Supplementary Information

Synthesis of α-Methylene-δ-Oxo-γ-Amino Esters *via* Rh(II)-Catalyzed Coupling of 1-Sulfonyl-1,2,3-Triazoles with Morita-Baylis-Hillman Adducts

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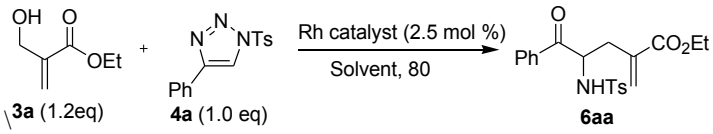
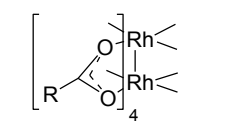
1. Optimization table of 6aa[a]

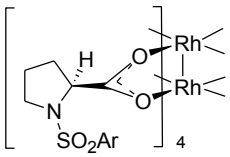


Entry	Rh catalyst	Solvent	Time[b]	Yield (%)[c]
1	$Rh_2(OAc)_4$	Toluene	12 h	52[d]
2	$Rh_2(Oct)_4$	Toluene	4 h	86
3	$Rh_2(TPA)_4$	Toluene	12 h	66[d]
4	$Rh_2((S)\text{-}DOSP)_4$	Toluene	12 h	16[d]
5	$Rh_2((S)\text{-}PTPA)_4$	Toluene	6 h	70
6	$Rh_2((S)\text{-}NTTL)_4$	Toluene	45 m	76
7	$Rh_2(^t\text{BuCO2})_4$	Toluene	15 m	94
8[e]	$Rh_2(^t\text{BuCO2})_4$	Toluene	30 m	86
9[f]	$Rh_2(^t\text{BuCO2})_4$	Toluene	1 h	75
10	$Rh_2(^t\text{BuCO2})_4$	Chlorobenzene	15 m	91
11	$Rh_2(^t\text{BuCO2})_4$	1,2-DCE	30 m	77
12	$Rh_2(^t\text{BuCO2})_4$	$CHCl_3$	2 h	77
13[g]	$Rh_2(^t\text{BuCO2})_4$	Toluene	1.5 h	87
14[h]	$Rh_2(^t\text{BuCO2})_4$	Toluene	2d	< 5

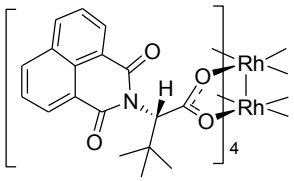
[a]Condition : Triazole **4a** (0.2 mmol), Morita-Baylis-Hillman adduct **3a** (0.24 mmol), Rh catalyst (2.5 mol %), and solvent (1.0 mL) were added into a flame-dried vial reactor. The mixure was then heated at 80 °C. After cooling to room temperature, the reaction mixture was concentrated under reduced pressure. The residue was purified by silica chromatography to afford the corresponding α-methylene δ-oxo-γ-amino ester **6aa.** [b]Time for complete conversion of triazole by TLC. [c]Isolated yield after silica-gel column chromatography. [d]After the given time, the starting materials was remained. [e]Reaction was carried using 2.0 mol % Rh catalyst. [f]Reaction was carried using 1.5 mol % Rh catalyst. [g]Reaction temperature was 60 °C. [h]Reaction was carried out at room temperature.



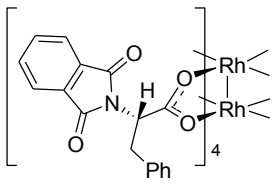
R = Me: $Rh_2(OAc)_4$
R = *n*-Heptyl: $Rh_2(Oct)_4$
R = *t*-Bu: $Rh_2(^t\text{BuCO}_2)_4$



Ar = 4-$C_{12}H_{25}C_6H_4$-
$Rh_2(S\text{-}DOSP)_4$



$Rh_2(S\text{-}NTTL)_4$



$Rh_2(S\text{-}PTPA)_4$

2. X-ray Crystal Structures and Data for 6aa and (*E*)-6ab.

1) X-ray crystal of 6aa

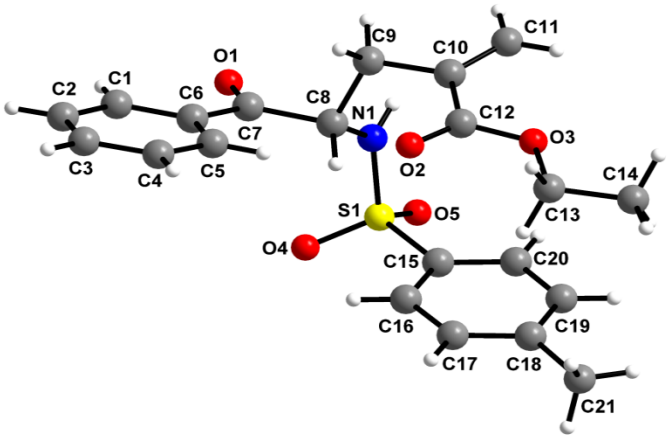


Table S2-1. Crystal data and structure refinement for 6aa.

Empirical formula	$C_{21}H_{23}NO_5S$	
Formula weight	401.46	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 9.9971(2) Å	α= 90°.
	b = 10.9922(2) Å	β= 93.6089(10)°.
	c = 18.9189(3) Å	γ = 90°.
Volume	2074.88(7) $Å^3$	
Z	4	
Density (calculated)	1.285 Mg/m^3	
Absorption coefficient	0.187 mm^{-1}	
F(000)	848	
Crystal size	0.320 x 0.200 x 0.200 mm^3	
Theta range for data collection	2.144 to 28.337°.	
Index ranges	-13<=h<=13, -14<=k<=14, -25<=l<=25	
Reflections collected	72298	
Independent reflections	5175 [R(int) = 0.0644]	
Completeness to theta = 25.242°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5175 / 0 / 255	
Goodness-of-fit on F^2	1.036	
Final R indices [I>2sigma(I)]	R_1 = 0.0507, wR_2 = 0.1110	
R indices (all data)	R_1 = 0.0946, wR_2 = 0.1301	
Largest diff. peak and hole	0.252 and -0.302 $e.Å^{-3}$	

2) X-ray crystal of (*E*)-6ab

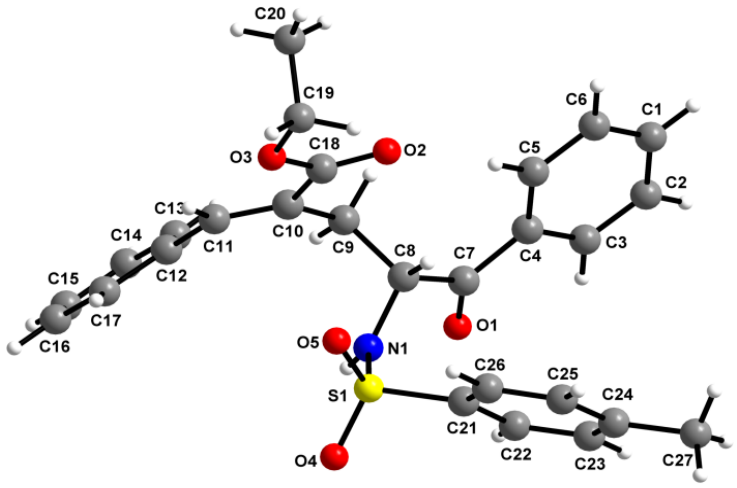
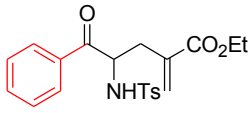


Table S2-2. Crystal data and structure refinement for (*E*)-6ab

Empirical formula	$C_{27}H_{27}NO_5S$	
Formula weight	477.55	
Temperature	170(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.1944(8) Å	α = 70.003(4)°
	b = 10.8330(9) Å	β = 83.089(4)°
	c = 13.2249(12) Å	γ = 89.062(4)°
Volume	1228.40(19) Å3	
Z	2	
Density (calculated)	1.291 g/cm3	
Absorption coefficient	0.170 mm-1	
F(000)	504	
Crystal size	0.200 x 0.400 x 0.400 mm^3	
Theta range for data collection	2.00 to 25.49°	
Index ranges	-11<=h<=11, -13<=k<=13, -16<=l<=16	
Reflections collected	20790	
Independent reflections	4272 [R(int) = 0.0503]	
Coverage of independent reflections	93.7 %	
Refinement method	Full-matrix least-squares on F2	
Data / restraints / parameters	4272 / 0 / 309	
Goodness-of-fit on F2	1.167	
Final R indices [I>2sigma(I)]	R1 = 0.0892, wR2 = 0.1579	
R indices (all data)	R1 = 0.1087, wR2 = 0.1674	
Largest diff. peak and hole	0.325 and -0.491 $eÅ^{-3}$	

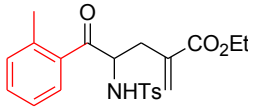
3. Characterization data for 6aa-6na, 6ab-6ah and 6nb

Ethyl 2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenylpentanoate (6aa). Yield : 94 % (76 mg);



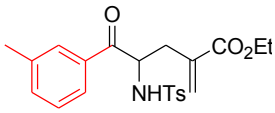
Eluents : *n*-hexane/EtOAc = 7/1; pale yellow solid; mp: 96-98°C; ^{1}H NMR (300 MHz, $CDCl_3$), δ 1.30-1.36 (m, 3H), 2.17-2.27 (m, 4H), 2.89 (dd, *J* = 13.7 Hz, 2.7 Hz, 1H), 4.18-4.29 (m, 2H), 5.14-5.29 (m, 1H), 5.71(s, 1H), 5.77 (d, *J* = 9.2 Hz, 1H), 6.29 (s, 1H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.43-7.49 (m, 2H), 7.55-7.63 (m, 3H), 7.94-7.97 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.5, 37.9, 56.3, 61.1, 127.3, 128.8, 128.9, 129.6, 130.2, 133.6, 134.3, 134.6, 136.8, 143.5, 166.7, 197.8 ppm. HRMS Calcd *m/z* for $C_{21}H_{23}NO_5S$ $[M]^+$: 401.1297. Found (FAB, $[M+H]^+$): 402.1373.

Ethyl 2-methylidene-5-(2-methylphenyl)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6ba). Yield :



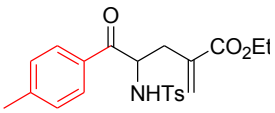
88% (73mg); Elunent : *n*-hexane/EtOAc = 7/1; white solid; mp: 102-104°C; ^{1}H NMR (300 MHz, $CDCl_3$), δ 1.27-1.33 (m, 3H), 2.18-2.31 (m, 4H), 2.33 (s, 3H), 2.74-2.80 (m, 1H), 4.13-4.24 (m, 2H), 5.08-5.17 (m, 1H), 5.67(s, 1H), 5.81 (d, *J* = 9.0 Hz, 1H), 6.24 (d, *J* = 0.9 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 7.26-7.32 (m, 1H), 7.37-7.43 (m, 1H), 7.72 (d, *J* = 0.9 Hz, 2H), 7.74 (d, *J* = 0.9 Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.5(21.50), 21.5(21.54), 37.3, 57.7, 61.0, 126.1, 127.3, 129.4, 129.6, 129.8, 132.3, 132.7, 133.6, 134.7, 137.0, 140.0, 143.5, 166.5, 200.3 ppm. HRMS Calcd *m/z* for $C_{22}H_{25}NO_5S$ $[M]^+$: 415.1453. Found (FAB, $[M+H]^+$): 416.1529.

Ethyl 2-methylidene-5-(3-methylphenyl)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6ca).



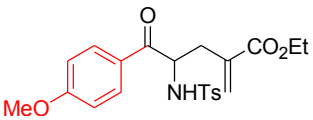
Yield : 84% (70 mg); Eluents : *n*-hexane/EtOAc = 7/1;pale yellow solid; mp: 90-92 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.30-1.35 (m, 3H), 2.18-2.28 (m, 4H), 2.39 (s, 3H), 2.85-2.92 (m, 1H), 4.19-4.27 (m, 2H), 5.15-5.23 (m, 1H), 5.70 (s, 1H), 5.79 (d, *J* = 9.2 Hz, 1H), 6.28 (d, *J* = 0.9 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.31-7.41 (m, 2H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.72-7.80 (m, 2H) ppm; ^{13}C NMR (75 MHz,$CDCl_3$) δ 14.3, 21.4(21.35), 21.4(21.44), 37.8, 56.3, 61.0, 126.0, 127.2, 128.7, 129.2, 129.5, 130.0, 133.6, 134.6, 135.0, 136.9, 138.7, 143.4, 166.5, 197.9 ppm. HRMS (FAB) Calcd *m/z* for $C_{22}H_{26}NO_5S$ $[M+H]^+$: 416.1531. Found:416.1530.

Ethyl 2-methylidene-5-(4-methylphenyl)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6da).



Yield: 85% (71 mg); Eluents: *n*-hexane/EtOAc = 7/1; pale yellow solid; mp: 119-120 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.30-1.36 (m, 3H), 2.16-2.27 (m, 4H), 2.40 (s, 3H), 2.87 (dd, *J* = 13.7, 2.6 Hz, 1H), 4.19-4.27 (m, 2H), 5.13-5.21 (m, 1H), 5.70 (s, 1H),5.81 (d, *J* = 9.2 Hz, 1H), 6.28 (d, *J* = 1.0 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.59-7.62 (m, 2H), 7.86 (d, *J* = 8.3 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 21.4, 21.8, 37.9, 56.1, 61.0, 127.2, 128.9, 129.5, 129.6, 130.0, 131.1, 134.6, 136.9, 143.3, 145.3, 166.6, 197.2 ppm. HRMS (FAB) Calcd *m/z* for $C_{22}H_{26}NO_5S$ $[M+H]^+$: 416.1531. Found: 416.1533.

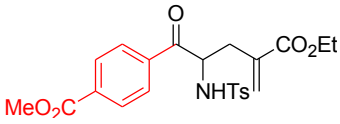
Ethyl 5-(4-methoxyphenyl)-2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6ea).



Yield: 86% (74mg); Eluents: *n*-hexane/EtOAc = 7/1; yellow solid; mp: 126-128 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.31-1.37 (m, 3H), 2.14-2.32 (m, 4H), 2.80-2.93 (m, 1H), 3.87 (s, 1H), 4.24 (dd, *J* = 14.0, 7.1 Hz, 2H), 5.08-5.20 (m, 1H), 5.70 (s, 1H), 5.79 (d, *J* = 9.2 Hz, 1H), 6.29 (s,1H), 6.93 (d, *J* = 8.9 HZ, 2H), 7.09 (d, *J* = 8.1 HZ, 2H), 7.60 (d, *J* = 8.3 HZ, 2H), 7.96 (d, *J* = 8.9 HZ, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.5, 38.2, 55.7, 56.0, 61.1, 114.1,

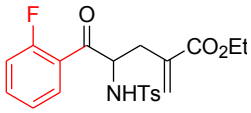
126.5, 127.2, 129.5, 130.0, 131.3, 134.7, 136.9, 143.4, 164.4, 166.7, 196.0 ppm. HRMS (FAB) Calcd *m/z* for $C_{22}H_{26}NO_6S$ $[M+H]^+$: 432.1481. Found: 432.1479.

Methyl 4-{4-(ethoxycarbonyl)-2-{[(4-methylphenyl)sulfonyl]amino}-pent-4-enoyl}benzoate (6fa). Yield:



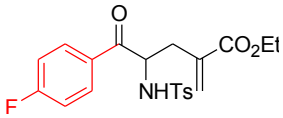
97% (89mg); Eluents: *n*-hexane/EtOAc = 7/1; white solid; mp: 116-118 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.33 (t, *J*= 7.1 Hz, 3H), 2.20-2.32 (m, 4H), 2.82-2.90 (m, 1H), 3.96 (s, 3H), 4.18-4.27 (m, 2H), 5.17-5.25 (m, 1H), 5.72 (s, 1H), 5.81 (d, *J* = 9.3 Hz, 1H), 6.29 (d, *J* = 0.9 Hz,1 Hz), 7.10 (d, *J* = 8.0 Hz, 2H), 7.61 (d, *J* = 8.3 Hz, 2H), 8.00-8.09 (m, 2H), 8.09-8.14(m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 21.5, 37.5, 52.7, 56.5, 61.1, 127.2, 128.7, 129.6, 130.0, 130.3, 134.3, 134.8, 136.8(136.76), 136.8(136.81), 143.6, 166.0, 166.5, 197.5 ppm. HRMS (FAB) Calcd *m/z* for $C_{23}H_{26}NO_7S$ $[M+H]^+$: 460.1430. Found: 460.1433.

Ethyl 5-(2-fluorophenyl)-2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6ga).



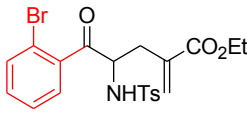
Yield: 96% (80mg); Eluents: *n*-hexane/EtOAc = 7/1; white solid; mp: 97-99 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.25 (t, *J* = 7.1 Hz, 3H), 2.30 (s, 3H), 2.48-2.57 (m, 1H), 2.79 (dd, *J* = 14.1, 4.5 Hz, 1H), 4.07-4.20 (m, 2H), 5.03-5.12 (m, 1H), 5.68-5.76 (m, 2H), 6.28 (d, *J* = 0.75Hz), 7.08-7.25 (m, 4H), 7-50 (m, 1H), 7.61-7.70 (m, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 21.5, 35.6, 59.7 (d, *J* = 8.25 Hz), 61.1, 116.9 (d, *J* = 23.8 Hz), 122.9 (d, *J* = 11.3 Hz), 124.7 (d, *J* = 3.8 Hz), 127.3, 129.6, 129.9, 131.2 (d, *J* = 2.3 Hz), 134.6, 135.8 (d, *J* = 9.0 Hz), 136.8, 143.6, 161.7 (d, *J* = 254.3 Hz), 166.5, 196.0 (d, *J* = 3.8 Hz) ppm. HRMS (FAB) Calcd *m/z* for $C_{21}H_{23}FNO_5S$ $[M+H]^+$: 420.1281. Found: 420.1279.

Ethyl 5-(4-fluorophenyl)-2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6ha).



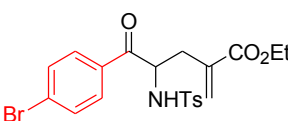
Yield: 75% (63 mg); Eluents: *n*-hexane/EtOAc = 7/1; yellow solid, mp: 92-94 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.29-1.36 (m, 3H), 2.10-2.35 (m, 4H), 2.86 (dd, *J* = 13.7, 2.5 Hz, 1H), 4.19-4.28 (m, 2H), 5.11-5.22 (m, 1H), 5.72 (s, 1H), 5.80 (d, *J* = 9.3Hz, 1H), 6.28 (s, 1H), 7.05-7.20 (m, 4H), 7.61 (d, *J* = 8.2Hz, 2H), 7.98-8.10 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.5, 37.9, 56.2, 61.2, 116.2 (d, *J* = 21.8 Hz), 127.3, 129.6, 130.0 (d, *J* = 3.0 Hz), 130.3, 131.7(d, *J*= 9.8 Hz), 134.4, 136.8, 143.6, 166.4 (d, *J* = 255.0 Hz), 166.7, 196.3 ppm. HRMS Calcd *m/z* for $C_{21}H_{23}FNO_5S$ $[M+H]^+$: 420.1281. Found: 420.1280.

Ethyl 5-(2-bromophenyl)-2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6ia).



Yield: 94% (90mg); Eluents: *n*-hexane/EtOAc = 7/1; brown solid;mp: 70-72 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.24-1.32 (m, 3H), 2.28-2.42 (m, 4H), 2.70-2.79 (m, 1H), 4.11-4.20 (m, 2H), 5.07-5.15 (m, 1H), 5. 68 (s, 1H), 5.79 (d, *J* = 8.8 Hz, 1H), 6.21 (d, *J* = 0.8 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.28-7.42 (m, 3H), 7.57-7.61 (m, 1H), 7.71 (d, *J* = 8.3 Hz, 2H) ppm;^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.6, 36.3, 59.1, 61.1, 120.2, 127.4, 127.6, 129.7(129.71), 129.7(129.74), 129.9, 132.9, 134.4, 134.5, 137.0, 137.2, 143.7, 166.4, 199.6 ppm. HRMS (FAB) Calcd *m/z* for $C_{21}H_{23}{}^{79}BrNO_5S$ $[M+H]^+$: 480.0480. Found: 480.0482.; $C_{21}H_{23}{}^{81}BrNO_5S$ $[M+H]^+$: 482.0460. Found: 482.0461.

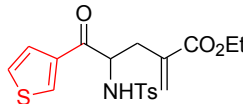
Ethyl 5-(4-bromophenyl)-2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6ja).



Yield: 83% (80 mg); Eluents: *n*-hexane/EtOAc = 7/1; pale yellow solid; mp: 106-108 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.33 (t, *J* = 7.1 Hz, 3H), 2.19 (dd, *J* = 13.7,

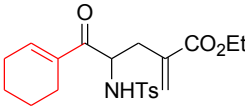
10.2 Hz, 1H), 2.29 (s, 3H), 2.81-2.87 (m, 1H), 4.17-4.30 (m, 2H), 5.09-5.17 (m, 1H), 5.68-5.74 (m, 2H), 6.29 (d, *J* = 0.8 Hz), 7.11 (d, *J* = 8.1 Hz, 2H), 7.58-7.68 (m, 4H), 7.82-7.90 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.5, 37.8, 56.3, 61.2, 127.3, 129.7(129.65), 129.7(129.72), 130.3, 132.3(132.31), 132.3(132.34), 134.4, 136.8, 143.6, 166.7, 197.0 ppm. HRMS (FAB) Calcd *m/z* for $C_{21}H_{23}{}^{79}BrNO_5S$ $[M+H]^+$: 480.0480. Found: 480.0483.; $C_{21}H_{23}{}^{81}BrNO_5S$ $[M+H]^+$: 482.0460. Found: 482.0460.

