Electronic Supplementary Information

Ruthenium(II) Catalysed Direct Synthesis of Mono-allylation Products of 1,3-diketones by Cinnamyl Alcohols

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Table S1 Crystal data and structure refinement for 1

Complex	**1**
Empirical formula	$C_{43}H_{46}ClF_6P_3Ru$
Formula weight	906.23
Temperature, K	100(3)
Wavelength (Å)	0.71073
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
a (Å)	10.4015(6)
b (Å)	12.1513(6)
c (Å)	31.7163(16)
α, *β*, *γ* (°)	90, 90, 90
V (Å^3)	4008.7(4)
Z	4
Dcalc. (Mg/m^3)	1.480
μ (Mo-Kα) (mm^{-1})	0.637
F(000)	1856
θ Range (°)	1.795 to 24.994
Reflections collected	46642
Unique reflections R(int) Restraints	7086 0.0646 0
parameters	491
Goodness of fit (F^2)	1.024
Absolute structure (Flack) parameter	-0.02(2)
Final R indices [I>2σ(I)]	*R1*= 0.0313,*wR2* = 0.0677
R indices (all data)	*R1* = 0.0354,*wR2* =0.0699

Table S2 Important bond distances (Å) and bond angles (°) for 1

Selected bond lengths (Å)		Selected angles (°)	
P(1)-Ru(1)	2.3091(13)	C(7)-C(2)-Ru(1)	70.7(5)
P(2)-Ru(1)	2.3250(13)	C(3)-C(2)-Ru(1)	71.3(5)
Cl(1)-Ru(1)	2.3938(11)	C(1)-C(2)-Ru(1)	133.5(6)
C(1)-Ru(1)	2.201(5)	C(4)-C(3)-Ru(1)	72.8(5)
C(2)-Ru(1)	2.245(8)	C(2)-C(3)-Ru(1)	72.3(5)
C(3)-Ru(1)	2.263(9)	C(3)-C(4)-Ru(1)	71.4(5)
C(4)-Ru(1)	2.341(8)	C(5)-C(4)-Ru(1)	74.6(5)
C(5)-Ru(1)	2.239(5)	C(6)-C(5)-Ru(1)	70.7(4)
C(6)-Ru(1)	2.222(8)	C(4)-C(5)-Ru(1)	68.7(5)
Centroid-Ru(1)	1.757	C(8)-C(5)-Ru(1)	132.3(7)
		C(7)-C(6)-Ru(1)	68.7(4)
		C(5)-C(6)-Ru(1)	73.7(4)
		C(2)-C(7)-Ru(1)	73.6(5)
		C(6)-C(7)-Ru(1)	74.8(5)
		P(2)-Ru(1)-P(1)	83.80(8)
		P(2)-Ru(1)-Cl(1)	80.88(7)
		P(1)-Ru(1)-Cl(1)	85.63(8)

