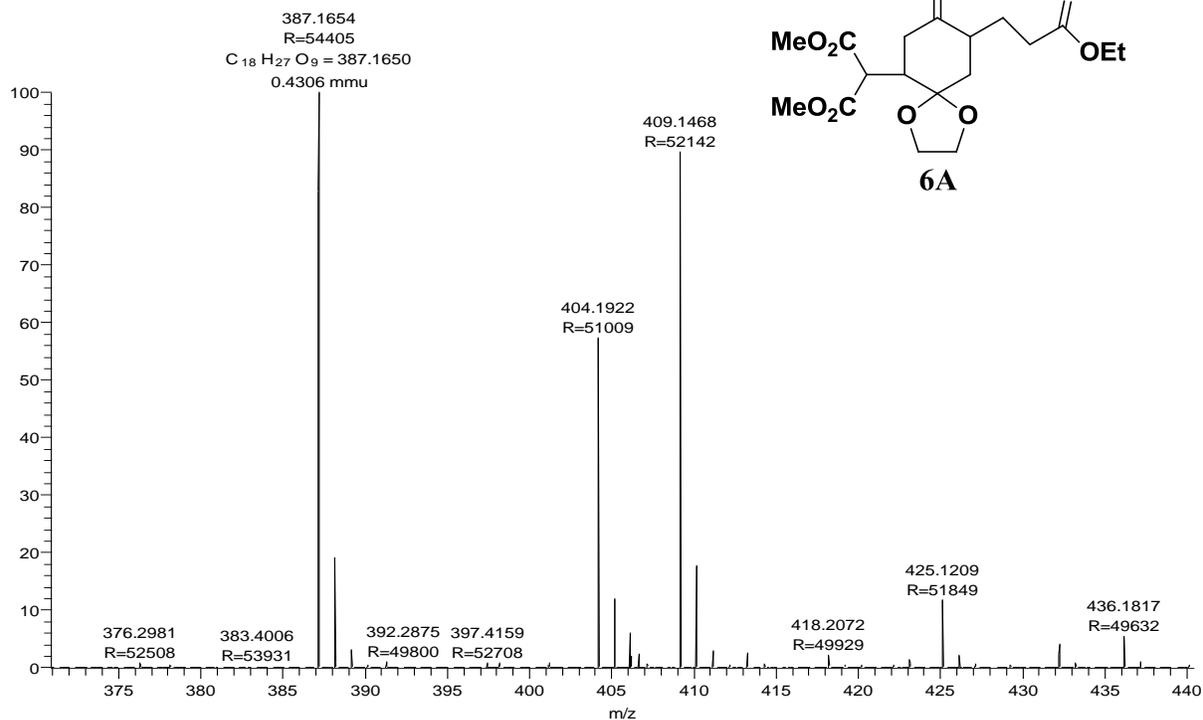
Acquisition Time (sec)	1.1010	Comment	13C	Date	10 Sep 2011 15:41:20
Date Stamp	10 Sep 2011 15:41:20	File Name	E:\paper-1\DATA\16\Sat2av500#002\3\pdata1\11r		
Frequency (MHz)	125.76	Nucleus	13C	Number of Transients	3397
Original Points Count	32768	Owner	nmr	Points Count	32768
Receiver Gain	2050.00	SW(cyclical) (Hz)	29761.90	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	12572.9824	Spectrum Type	STANDARD	Sweep Width (Hz)	29761.00
				Temperature (degree C)	25.800
VerticalScaleFactor = 1					

Sat2av500#002.003.001.1r.esp

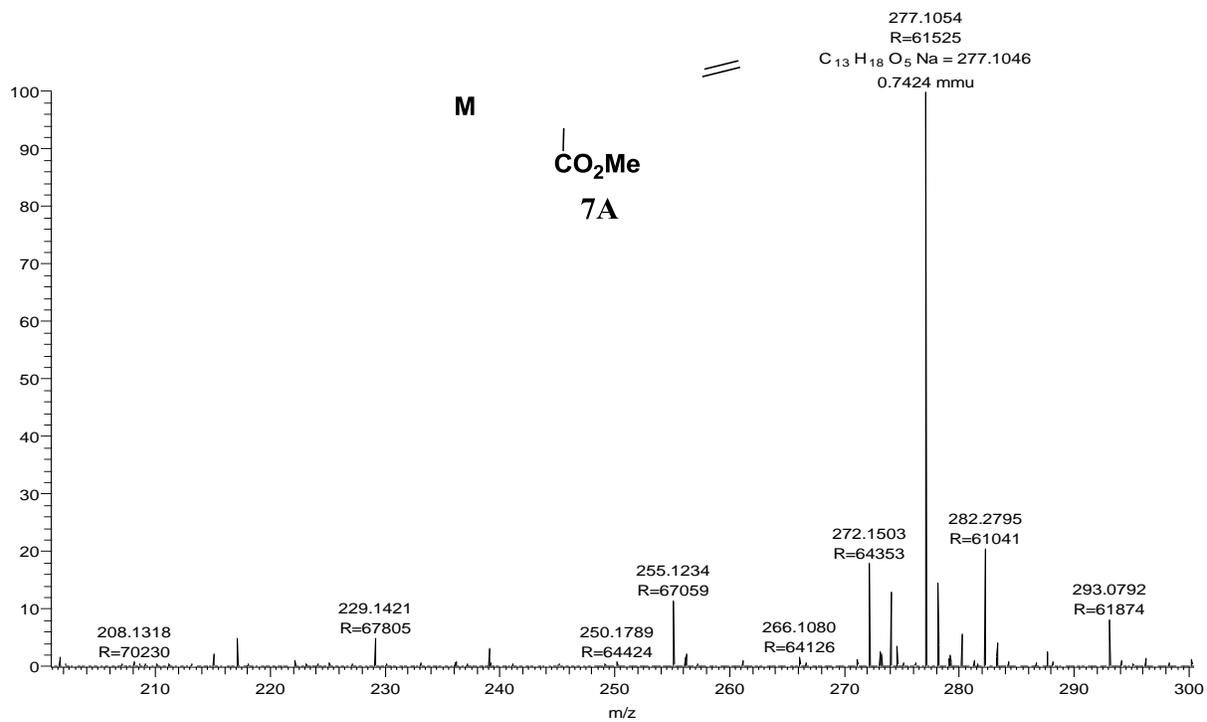


HRMS SPECTRAS

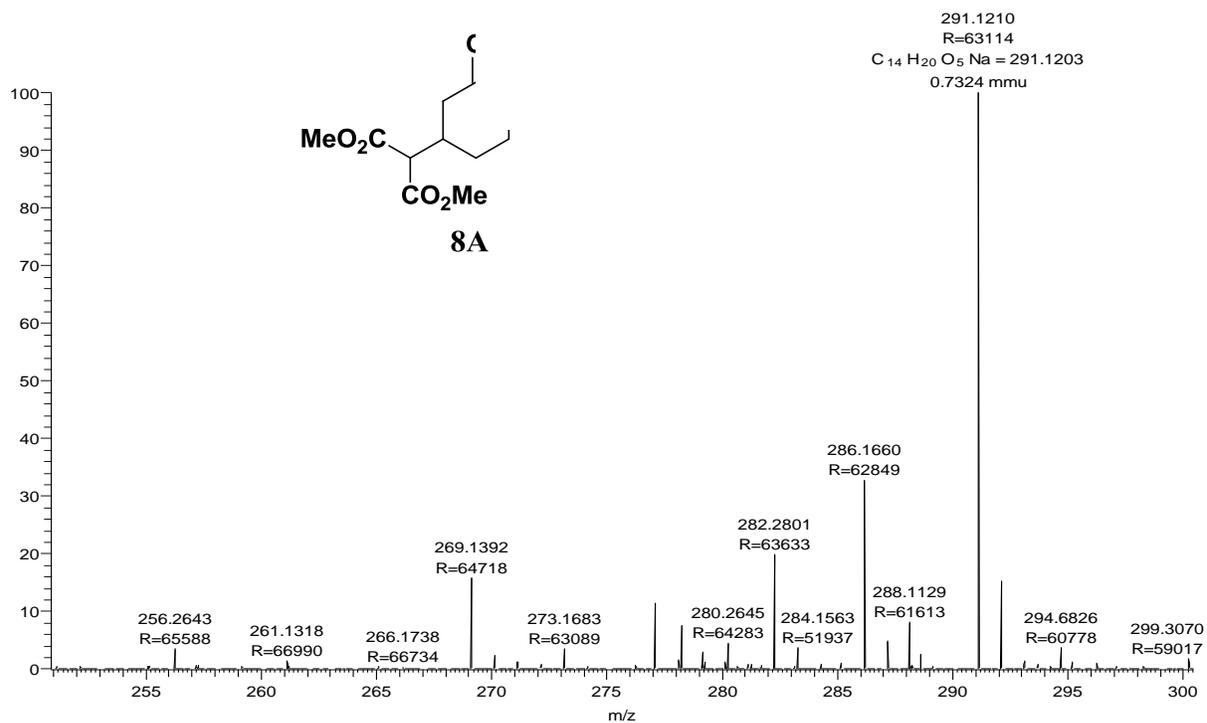
6A #1-19 RT: 0.01-0.21 AV: 19 NL: 1.53E7
T: FTMS + p ESI Full ms [200.00-800.00]