Ethyl 2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}]-5-oxo-5-(thiophen-3-yl)pentanoate (6ka).



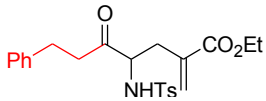
Yield: 86% (70mg); Eluents: *n*-hexane/EtOAc = 7/1; pale yellow solid; mp: 94-96 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 1.30-1.38 (m, 3H), 2.14-2.35 (m, 4H), 2.89-2.96 (m, 1H), 4.19-4.28 (m, 2H), 4.94-5.03 (m, 1H), 5.72 (s, 1H), 5.80 (d, *J* = 9.3Hz, 1H), 6.27 (d, *J* = 1.0Hz, 1H), 7.11 (d, *J* = 8.0Hz, 2H), 7.30 (dd, *J* = 5.1, 2.9Hz, 1H), 7.48-7.52 (m, 1H), 7.59-7.65 (m, 2H), 8.42 (dd, *J* =2.9, 1.3Hz, 1H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.5, 38.4, 57.6, 61.2, 126.8, 127.1, 127.3, 129.6, 130.1, 134.6, 134.7, 136.9, 138.6, 143.5, 166.9, 191.6 ppm. HRMS (FAB) Calcd *m/z* for $C_{19}H_{22}NO_5S_2$ $[M+H]^+$: 408.0939. Found: 408.0942.

Ethyl 5-(cyclohex-1-en-1-yl)-2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxopentanoate (6la).



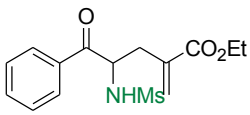
Yield: 95% (77mg); Eluents: *n*-hexane/EtOAc = 5/1; white solid;mp: 120-122 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.30-1.40 (m, 3H), 1.42-1.65 (m, 4H), 1.75-2.08 (m, 2H), 2.12-2.232 (m, 3H), 2.38 (s, 3H), 2.65-2.74 (m, 1H), 4.16-4.30 (m, 2H), 4.81-4.92 (m, 1H), 5.59 (d, *J* = 9.4 Hz, 1H), 5.67 (s, 1H), 6.25 (d, *J* = 1.1 Hz, 1H), 7.04-7.11 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.60 (dd, *J* = 6.6, 1.7 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 21.4, 21.6, 21.7, 22.9, 26.5, 38.2, 54.6, 61.0, 127.5, 130.0, 134.9, 136.8, 137.0, 143.4, 143.7, 166.6, 198.5 ppm. HRMS (FAB) Calcd *m/z* for $C_{21}H_{28}NO_5S$ $[M+H]^+$: 406.1688. Found: 406.1689.

Ethyl 2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-7-phenylheptanoate (6ma). Yield: 20%



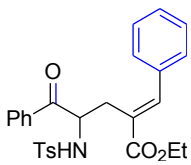
(17mg); Eluents: *n*-hexane/EtOAc = 10/1; pale yellow solid; mp: 69-71 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.28 (t, *J* = 7.1 Hz, 3H), 2.29-2.44 (m, 4H), 2.48-2.80 (m, 4H), 2.88-3.01 (m, 1H), 4.02-4.12 (m, 1H), 4.12-4.21 (m, 2H), 5.60-5.64 (m, 2H), 6.18 (d, *J* = 0.9Hz, 1H), 7.05-7.11 (m, 2H), 7.15-7.21 (m, 1H), 7.21-7.30 (m, 4H), 7.60-7.68 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.2, 21.7, 29.3, 35.2, 41.8, 60.4, 61.3, 126.3, 127.4, 128.3, 128.6, 129.8, 130.1, 134.4, 136.8, 140.5, 143.8, 166.8, 207.4 ppm. HRMS (FAB) Calcd *m/z* for $C_{23}H_{28}NO_5S$ $[M+H]^+$: 430.1688. Found: 430.1691.

Ethyl 2-methylidene-4-[(methylsulfonyl)amino]-5-oxo-5-phenylpentanoate (6na). Yield: 95% (62 mg);



Eluents: *n*-hexane/EtOAc = 5/1; pale yellow solid;mp: 64-66 °C; ^{1}H NMR (300 MHz, $CDCl_3$)δ1.34 (t, *J* = 7.1 Hz, 3H), 2.28 (dd, J = 13.9, 10.2 Hz, 1H), 2.84 (s, 3H), 3.00-3.07 (m, 1H), 4.24-4.32 (m, 2H), 5.34-5.41 (m, 1H), 5.54-5.58 (m, 1H), 5.74 (s, 1H), 6.36 (s, 1H), 7.53-7.59 (m, 2H), 7.64-7.70 (m, 1H), 8.17-8.21 (m, 2H) ppm;^{13}C NMR (75 MHz, $CDCl_3$) δ 14.3, 38.0, 41.5, 57.0, 61.3, 129.2(129.19), 129.2(129.24), 130.1, 133.6, 134.6, 135.1, 166.7, 198.0 ppm. HRMS (FAB) Calcd *m/z* for $C_{15}H_{20}NO_5S$ $[M+H]^+$: 326.1062. Found: 326.1066.

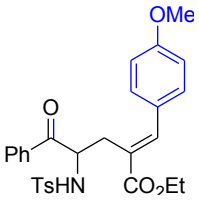
Ethyl (*E*)-2-benzylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenylpentanoate (6ab). Total



yield: 92% (88 mg); *E/Z* ratio = 77:23; Eluents: *n*-hexane/EtOAc = 7/1; white solid; mp: 104-106 °C;^{1}H NMR (300 MHz, $CDCl_3$) δ 1.39-1.45 (m, 3H), 2.26 (s, 3H), 2.70 (dd, *J* = 13.9, 10.7 Hz, 1H), 2.78-2.86 (m, 1H), 4.29-4.37 (m, 2H), 5.25-5.33 (m, 1H), 5.65 (d, *J* = 9.0Hz,

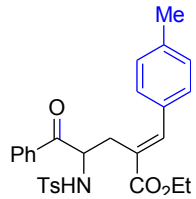
1H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.30-7.45 (m, 7H), 7.56-7.61 (m, 3H), 7.87-7.91 (m, 3H) ppm;^{13}C NMR (75 MHz, $CDCl_3$) δ 14.4, 21.5, 32.3, 56.7, 61.3, 127.3, 128.0, 128.6, 128.7, 128.9(128.85), 128.9(128.91), 129.6, 133.5, 134.2, 135.3, 136.8, 143.4(143.40), 143.4(143.44), 167.8, 198.0 ppm. HRMS (EI) Calcd *m/z* for $C_{27}H_{27}NO_5S$ $[M]^+$: 477.1610. Found: 477.1613

Ethyl (*E*)-2-(4-methoxybenzylidene)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenylpentanoate



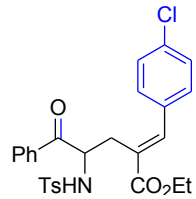
(6ac). Total yield: 83% (84mg); *E/Z* ratio = 75:25; Eluents: *n*-hexane/EtOAc = 7/1; white solid, mp: 80-82 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.35-1.41 (m, 3H), 2.25 (s, 3H), 2.74-2.90 (m, 2H), 3.83 (s, 3H), 4.28 (dd, *J* = 14.3, 7.1 Hz, 2H), 5.27-5.35 (m, 1H), 5.76 (d, *J* = 9.0 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 2H), 7.07 (d, *J* = 8.3Hz, 2H), 7.33 (d, *J* = 8.8Hz, 2H), 7.40-7.45 (m, 2H), 7.54-7.61 (m, 3H), 7.79 (s, 1H), 7.89-7.93 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ14.4, 21.5, 32.4, 55.4, 56.7, 61.2, 114.2, 125.9, 127.3, 127.6, 128.8, 128.9, 129.5, 130.9, 133.7, 134.2, 136.8, 143.1, 143.4, 160.1, 168.0, 198.2 ppm. HRMS (FAB) Calcd *m/z* for $C_{28}H_{30}NO_6S$ $[M+H]^+$: 508.1794. Found: 508.1794.

Ethyl (*E*)-2-(4-methylbenzylidene)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenylpentanoate



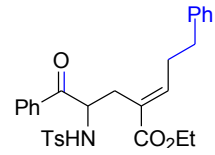
(6ad). Total yield: 86% (85 mg); *E/Z* ratio = 80:20; Eluents: *n*-hexane/EtOAc = 7/1; white solid, mp: 126-128 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.37-1.43 (m, 3H), 2.26 (s, 3H), 2.38(s, 3H), 2.68-2.90 (m, 2H), 4.26-4.34 (m, 2H), 5.20-5.44 (m, 1H), 5.66 (d,*J* = 9.1Hz, 1H), 7.08 (d, *J* = 8.0Hz, 2H), 7.17-7.26 (m, 2H), 7.39-7.45 (m, 2H), 7.53-7.61 (m, 3H) ,7.83-7.94 (m, 2H) ppm;^{13}C NMR (75 MHz, $CDCl_3$) δ14.5, 21.5, 21.5, 32.3, 56.7, 61.3, 127.2, 127.3, 128.8, 128.9, 190.1, 129.5, 129.6, 132.4, 133.7, 134.2, 136.8, 138.8, 143.4, 143.5, 167.9, 198.2 ppm. HRMS (FAB) Calcd *m/z* for $C_{28}H_{30}NO_5S$ $[M+H]^+$: 492.1844. Found: 429.1845.

Ethyl (*E*)-2-(4-chlorobenzylidene)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenylpentanoate (6ae)



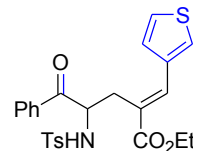
Total yield: 75% (77 mg); *E/Z* ratio = 87:13; Eluents: *n*-hexane/EtOAc = 7/1; white solid; mp: 112-114 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.39-1.45 (m, 3H), 2.25 (s, 3H), 2.58-2.71 (m, 1H), 2.75-2.86 (m, 1H), 4.30-4.39 (m, 2H), 5.24-5.32 (m, 1H), 5.76 (d, *J* = 8.9 Hz, 1H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.24-7.38(m, 4H), 7.40-7.46 (m, 2H), 7.55-7.60 (m, 3H), 7.83-7.92 (m, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ14.4, 21.5, 32.4, 56.6, 61.4, 127.2, 128.7, 128.8, 128.9(128.87), 128.9(128.93), 129.6, 130.3, 133.4, 133.8, 134.3, 134.6, 136.7, 142.0, 143.5, 167.5, 197.8 ppm. HRMS (FAB) Calcd *m/z* for $C_{27}H_{27}ClNO_5S$ $[M+H]^+$: 512.1298. Found: 512.1298.

Ethyl (*E*)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenyl-2-(3-phenylpropylidene) pentanoate



(6af). Total yield: 85% (86mg); *E/Z* ratio = 88:12; Eluents: *n*-hexane/EtOAc = 5/1; white solid; mp: 121-123 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.31 (t, *J* = 7.1 Hz, 3H), 2.10-2.22 (m, 1H), 2.25 (s, 3H), 2.62-2.86 (m, 5H), 4.15-4.28 (m, 2H), 5.11-5.20 (m, 1H), 5.68 (d, *J* = 9.2 Hz, 1H), 6.05-6.11 (m, 1H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.15-7.23 (m, 3H), 7.25-7.34 (m, 2H), 7.40-7.48 (m, 2H), 7.53-7.64 (m, 3H), 7.87-7.93 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ14.4, 21.5, 31.7, 35.2, 40.1, 56.7, 60.7, 126.0, 126.1, 127.2, 128.5(128.50), 128.5(128.51), 128.7, 128.8, 129.6, 133.9, 134.2, 137.0, 141.4, 143.4, 148.5, 167.0, 198.1 ppm. HRMS (FAB) Calcd *m/z* for $C_{29}H_{32}NO_5S$ $[M+H]^+$: 506.2001. Found: 506.2001.

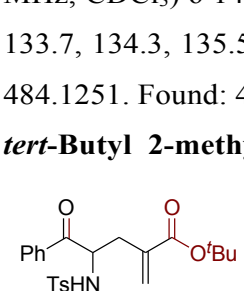
Ethyl (*E*)-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenyl-2-(thiophen-3-ylmethylidene)pentano-



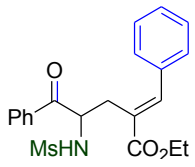
ate (6ag). Total yield: 64% (62mg); *E/Z* ratio = 56:44; Eluents: *n*-hexane/EtOAc = 7/1; white

solid; mp: 104-106 °C; ^{1}H NMR (300 MHz, $CDCl_3$)δ 1.35-1.42 (m, 3H), 2.26 (d, *J* = 8.3 Hz, 3H), 2.98 (d, *J* = 7.5 Hz, 2H), 4.20-4.32 (m, 2H), 5.25-5.38 (m, 1H), 5.79 (d, *J* =9.3 Hz, 1H), 7.03-7.12 (m, 3H), 7.28 (d, *J* = 3.4 Hz, 1H), 7.41-7.50 (m, 3H), 7.51-7.86 (m, 3H), 7.99 (s, 1H), 8.00, (d, *J* = 7.1 Hz, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.5, 21.5, 33.3, 56.7, 61.3, 123.3, 127.3, 127.5, 128.9(128.87), 128.9(128.94), 129.4, 129.5, 133.7, 134.3, 135.5, 136.9, 137.8, 143.4, 167.8, 198.2 ppm. HRMS (FAB) Calcd *m/z* for $C_{25}H_{26}NO_5S_2$ $[M]^+$: 484.1251. Found: 484.1252.

***tert*-Butyl 2-methylidene-4-{[(4-methylphenyl)sulfonyl]amino}-5-oxo-5-phenylpentanoate (6ah).** Yield: 95% (82 mg); Eluents: *n*-hexane/EtOAc = 5/1; white solid; mp: 90-92 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.52 (s, 9H), 2.20-2.32 (m, 4H), 2.78-2.90 (m, 1H), 5.12-5.24 (m, 1H), 5.61 (s, 1H), 5.76 (d, *J* = 9.2Hz, 1H), 6.19 (d, *J* = 1.2Hz, 1H), 7.07 (d, *J* = 8.0Hz, 2H), 7.39-7.48 (m, 2H), 7.52-7.64 (m, 3H), 7.90-7.98 (m, 2H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 21.4, 28.1, 37.7, 56.3, 81.2, 127.2,128.8(128.76), 128.8(128.83), 129.2, 129.6, 133.7, 134.2, 136.0, 136.9, 143.4, 165.7, 198.0 ppm. HRMS (FAB) Calcd *m/z* for $C_{23}H_{28}NO_5S$ $[M+H]^+$: 430.1688. Found: 430.1688.

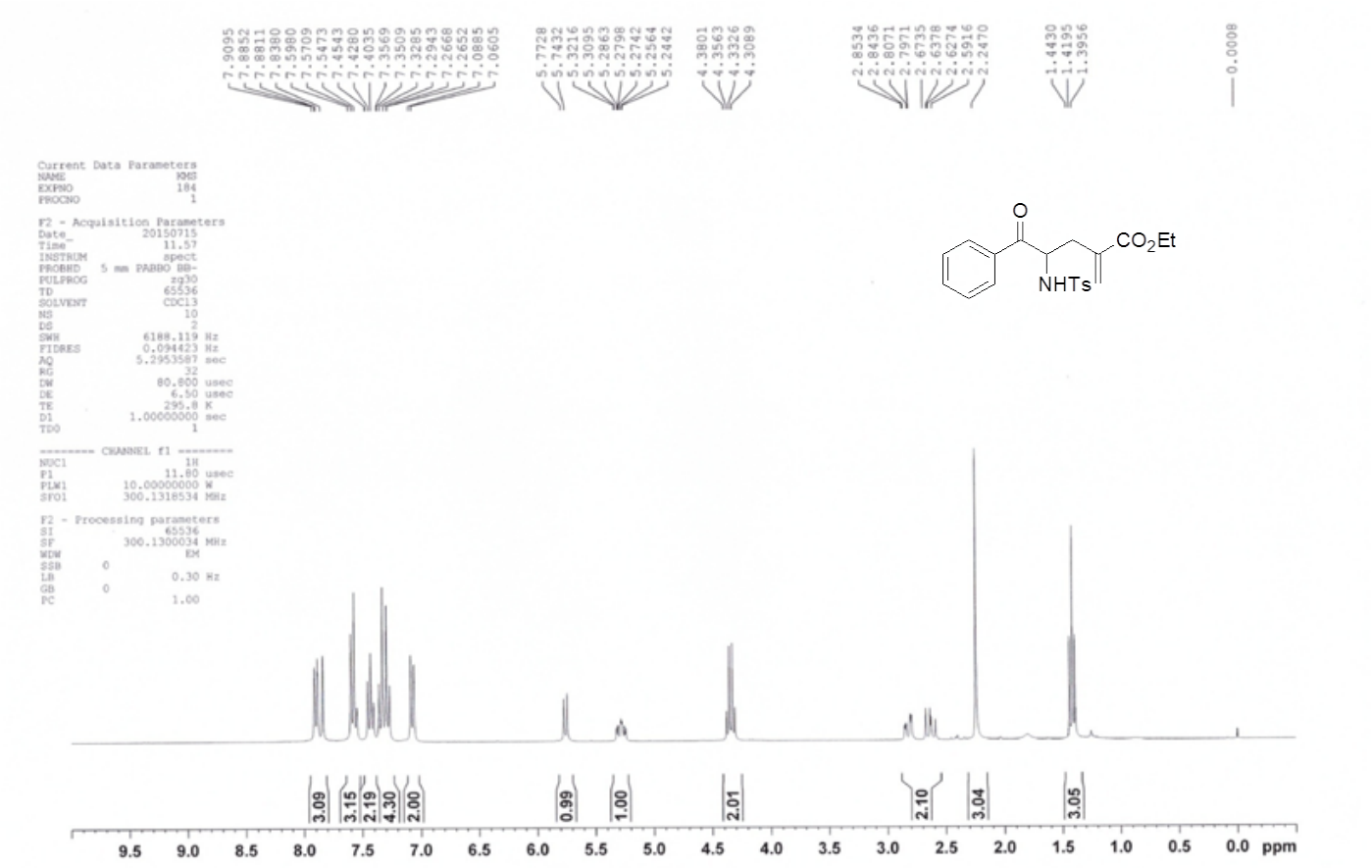


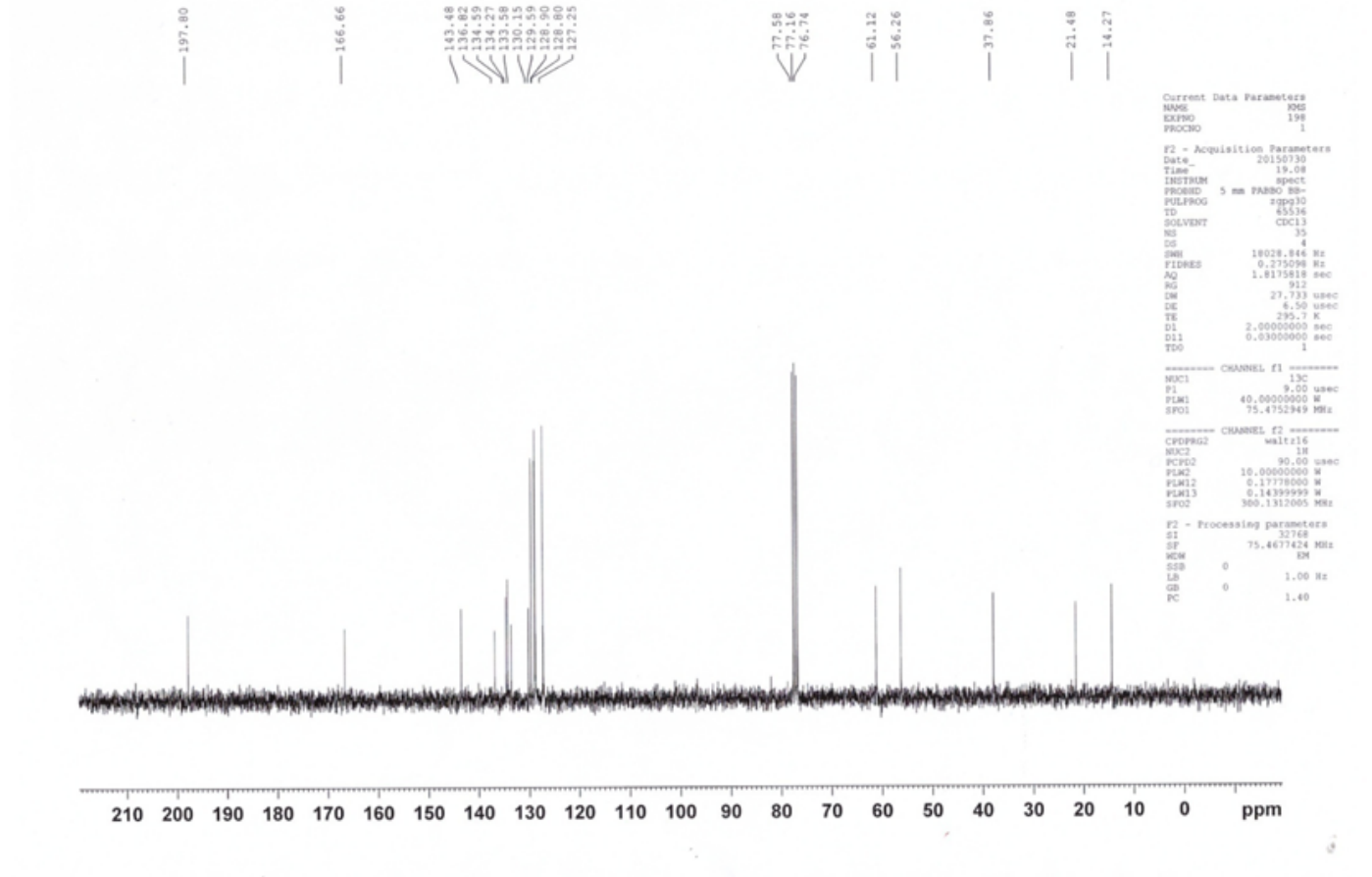
Ethyl (*E*)-2-benzylidene-4-[(methylsulfonyl)amino]-5-oxo-5-phenylpentanoate (6nb). Total yield: 77% (62mg); *E/Z* ratio = 78:22; Eluents: *n*-hexane/EtOAc = 7/1; white solid; mp: 108-110 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ1.41 (t, *J* = 7.1Hz, 3H), 2.71-2.90 (m, 4H), 2.90-3.01 (m, 1H), 4.36 (q, *J* =7.1Hz, 2H), 5.40-5.52 (m, 2H), 7.28-7.42 (m, 5H), 7.45-7.54 (m, 2H), 7.58-7.67 (m, 1H), 7.95 (s, 1H), 8.05-8.12 (m, 2H) ppm; ; ^{13}C NMR (75 MHz, $CDCl_3$) δ 14.5, 32.3, 41.5, 57.5, 61.5, 128.5, 128.8, 128.9,129.2(129.16), 129.2(129.21), 133.6, 134.6, 135.2, 143.4, 167.8, 198.1 ppm. HRMS (FAB) Calcd *m/z* for $C_{21}H_{24}NO_5S$ $[M+H]^+$: 402.1375. Found: 402.1375.