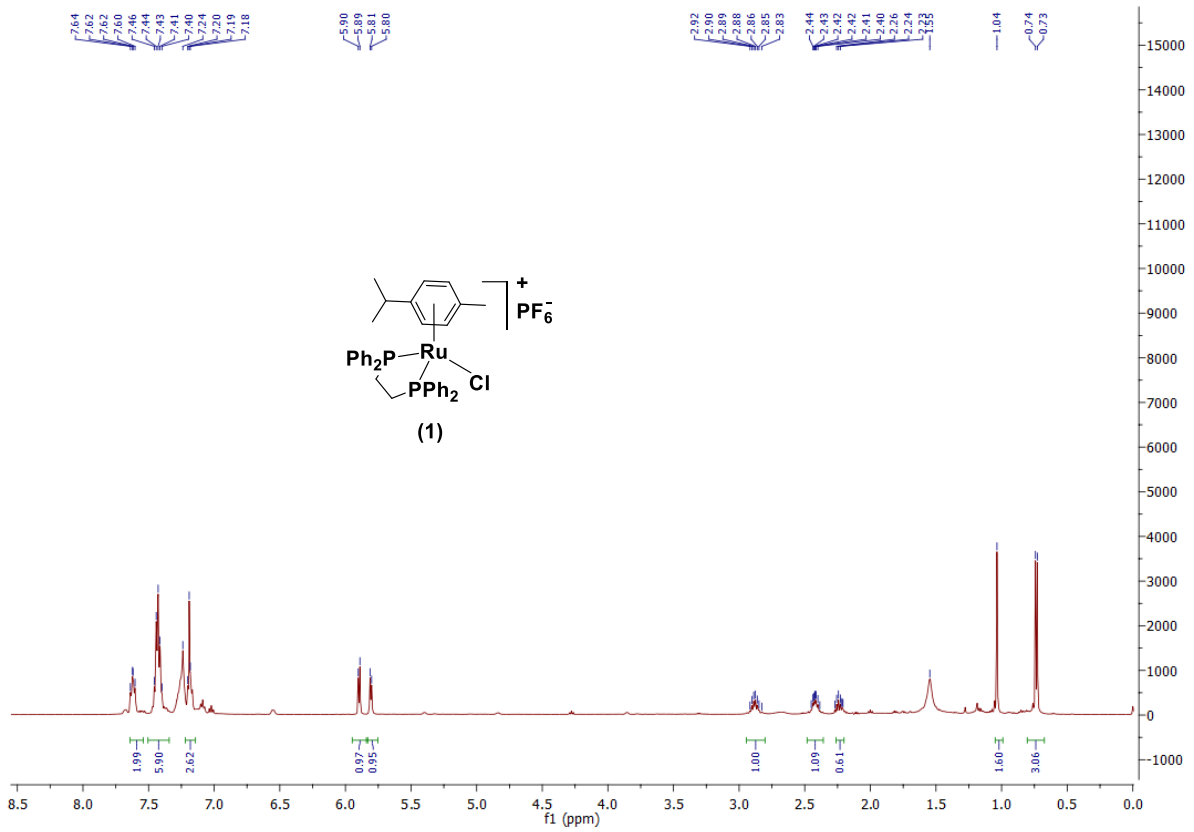

Figure S1 ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of **1**

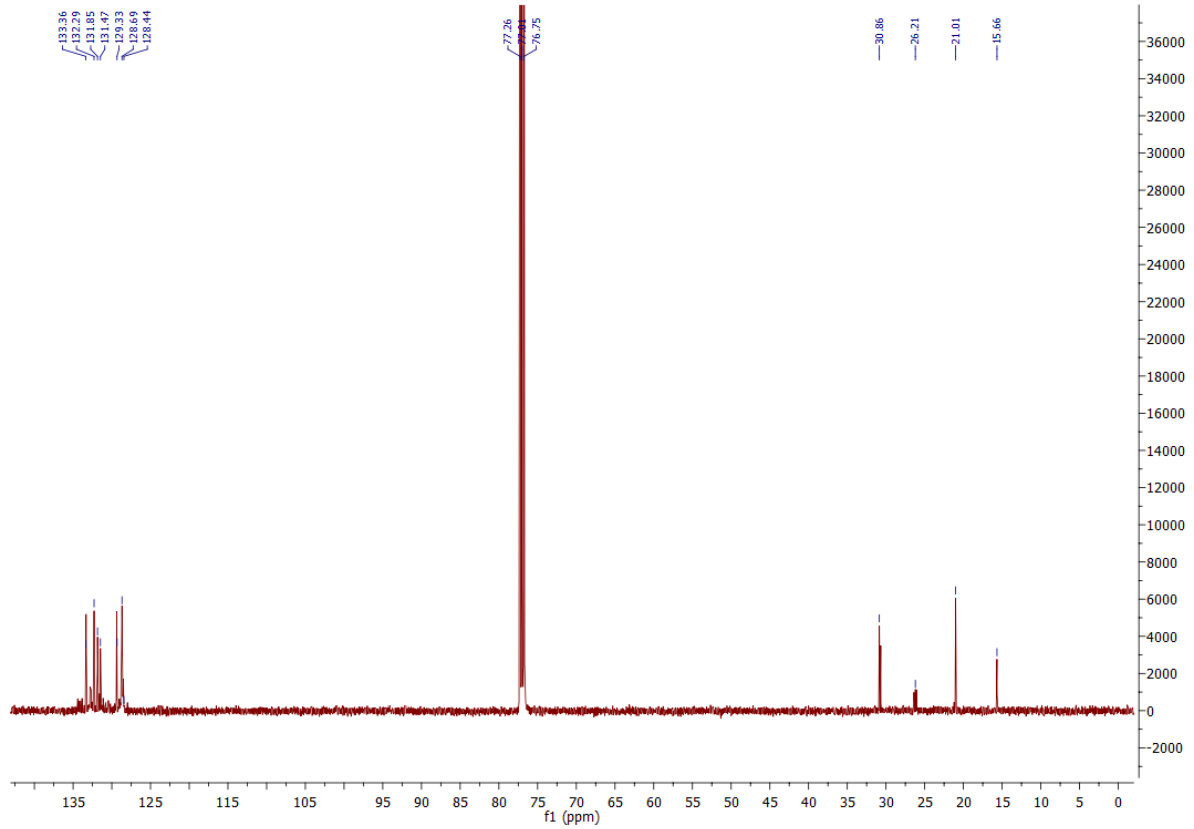

Figure S2 ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of **1**

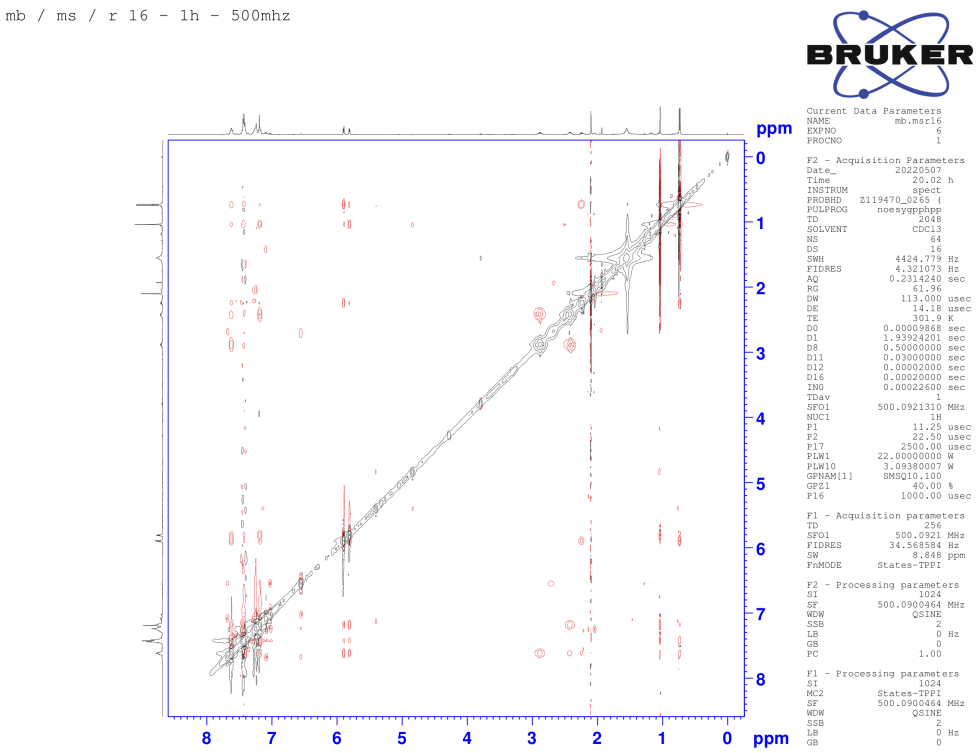

Figure S3 NOSEY spectrum of **1**

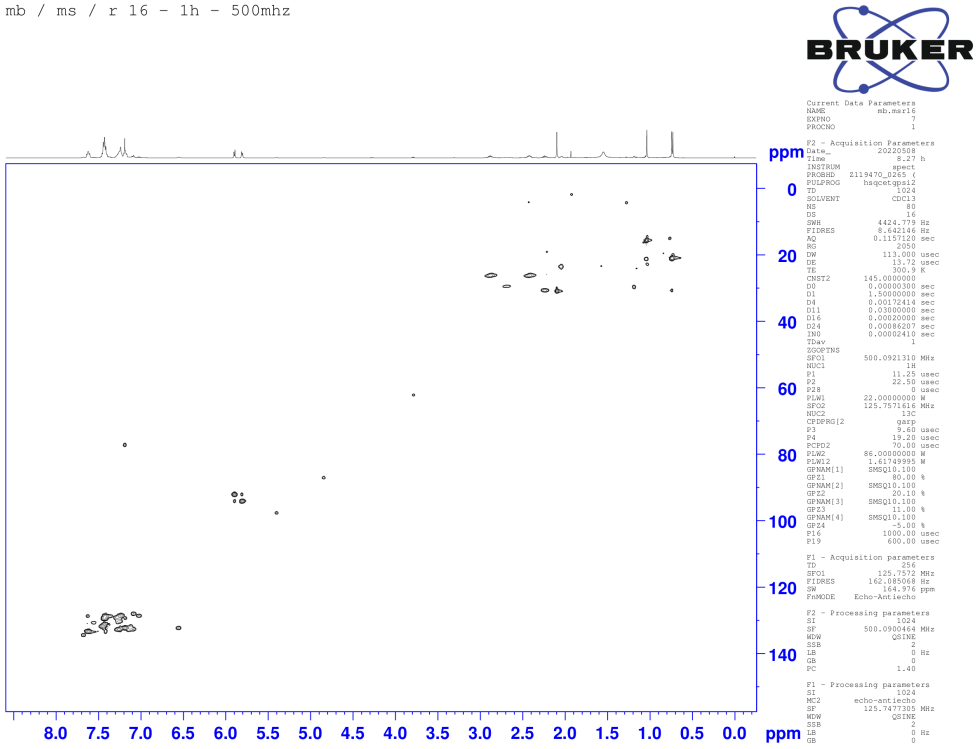

Figure S4 HSQC spectrum of **1**

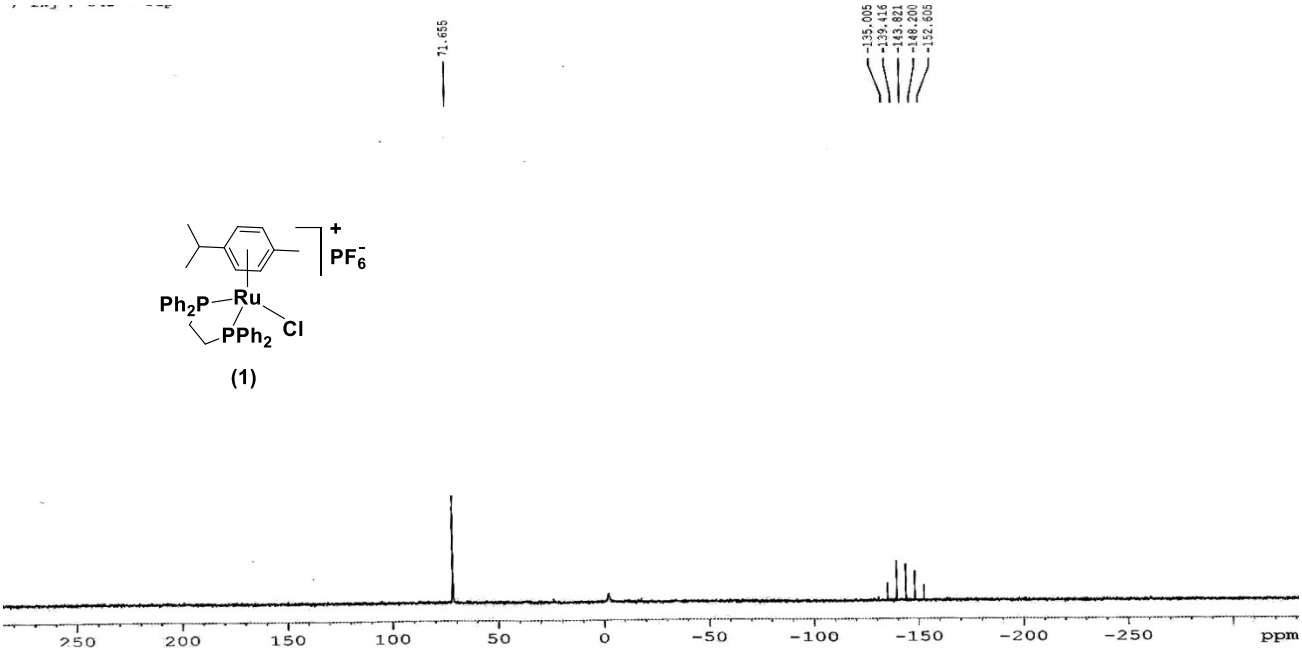

Figure S5 ^{31}P NMR (161.98 MHz, $CDCl_3$) spectrum of **1**

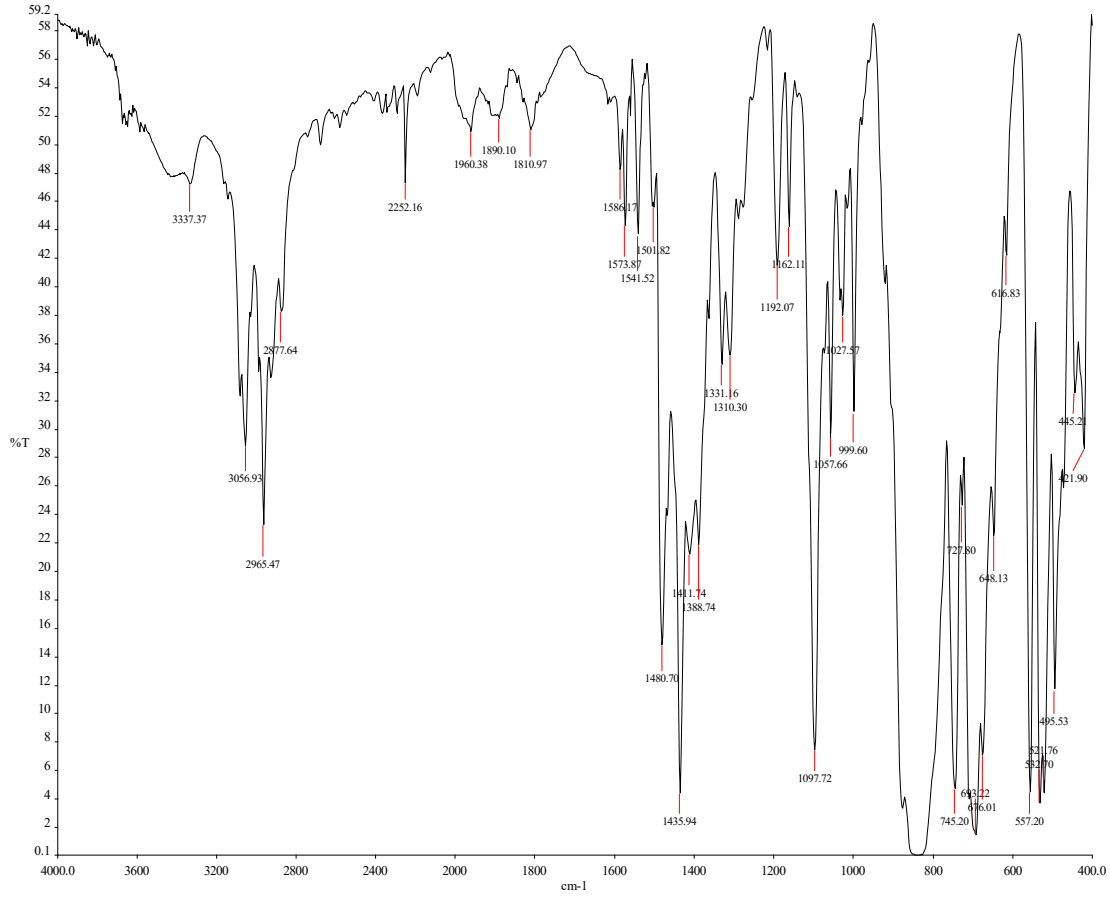

Figure S6 IR spectra of complex **1**