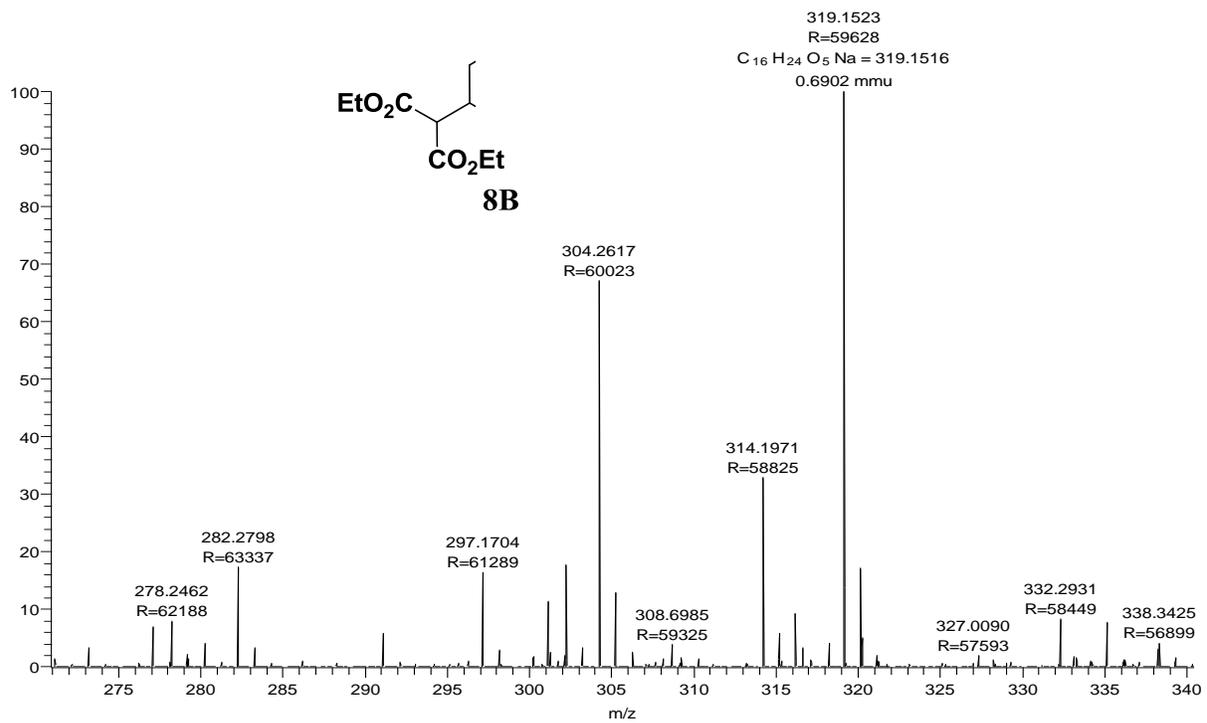
7A #1-18 RT: 0.01-0.20 AV: 18 NL: 7.36E6
T: FTMS + p ESI Full ms [200.00-800.00]



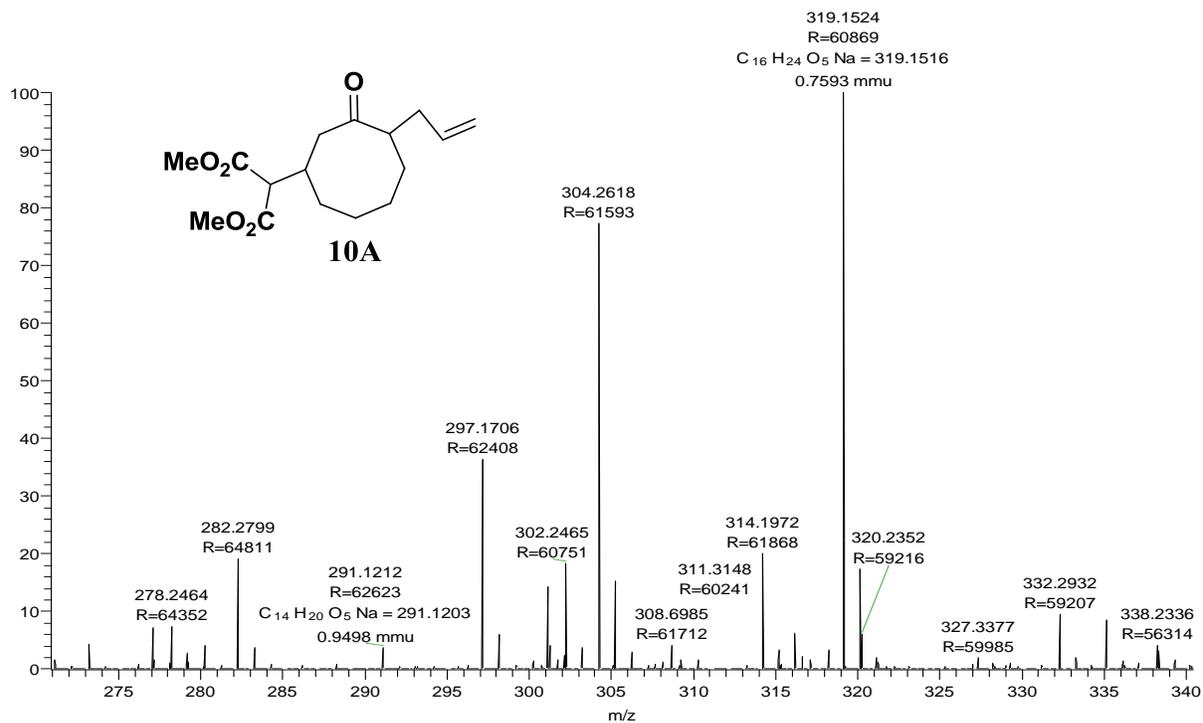
8A #1-17 RT: 0.01-0.21 AV: 17 NL: 3.12E6
T: FTMS + p ESI Full ms [200.00-800.00]