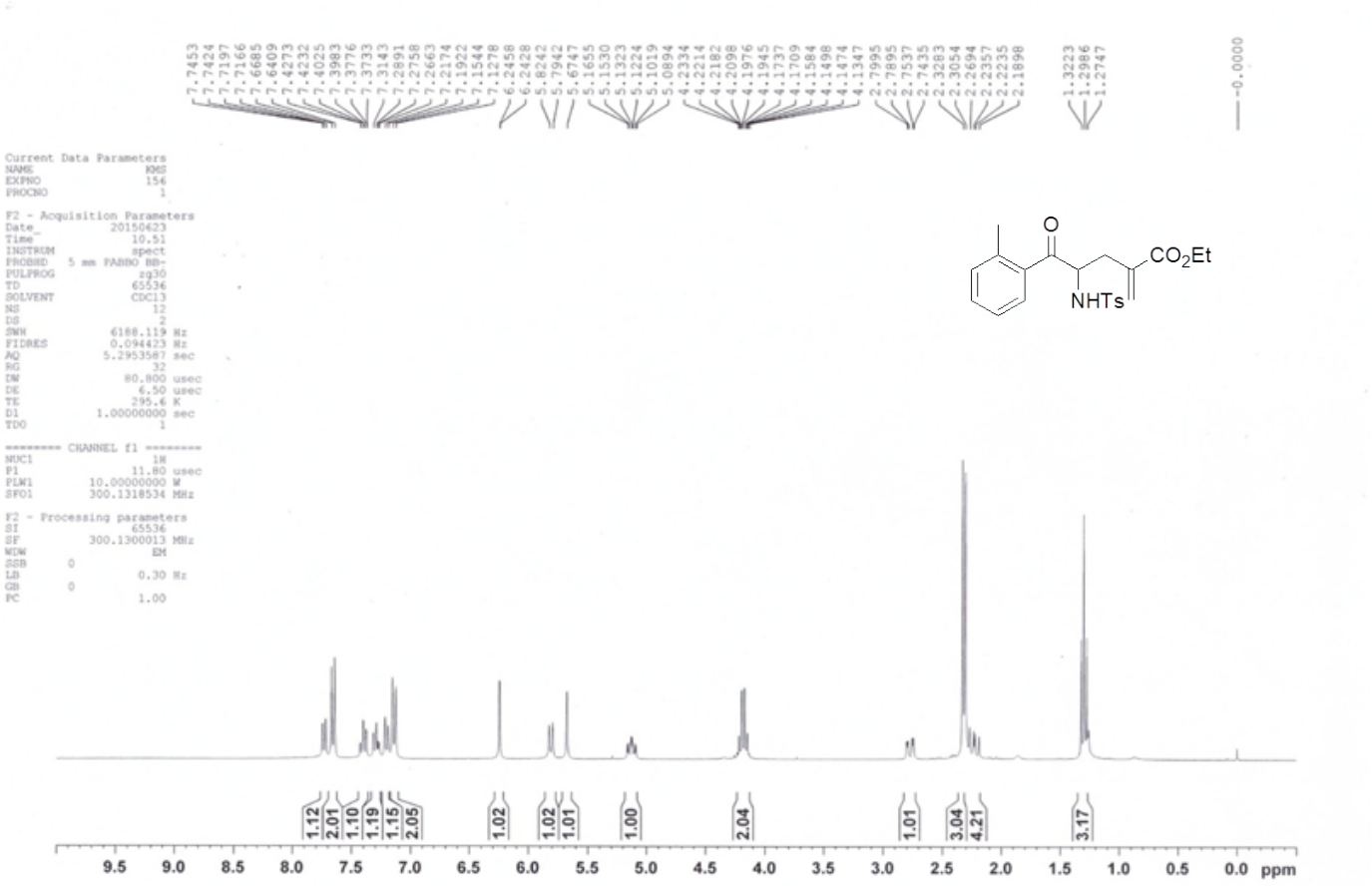
4. Copies of ^{1}H and ^{13}C NMR Spectra for All Compounds.

$^{1}H/^{13}C$ spectra of compound **6aa**

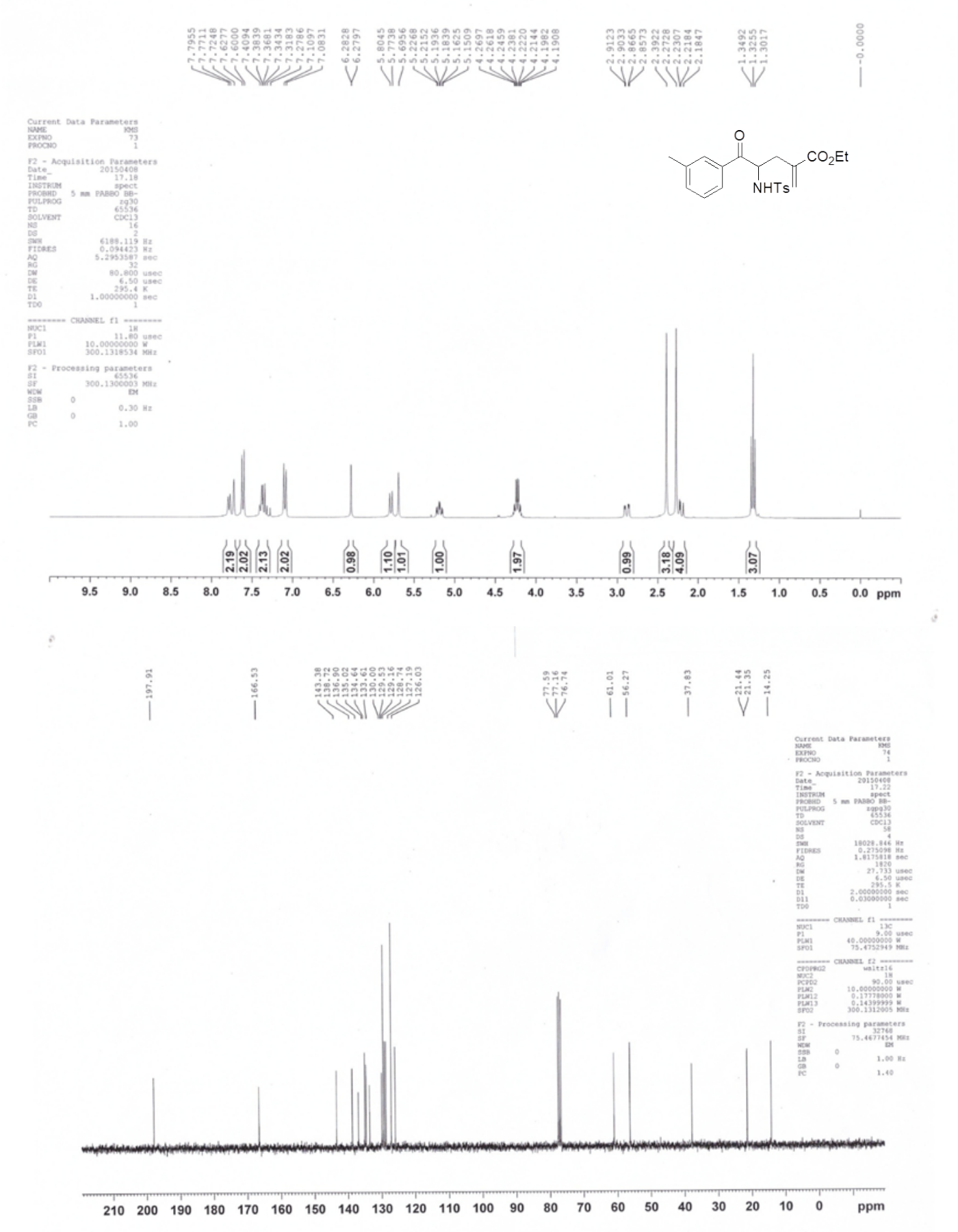




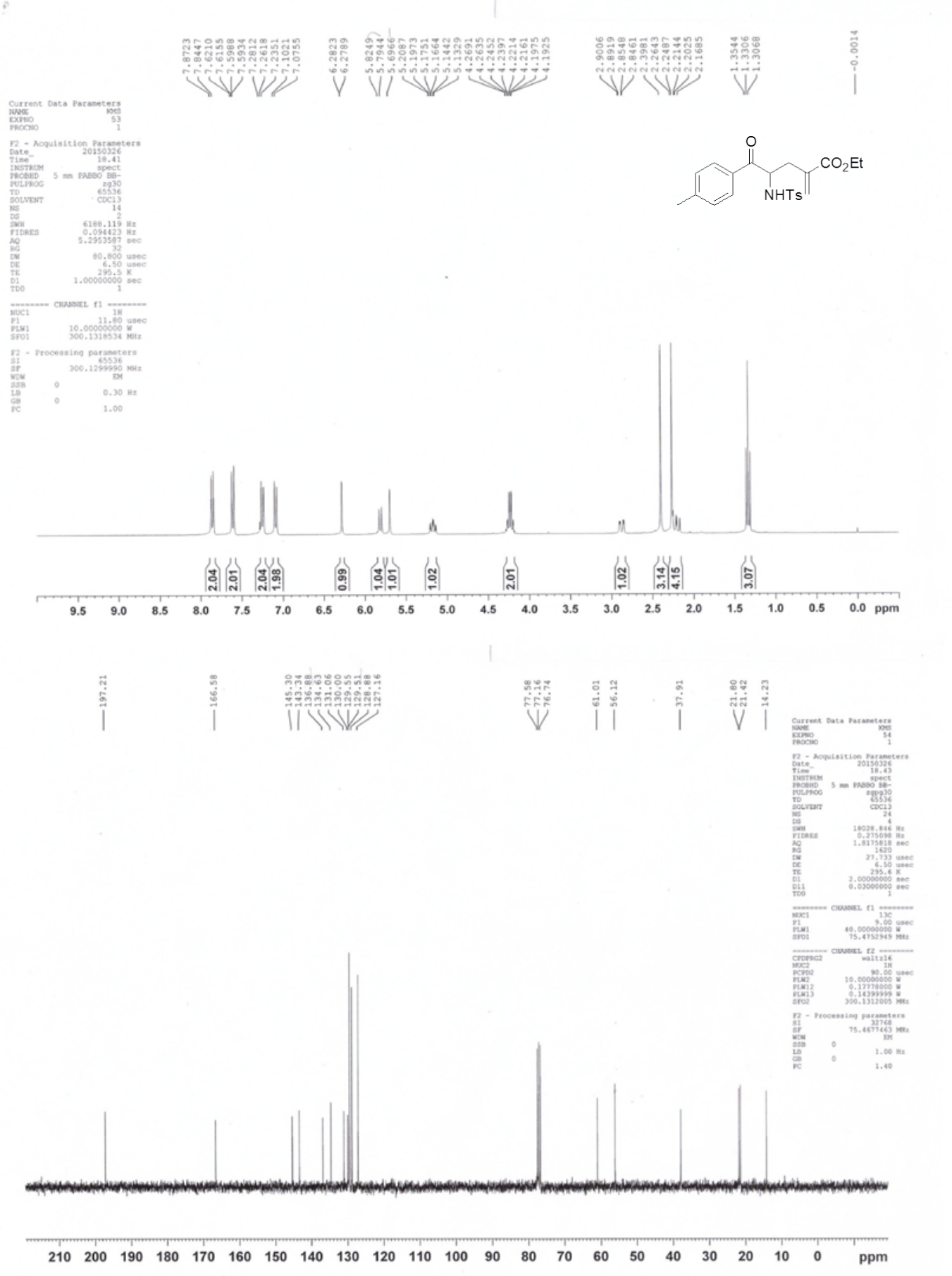
$^{1}H/^{13}C$ spectra of compound **6ba.**



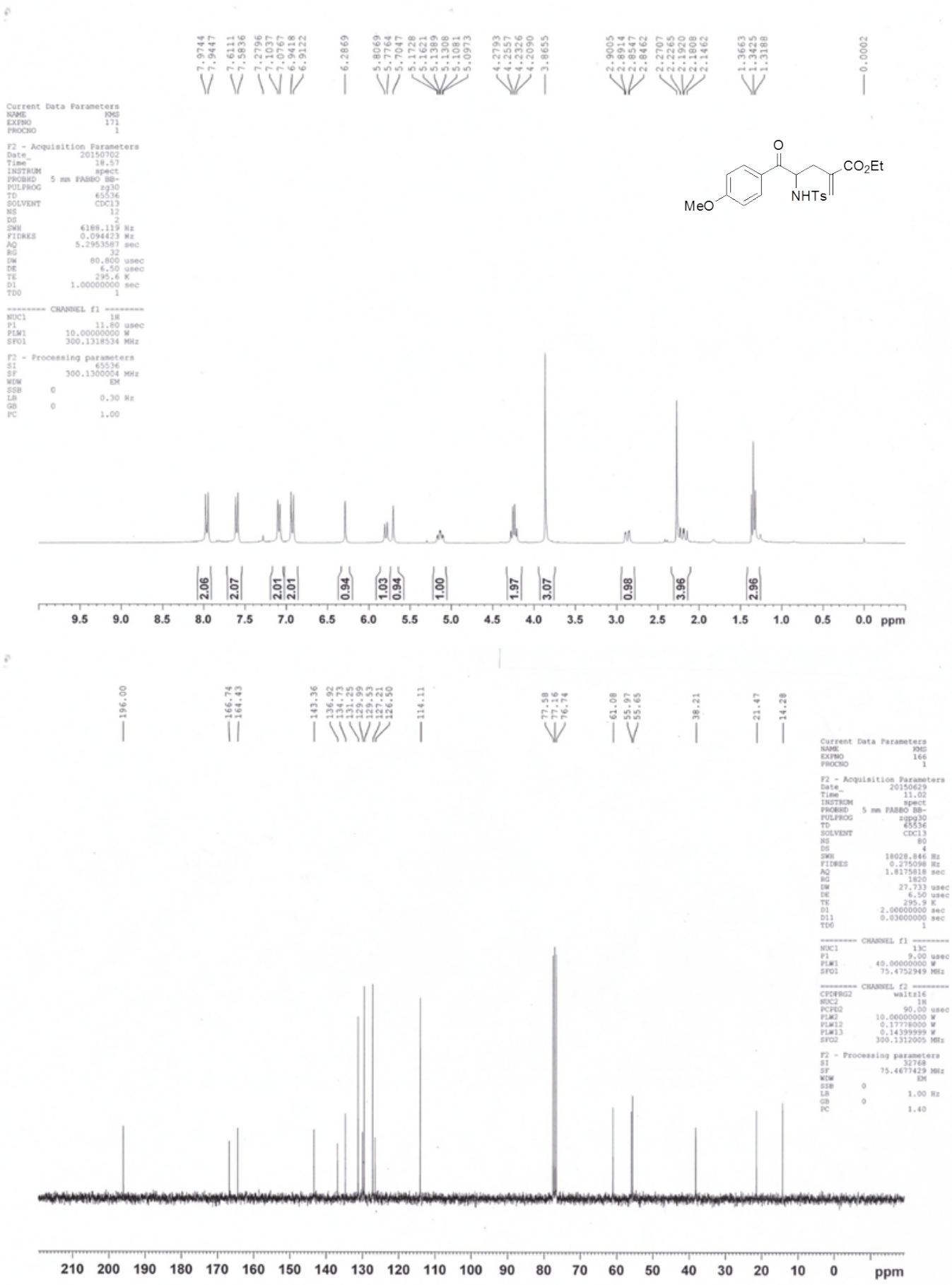
^{1}H /^{13}C spectra of compound **6ca.**



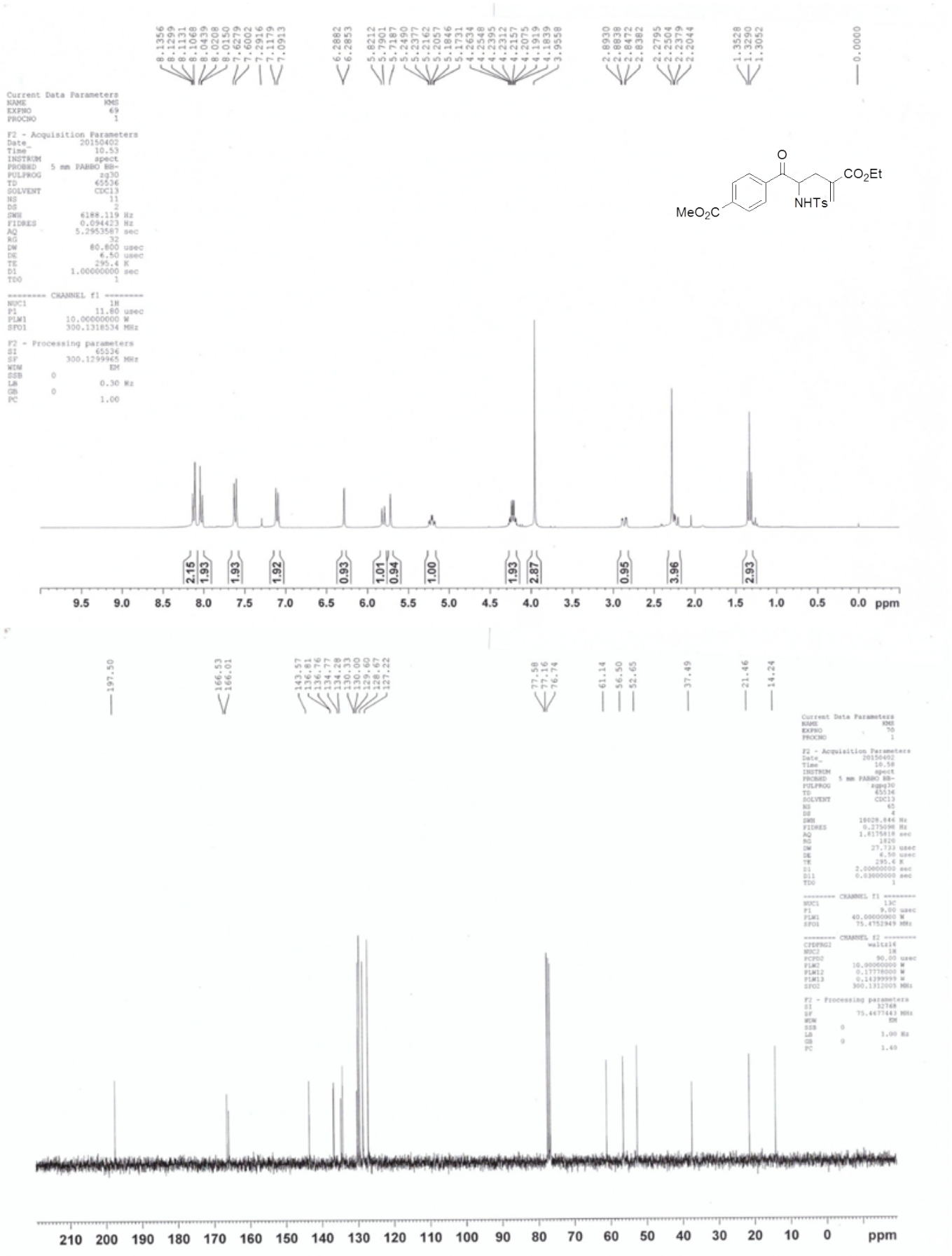
$^{1}H/^{13}C$ spectra of compound **6da.**