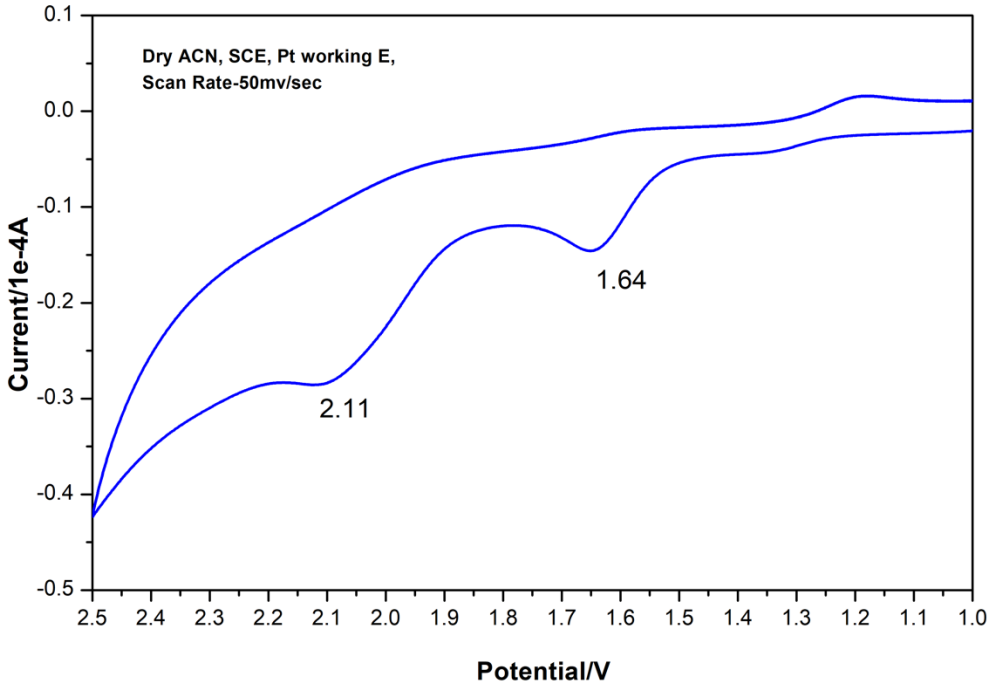

Figure S7 Cyclic voltammogram of complex **1**

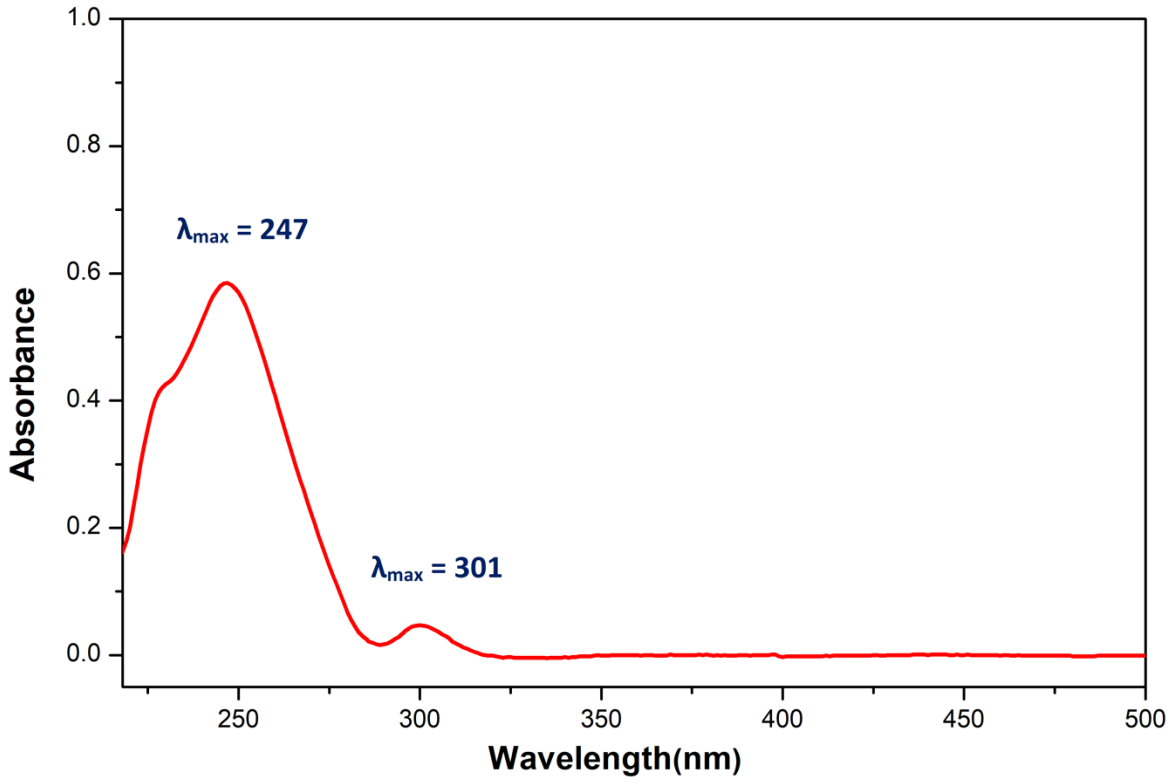

Figure S8 UV-vis spectrum of complex **1**

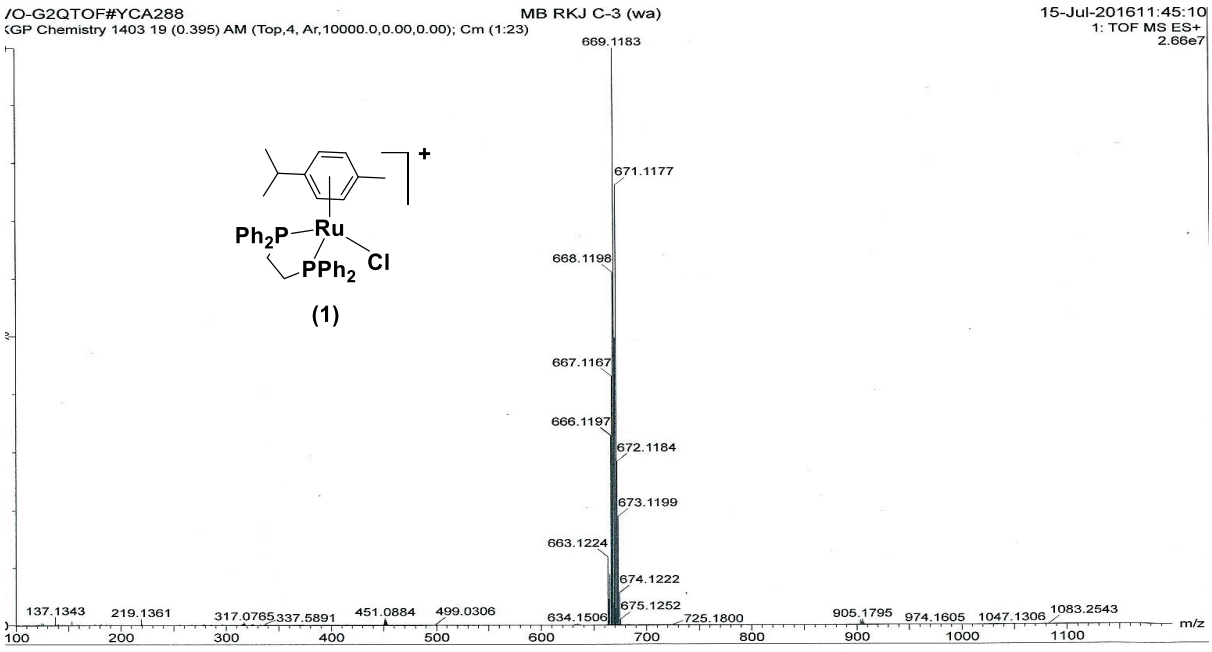

Figure S9 HRMS of complex **1**

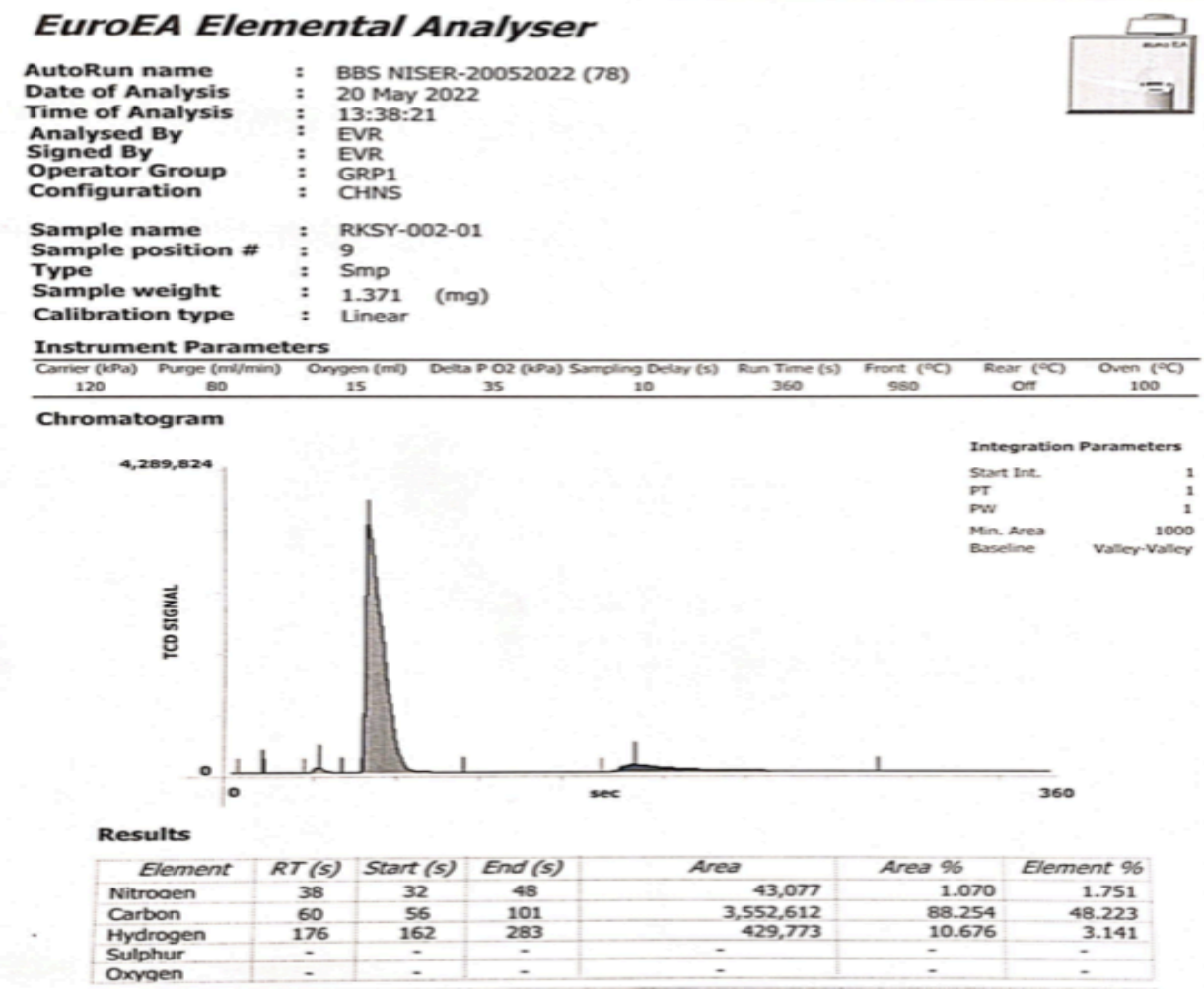

Figure S10 Elemental analysis of complex **1**

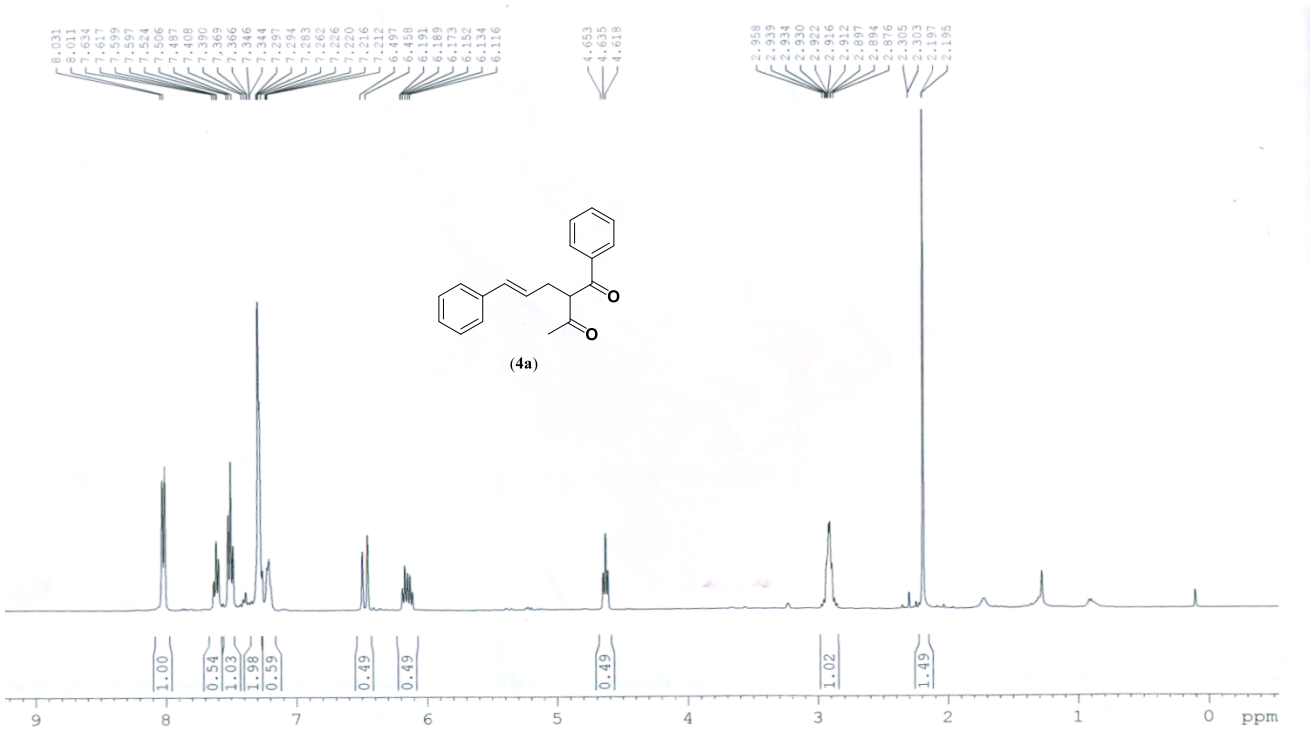

Figure S11 ^{1}H NMR (400 MHz) spectrum of compound **4a** in $CDCl_3$

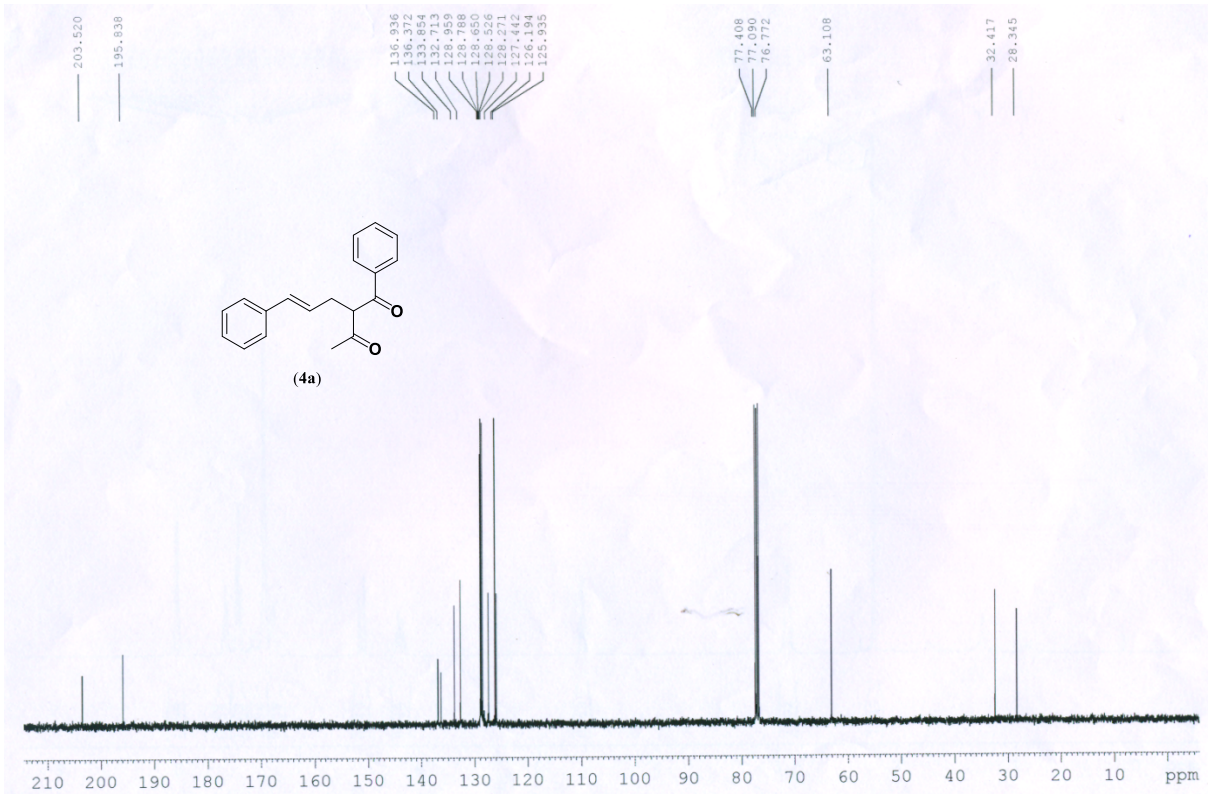

Figure S12 ^{13}C NMR (100 MHz) spectrum of compound **4a** in $CDCl_3$

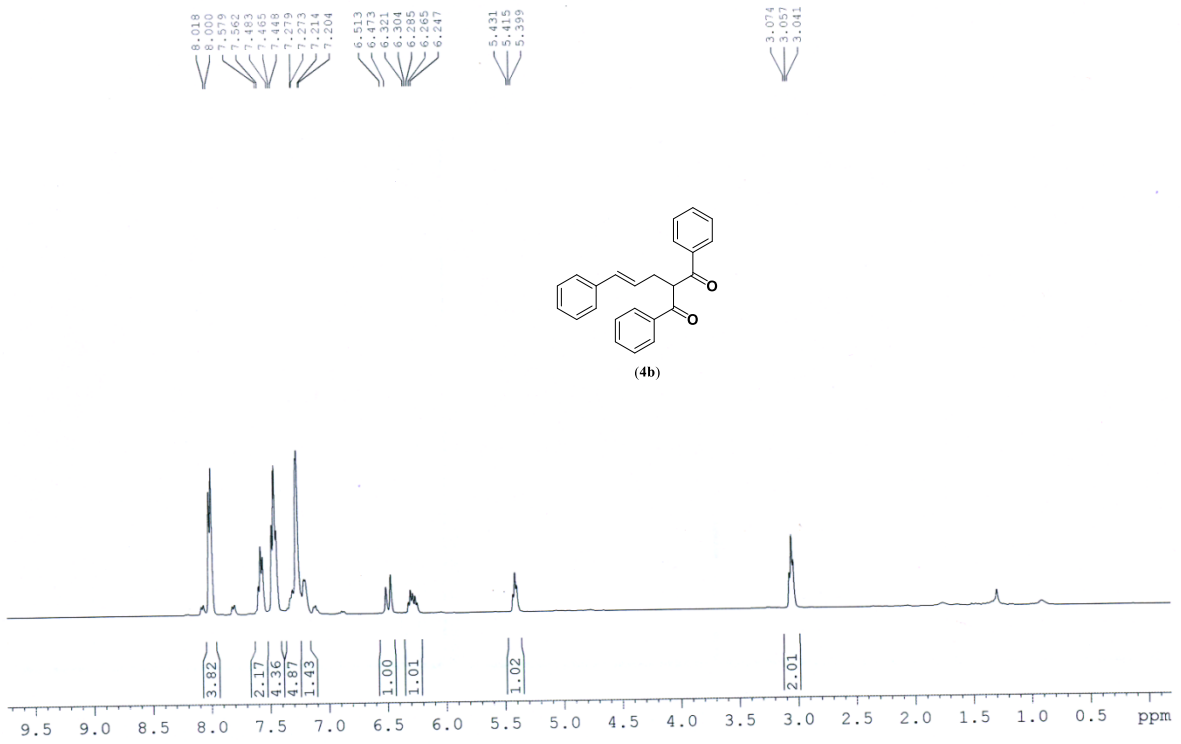