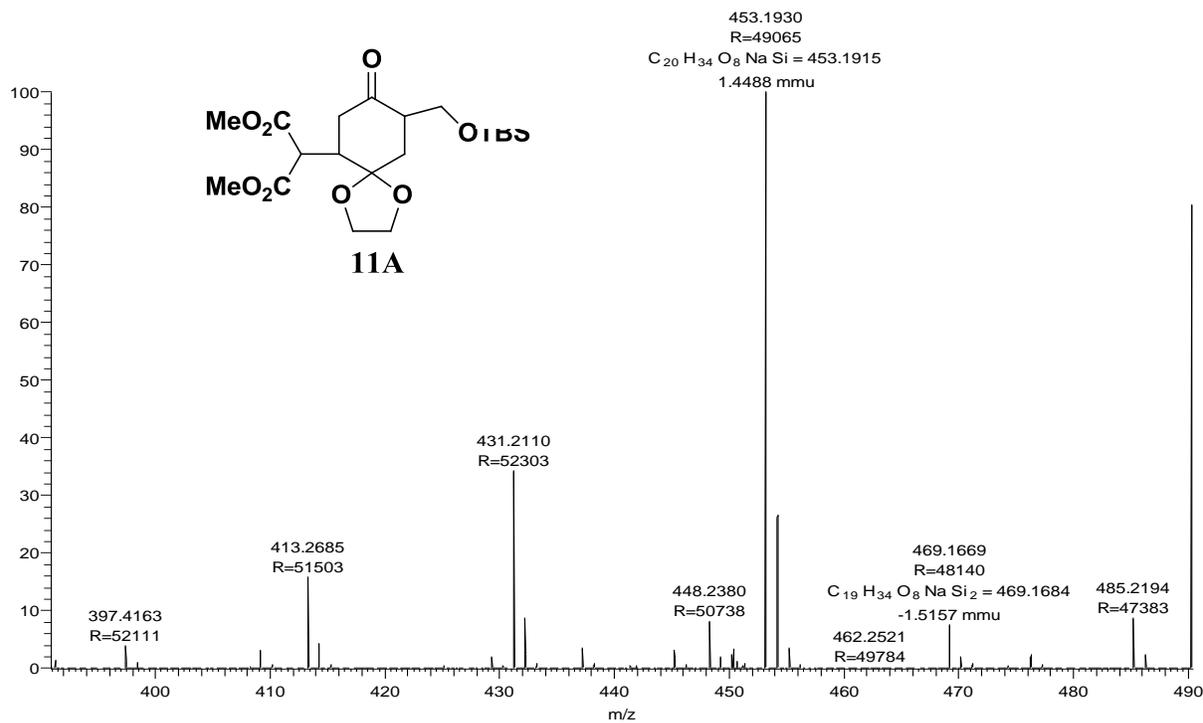
8B #1-18 RT: 0.01-0.21 AV: 18 NL: 3.27E6
T: FTMS + p ESI Full ms [200.00-800.00]



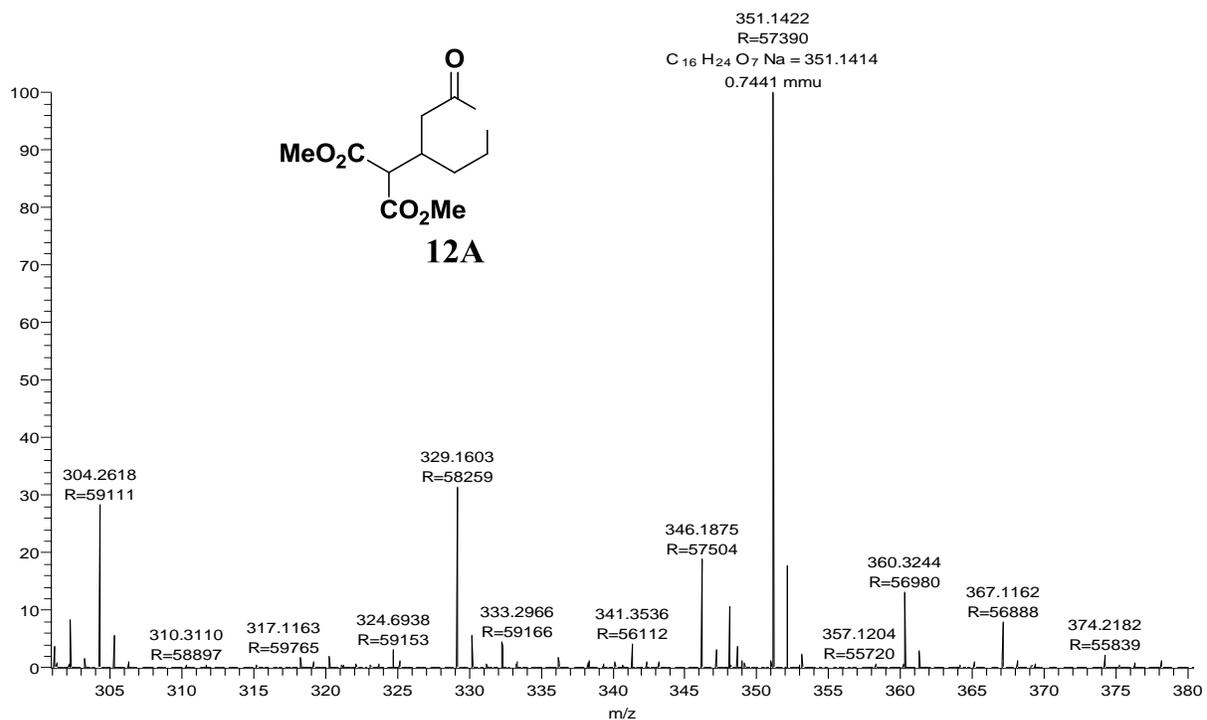
10A #1-18 RT: 0.01-0.21 AV: 18 NL: 2.84E6
T: FTMS + p ESI Full ms [200.00-800.00]



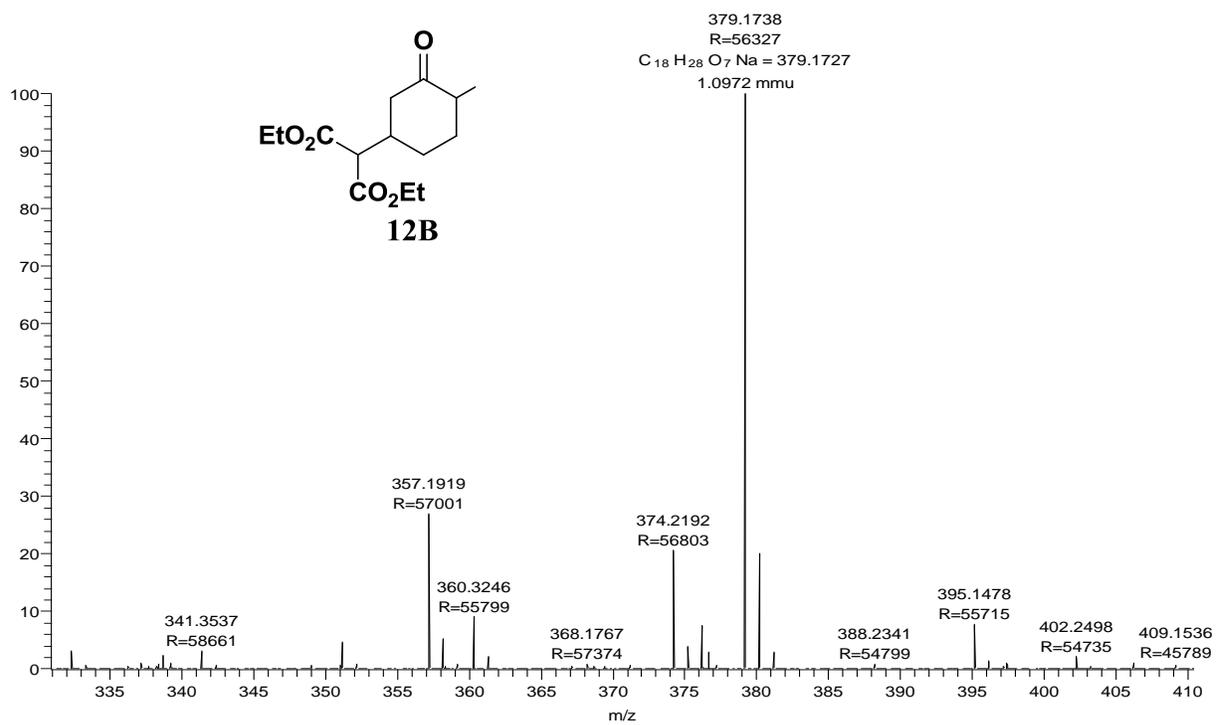
11A #1-18 RT: 0.01-0.21 AV: 18 NL: 6.49E6
T: FTMS + p ESI Full ms [200.00-800.00]