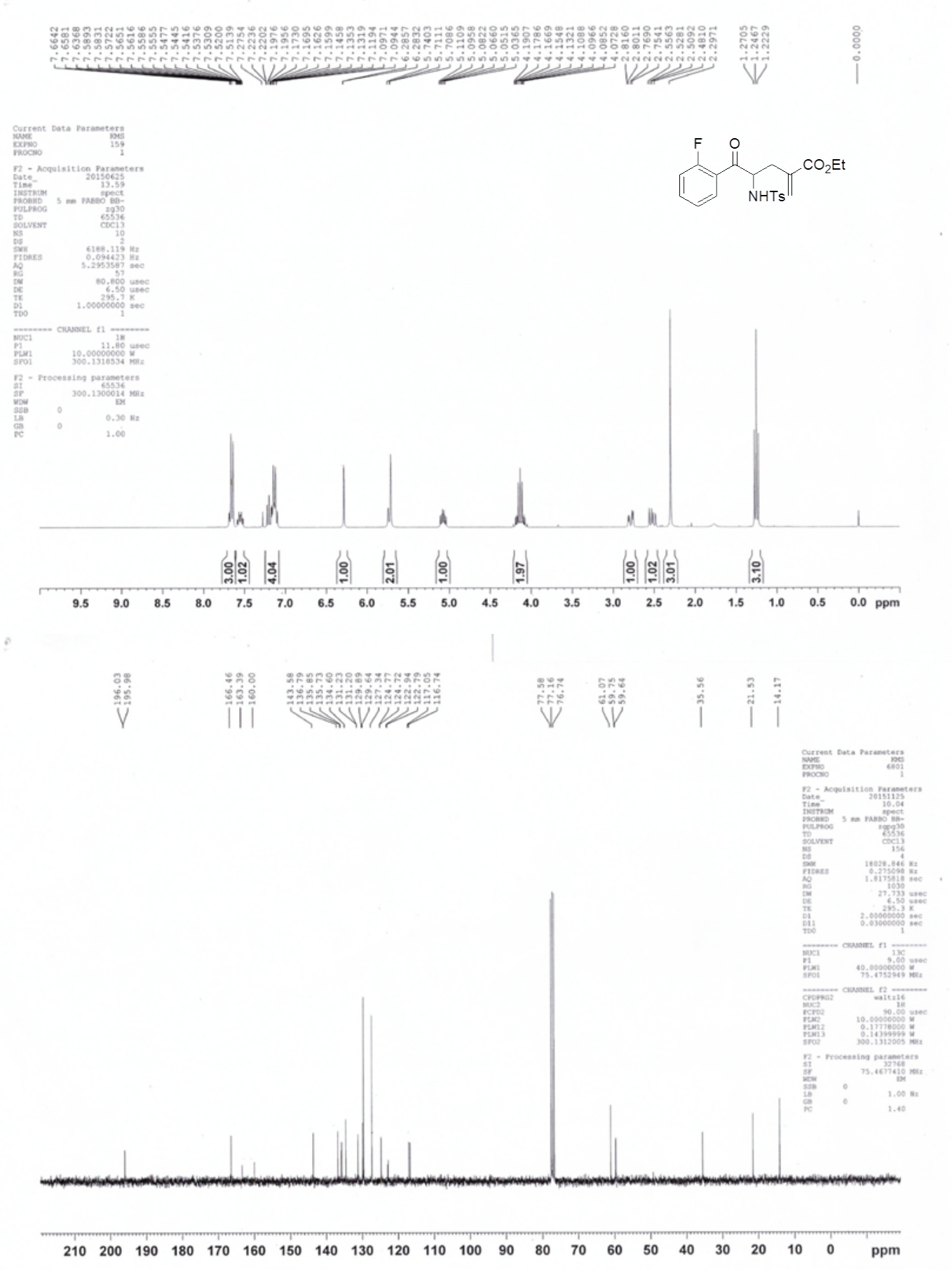
$^{1}H/^{13}C$ spectra of compound **6ea.**



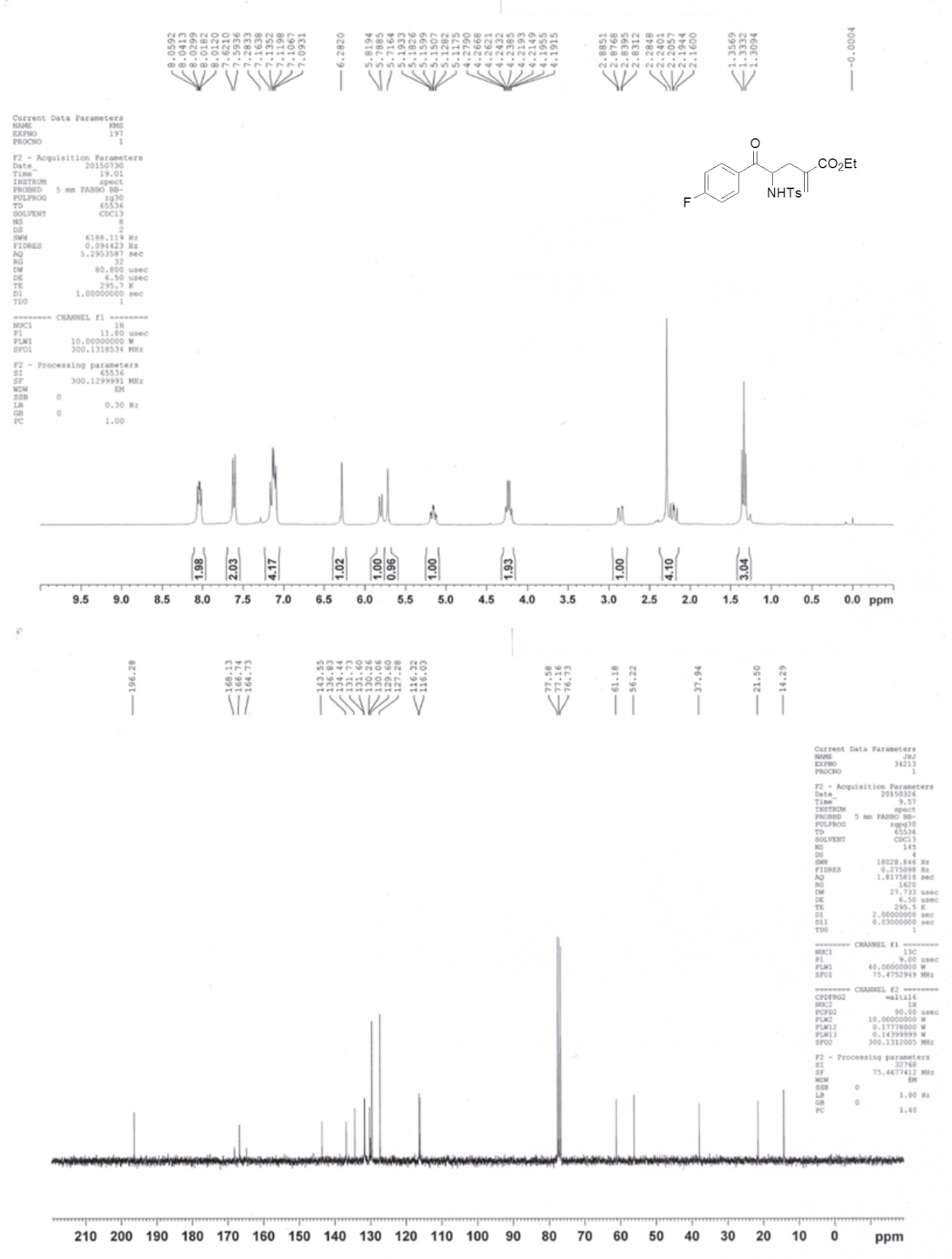
$^{1}H/^{13}C$ spectra of compound **6fa.**



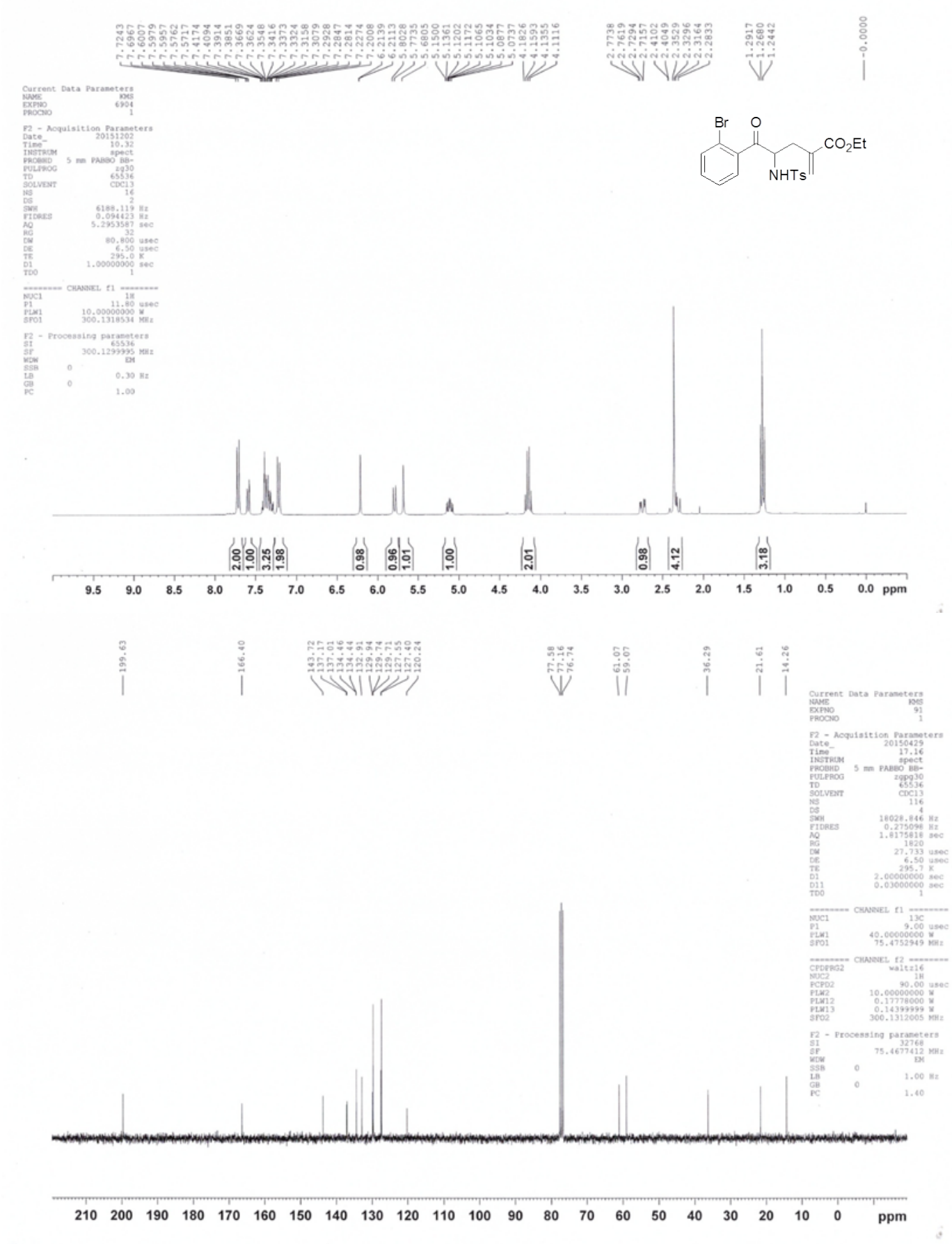
$^{1}H/^{13}C$ spectra of compound **6ga.**



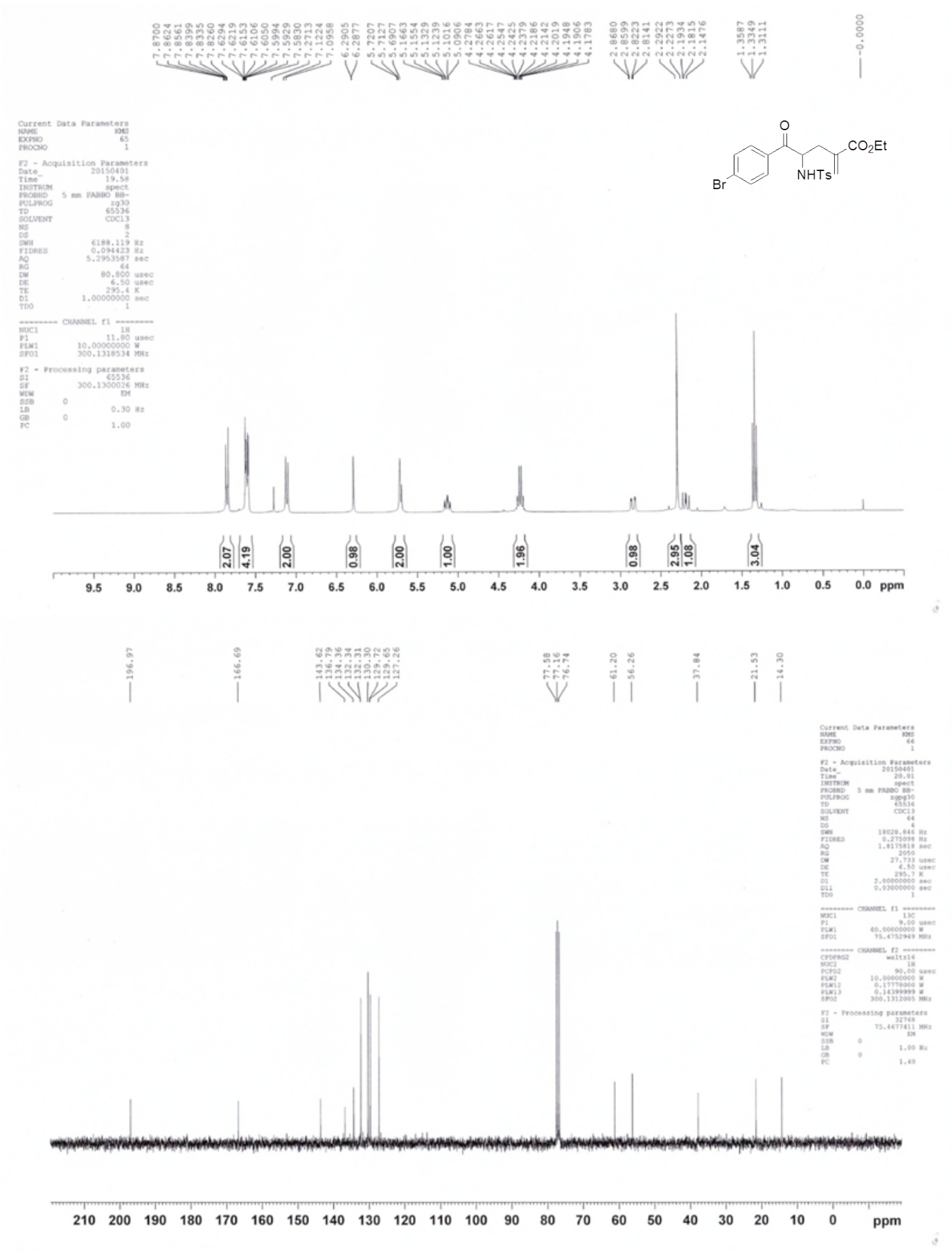
$^{1}H/^{13}C$ spectra of compound **6ha.**



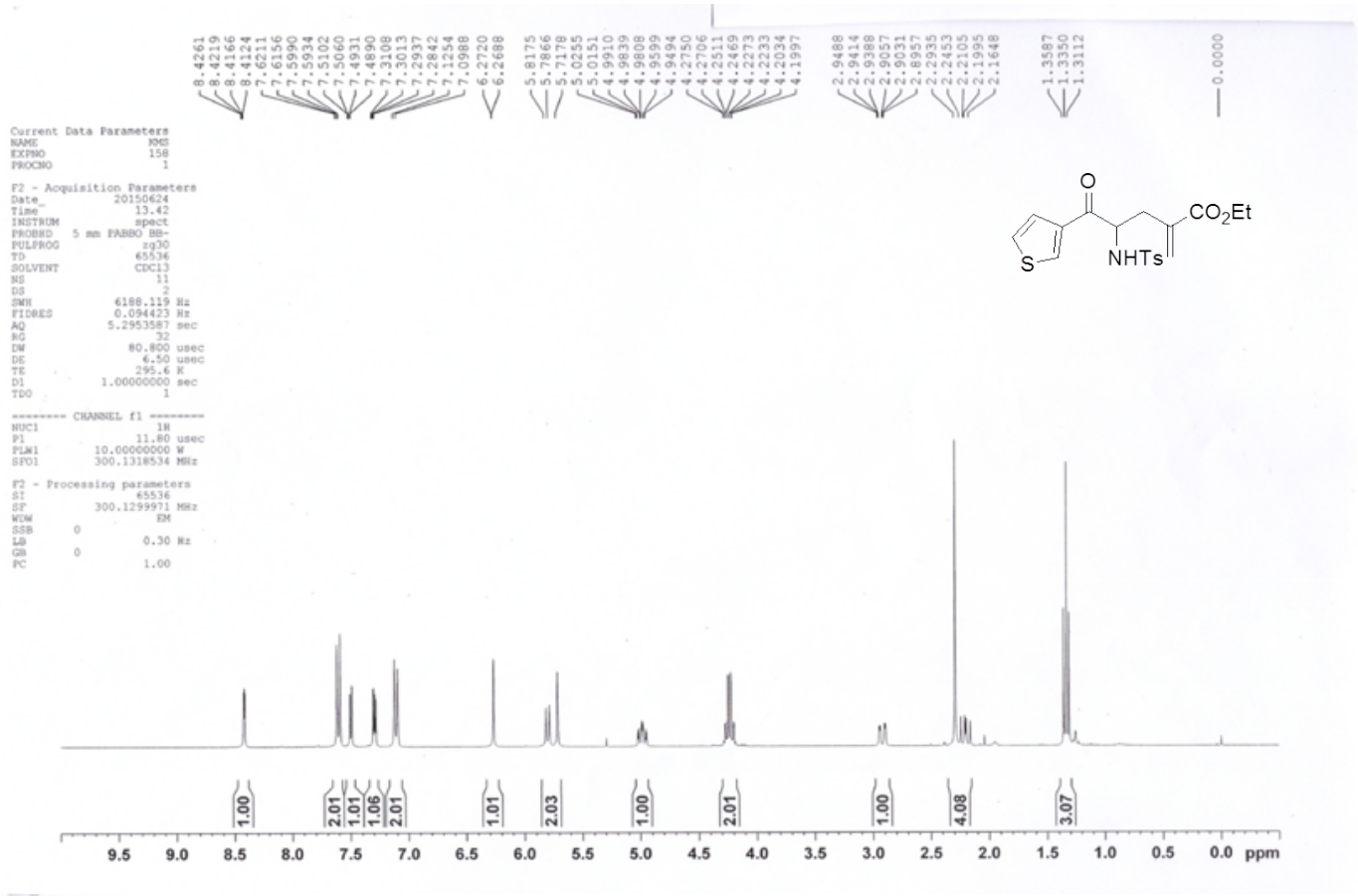
$^{1}H/^{13}C$ spectra of compound **6ia.**