Figure S13 ^{1}H NMR (400 MHz) spectrum of compound **4b** in $CDCl_3$

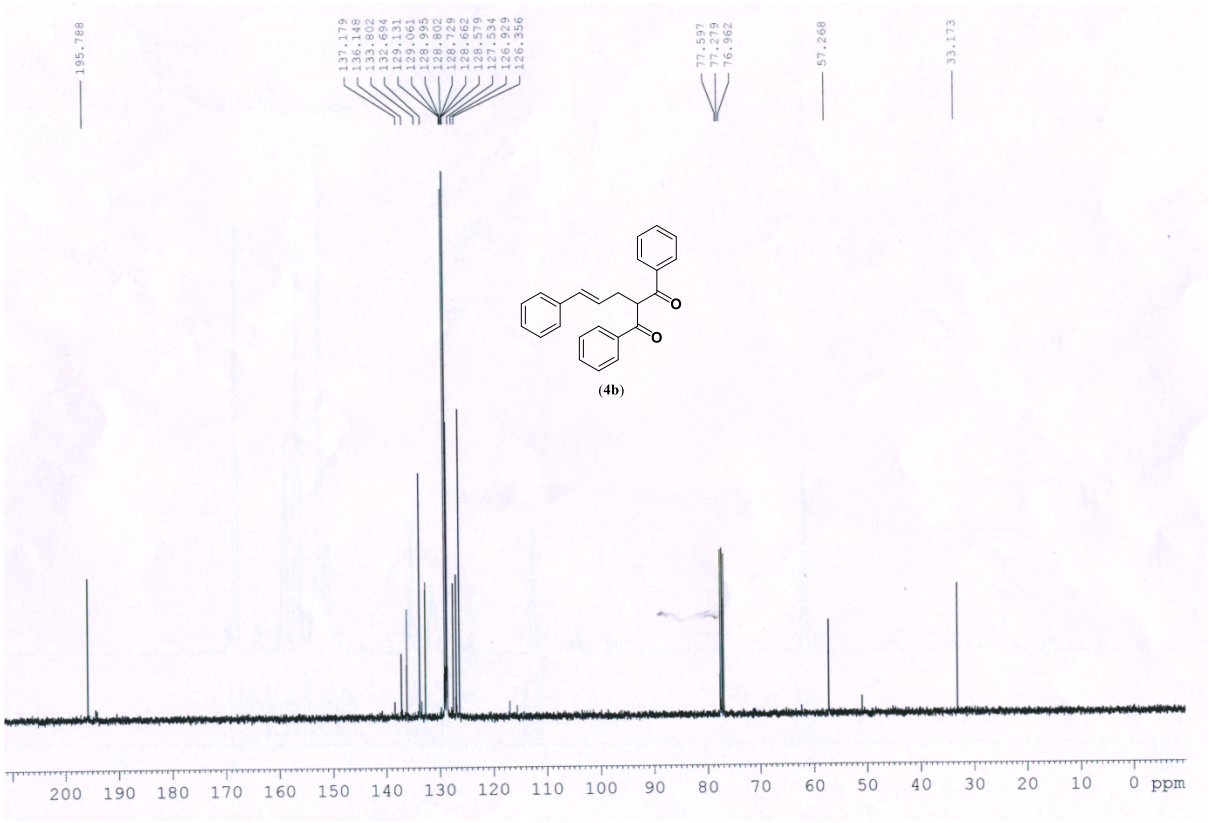

Figure S14 ^{13}C NMR (100 MHz) spectrum of compound **4b** in $CDCl_3$

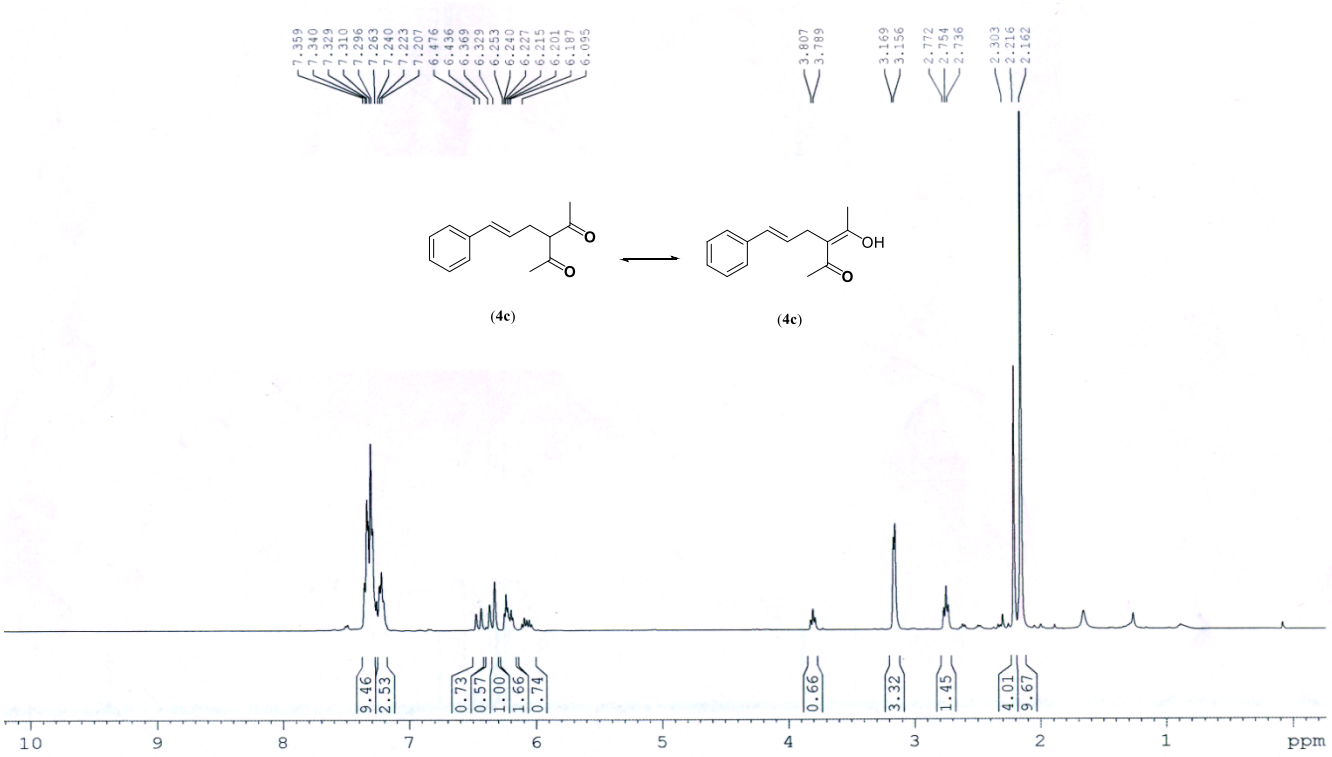

Figure S15 ^{1}H NMR (400 MHz) spectrum of compound **4c** in $CDCl_3$

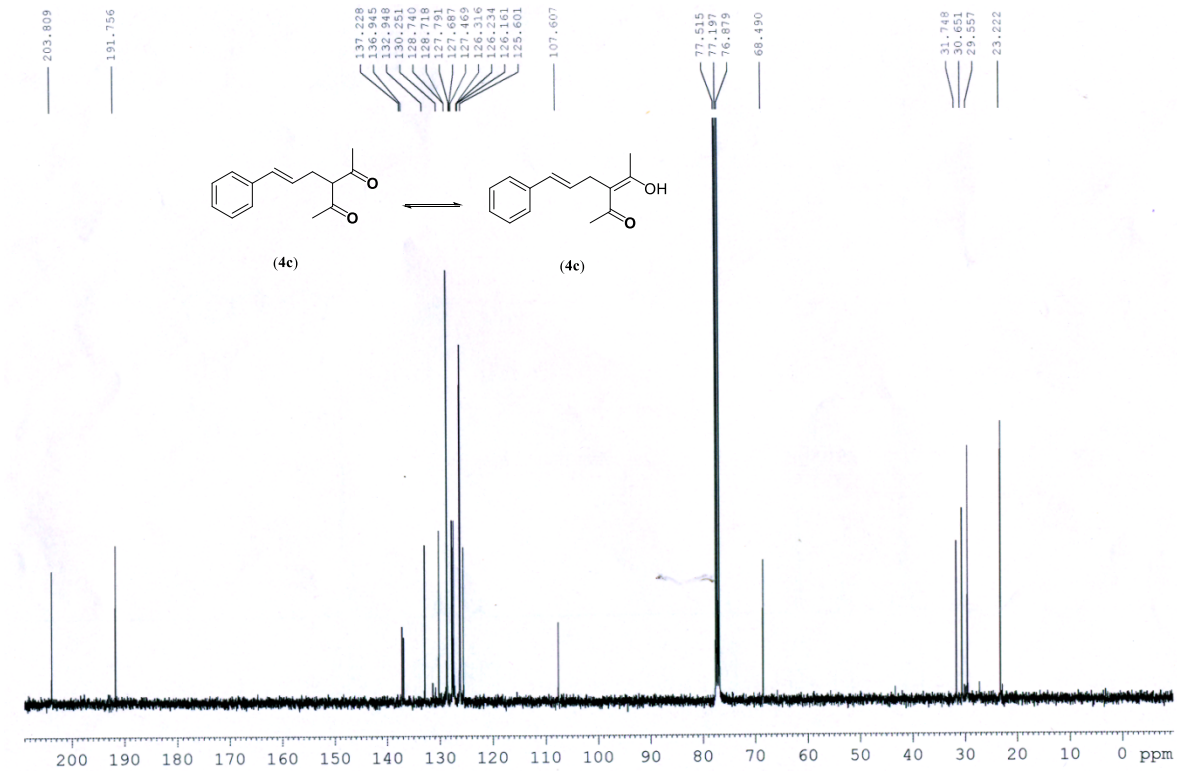

Figure S16 ^{13}C NMR (100 MHz) spectrum of compound **4c** in $CDCl_3$

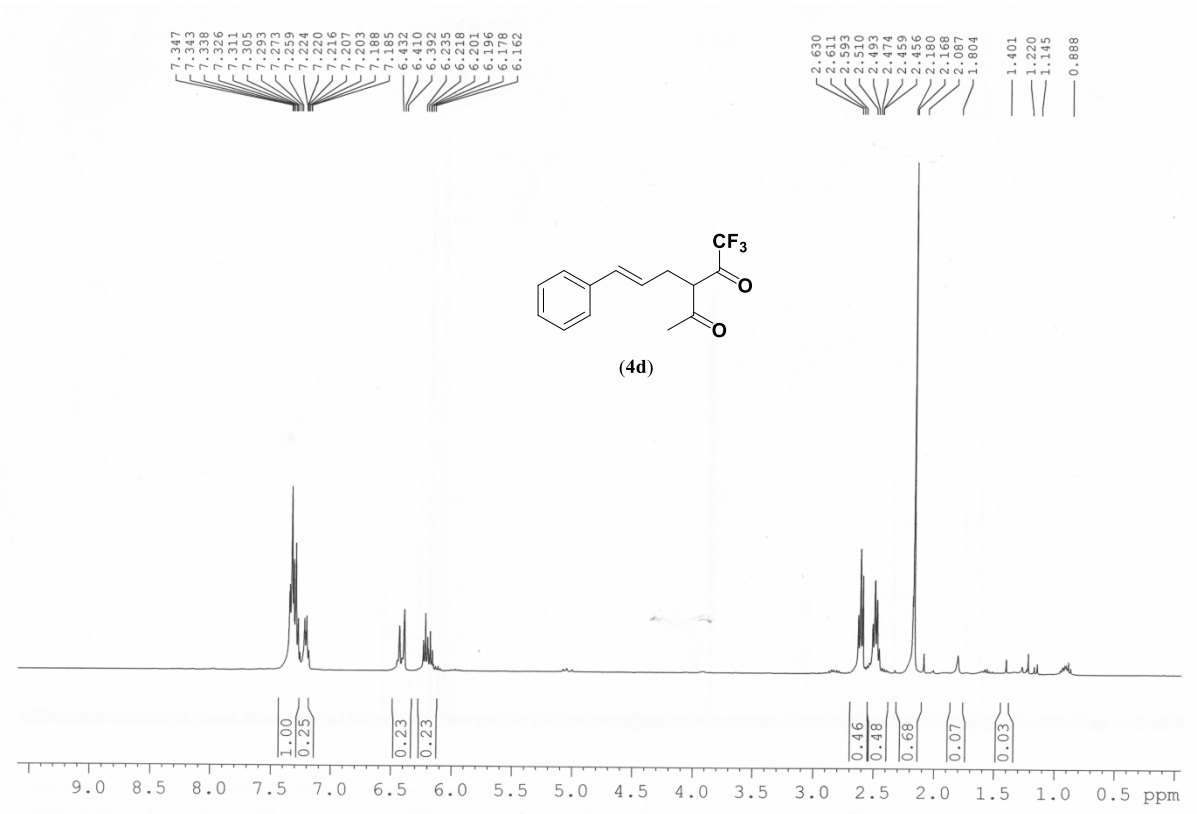

Figure S17 ^{1}H NMR (400 MHz) spectrum of compound **4d** in $CDCl_3$

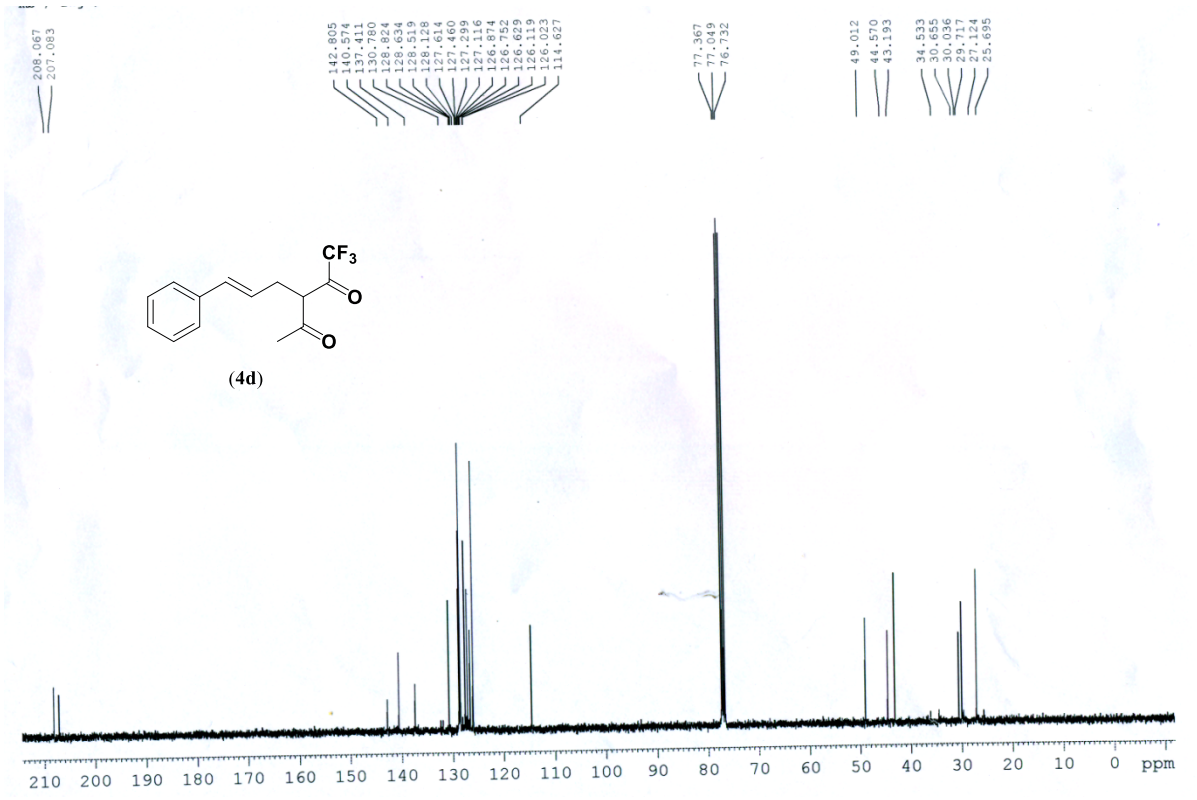