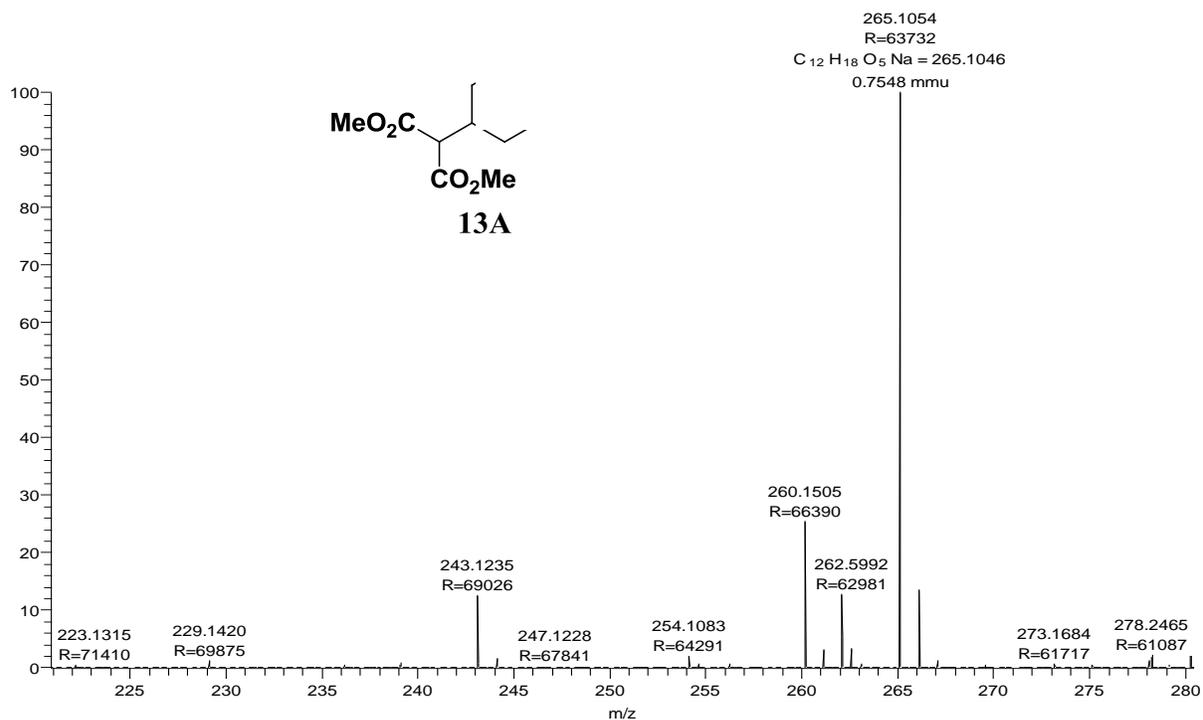
12A #1-19 RT: 0.01-0.21 AV: 19 NL: 1.08E7
T: FTMS + p ESI Full ms [200.00-800.00]



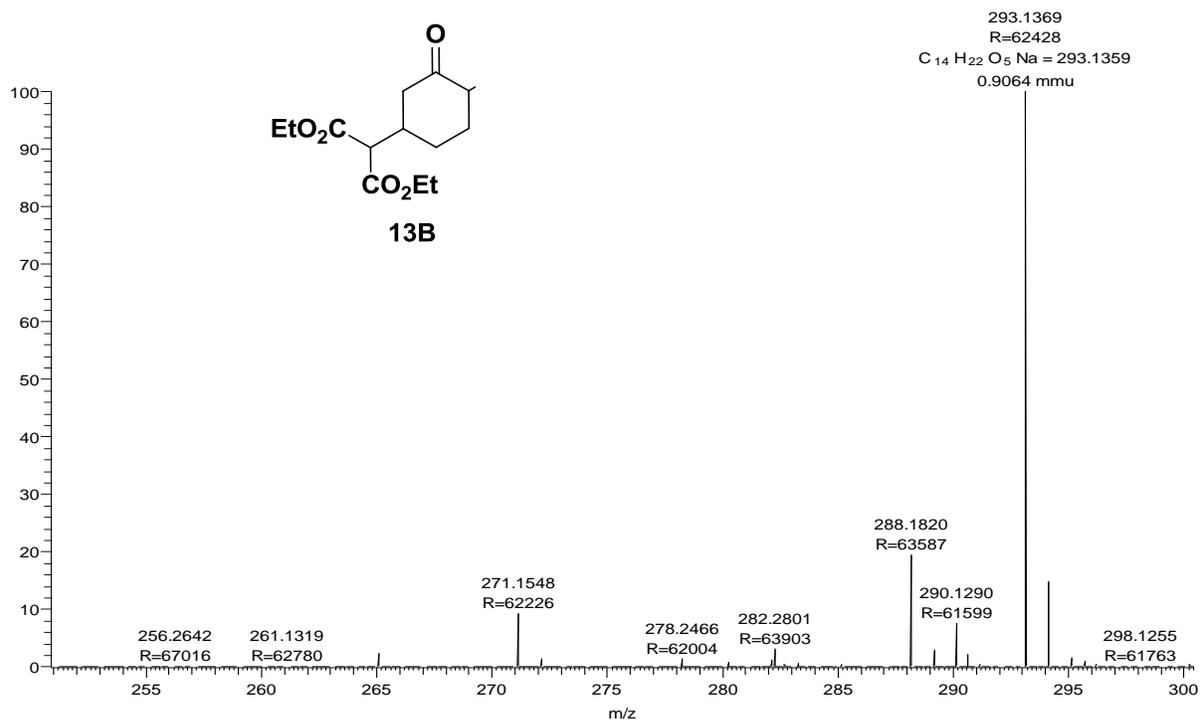
12B #1-19 RT: 0.01-0.22 AV: 19 NL: 1.36E7
T: FTMS + p ESI Full ms [200.00-800.00]



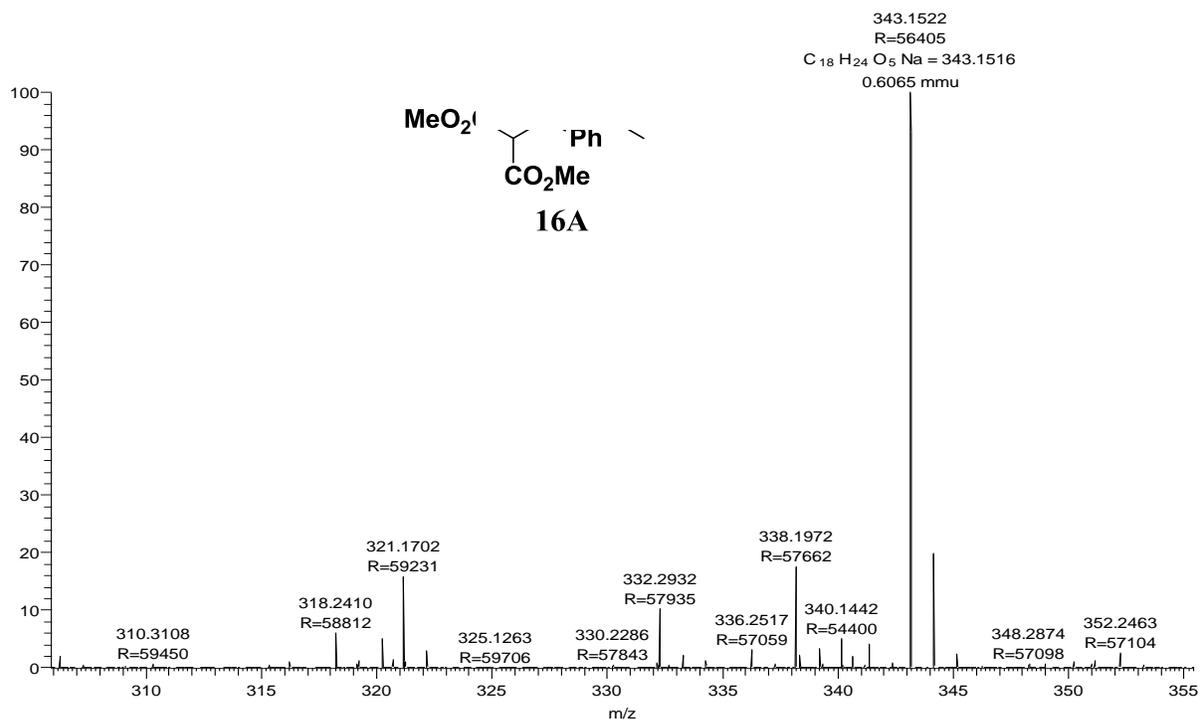
13A #1-18 RT: 0.01-0.20 AV: 18 NL: 1.23E7
T: FTMS + p ESI Full ms [200.00-800.00]