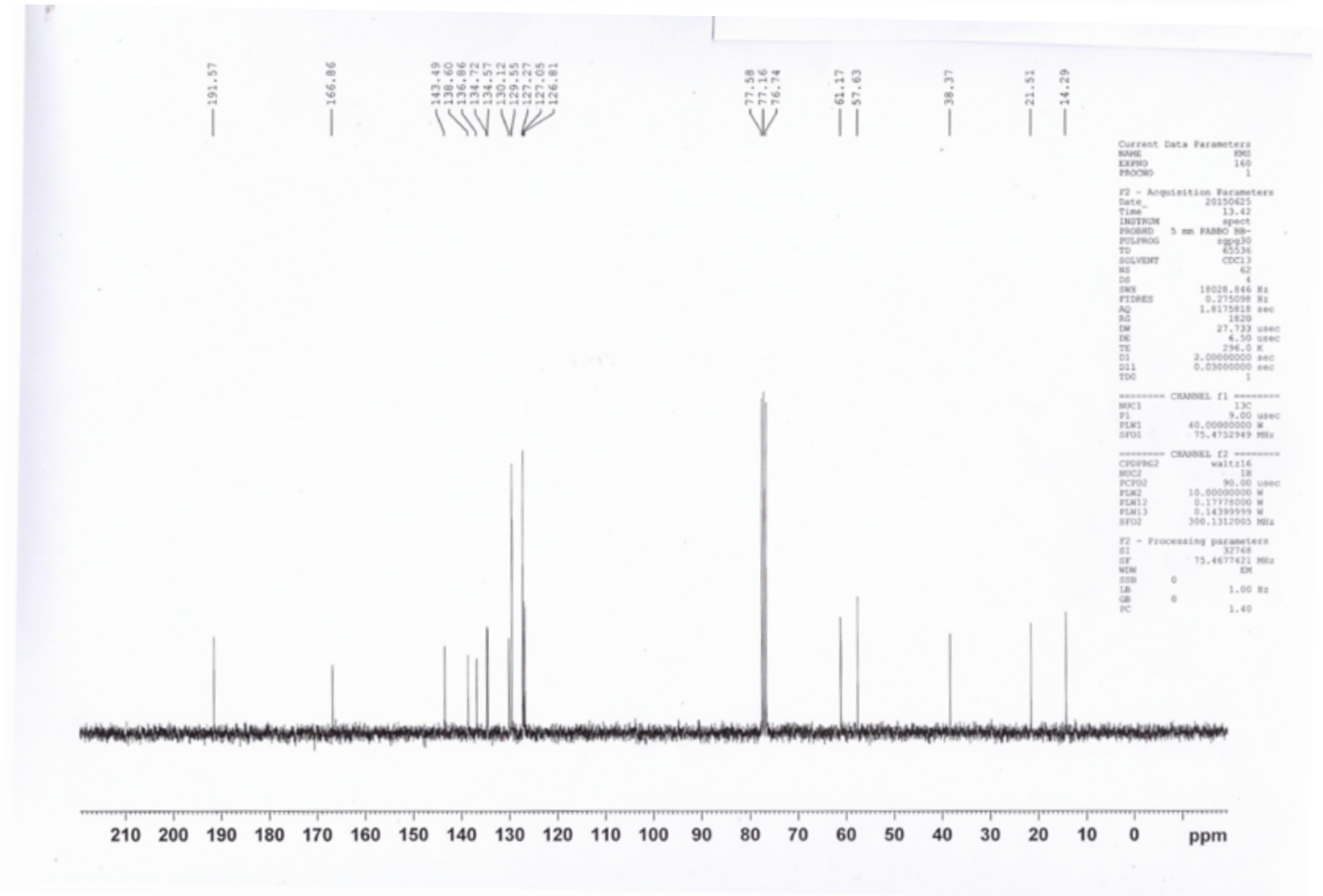


$^{1}H/^{13}C$ spectra of compound **6ja.**

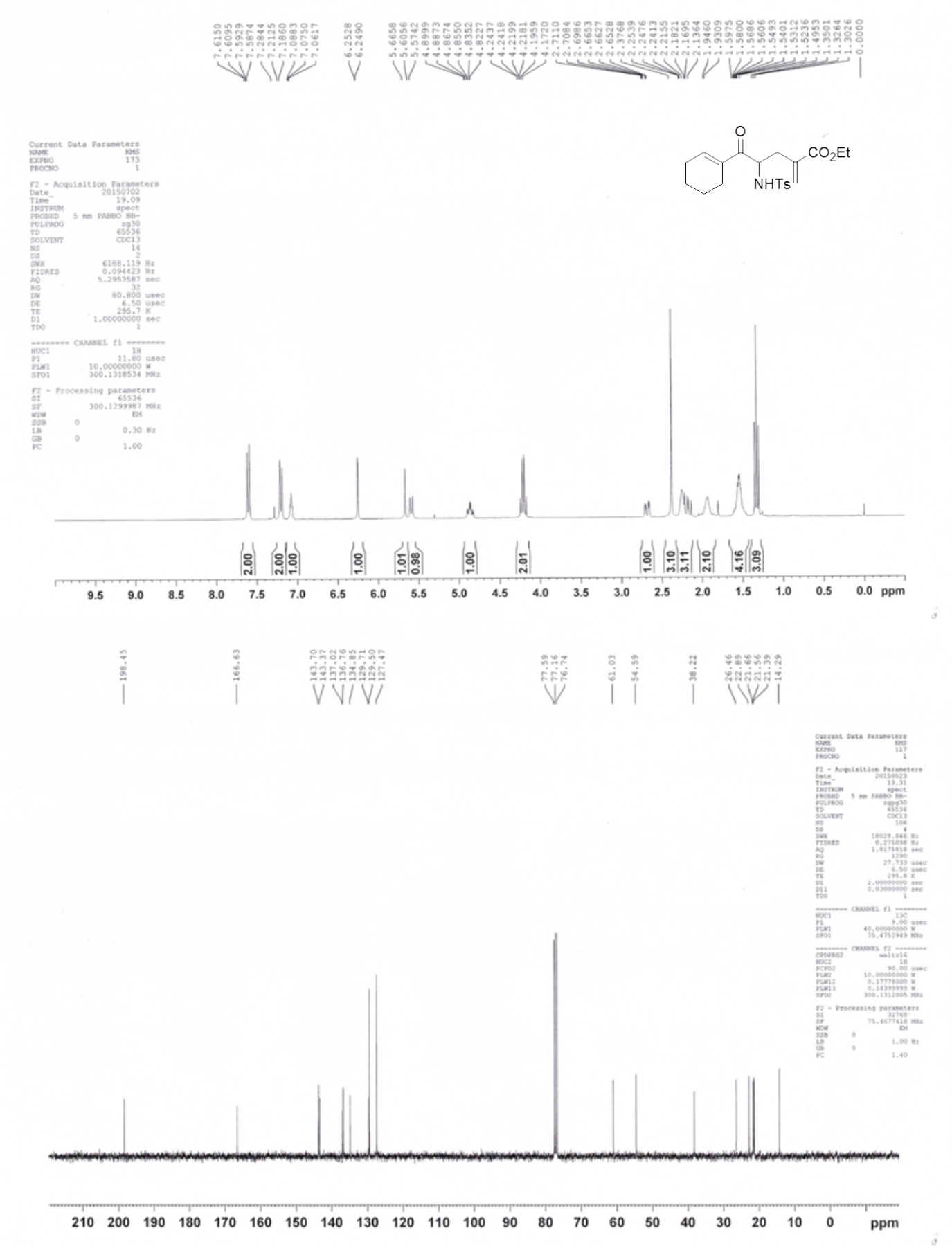


$^{1}H/^{13}C$ spectra of compound **6ka.**

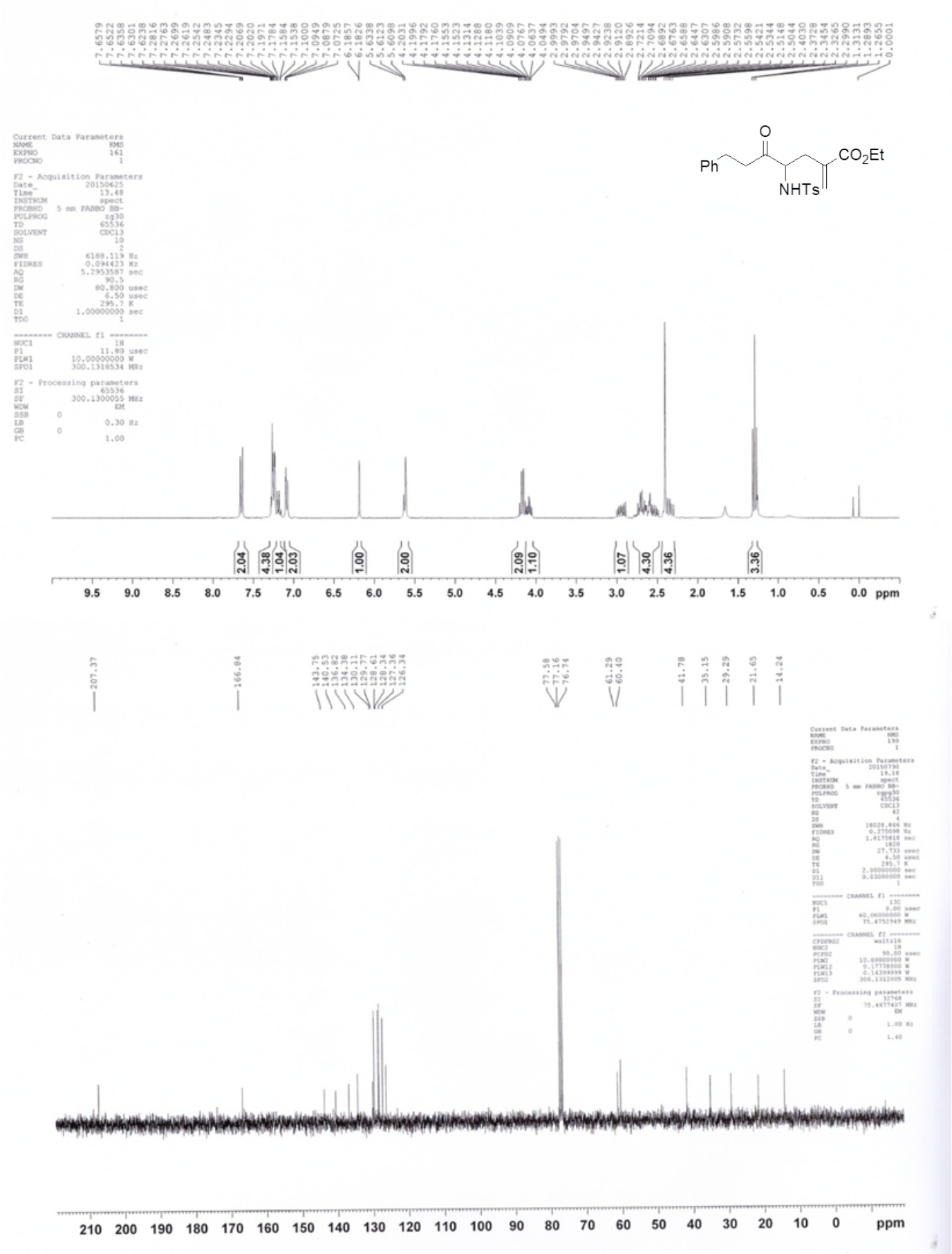




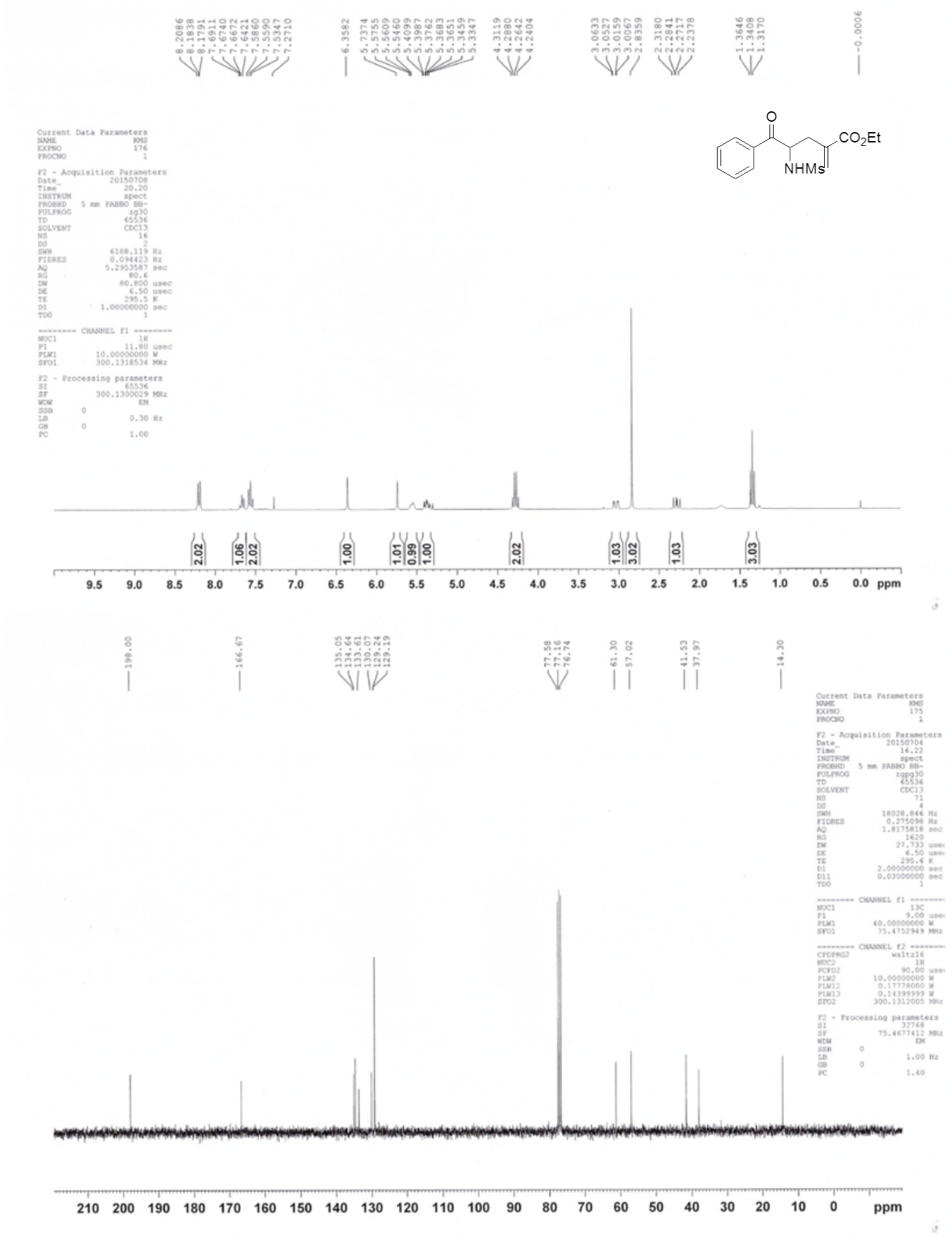
$^{1}H/^{13}C$ spectra of compound **6la.**



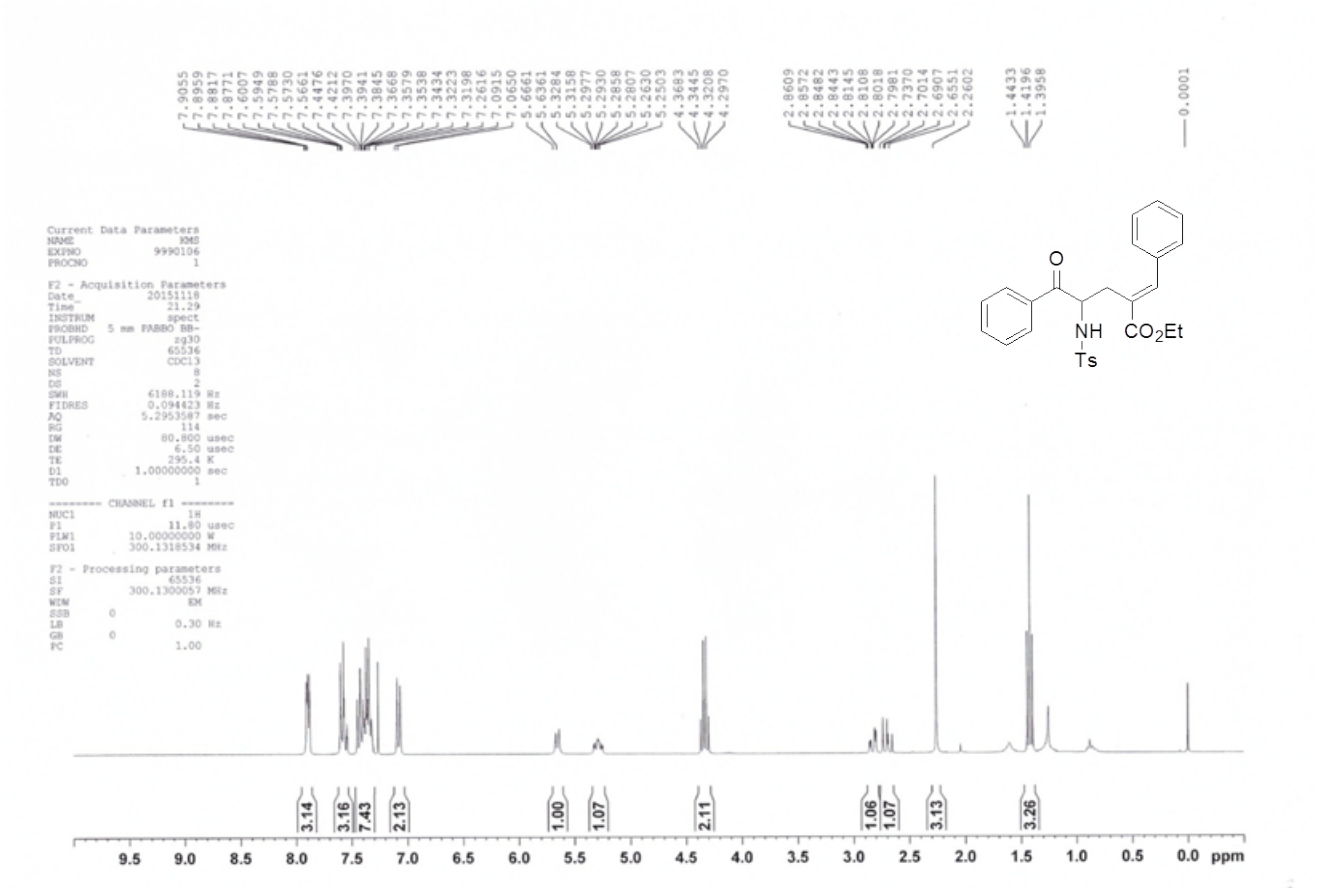
$^{1}H/^{13}C$ spectra of compound **6ma.**