Figure S18 ^{13}C NMR (100 MHz) spectrum of compound **4d** in $CDCl_3$

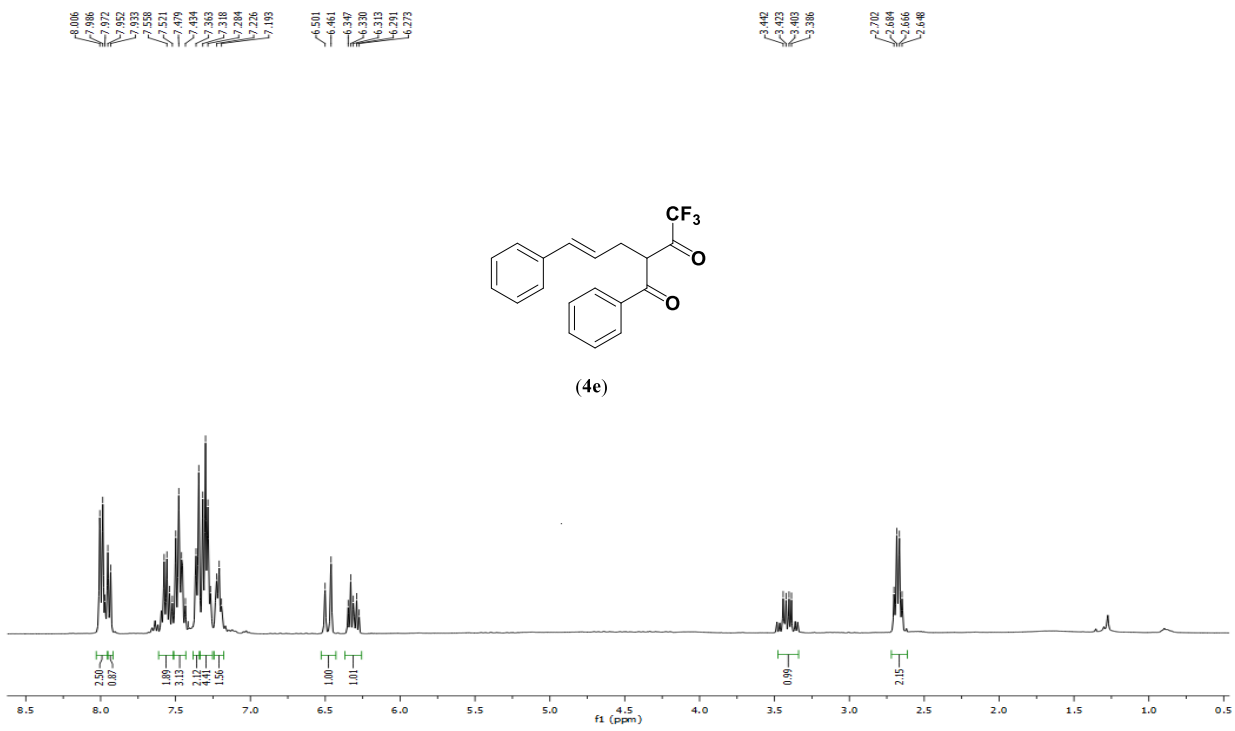

Figure S19 ^{1}H NMR (400 MHz) spectrum of compound **4e** in $CDCl_3$

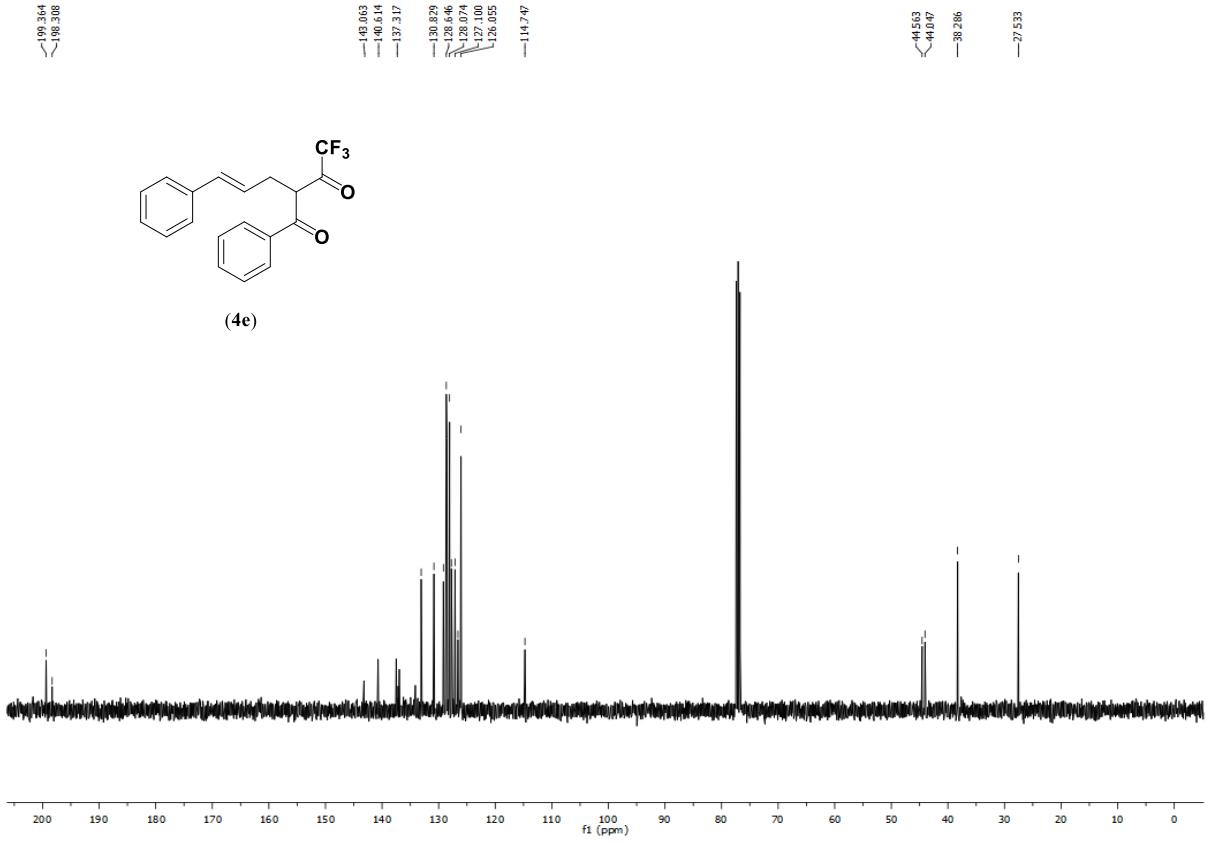

Figure S20 ^{13}C NMR (100 MHz) spectrum of compound **4e** in $CDCl_3$

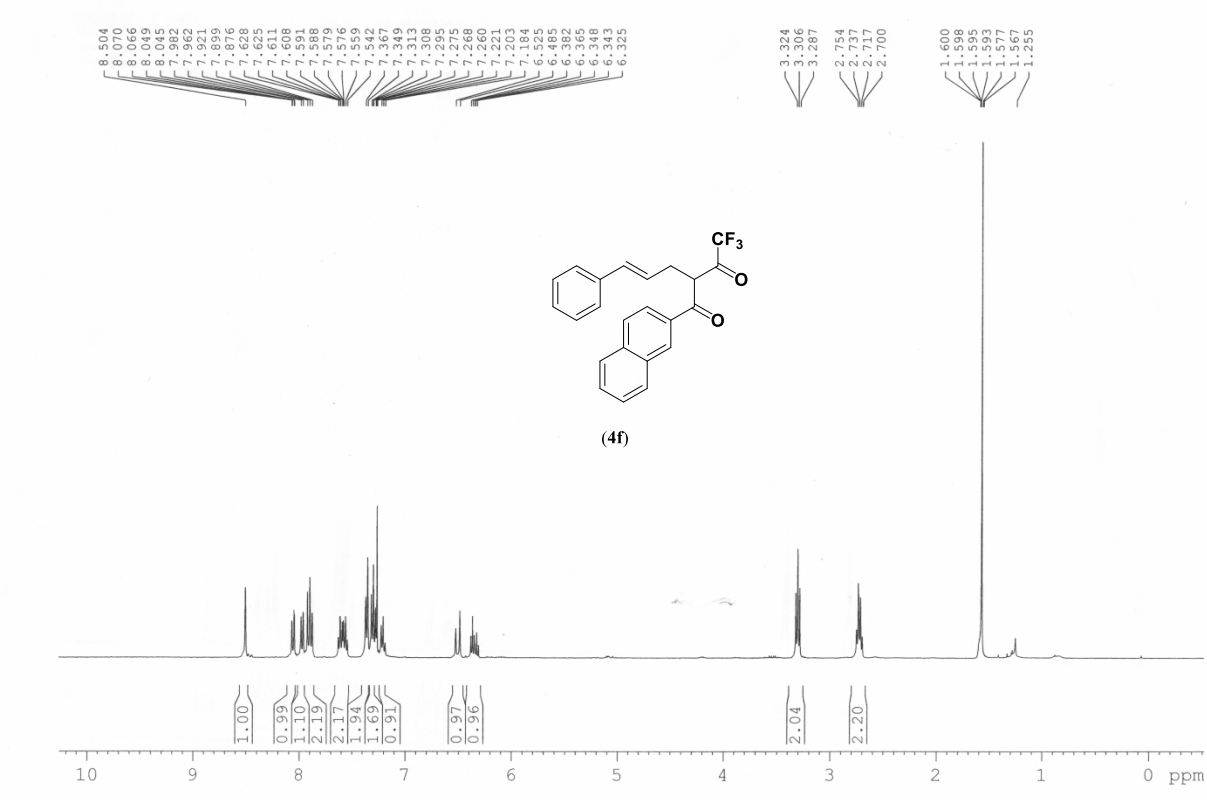

Figure S21 ^{1}H NMR (400 MHz) spectrum of compound **4f** in $CDCl_3$

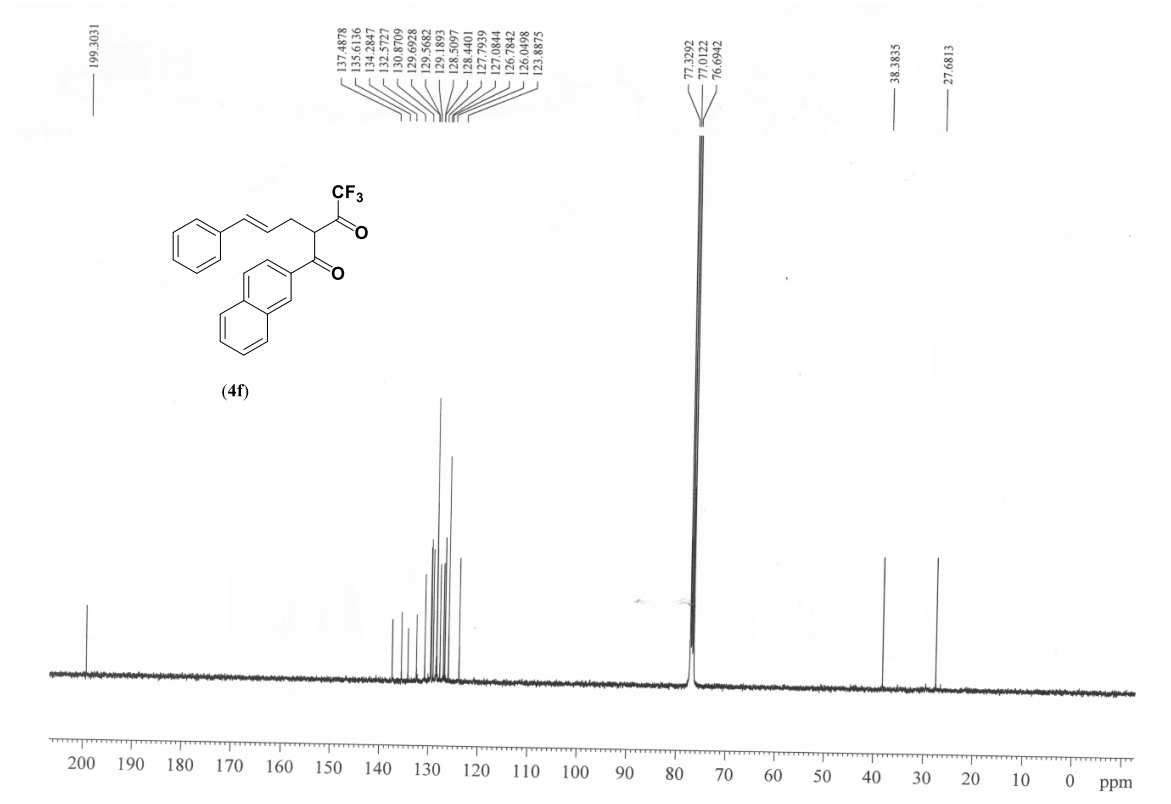

Figure S22 ^{13}C NMR (100 MHz) spectrum of compound **4f** in $CDCl_3$

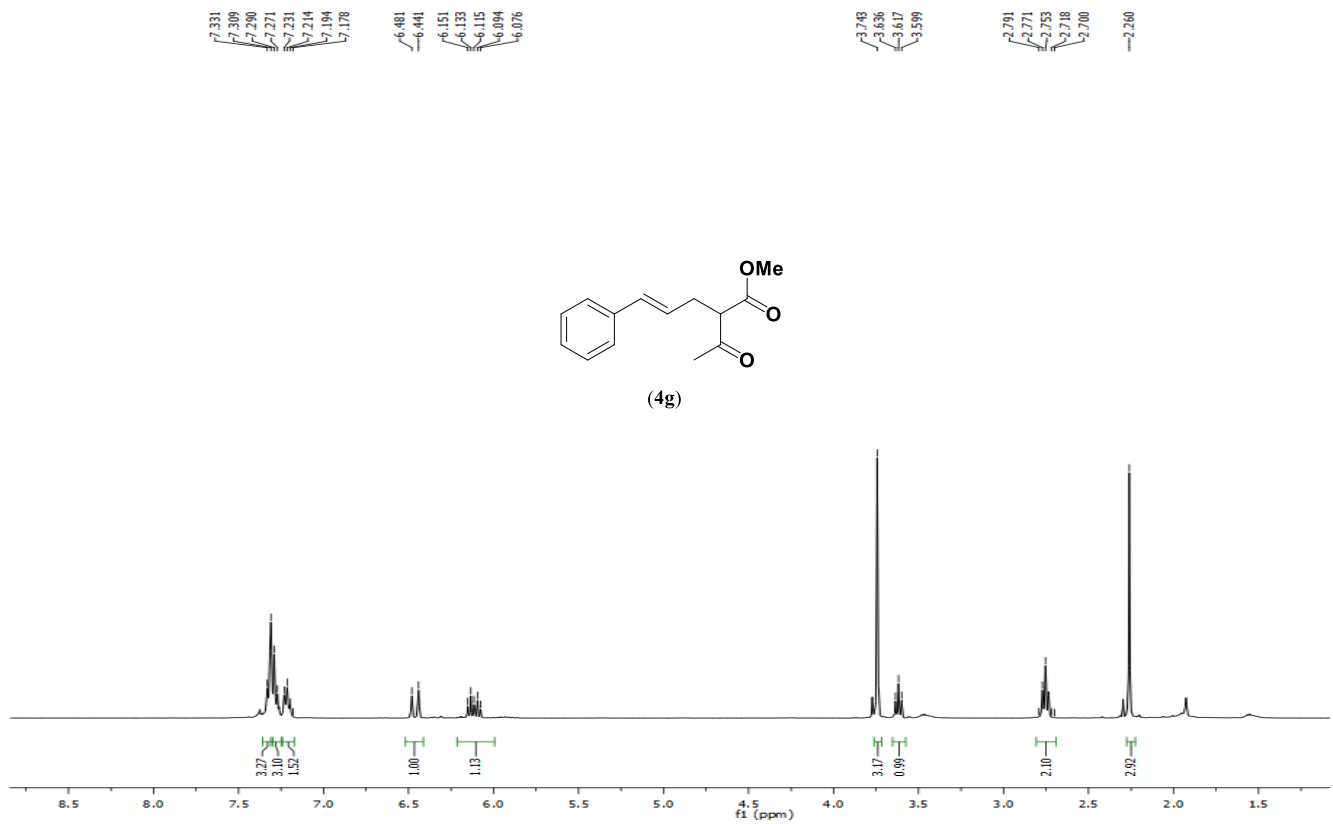