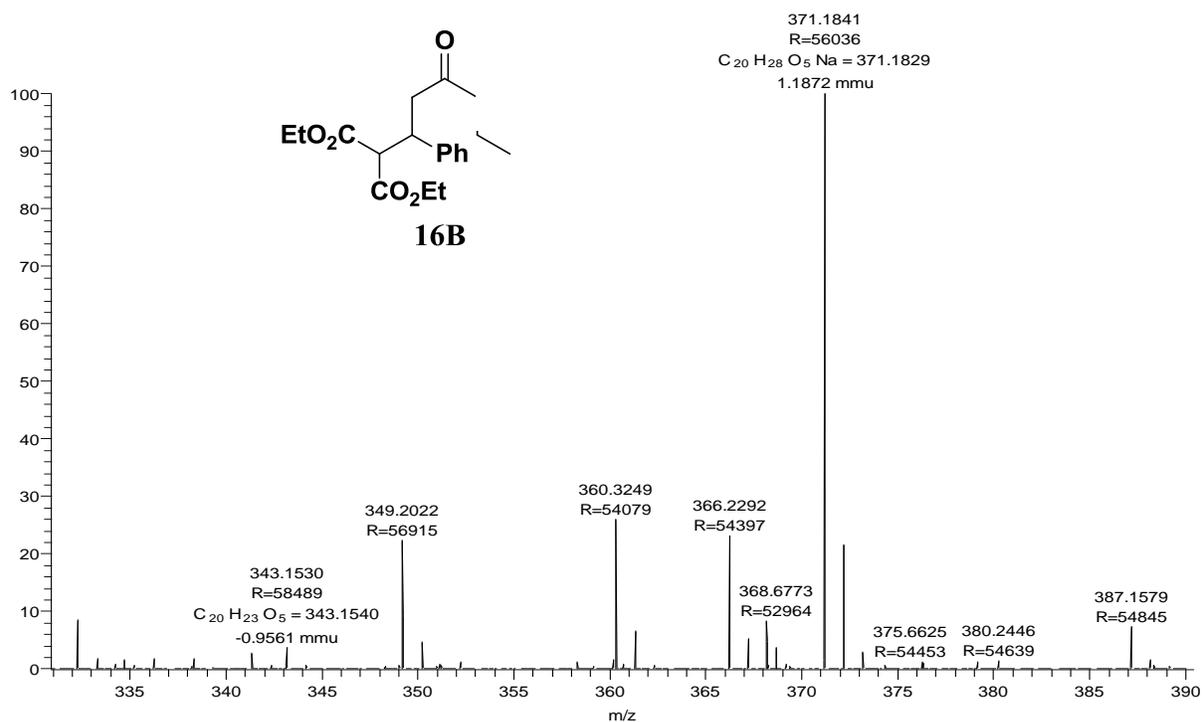
13B #1-19 RT: 0.01-0.21 AV: 19 NL: 2.28E7
T: FTMS + p ESI Full ms [200.00-800.00]



16A #1-19 RT: 0.01-0.21 AV: 19 NL: 1.22E7
T: FTMS + p ESI Full ms [200.00-800.00]



16B #1-19 RT: 0.01-0.21 AV: 19 NL: 1.21E7
T: FTMS + p ESI Full ms [200.00-800.00]



HPLC spectras:

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met

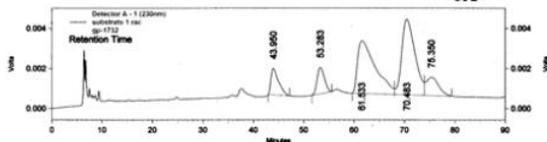
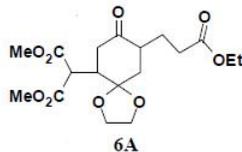
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1732

User: System

Acquired: 12/27/11 11:05:15 AM

Printed: 12/30/11 5:58:37 PM

Sample Name: substrate 1 rac



Retention Time	C Area	Area %
43.950	141005	7.954
53.283	133311	7.520
61.533	645879	36.434
70.483	696431	39.286
75.350	156110	8.806
Totals	1772736	100.000

Project Leader :Dr.Ganesh Pandey
 Column :Chiralcel OJ-H(250x4.6 mm)
 Mobile Phase :IPA:Pet Ether (20:80)
 Wavelength :220 nm
 Flow Rate :0.5 ml/min (23Kgf)
 conc. :1 mg/1.0mL
 Inj vol :5 ul

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met

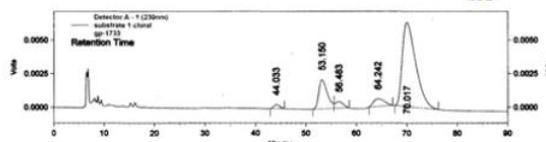
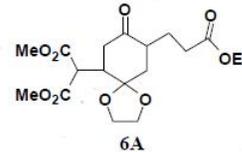
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1733

User: System

Acquired: 12/27/11 12:52:31 PM

Printed: 12/30/11 6:05:20 PM

Sample Name: substrate 1 chiral



Retention Time	C Area	Area %
44.033	23712	1.497
53.150	253647	16.009
56.483	54286	3.426
64.242	86270	5.445
70.017	1166456	73.623
Totals	1584371	100.000

Project Leader :Dr.Ganesh Pandey
 Column :Chiralcel OJ-H(250x4.6 mm)
 Mobile Phase :IPA:Pet Ether (20:80)
 Wavelength :220 nm
 Flow Rate :0.5 ml/min (23Kgf)
 conc. :1 mg/1.0mL
 Inj vol :5 ul

Sample Name: paa-roc enone

Method Name: C:\CLASS-VP\Method ch 1.met

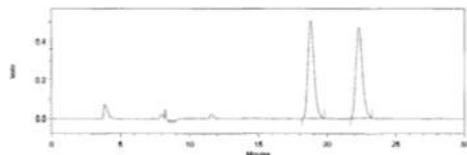
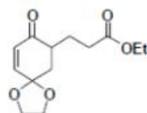
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1320

User: System

Acquired: 3/16/11 2:42:40 PM

Printed: 3/16/11 3:14:09 PM

Area % Report



PK.#	Retention Time	Area	Area %
1	18.800	15798626	50.426
2	22.308	15502311	49.574
Totals		31300937	100.000

Project Leader : Dr. Ganesh Pandey
 Column :Kromasil-3-Amcoat (250x4.6mm)
 M.P. : IPA:PE (05:95)
 Wavelength :220nm
 Flow :1 ml/min (630psi)
 conc. :1 mg/1 ml IPA
 Injection vol :5 ul

Sample Name: paa-roc enone

Method Name: C:\CLASS-VP\Method ch 1.met

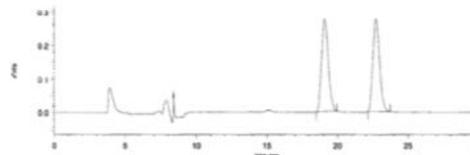
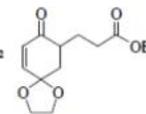
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1322

User: System

Acquired: 3/16/11 3:44:17 PM

Printed: 3/16/11 4:17:10 PM

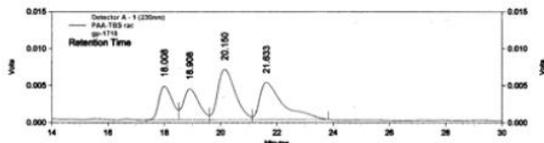
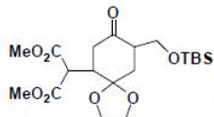
Area % Report



PK.#	Retention Time	Area	Area %
1	19.083	9246646	50.164
2	22.773	9188293	49.836
Totals		18434941	100.000

Project Leader : Dr. Ganesh Pandey
 Column :Kromasil-3-Amcoat (250x4.6mm)
 M.P. : IPA:PE (05:95)
 Wavelength :220nm
 Flow :1 ml/min (630psi)
 conc. :1 mg/1 ml IPA
 Injection vol :5 ul

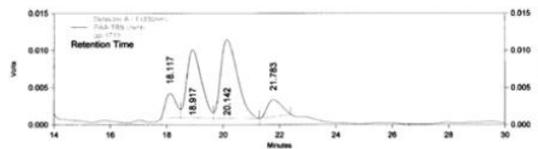
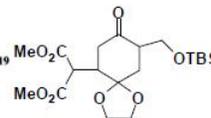
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1718
 User: System
 Acquired: 11/22/11 3:06:23 PM
 Printed: 12/30/11 5:41:09 PM
 Sample Name: PAA-TBS rac



Retention Time	C Area	Area %
18.008	149958	16.803
18.908	158394	17.835
20.150	292322	32.952
21.633	287336	32.390
Totals	887110	100.000