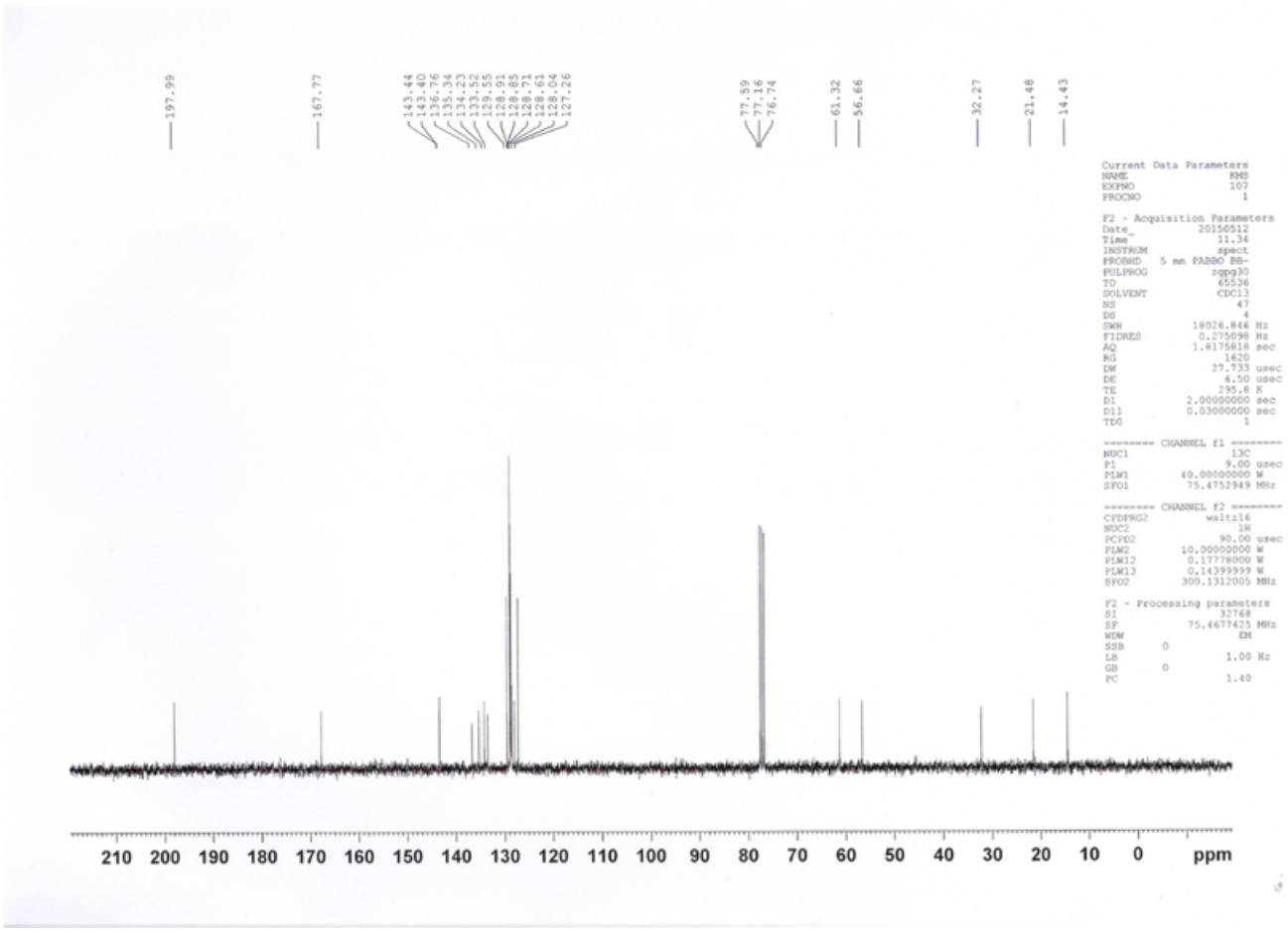


$^{1}H/^{13}C$ spectra of compound **6na.**

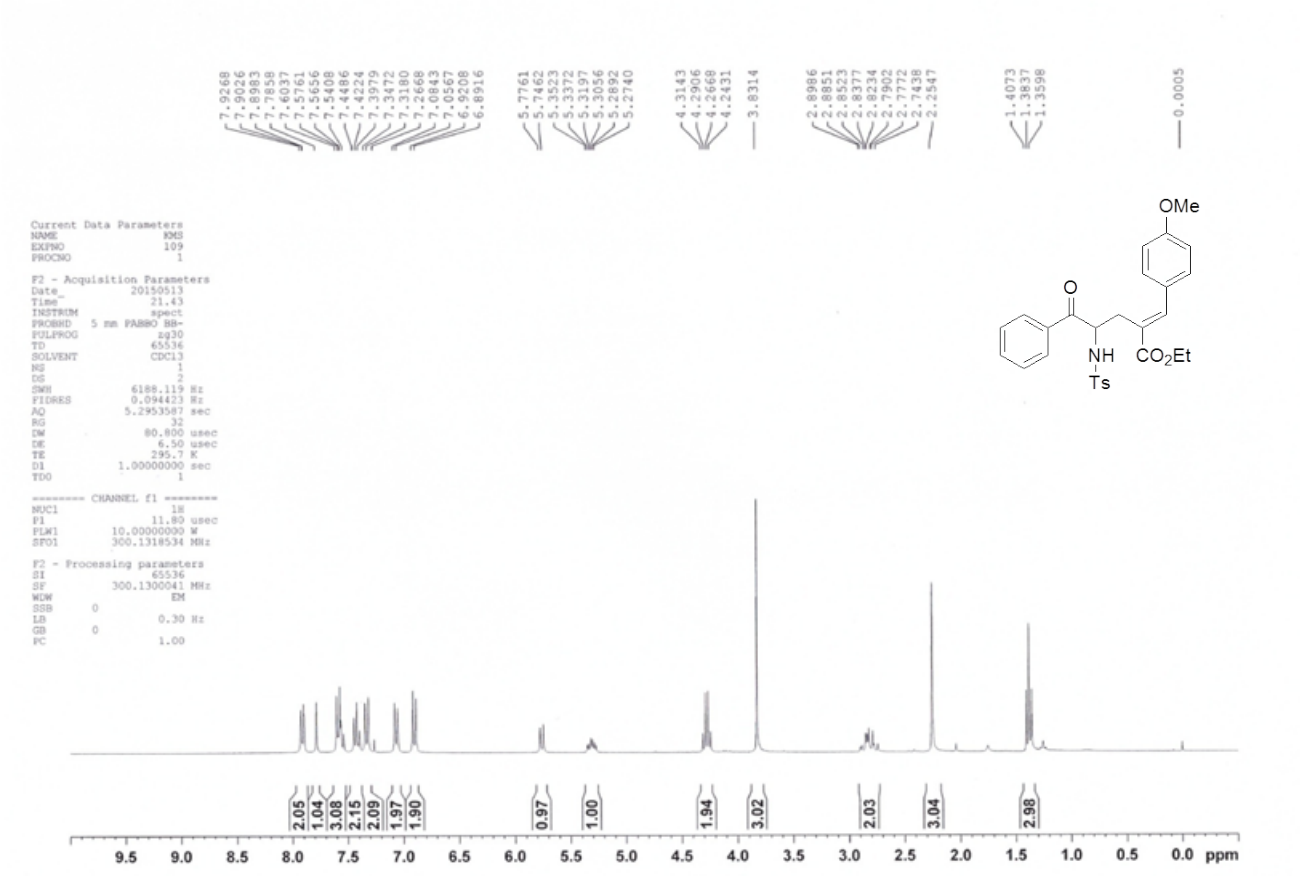


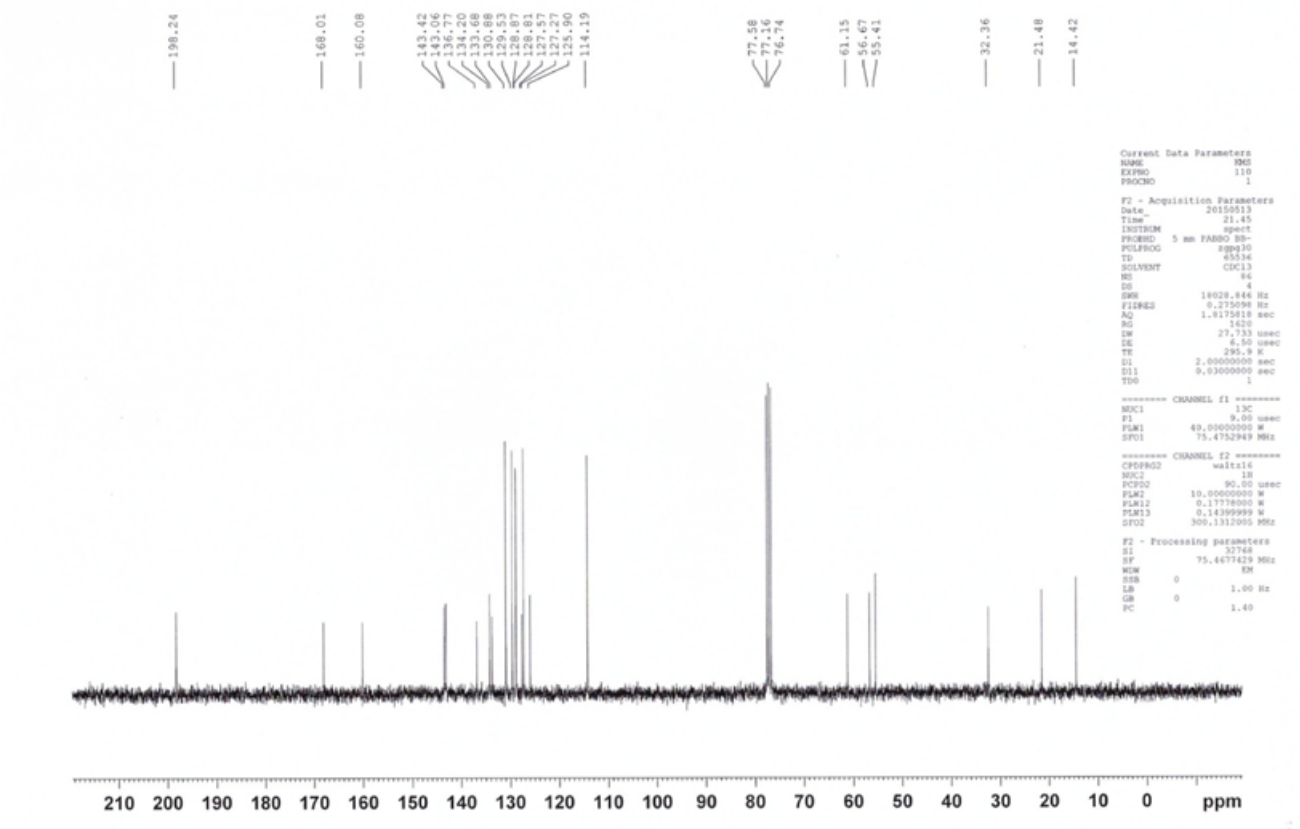
$^{1}H/^{13}C$ spectra of compound **6ab.**



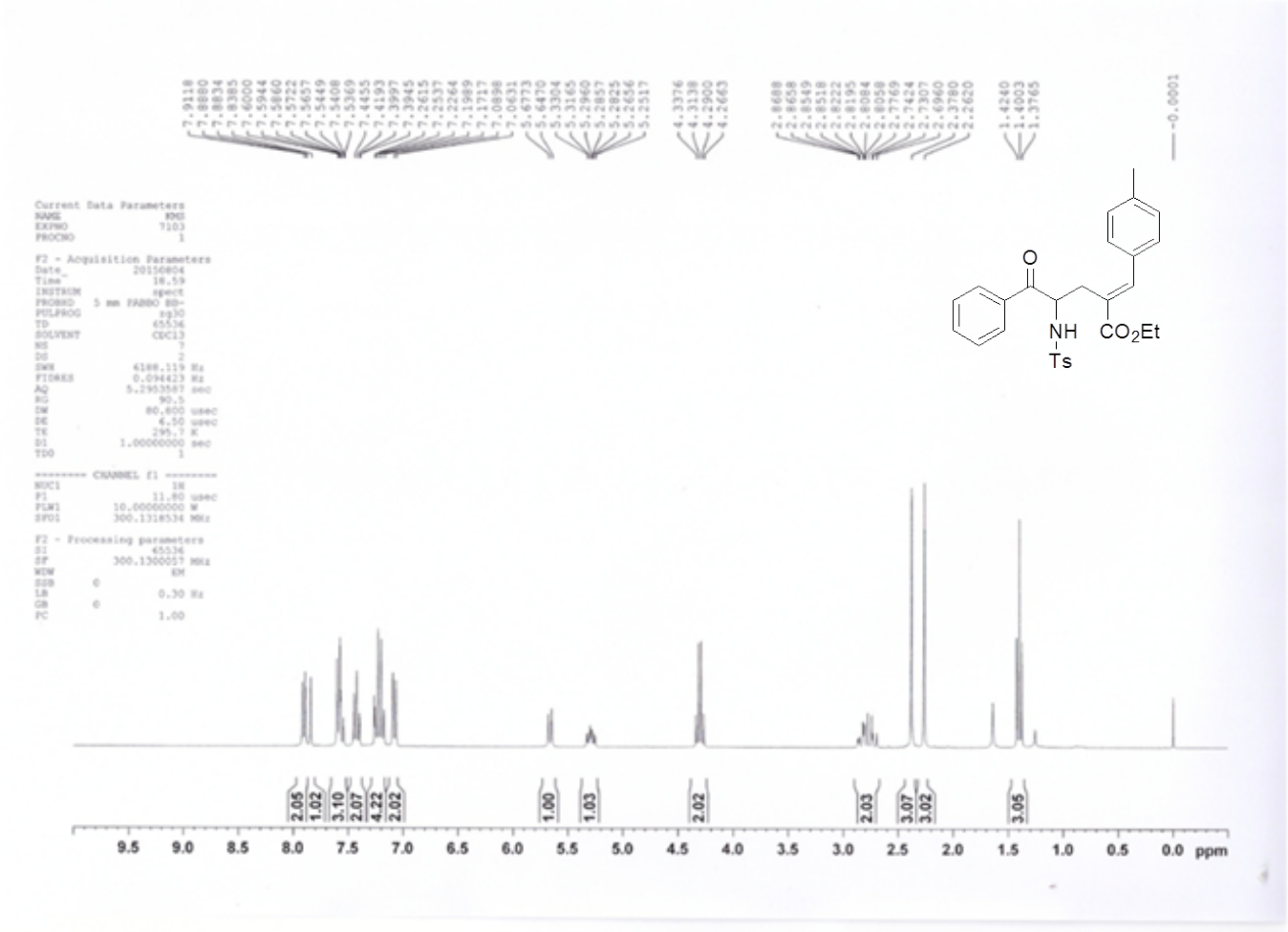


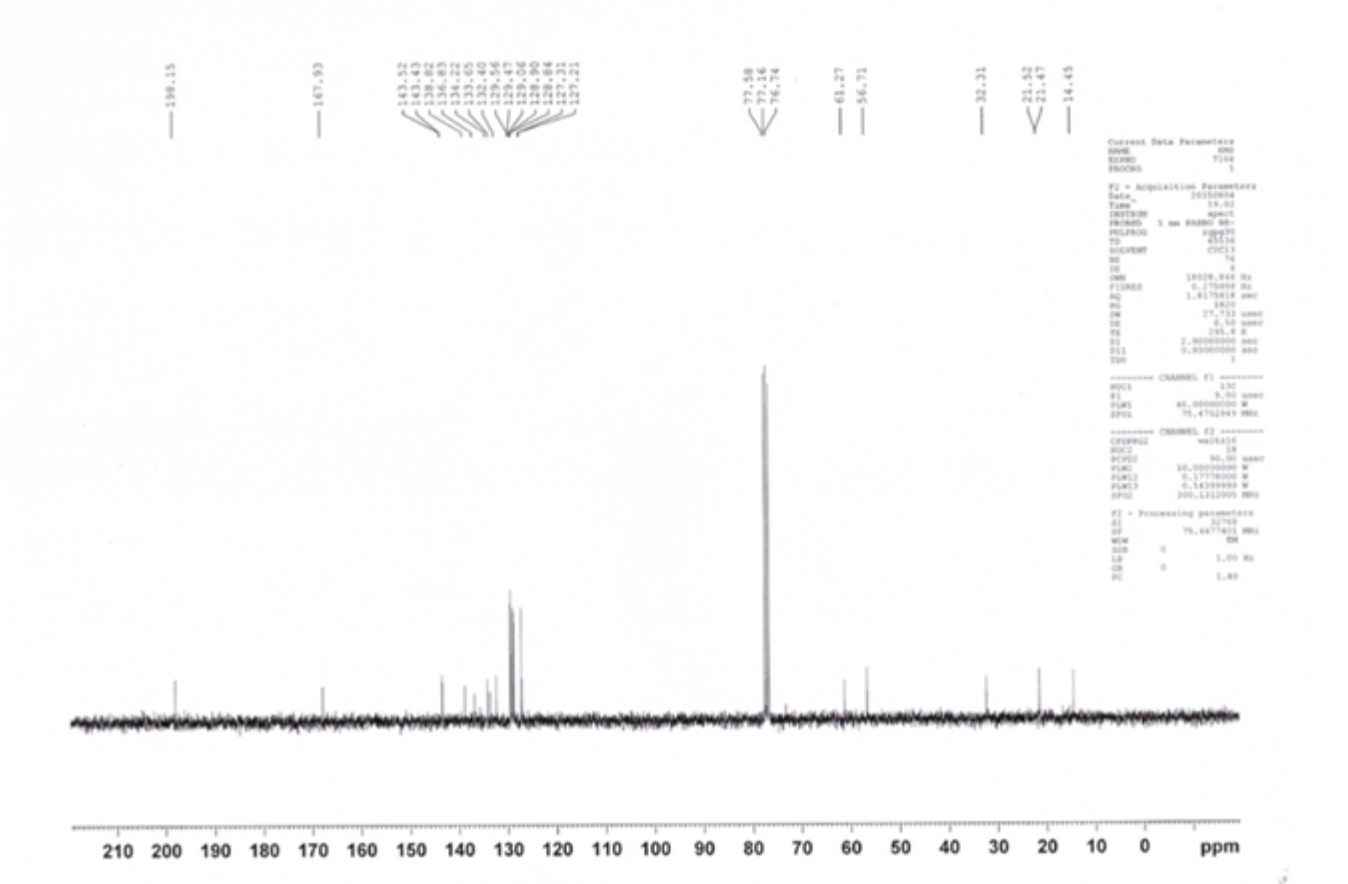
$^{1}H/^{13}C$ spectra of compound **6ac.**



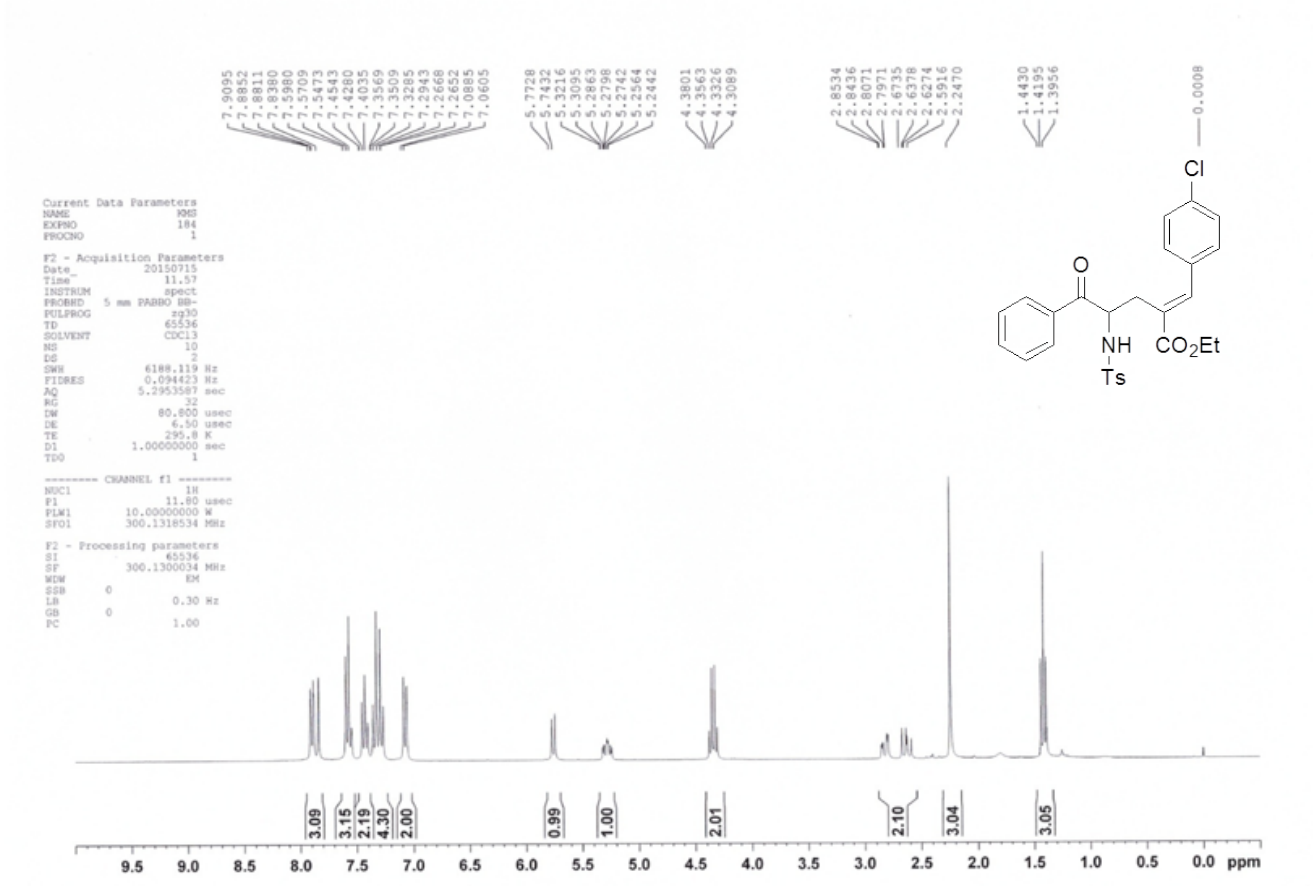


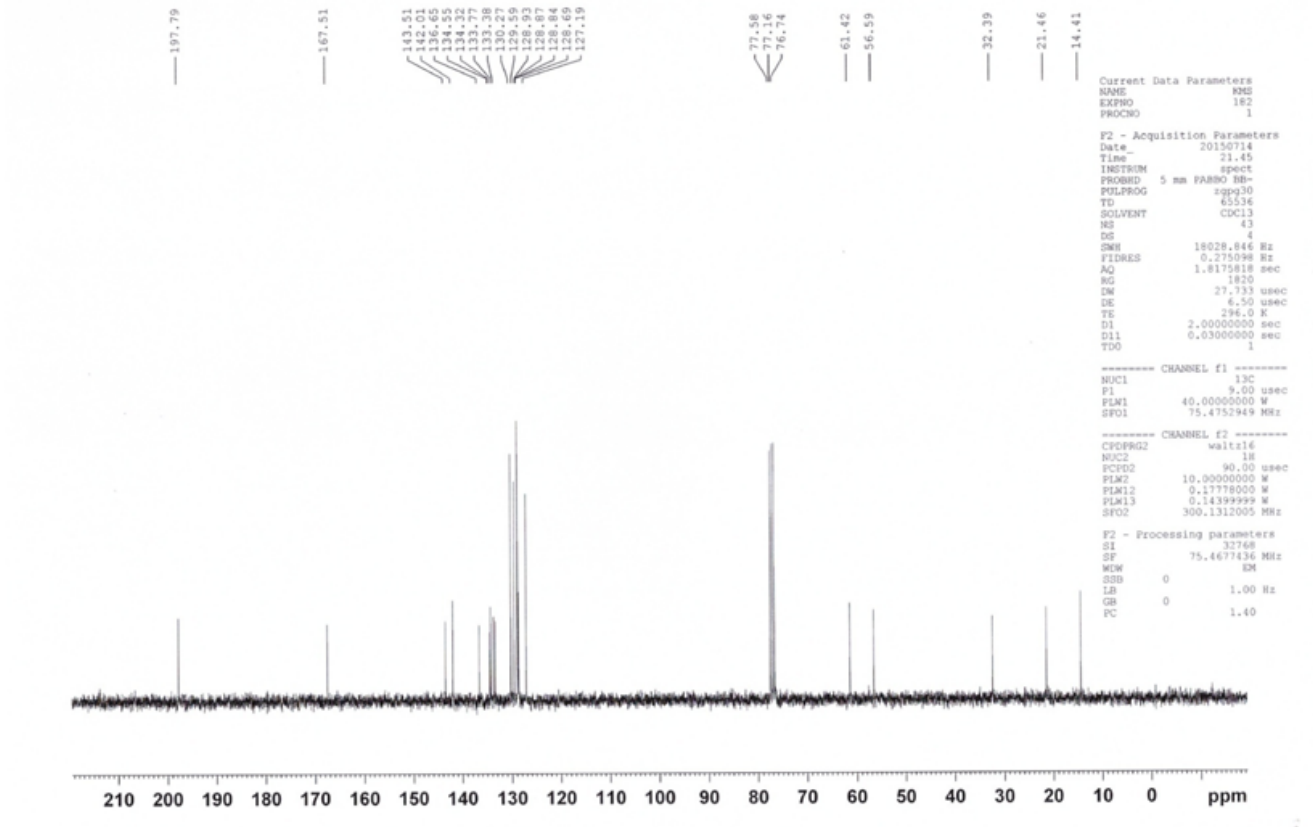
$^{1}H/^{13}C$ spectra of compound **6ad.**