Figure S23 ^{1}H NMR (400 MHz) spectrum of compound **4g** in $CDCl_3$

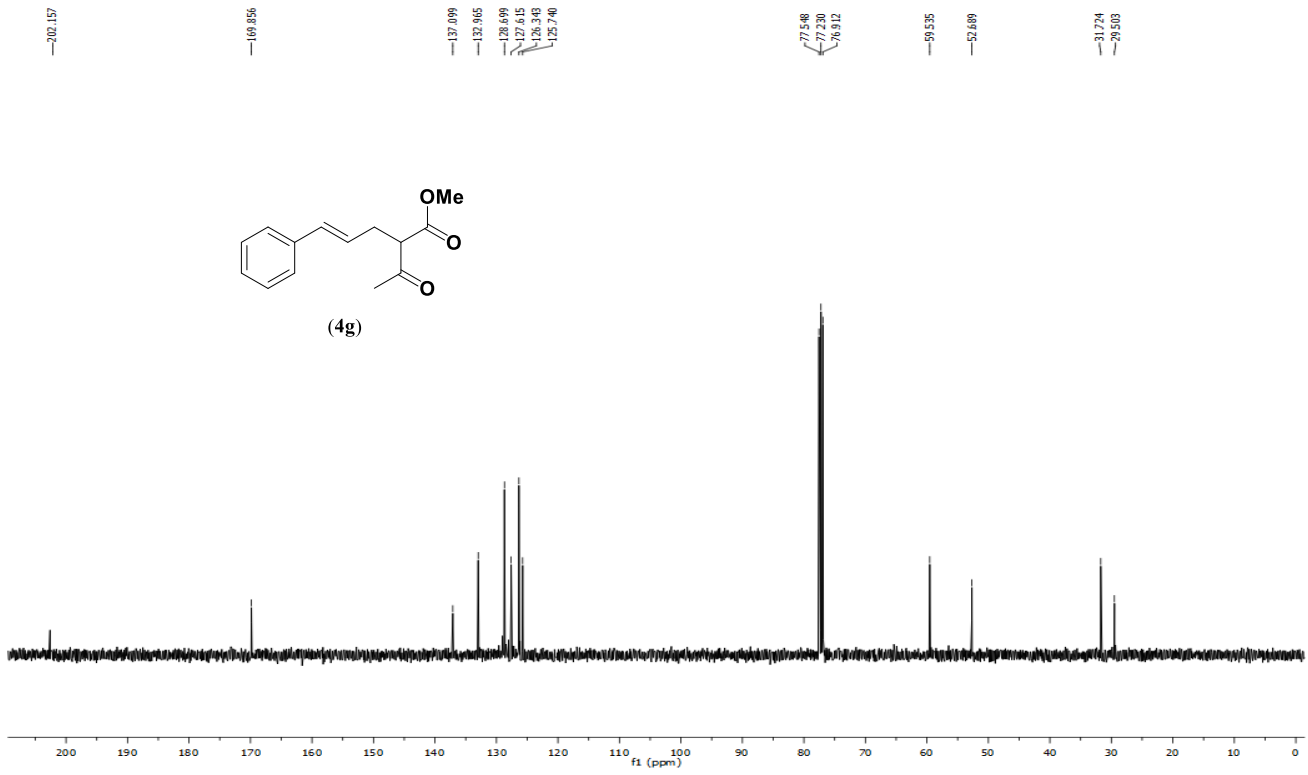

Figure S24 ^{13}C NMR (100 MHz) spectrum of compound **4g** in $CDCl_3$

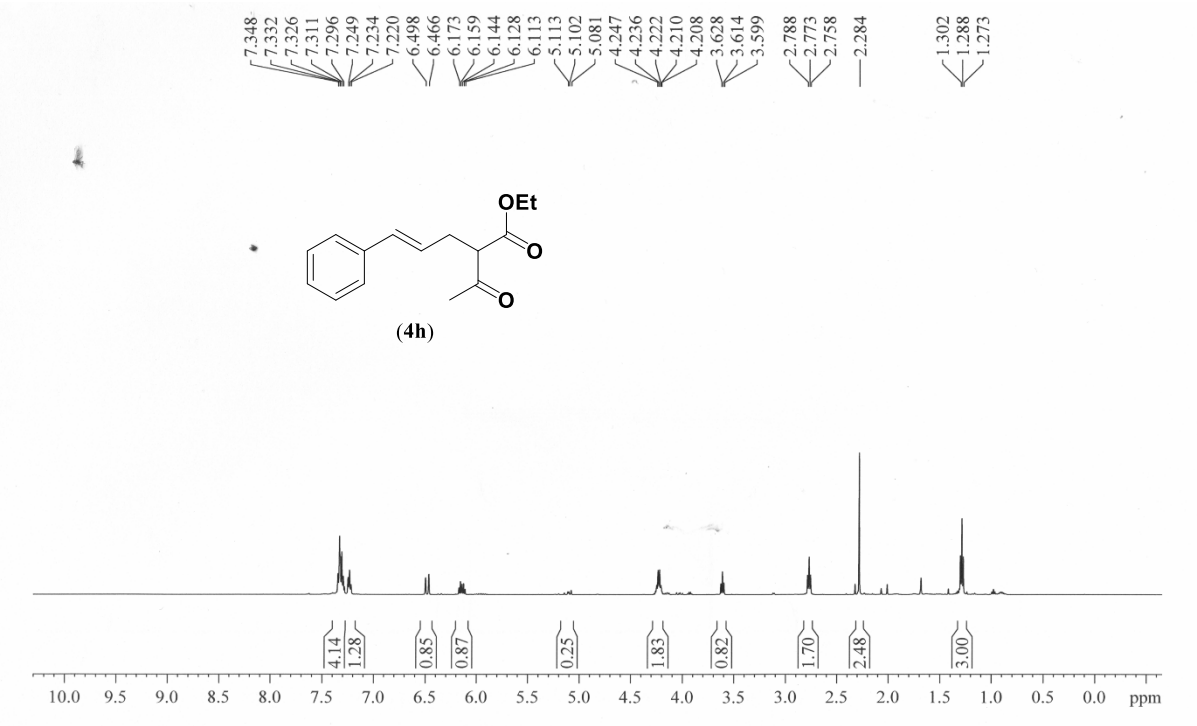

Figure S25 ^{1}H NMR (500 MHz) spectrum of compound **4h** in $CDCl_3$

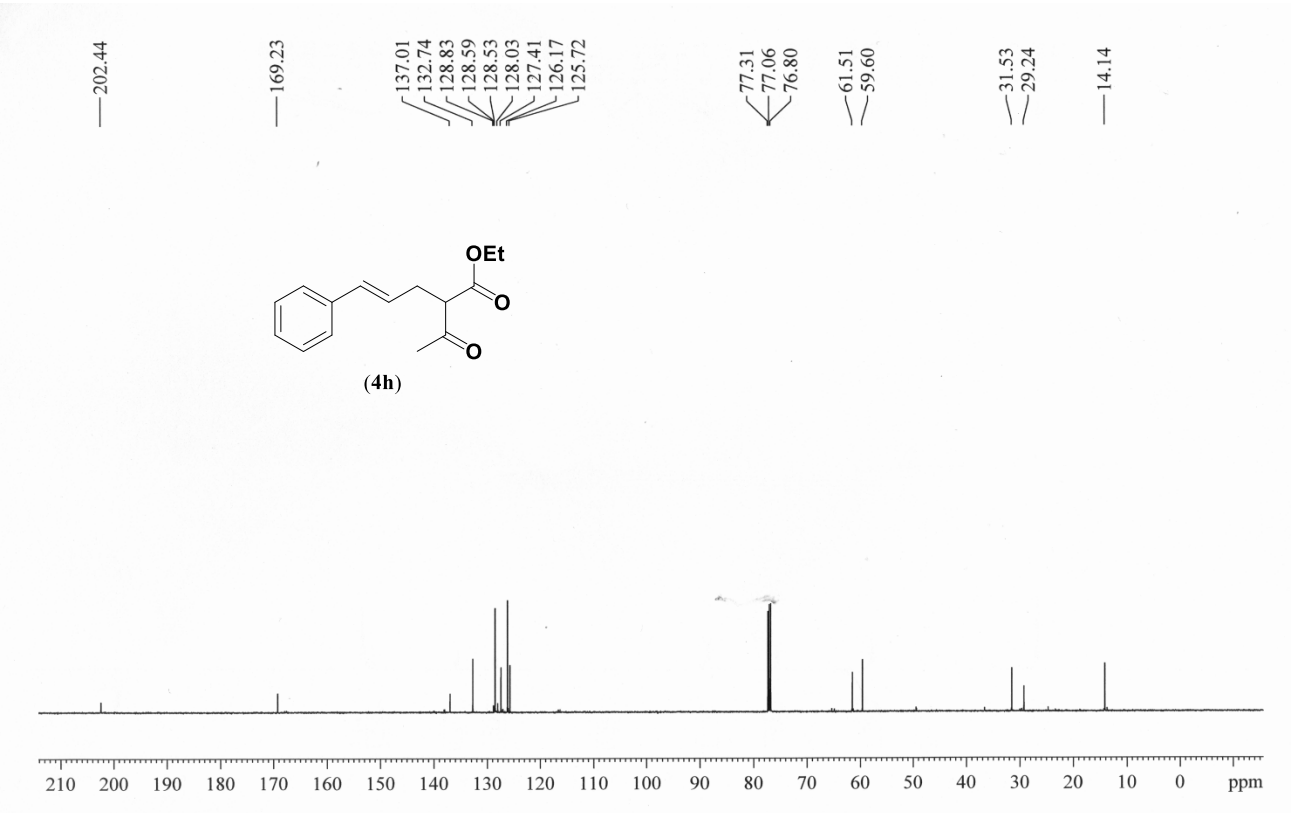

Figure S26 ^{13}C NMR (125 MHz) spectrum of compound **4h** in $CDCl_3$

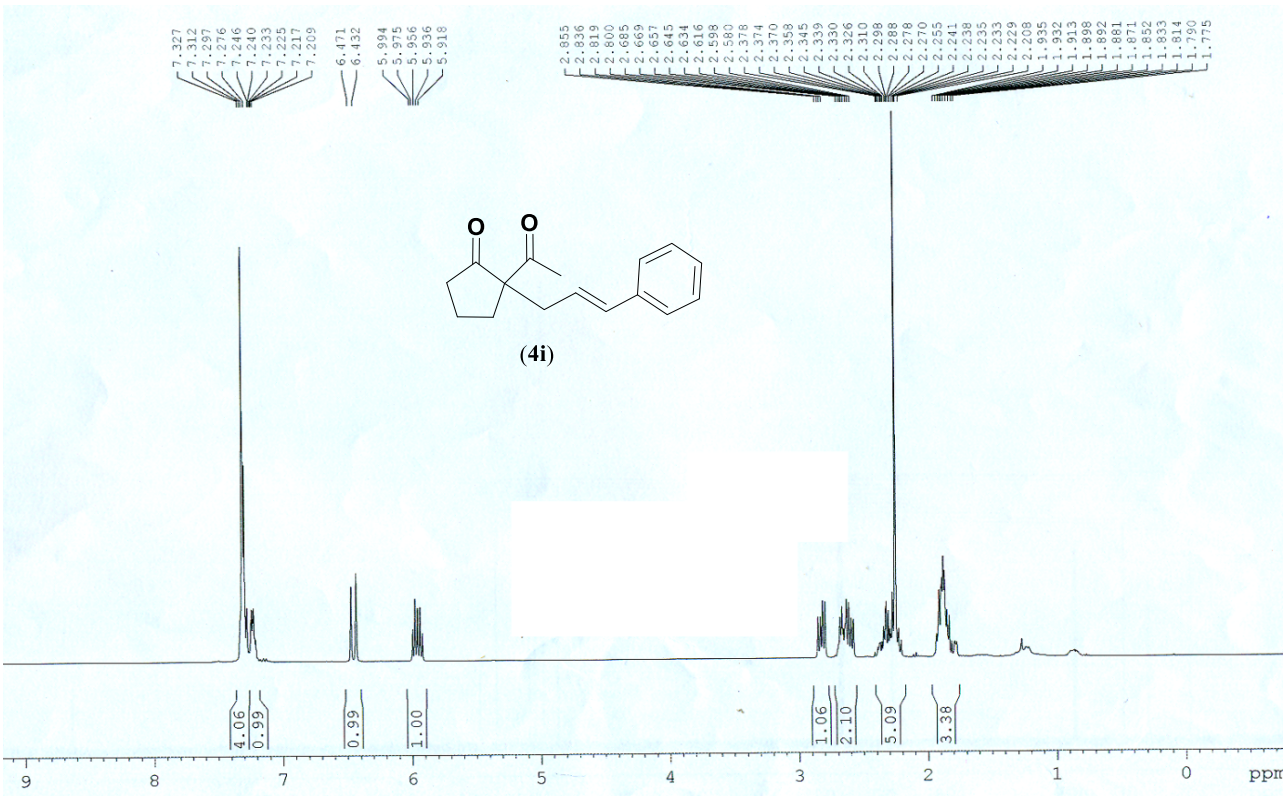

Figure S27 ^{1}H NMR (400 MHz) spectrum of compound **4i** in $CDCl_3$

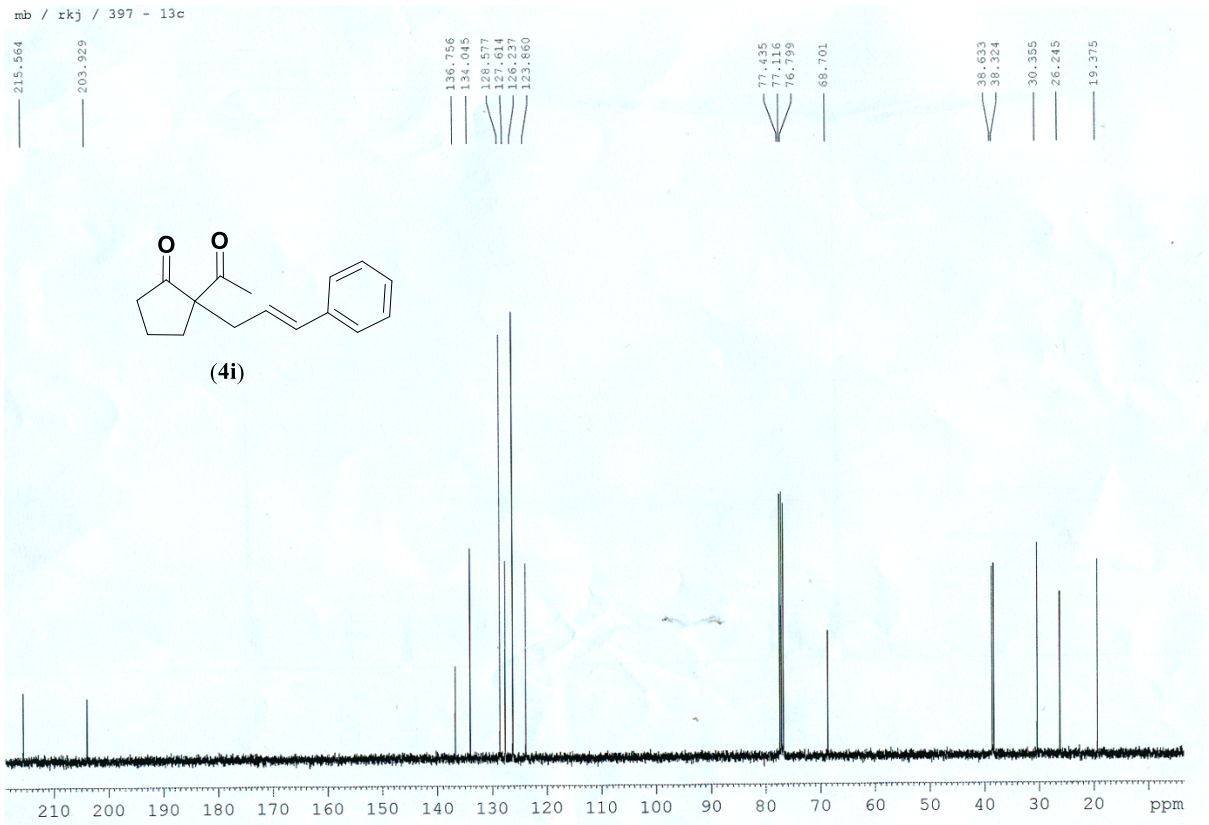