Project Leader :Dr.Ganesh Pandey
 Column :Chiralcel OI-H(250x4.6 mm)
 Mobile Phase :IPA:Pet Ether (10:90)
 Wavelength : 220 nm
 Flow Rate :0.5 ml/min (23Kg)
 conc. :.1 mg/1.0mL
 Inj vol- : 5 ul

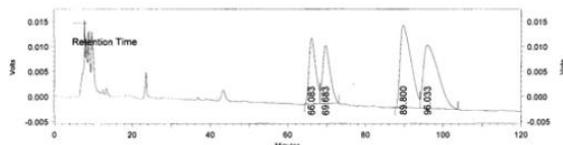
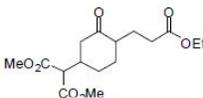
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1719
 User: System
 Acquired: 11/22/11 3:42:30 PM
 Printed: 12/30/11 5:43:23 PM
 Sample Name: PAA-TBS chiral



Retention Time	C Area	Area %
18.117	86017	9.233
18.917	331907	35.627
20.142	434420	46.631
21.783	79261	8.508
Totals	931605	100.000

Project Leader :Dr.Ganesh Pandey
 Column :Chiralcel OI-H(250x4.6 mm)
 Mobile Phase :IPA:Pet Ether (10:90)
 Wavelength : 220 nm
 Flow Rate :0.5 ml/min (23Kg)
 conc. :.1 mg/1.0mL
 Inj vol- : 5 ul

Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1395
 User: System
 Acquired: 6/4/11 8:00:43 PM
 Printed: 6/6/11 5:11:16 PM
 Sample Name: paa-2741 RAC



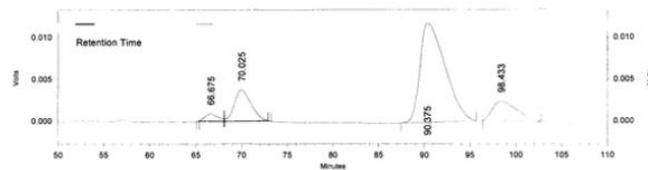
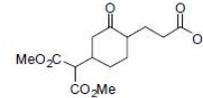
Retention Time	C Area	Area %
66.083	1556456	16.097
69.683	1542824	15.956
89.800	3235931	33.466
96.033	3334098	34.481
Totals	9669309	100.000

Project Leader : Dr.G Pandey
 Column :Chiralcel OD-H (250x4.6mm)
 Mobile Phase :Ethanol:n-Hexane (0.4:99.6)
 Wavelength : 230nm
 Flow Rate : 0.5ml/min 235 kgf
 conc. : xmg/0.5ml
 Inj vol- :.5ul

Shimadzu CLASS-VP V6.12 SP5
 Page 1 of 1 paa-2741 B

Area % Report

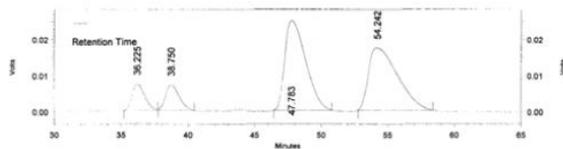
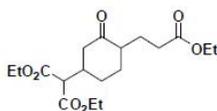
Method Name: C:\CLASS-VP\Methods\Date6\June.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1396
 User: System
 Acquired: 6/4/11 10:16:02 PM
 Printed: 6/6/11 11:56:15 AM



PK #	Retention Time	Area	Area %	Height	Height %
1	66.675	81950	2.533	823	4.384
2	70.025	457712	14.149	3699	19.703
3	90.375	2264268	69.993	11919	63.487
4	98.433	431050	13.325	2333	12.427
Totals		3234980	100.000	18774	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralcel OD-H0 0.46cm X 25cm
 Mobile Phase :Ethanol: n-Hexane (1.5:98.5)
 Flow Rate : 0.5 ml/min
 Wavelength : 230nm
 Con. :4mg 0.5ml
 Inject vol. :.15ul.

Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1478
 User: System
 Acquired: 6/28/11 4:30:42 PM
 Printed: 6/29/11 5:20:55 PM
 Sample Name: PAA-286-10 RAC

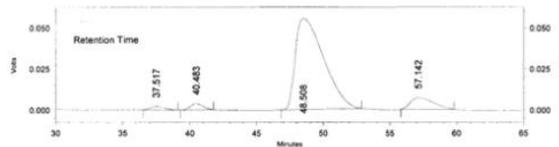
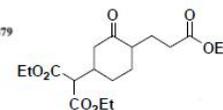


Retention Time	C Area	Area %
36.225	484977	7.674
38.750	502208	7.946
47.783	2710434	42.887
54.242	2622304	41.493
Totals	6319923	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralcel OD-H (4.6x250 mm)
 Mobile Phase :EtOH : n-Hexane (1.5:98.5)
 Flow Rate : 0.5ml/min (Pressure 235kgf)
 Wavelength : 230nm
 Con. : 2mg/0.5ml

Inject vol. :20uL

Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1479
 User: System
 Acquired: 6/28/11 5:39:16 PM
 Printed: 6/29/11 5:25:49 PM
 Sample Name: PAA-286-10 CHIRAL

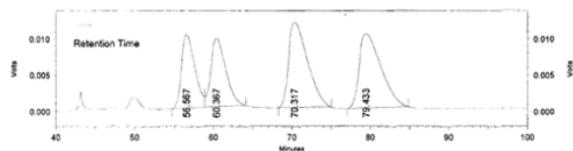
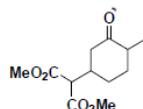


Retention Time	C Area	Area %
37.817	152120	1.612
40.483	245139	2.598
48.808	8193019	86.846
57.142	843705	8.943
Totals	9433983	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralcel OD-H (4.6x250 mm)
 Mobile Phase :EtOH : n-Hexane (1.5:98.5)
 Flow Rate : 0.5ml/min (Pressure 235kgf)
 Wavelength : 230nm
 Con. : 2mg/0.5ml

Inject vol. :20uL

Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1486
 User: System
 Acquired: 6/30/11 12:34:35 PM
 Printed: 6/30/11 2:54:17 PM
 Sample Name: PAA-287 iii Rac

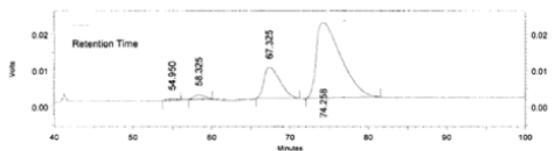
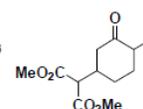


Retention Time	C Area	Area %
56.567	1185498	18.610
60.367	1233708	19.388
70.317	1974666	31.032
79.433	1969409	30.950
Totals	6363281	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralpalpak OD-H (4.6x250 mm)
 Mobile Phase :EtOH : n-Hexane (0.4:99.6)
 Flow Rate : 0.5ml/min (Pressure 235kgf)
 Wavelength : 230nm
 Con. : 2mg/0.5ml

Inject vol. :20uL

Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1485
 User: System
 Acquired: 6/30/11 10:51:34 AM
 Printed: 6/30/11 2:49:57 PM
 Sample Name: PAA-287 iii Chiral

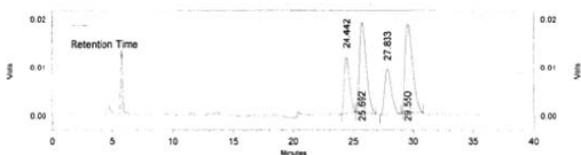
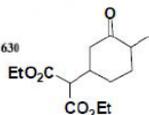


Retention Time	C Area	Area %
54.950	27708	0.465
58.325	115886	1.946
67.325	1227209	20.613
74.258	4582908	76.976
Totals	5953711	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralpalpak OD-H (4.6x250 mm)
 Mobile Phase :EtOH : n-Hexane (0.4:99.6)
 Flow Rate : 0.5ml/min (Pressure 235kgf)
 Wavelength : 230nm
 Con. : 2mg/0.5ml