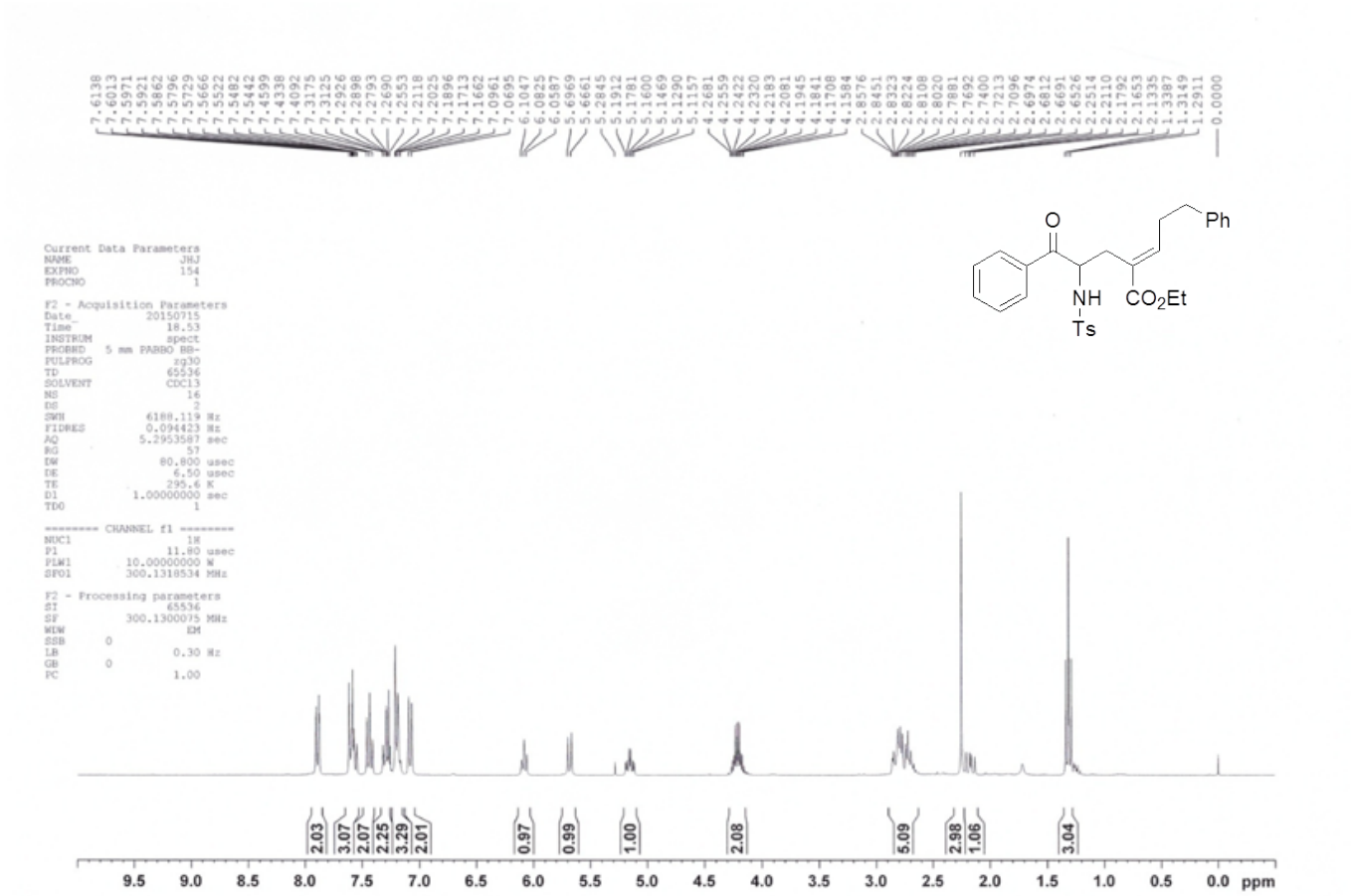


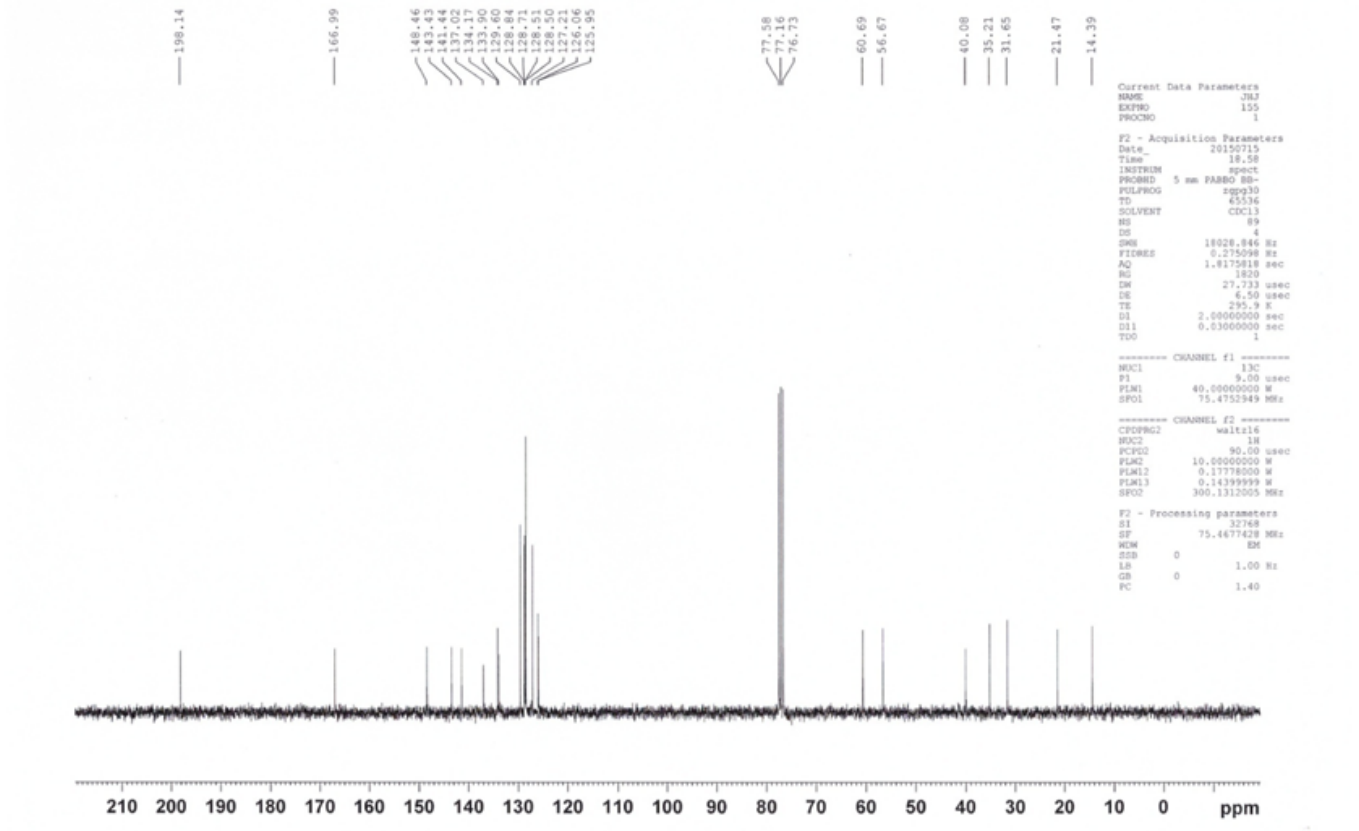
$^{1}H/^{13}C$ spectra of compound **6ae.**



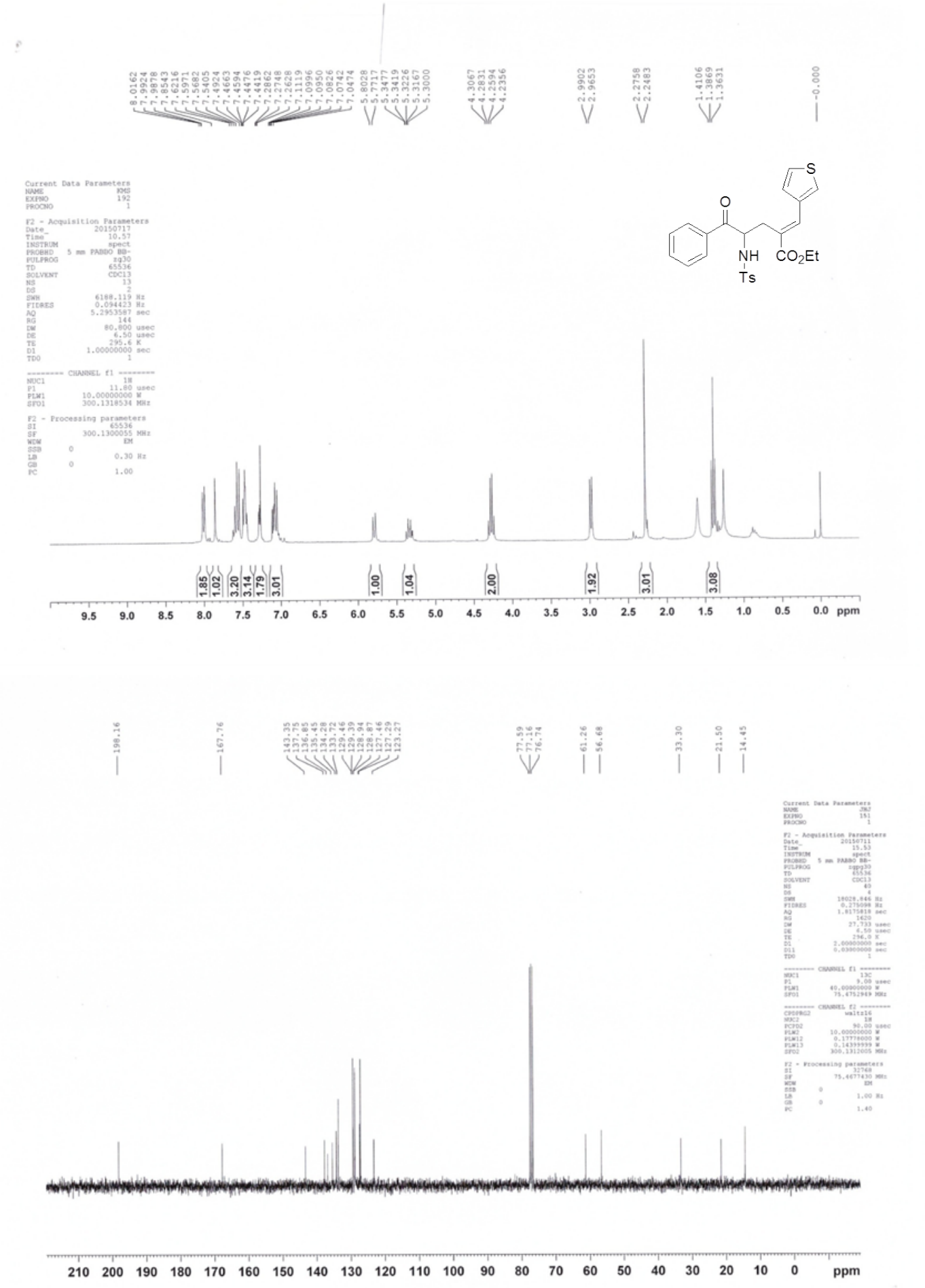


$^{1}H/^{13}C$ spectra of compound **6af.**

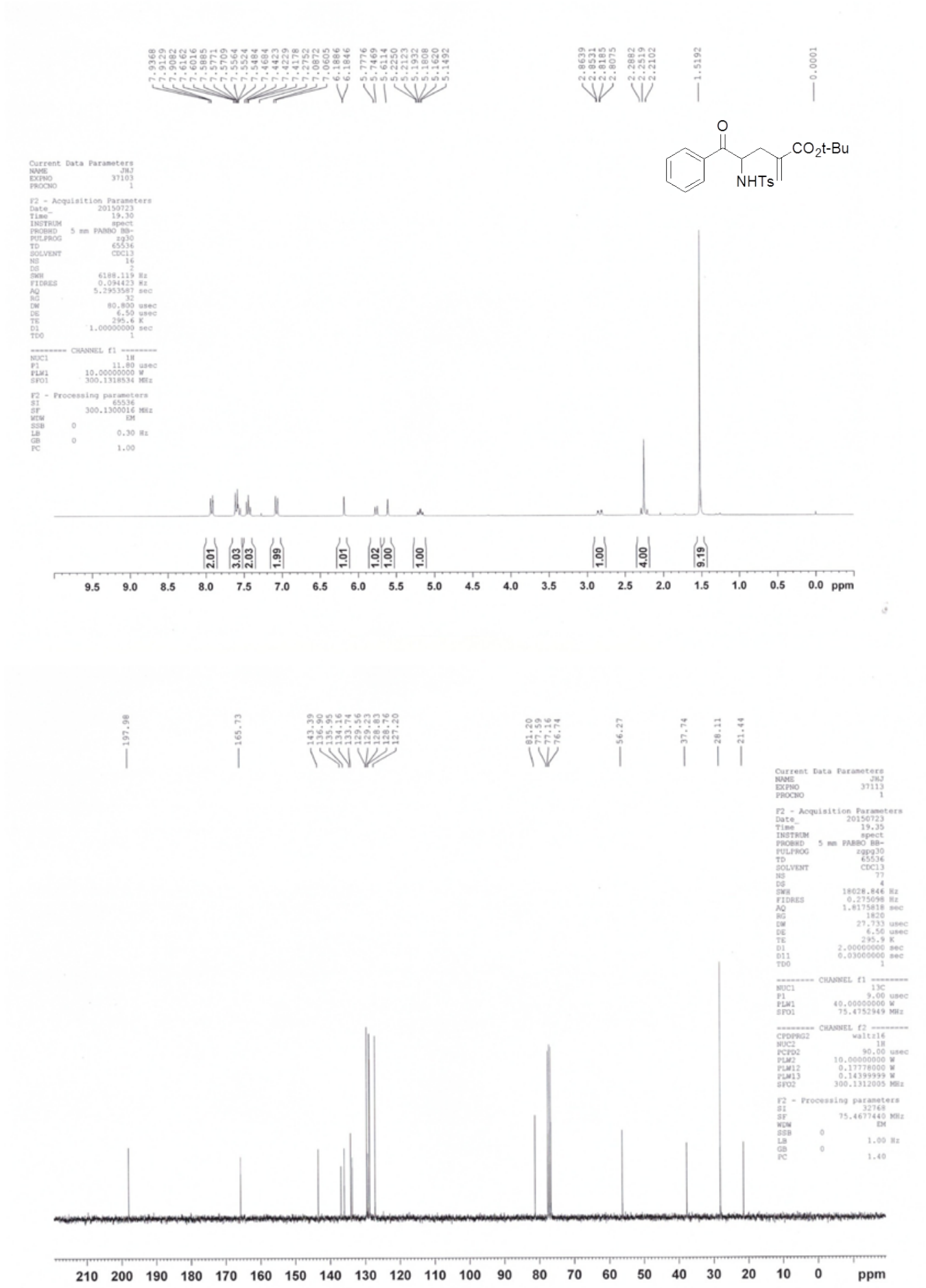




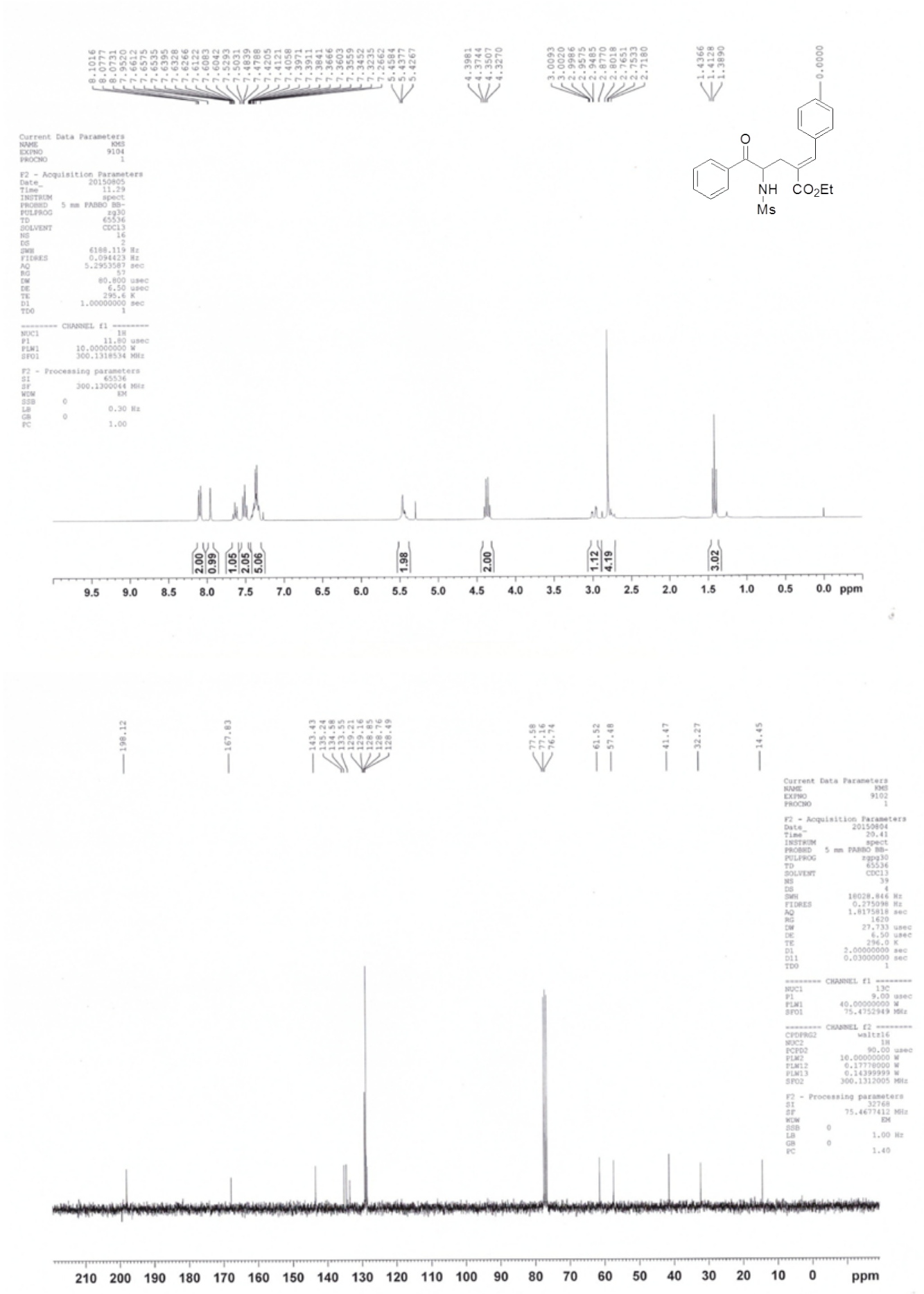
$^{1}H/^{13}C$ spectra of compound **6ag.**



$^{1}H/^{13}C$ spectra of compound **6ah.**



$^{1}H/^{13}C$ spectra of compound **6nb.**

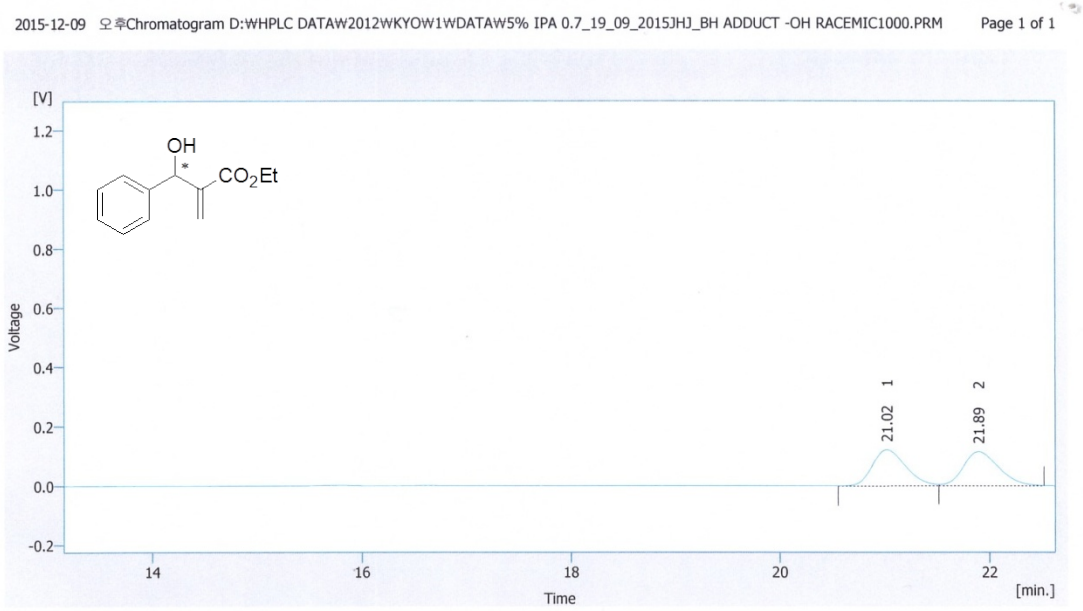


5. Copies of HPLC Spectra for racemic and chiral MBH alcohol 3b.

-HPLC analysis using chiral stationary phase columns (Daicel Chiralpak AD-H 250 x 4.6 mm ID).