Figure S28 ^{13}C NMR (100 MHz) spectrum of compound **4i** in $CDCl_3$

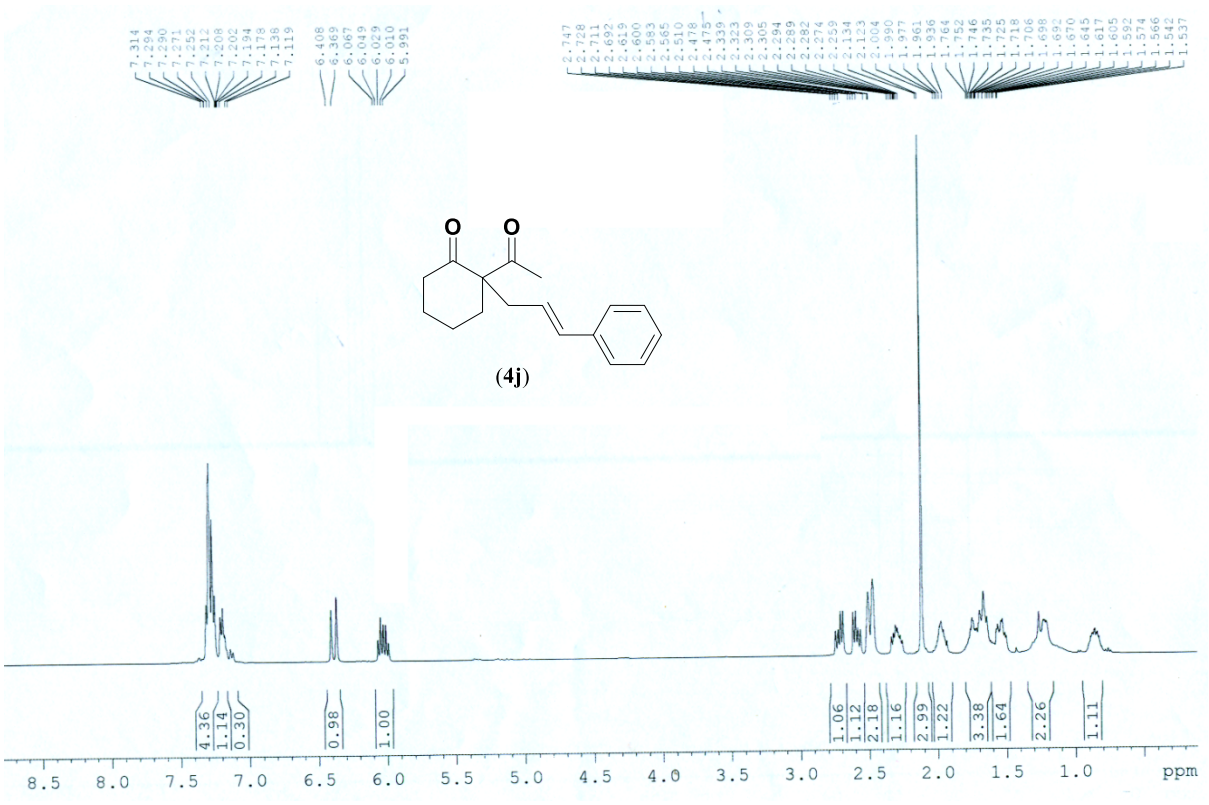

Figure S29 ^{1}H NMR (400 MHz) spectrum of compound **4j** in $CDCl_3$

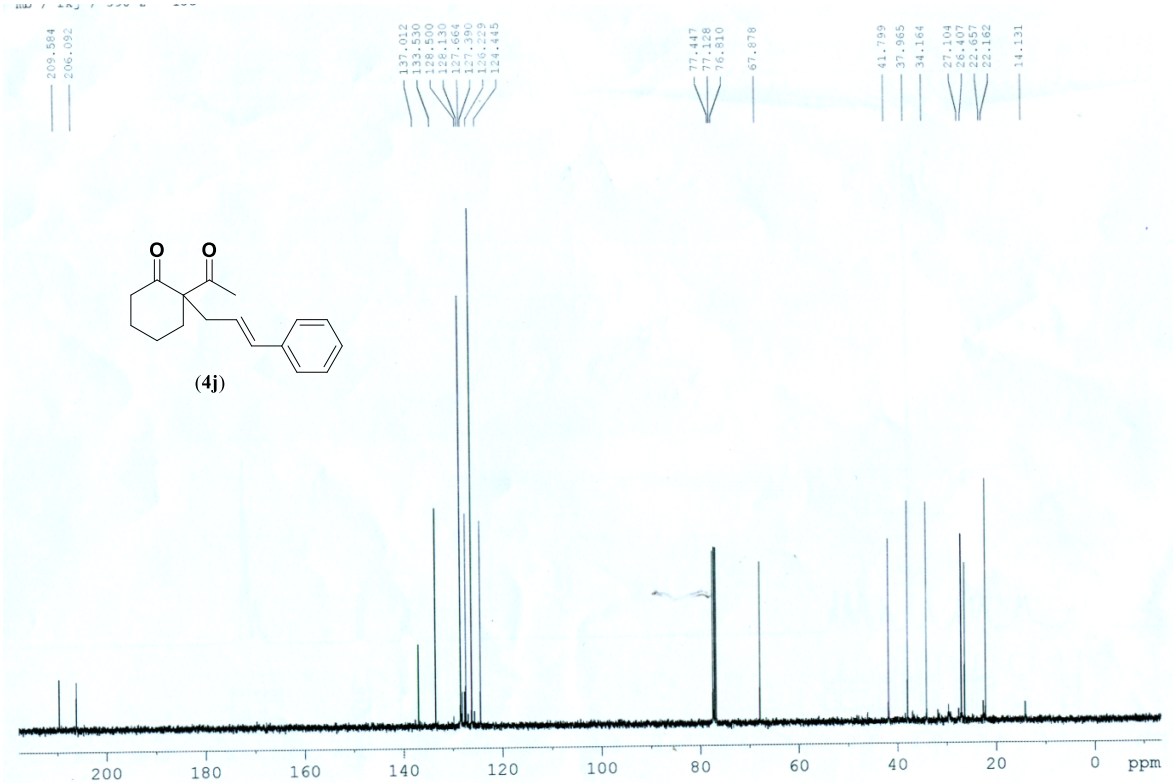

Figure S30 ^{13}C NMR (100 MHz) spectrum of compound **4j** in $CDCl_3$

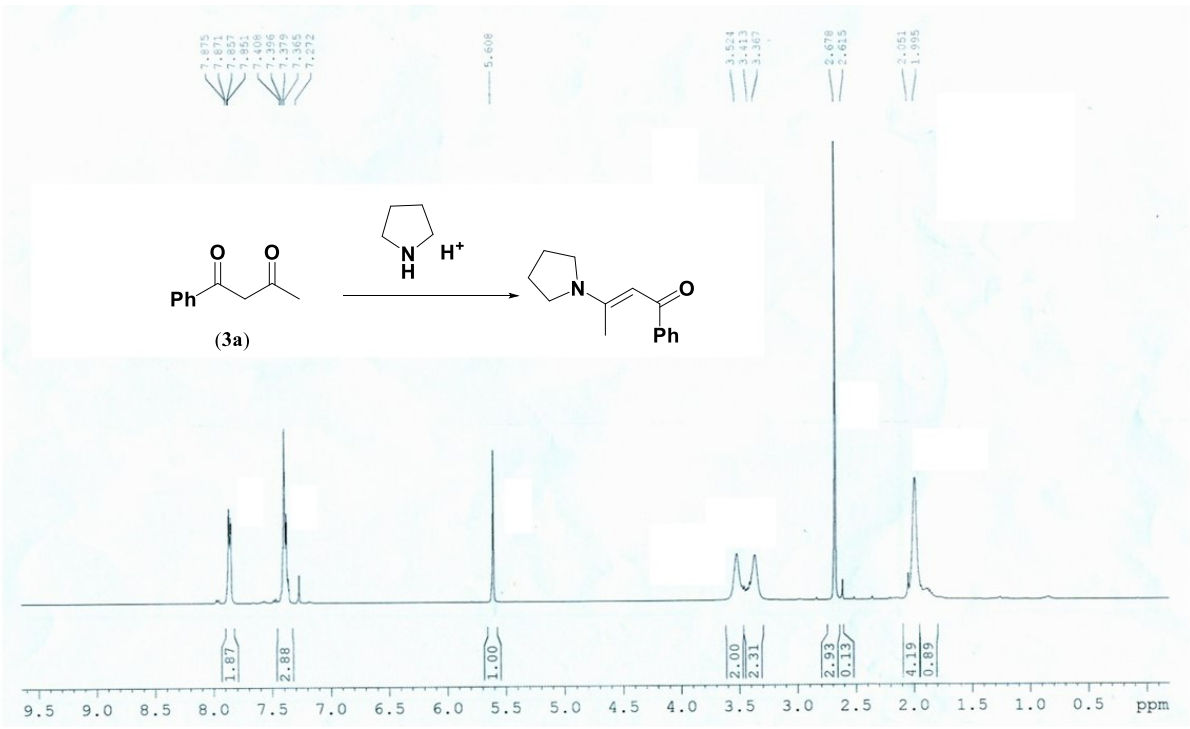

Figure S31 ^{1}H NMR (400 MHz) spectrum of 1-Phenyl-1,3-butanedione (**3a**) with pyrrolidine and acetic acid in $CDCl_3$

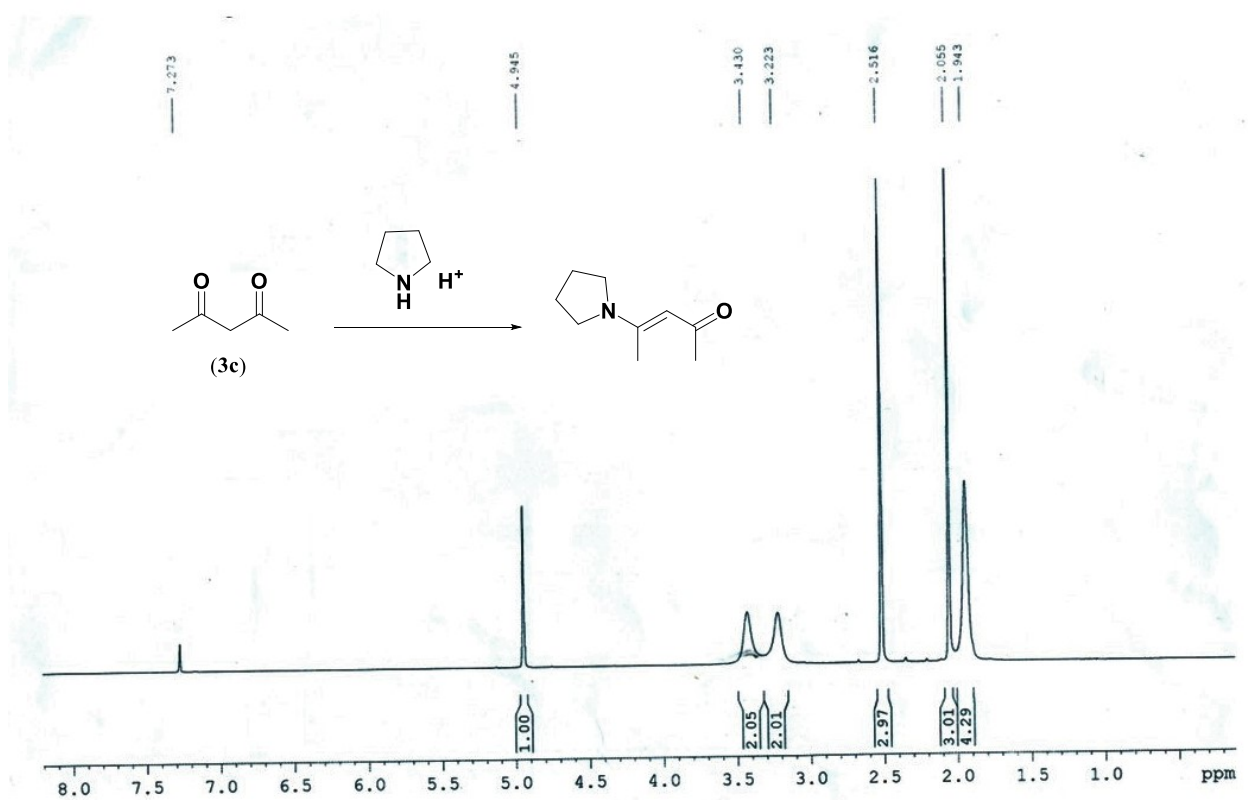

Figure S32 ^{1}H NMR (400 MHz) spectrum of Acetylacetone (**3c**) with pyrrolidine and acetic acid in $CDCl_3$