Inject vol. :20uL

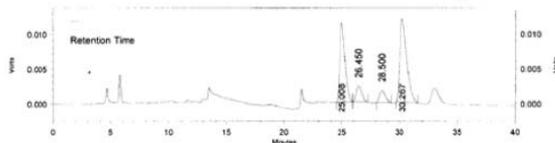
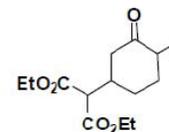
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1630
 User: System
 Acquired: 8/29/11 3:11:22 PM
 Printed: 8/29/11 4:29:07 PM
 Sample Name: PAA-ETHYL-METHYL racemic



Retention Time	C Area	Area %
24.442	375714	16.750
25.692	715707	31.908
27.833	344823	15.608
29.550	704763	30.433
Totals	2243007	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralcel OJ-H (4.6x250 mm)
 Mobile Phase :Ethanol:n-Hexane: (0.6:99.4)
 Flow Rate : 0.7ml/min (Pressure :51 psi)
 Wavelength : 230 nm
 Con. : 0.5mg/ml
 Inject vol. :5uL

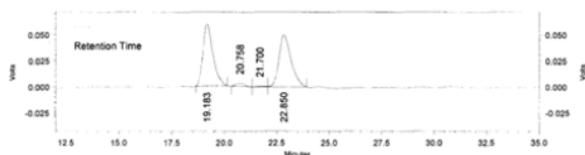
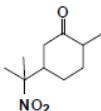
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1631
 User: System
 Acquired: 8/29/11 3:52:15 PM
 Printed: 8/29/11 5:33:31 PM
 Sample Name: PAA-ETHYL-METHYL Chiral



Retention Time	C Area	Area %
25.008	385026	36.811
26.450	75420	7.211
28.500	57735	5.520
30.267	527773	50.459
Totals	1045954	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralcel OJ-H (4.6x250 mm)
 Mobile Phase :Ethanol:n-Hexane: (0.6:99.4)
 Flow Rate : 0.7ml/min (Pressure 351 psi)
 Wavelength : 230 nm
 Con. : 0.5mg/ml
 Inject vol. :5uL

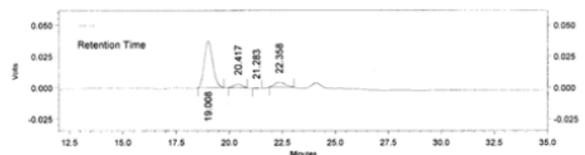
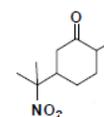
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1578
 User: System
 Acquired: 8/10/11 12:17:58 PM
 Printed: 8/10/11 1:03:36 PM
 Sample Name: PAA- NITRO-METHYL-RACEMIC



Retention Time	C Area	Area %
19.183	1994552	48.729
20.758	81851	2.000
21.700	20552	0.502
22.850	1996232	48.770
Totals	4093187	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralcel-OD-H (4.6x250 mm)
 Mobile Phase :IPA:PE (5:95)
 Flow Rate : 0.5ml/min (Pressure:24Kgf)
 Wavelength : 230nm
 Con. : 1mg/0.2ml
 Inject vol. : 10 uL

Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1576
 User: System
 Acquired: 8/10/11 11:08:07 AM
 Printed: 8/10/11 1:08:35 PM
 Sample Name: PAA- NITRO-METHYL-CHIRAL



Retention Time	C Area	Area %
19.008	1035975	82.852
20.417	76093	6.086
21.283	2147	0.172
22.358	136170	10.890
Totals	1250385	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralcel-OD-H (4.6x250 mm)
 Mobile Phase :IPA:PE (5:95)
 Flow Rate : 0.5ml/min (Pressure:24Kgf)
 Wavelength : 230nm
 Con. : 1mg/0.2ml
 Inject vol. : 10 uL

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met

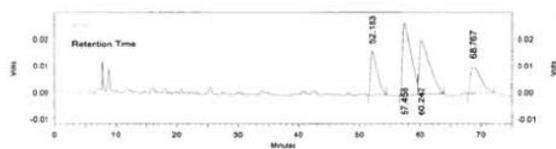
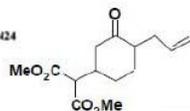
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1424

User: System

Acquired: 6/10/11 12:52:31 PM

Printed: 6/10/11 3:35:33 PM

Sample Name: PAA-ALLYLCYCLOHEXANONE RAC



Detector A - 1 (230nm)

Retention Time	C Area	Area %
52.183	1222115	16.603
57.428	2479045	33.643
60.242	2481126	33.671
68.767	1185132	16.083

Totals	C Area	Area %
	7368718	100.000

Project Leader :Dr.Ganesh Pandey

Column :Chiralcel OJ-H (0.46cm X 25cm)

Mobile Phase :IPA:PE (2:98)

Flow Rate :0.5 ml/min 246psi

Wavelength :230nm

Con. :3mg /0.5ml

Inject vol. :20uL

Kunte

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met

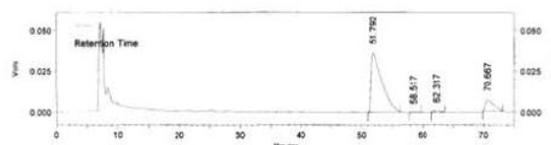
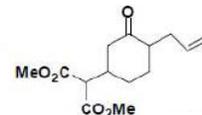
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1416

User: System

Acquired: 6/10/11 2:09:18 PM

Printed: 6/10/11 3:31:32 PM

Sample Name: PAA-ALLYLCYCLOHEXANONE CHIRAL



Detector A - 1 (230nm)

Retention Time	C Area	Area %
51.792	4738840	85.350
58.517	10641	0.192
62.317	76365	1.375
70.667	726393	13.083

Totals	C Area	Area %
	5552239	100.000

Project Leader :Dr.Ganesh Pandey

Column :Chiralcel OJ-H (0.46cm X 25cm)

Mobile Phase :IPA:PE (2:98)

Flow Rate :0.5 ml/min 246psi

Wavelength :230nm

Con. :3mg /0.5ml

Inject vol. :20uL

Kunte

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met

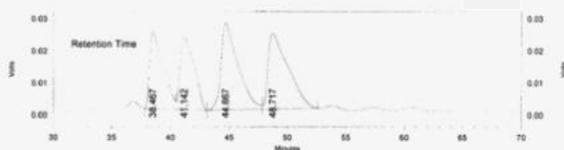
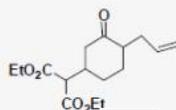
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1566

User: System

Acquired: 8/8/11 12:07:22 PM

Printed: 8/10/11 10:53:11 AM

Sample Name: PAA-ETHYL-ALLYL HEX RAC



Detector A - 1 (230nm)

Retention Time	C Area	Area %
38.467	1973417	21.016
41.142	1870465	19.920
44.667	2722438	29.190
48.717	2813570	29.964

Totals	C Area	Area %
	9389890	100.000

Project Leader :Dr. Ganesh Pandey

Column :Chiralcel-OJ-H (4.6x250 mm)

Mobile Phase :IPA:PE (0.5:99.5)

Flow Rate :0.5ml/min (Pressure25Kgf)

Wavelength :230nm

Con. :1mg/0.2ml

Inject vol. :20 uL

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met

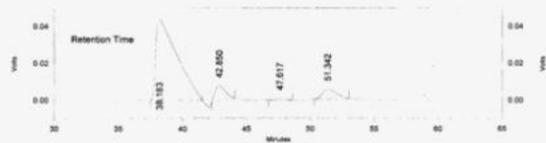
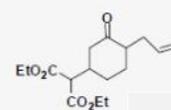
Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1568

User: System

Acquired: 8/8/11 2:32:43 PM

Printed: 8/10/11 11:00:58 AM

Sample Name: PAA-ETHYL-ALLYL HEX chiral



Detector A - 1 (230nm)

Retention Time	C Area	Area %
38.183	5013488	84.724
42.850	462574	7.817
47.617	51877	0.877
51.342	389518	6.583

Totals	C Area	Area %
	5917457	100.000

Project Leader :Dr. Ganesh Pandey

Column :Chiralcel-OJ-H (4.6x250 mm)

Mobile Phase :IPA:PE (0.5:99.5)

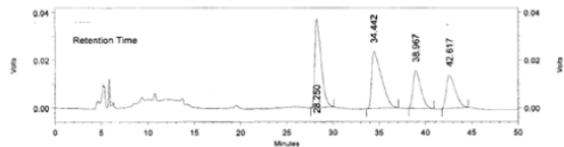
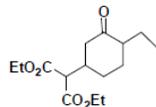
Flow Rate :0.5ml/min (Pressure25Kgf)

Wavelength :230nm

Con. :1mg/0.2ml

Inject vol. :20 uL

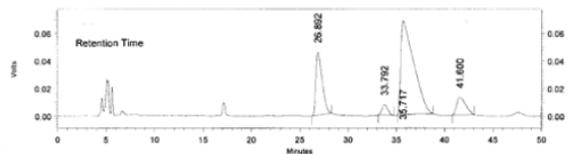
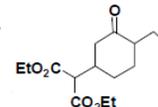
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1605
 User: System
 Acquired: 8/24/11 2:19:58 PM
 Printed: 8/24/11 4:29:12 PM
 Sample Name: PAA-ETHYL-ETHYL RAC



Retention Time	C Area	Area %
28.250	1785509	33.076
34.442	1757288	32.553
38.967	927855	17.188
42.817	927540	17.182
Totals	5398192	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Kromasil 5-AmyCoat (4.6x250 mm)
 Mobile Phase :EtOH:n-Hexane (02:98.0)
 Flow Rate : 0.7ml/min (Pressure 445psi)
 Wavelength : 230 nm
 Con. : 1mg/0.2ml
 Inject vol. :20uL

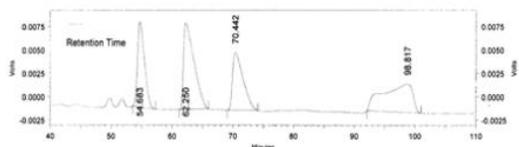
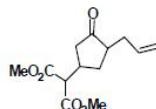
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1606
 User: System
 Acquired: 8/24/11 3:12:11 PM
 Printed: 8/24/11 4:31:51 PM
 Sample Name: PAA-ETHYL-ETHYL Chiral



Retention Time	C Area	Area %
26.892	2072160	21.747
33.792	314032	3.296
35.717	6312377	66.246
41.600	830067	8.711
Totals	9528636	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Kromasil 5-AmyCoat (4.6x250 mm)
 Mobile Phase :EtOH:n-Hexane (02:98.0)
 Flow Rate : 0.7ml/min (Pressure 445psi)
 Wavelength : 230 nm
 Con. : 1mg/0.2ml
 Inject vol. :20uL

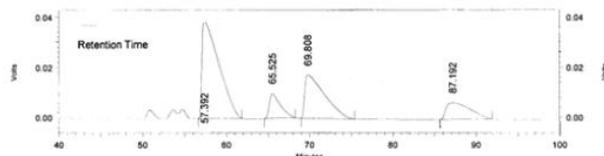
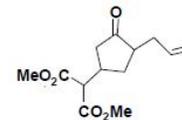
Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1474
 User: System
 Acquired: 6/28/11 9:59:46 AM
 Printed: 6/29/11 5:45:33 PM
 Sample Name: PAA- pentane racemic



Retention Time	C Area	Area %
54.683	712108	20.003
62.250	1094488	30.744
70.442	740369	20.797
98.817	1013077	28.457
Totals	3560042	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralpak AS-H (4.6x250 mm)
 Mobile Phase :IPA : PE (2.0:98.0)
 Flow Rate : 0.5ml/min (Pressure 235kgf)
 Wavelength : 230nm
 Con. : 2mg/0.5ml
 Inject vol. :20uL

Shimadzu CLASS-VP V6.12 SP5
 Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1473
 User: System
 Acquired: 6/28/11 8:17:10 AM
 Printed: 6/29/11 5:37:39 PM
 Sample Name: PAA- pentane chiral

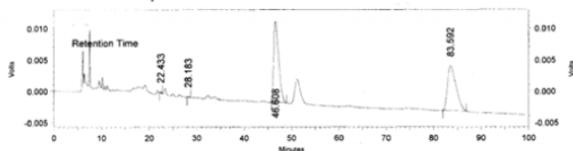
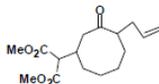


Retention Time	C Area	Area %
57.392	5475348	51.559
65.525	917351	8.638
69.808	2865756	26.985
87.192	1361180	12.818
Totals	10619635	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Chiralpak AS-H (4.6x250 mm)
 Mobile Phase :IPA : PE (2.0:98.0)
 Flow Rate : 0.5ml/min (Pressure 235kgf)
 Wavelength : 230nm
 Con. : 2mg/0.5ml
 Inject vol. :20uL

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1525
 User: System
 Acquired: 7/14/11 3:13:26 PM
 Printed: 7/14/11 5:27:44 PM
 Sample Name: PAA-OCTANE Rac



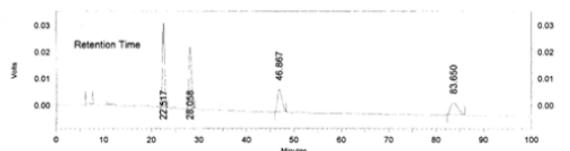
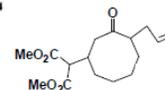
Retention Time	C Area	Area %
22.433	3700	0.207
28.183	3500	0.196
46.608	895689	50.118
83.592	884283	49.479
Totals	1787172	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Kromasil 5-AmyCoat (4.6x250 mm)
 Mobile Phase :EtOH : n-Hexane (02:98)
 Flow Rate : 0.5ml/min (Pressure 26kgf)
 Wavelength : 230nm
 Con. : 1mg/0.2ml
 Inject vol. :20uL

Kunte

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1524
 User: System
 Acquired: 7/14/11 1:27:55 PM
 Printed: 7/14/11 3:11:25 PM
 Sample Name: PAA-OCTANE CHIRAL



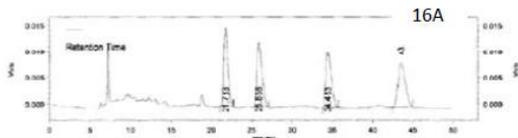
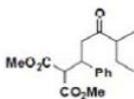
Retention Time	C Area	Area %
22.517	887523	31.971
28.058	873897	31.480
46.867	529112	19.060
83.650	485489	17.489
Totals	2776021	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Kromasil 5-AmyCoat (4.6x250 mm)
 Mobile Phase :EtOH : n-Hexane (02:98)
 Flow Rate : 0.5ml/min (Pressure 26kgf)
 Wavelength : 230nm
 Con. : 1mg/0.2ml
 Inject vol. :20uL

Kunte

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1595
 User: System
 Acquired: 8/19/11 11:40:18 AM
 Printed: 8/19/11 6:05:23 PM
 Sample Name: PAA-methyl acyclic

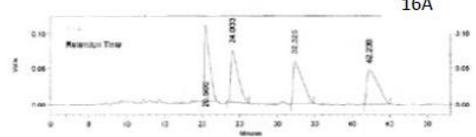
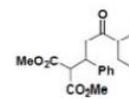


Retention Time	C Area	Area %
21.733	505982	25.065
24.838	335493	16.041
34.433	497050	24.623
43.542	310137	15.271
Totals	2018662	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Kromasil 5-Amycoat (4.6x250 mm)
 Mobile Phase :EtOH:n-Hexane (07:93)
 Flow Rate : 0.5ml/min (Pressure 30 kgf)
 Wavelength : 230 nm
 Con. : 2mg/0.5ml
 Inject vol. :20uL

Shimadzu CLASS-VP V6.12 SP5

Method Name: C:\CLASS-VP\Method ch 2.met
 Data Name: C:\CLASS-VP\Data\Dr.Ganesh Pandey\gp-1596
 User: System
 Acquired: 8/19/11 12:39:24 PM
 Printed: 8/19/11 6:09:14 PM
 Sample Name: PAA-methyl acyclic-Chiral



Retention Time	C Area	Area %
20.500	4952682	25.245
24.037	4816357	24.550
32.322	3103221	16.012
42.233	4745929	24.191
Totals	19618189	100.000

Project Leader :Dr. Ganesh Pandey
 Column :Kromasil 5-Amycoat (4.6x250 mm)
 Mobile Phase :EtOH:n-Hexane (07:93)
 Flow Rate : 0.5ml/min (Pressure 30 kgf)
 Wavelength : 230 nm
 Con. : 2mg/0.5ml
 Inject vol. :20uL

Reference:

1. K. C. Nicolaou, D. L. F. Gray, T. Montagnon, S. T. Harrison, *Angew. Chem. Int. Ed.*, 2002, **41**, 996.