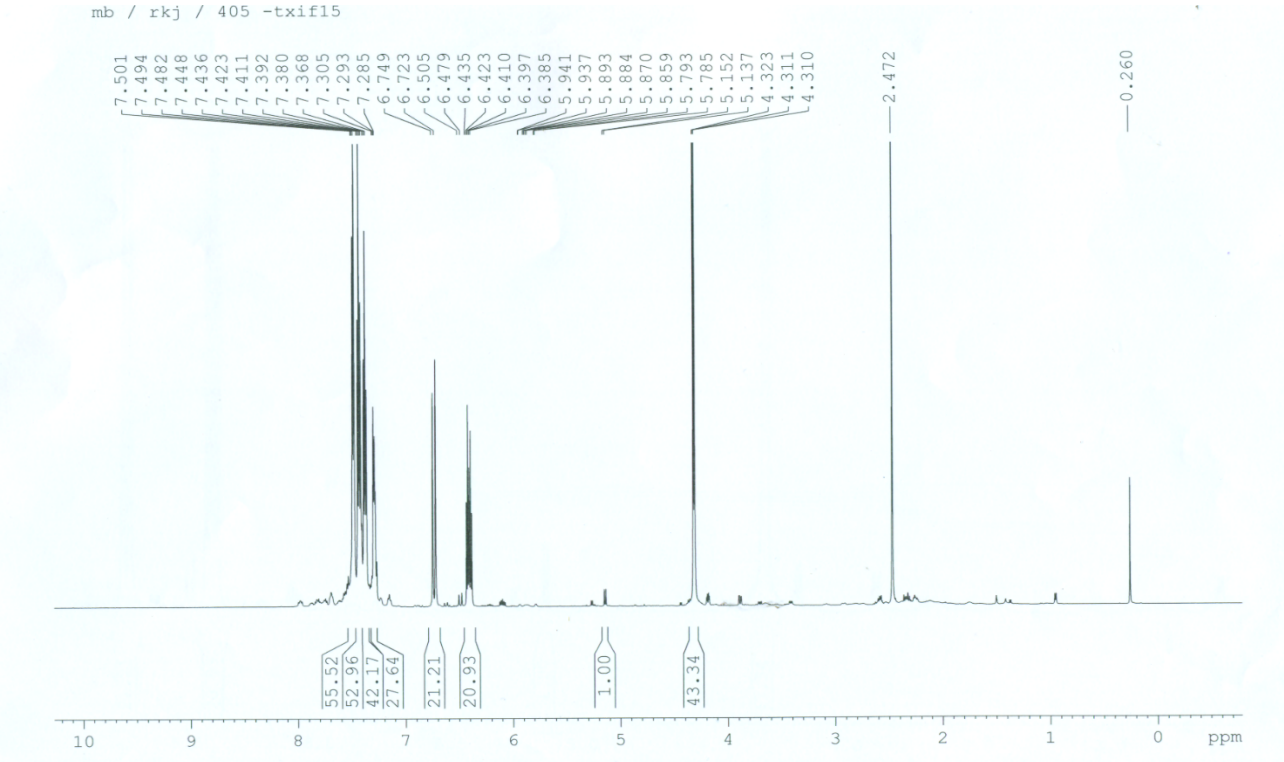

Figure S33 ^{1}H NMR (400 MHz) spectrum of **1** + Cinnamyl alcohol (**2**) in Toluene-D_8

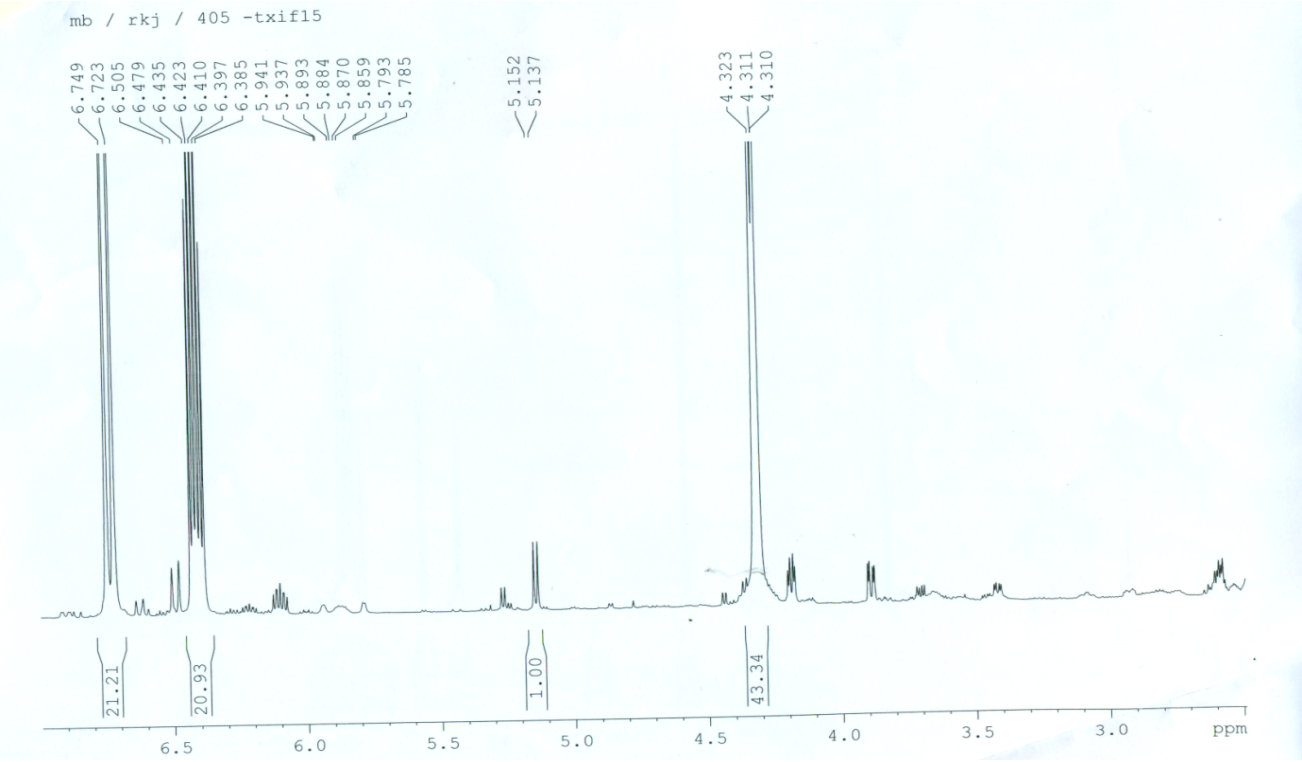

Figure S34 ^{1}H NMR (400 MHz) spectrum of **1** + Cinnamyl alcohol (**2**) in Toluene-D_8 (expanded)

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                                               Inj Volume : Manually
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Last changed    : 25-01-2017 09:56:04 by BIBEK
                  (modified after loading)

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Additional Info : Peak(s) manually integrated
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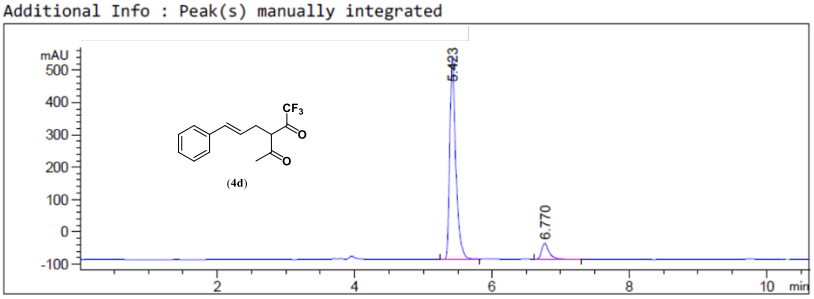


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Use Multiplier & Dilution Factor with ISTDs


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Totals :                  4183.09152  674.25923
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Figure S35 Chiral HPLC of **4d**

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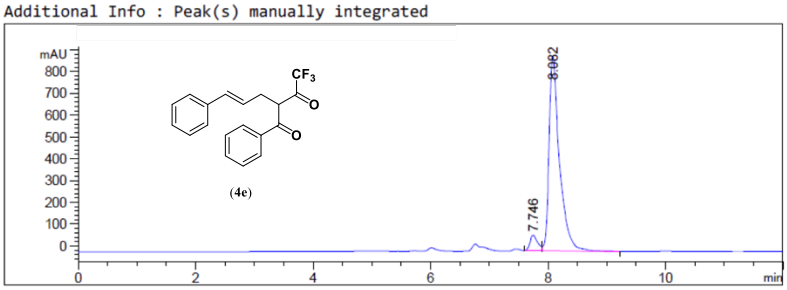
Additional Info : Peak(s) manually integrated



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Totals :				1.15480e4	964.25969	

Figure S36 Chiral HPLC of **4e**

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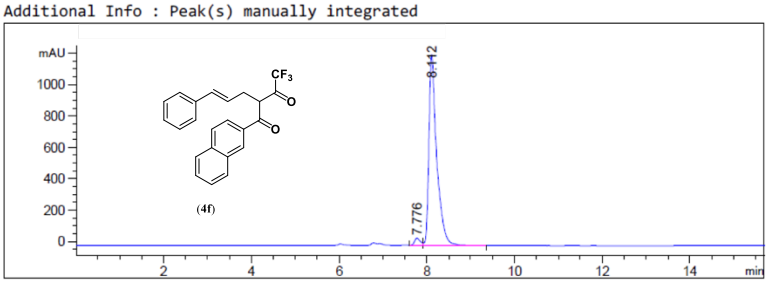
Additional Info : Peak(s) manually integrated



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Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

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2	8.112	VB	0.1781	1.50035e4	1214.52356	97.2300
Totals :				1.54310e4	1260.81589	

Figure S37 Chiral HPLC of **4f**

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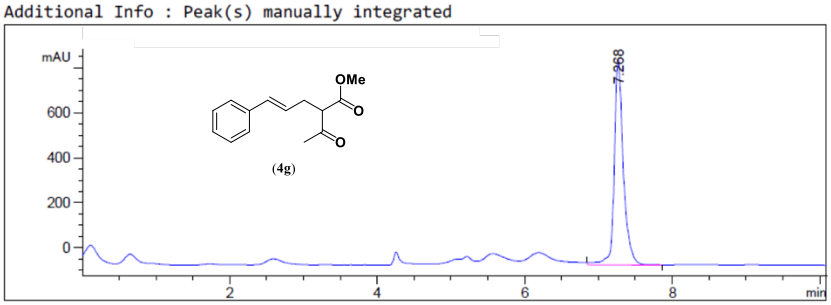
                  (modified after loading)
Analysis Method : C:\CHEM32\1\DATA\SUSIT\08122016000004.D\DA.M (METH1.M, From Data File)
Last changed    : 26-01-2017 11:52:49 by BIBEK
                  (modified after loading)

                  CHIRALPAK IA-3 250MM , 10 % iPrOH/HEXANE 1.0 ml/min flow rate, 254 nm

Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.268 VB    0.1274 7779.70801  913.29669 100.0000

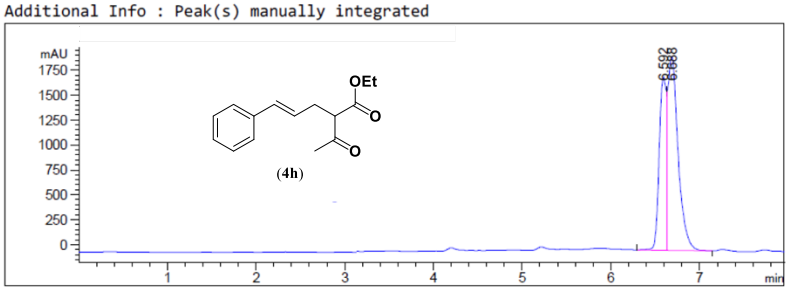
Totals :                  7779.70801  913.29669
```

Figure S38 Chiral HPLC of **4g**

```
================================================================================
Acq. Operator   : BIBEK
                                                    Location : Vial 1
Injection Date  : 08-12-2016 22:58:02
Acq. Method     : METH1.M
Analysis Method : C:\CHEM32\1\DATA\SUSIT\08122016000005.D\DA.M (METH1.M, From Data File)
Last changed    : 26-01-2017 11:50:54 by BIBEK
                  (modified after loading)

                  CHIRALPAK IA-3 250MM , 10 % iPrOH/HEXANE 1.0 ml/min flow rate, 254 nm

Additional Info : Peak(s) manually integrated
```




```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.592 BV    0.0839 9504.08594 1736.27625  37.3413
   2   6.688 VB    0.1198 1.59478e4  1942.84363  62.6587

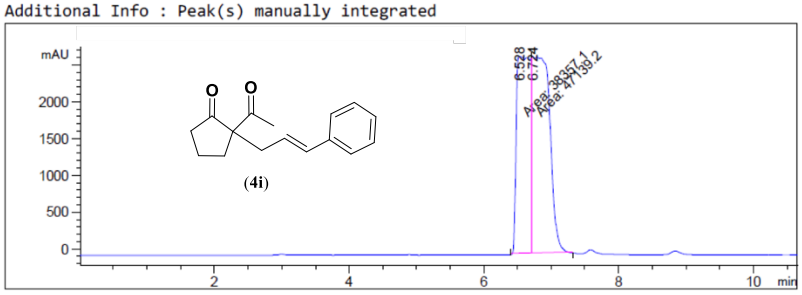
Totals :                  2.54519e4  3679.11987
```

Figure S39 Chiral HPLC of **4h**

```
Acq. Operator   : BIBEK
Acq. Instrument : HPLC                          Location : Vial 1
Injection Date  : 08-12-2016 23:35:15
                                               Inj Volume : Manually
Acq. Method     : C:\CHEM32\1\METHODS\METH1.M
Last changed    : 08-12-2016 23:33:59 by BIBEK
                  (modified after loading)
Analysis Method : C:\CHEM32\1\DATA\SUSIT\08122016000008.D\DA.M (METH1.M, From Data File)
Last changed    : 25-01-2017 09:54:57 by BIBEK
                  (modified after loading)

                  CHIRALPAK IA-3 250MM , 10 % iPrOH/HEXANE 1.0 ml/min flow rate, 254 nm

Additional Info : Peak(s) manually integrated
```




```
=====================================================================
                        Area Percent Report
=====================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]       [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.528 MF    0.2393 3.83571e4  2671.10107  44.8641
   2   6.724 FM    0.2951 4.71392e4  2662.14160  55.1359

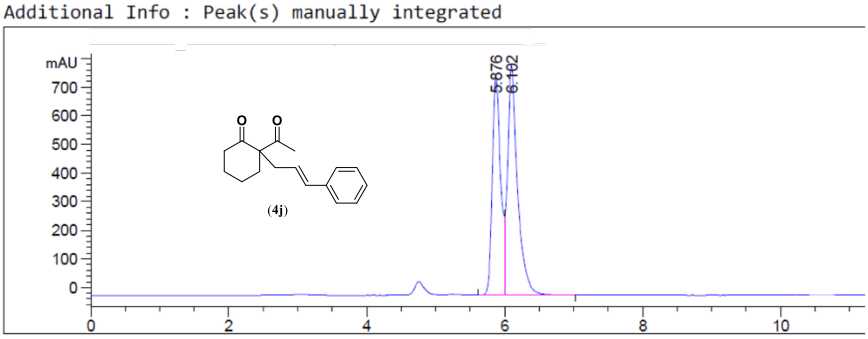
Totals :                  8.54964e4  5333.24268
```

Figure S40 Chiral HPLC of **4i**

```
Acq. Operator   : bibek
Acq. Instrument : HPLC                              Location : Vial 1
Injection Date  : 29-01-2018 20:32:32
                                                    Inj Volume : Manually
Acq. Method     : C:\CHEM32\1\METHODS\METH1.M
Last changed    : 29-01-2018 20:31:48 by bibek
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\METH1.M
Last changed    : 31-01-2018 13:01:46 by bibek
                  (modified after loading)

                  CHIRALPAK IA-3, 250 MM,   IPA/HEXANE : 10:90, 1.0 ml/min flc

Additional Info : Peak(s) manually integrated
```




```
================================================================================
                          Area Percent Report
================================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   5.876 BV    0.1240 6263.58252  761.51666  43.3013
   2   6.102 VB    0.1454 8201.54199  801.19952  56.6987

Totals :                 1.44651e4  1562.71619
```

Figure S41 Chiral HPLC of **4j**