Racemic **3b.**

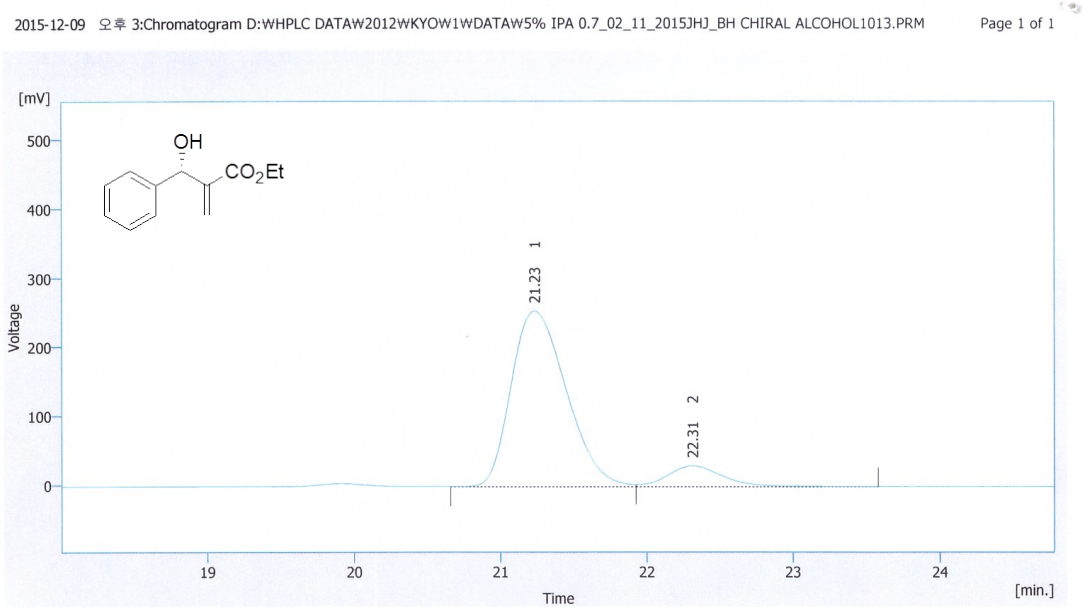
(HPLC condition : 95 % Hexane : 5 % IPA 0.7 ml/min)



Result Table (Uncal - 5% IPA 0.7_19_09_2015JHJ_BH ADDUCT -OH RACEMIC1000 - Channel 1)

	Reten. Time [min]	Area [%]	W05 [min]
1	21.017	49.8	0.35
2	21.893	50.2	0.37
	Total	100.0	

Chiral **3b.**



Result Table (Uncal - 5% IPA 0.7_02_11_2015JHJ_BH CHIRAL ALCOHOL1013 - Channel 1)

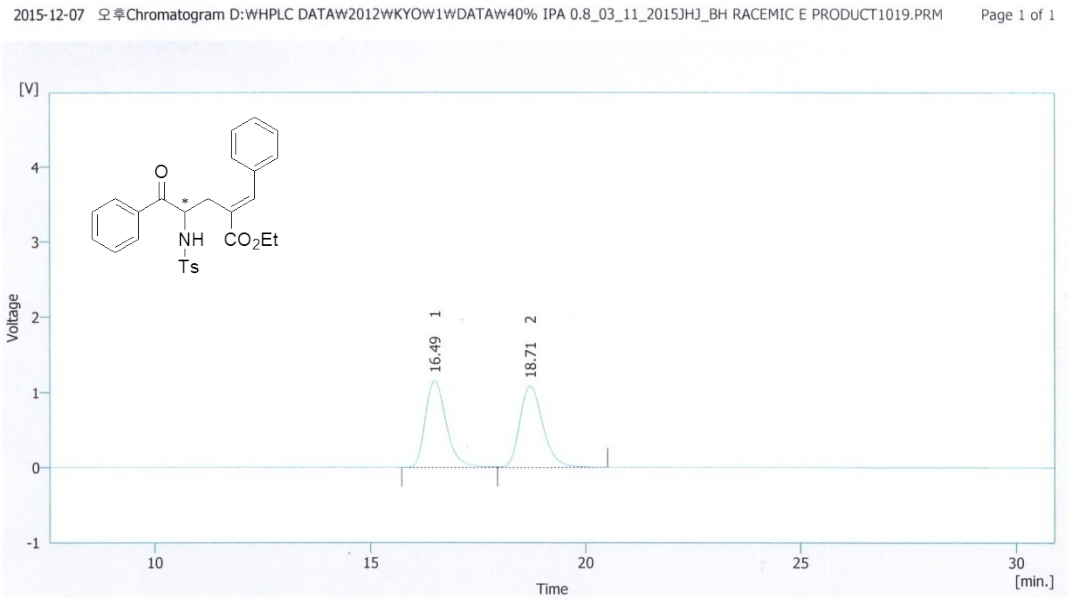
	Reten. Time [min]	Area [%]	W05 [min]
1	21.233	89.6	0.42
2	22.313	10.4	0.39
	Total	100.0	

6. Copies of HPLC Spectra for racemic and chiral (*E*)-6ab.

-HPLC analysis using chiral stationary phase columns (Daicel Chiralpak AD-H 250 x 4.6 mm ID).

Racemic **(*E*)-6ab**.

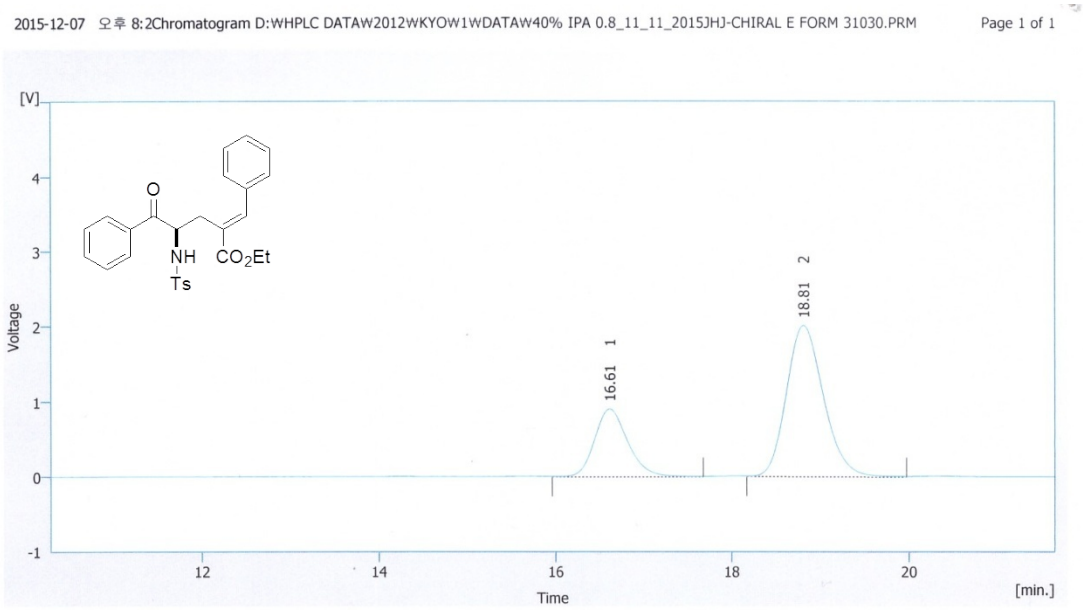
(HPLC condition : 60 % Hexane : 40 % IPA 0.4 ml/min)



Result Table (Uncal - 40% IPA 0.8_03_11_2015JHJ_BH RACEMIC E PRODUCT1019 - Channel 1)

	Reten. Time [min]	Area [%]	W05 [min]
1	16.487	49.3	0.52
2	18.707	50.7	0.57
	Total	100.0	

Chiral**(*E*)-6ab.**



Result Table (Uncal - 40% IPA 0.8_11_11_2015JHJ-CHIRAL E FORM 31030 - Channel 1)

	Reten. Time [min]	Area [%]	W05 [min]
1	16.610	28.6	0.40
2	18.810	71.4	0.45
	Total	100.0	

7. Computational Details.

Calculations were performed using Gaussian 09 package.[1] Optimizations were carried out with B3LYP/6-311G++(d,p) on a truncated model of intermediate **7ab'** featuring a methyl ester and a *N*-methanesulfonyl group in place of the ethyl ester and *N*-toluenesulfonyl group of **7ab**. Solvation effects were accounted using the polarizable continuum model (IEFPCM), with toluene as the solvent. Relative free energies are reported in kcal/mol. All vibrational frequencies were computed at the same level of theory to verify the transition state (one and only one imaginary frequency) and provide the thermal corrections. 3D Structures of the transition states were plotted with CYL view.[2]

(*Z*)-**7ab'**

Single Point Energy (A.U.): -1604.10456014
Sum of electronic and thermal Free Energies (A. U.) = -1603.787796
Imaginary Frequency (cm^{-1}) : n/a
Cartesian Coordinates :

C	-0.32399100	-1.01282200	-0.42565000
C	0.71942400	-1.66679500	0.11202600
O	-0.20831600	0.33355200	-0.77836700
C	-0.29930500	1.29657900	0.30768000
H	0.38302200	0.97831500	1.10273900
C	0.24370600	2.59429600	-0.27026600
C	-0.43999900	3.73783700	-0.35506900
H	0.01748500	4.62870200	-0.76470900
H	-1.46162800	3.81065900	-0.00587300
C	1.67962000	2.53978500	-0.68360900
O	2.46307600	1.68715000	-0.30391000
O	2.04124000	3.53877900	-1.49380700
C	3.42813000	3.56960700	-1.90054500
H	3.51004400	4.42358700	-2.56795800
H	4.07302900	3.69634300	-1.03078900
H	3.68831800	2.64687500	-2.41833300
N	1.93418800	-1.06530100	0.46624500
H	2.11958500	-0.12728800	0.09397100
H	0.65898200	-2.72572600	0.31732900
C	-1.57463800	-1.69186200	-0.82221200
C	-2.25871700	-1.28082600	-1.97717600
C	-2.09026300	-2.77490200	-0.09307200
C	-3.40877500	-1.94293400	-2.39721200
H	-1.87232800	-0.44674700	-2.54977800
C	-3.23870900	-3.43785100	-0.51739600
H	-1.60218600	-3.08707700	0.82302100
C	-3.90452800	-3.02639300	-1.67170800
H	-3.91654100	-1.61529400	-3.29797500

[1] *Gaussian 09, Revision C.01*: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

[2] Legault, C.Y. CYLView, version 1.0b; Université de Sherbrooke: Sherbrooke, Québec, Canada, 2009. http://www.cylview.org.

H	-3.62234600	-4.26902200	0.06405800
H	-4.80147100	-3.54009900	-1.99866600
C	-1.68894500	1.39702200	0.90452100
C	-1.83946000	1.38273400	2.29367500
C	-2.82809800	1.51951600	0.10196600
C	-3.10166800	1.49862200	2.87526800
H	-0.96404100	1.27675200	2.92657800
C	-4.09031200	1.63019500	0.67993100
H	-2.72693900	1.51573600	-0.97625900
C	-4.23058500	1.62283800	2.06811300
H	-3.20217000	1.48253100	3.95471000
H	-4.96597400	1.71727300	0.04658900
H	-5.21434700	1.70603100	2.51620400
S	3.33369900	-2.00455700	0.59092500
O	2.90402500	-3.39136900	0.77980200
O	4.25969800	-1.66851400	-0.49140100
C	4.04468900	-1.39847600	2.12537800
H	4.22852400	-0.33031900	2.02115900
H	3.34752300	-1.60804600	2.93383700
H	4.98172600	-1.93697200	2.26523700

(*E*)-**7ab'**

Single Point Energy (A.U.): -1604.09914383
Sum of electronic and thermal Free Energies (A. U.) = -1603.783968
Imaginary Frequency (cm^{-1}) : n/a
Cartesian Coordinates :

C	-0.36553100	0.70731200	0.45964800
C	-1.30644400	-0.09563100	-0.06380100
H	-1.09155100	-1.11314300	-0.35145700
N	-2.65329400	0.29324200	-0.28797100
H	-2.83930800	1.28921900	-0.35265100
O	0.95373300	0.32913300	0.61624500
C	1.46026900	-0.80229300	-0.11778600
H	1.00428900	-0.78919600	-1.11356300
C	2.94769600	-0.53146200	-0.28761400
C	3.91631300	-1.23742200	0.29917300
H	4.95790200	-0.99263900	0.13886500
H	3.68885900	-2.07840800	0.94200000
C	3.26135100	0.59807200	-1.21822600
O	2.45153800	1.09825300	-1.96878900
O	4.54505900	0.99654100	-1.14990800
C	4.93409400	2.04800900	-2.05672900
H	5.98764700	2.22653500	-1.85544200
H	4.78834800	1.73191100	-3.09014400
H	4.34958700	2.94868200	-1.86709900
C	1.14420700	-2.12215800	0.56485200
C	0.97064700	-3.27583100	-0.20568700
C	1.04377900	-2.21132200	1.95576900
C	0.70869900	-4.50180800	0.40344100
H	1.03383900	-3.21526900	-1.28764000
C	0.77690700	-3.43641300	2.56586000
H	1.16463600	-1.31684800	2.55533000
C	0.61159900	-4.58496100	1.79229700
H	0.57335300	-5.38816900	-0.20612700
H	0.69792600	-3.49323600	3.64590400
H	0.40342600	-5.53697300	2.26758800
C	-0.58349900	2.09945400	0.91553400
C	0.32467400	3.10493400	0.54984800
C	-1.67766000	2.44022900	1.72403900

C	0.13031900	4.41767000	0.96748800
H	1.17289800	2.84696800	-0.07158800
C	-1.86948700	3.75647600	2.14096600
H	-2.36780500	1.66944100	2.04715200
C	-0.96819700	4.74942900	1.76231400
H	0.83527400	5.18585300	0.66960400
H	-2.71701200	4.00212300	2.77107100
H	-1.11680200	5.77300800	2.08720900
S	-3.61984300	-0.55857200	-1.37917100
O	-4.49532800	0.43921200	-1.99610100
O	-2.78600800	-1.44023300	-2.19682700
C	-4.61992100	-1.59905100	-0.30724800
H	-3.95523200	-2.24099900	0.26855000
H	-5.20934100	-0.95389600	0.34096800
H	-5.26123700	-2.19314100	-0.95776900

(*E*)-**6ab'**

Single Point Energy (A.U.): -1604.13895058

Sum of electronic and thermal Free Energies (A. U.) = -1603.821548

Imaginary Frequency (cm^{-1}) : n/a

Cartesian Coordinates :

C	0.73401200	0.27725200	-1.32488000
O	0.11173200	-0.24305700	-2.23781900
C	1.05710700	-0.59766500	-0.09681200
H	1.75338700	-0.10292300	0.57260200
C	-0.22369100	-0.96673000	0.70360500
H	0.12642000	-1.54231500	1.56440100
H	-0.83136600	-1.63082400	0.09080100
C	-1.07031700	0.18071200	1.21020800
C	-2.38049900	0.38487200	0.94382000
C	-0.39781400	1.05815400	2.21167900
O	0.76460900	0.92171200	2.54623000
O	-1.18300000	2.02716300	2.72366000
C	-0.57493600	2.88892200	3.70463000
H	-1.35758900	3.58280500	4.00248100
H	-0.23048600	2.30843900	4.56099800
H	0.26734700	3.42752400	3.26898600
N	1.73250700	-1.78235900	-0.65205800
H	1.18279800	-2.31041900	-1.32300100
H	-2.84892600	1.18372600	1.50923200
C	1.17727300	1.69741200	-1.40569400
C	1.87905700	2.34525600	-0.37784700
C	0.87512800	2.40977900	-2.57949800
C	2.27067800	3.67429700	-0.52458700
H	2.11066800	1.83378700	0.54663700
C	1.26855500	3.73265100	-2.72291200
H	0.33243800	1.90376200	-3.36795400
C	1.96911900	4.36826300	-1.69436200
H	2.81129400	4.16587700	0.27586300
H	1.03220500	4.27199400	-3.63289200
H	2.27716300	5.40177500	-1.80628000
C	-3.32090000	-0.34073400	0.07804800
C	-4.66318700	-0.39334900	0.50038100
C	-2.98773600	-0.94657400	-1.14590500
C	-5.62580300	-1.06901800	-0.24109700
H	-4.94496900	0.09292900	1.42841100
C	-3.95768600	-1.60783400	-1.89505100
H	-1.98366900	-0.86944400	-1.53982500
C	-5.27468700	-1.68326400	-1.44324800

H	-6.64969000	-1.10834100	0.11305500
H	-3.68232600	-2.05887500	-2.84175800
H	-6.02379000	-2.20322700	-2.02957900
S	2.67932700	-2.80185800	0.28032000
O	2.34087900	-2.67142900	1.69996200
O	2.61219600	-4.10887200	-0.37824700
C	4.33722000	-2.14078500	0.06143800
H	4.58770500	-2.19138800	-0.99600000
H	4.35520500	-1.11515600	0.42679000
H	5.00272600	-2.76729500	0.65452900

(*Z*)-**6ab'**

Single Point Energy (A.U.): -1604.12940773
Sum of electronic and thermal Free Energies (A. U.) = -1603.814634
Imaginary Frequency (cm^{-1}) : n/a
Cartesian Coordinates :

C	1.35072600	0.48010800	-0.64402300
O	1.04986500	0.16933100	-1.78213200
C	1.21200800	-0.55961100	0.49312500
H	0.97950000	-0.02369800	1.41448700
C	0.08056400	-1.57467700	0.23554500
H	0.17643100	-2.36334900	0.98682200
H	0.20838800	-2.03096100	-0.74250800
C	-1.30176900	-0.96248500	0.34783800
C	-2.11786000	-0.91330400	-0.72323000
H	-1.66986800	-1.23163400	-1.66226200
C	-1.64931000	-0.48380900	1.71993700
O	-1.17795700	-0.96354900	2.73333500
O	-2.47293600	0.57713400	1.73127900
C	-2.85689800	1.07779100	3.02722900
H	-3.51752800	1.91764300	2.82641500
H	-3.37886800	0.30628600	3.59479700
H	-1.97879400	1.40451700	3.58534900
N	2.54910800	-1.13536400	0.77007800
H	2.65875100	-1.46288800	1.72479400
C	-3.53577600	-0.53216500	-0.84069300
C	-3.95086700	0.17316400	-1.98131900
C	-4.50648800	-0.91417200	0.09747200
C	-5.28530700	0.53027800	-2.15439100
H	-3.21675100	0.45155700	-2.73006000
C	-5.84290100	-0.57275300	-0.08381600
H	-4.21678500	-1.50377600	0.95916700
C	-6.23654200	0.15936100	-1.20485000
H	-5.58373400	1.08788200	-3.03503800
H	-6.58118000	-0.88688100	0.64561700
H	-7.27845900	0.42474900	-1.34392400
C	1.87172000	1.84677900	-0.33125600
C	2.34299600	2.21778700	0.93679300
C	1.88200800	2.79720300	-1.36488700
C	2.81459700	3.50820000	1.16321500
H	2.36248500	1.50499800	1.75056900
C	2.34605800	4.08604900	-1.13551300
H	1.51575100	2.50599300	-2.34143900
C	2.81417300	4.44439100	0.13036100
H	3.18159800	3.78208600	2.14550000
H	2.34249000	4.81336700	-1.93916600
H	3.17705200	5.45004700	0.31028800
S	3.36710100	-2.23390500	-0.22673300
O	4.29629700	-2.90675100	0.68594700

O	2.44819600	-3.02769300	-1.04337200
C	4.31389600	-1.18138900	-1.33350100
H	3.62548200	-0.61111900	-1.95399200
H	4.95152800	-0.53660300	-0.73304100
H	4.90725100	-1.85644200	-1.94983200

(*Z*) Chair 1 TS‡

Single Point Energy (A.U.): -1604.07190006
Sum of electronic and thermal Free Energies (A. U.) = -1603.756772
Imaginary Frequency (cm^{-1}) : -228.79
Cartesian Coordinates :

C	-0.44216600	-0.01264600	1.96481300
C	-2.00813800	-0.11888200	-0.31150900
C	-1.20188300	1.00769500	-0.47525800
C	1.37644200	0.81408800	0.60507700
C	0.76582100	-0.23217200	1.34612600
H	-0.80377000	0.99170300	2.13311600
H	-0.95318800	-0.81430400	2.48263900
H	1.07259100	1.81261000	0.89607900
O	-0.01939000	0.86850000	-0.96433600
C	1.32106300	-1.62348500	1.42213100
O	0.67865300	-2.64045600	1.25761400
O	2.61374200	-1.62211600	1.77505300
C	3.25304100	-2.91092000	1.89179600
H	3.20895100	-3.44278600	0.94086300
H	4.28347800	-2.69608600	2.16311800
H	2.76667500	-3.50569200	2.66531300
H	-3.03671800	-0.06113300	0.01433800
N	-1.63323800	-1.32416700	-0.85557300
H	-0.69763500	-1.40890400	-1.23813700
C	2.61425900	0.76907700	-0.16918000
C	3.45988500	1.89097600	-0.14733800
C	2.97301500	-0.32200300	-0.97847000
C	4.64774600	1.90501400	-0.87180500
H	3.18529800	2.75162400	0.45332700
C	4.15086500	-0.30118300	-1.71463000
H	2.31288200	-1.17701600	-1.05874600
C	4.99769500	0.80794200	-1.65763700
H	5.29382100	2.77458200	-0.83134100
H	4.40626100	-1.14600400	-2.34423800
H	5.91635600	0.82072500	-2.23309100
C	-1.68414400	2.36494300	-0.08512900
C	-0.95020700	3.47665100	-0.52501600
C	-2.83097400	2.59142300	0.69385700
C	-1.35152200	4.77150200	-0.20419800
H	-0.07065300	3.30801500	-1.13372200
C	-3.23039400	3.88525600	1.01430200
H	-3.41779700	1.76004400	1.06695200
C	-2.49333300	4.98275800	0.56646100
H	-0.77377700	5.61654700	-0.56226900
H	-4.11819000	4.03724700	1.61804600
H	-2.80767300	5.98972200	0.81629300
S	-2.59734700	-2.70209400	-0.89630300
O	-3.98455900	-2.24462400	-0.95405800
O	-2.02514700	-3.53379000	-1.95099900
C	-2.35424500	-3.52721300	0.68061600
H	-1.29017500	-3.70592900	0.81271900
H	-2.74543300	-2.88077400	1.46462100
H	-2.92442200	-4.45457200	0.62772600

(Z) Chair 2 TS‡

Single Point Energy (A.U.): -1604.07511402

Sum of electronic and thermal Free Energies (A. U.) = -1603.759348

Imaginary Frequency (cm^{-1}) : -218.91

Cartesian Coordinates :

C	-0.10433300	-0.72960800	1.61548900
C	-1.05090800	1.25152900	0.05753800
C	0.22682800	1.06390200	-0.46571800
C	0.74718800	-1.75704400	-0.45296900
C	-0.20959200	-1.63500400	0.59051400
H	0.81739800	-0.20560500	1.81716200
H	-0.90588400	-0.61488200	2.33163000
O	0.39702800	0.15321100	-1.36089800
C	-1.51050000	-2.34307700	0.34466500
O	-1.78351400	-2.93263500	-0.68094000
O	-2.33603700	-2.28108600	1.40077600
C	-3.63413200	-2.89453400	1.23770300
H	-3.52512800	-3.94592100	0.97135500
H	-4.12124900	-2.79132900	2.20446900
H	-4.19684400	-2.36737800	0.46741400
H	-1.30602400	2.00407400	0.78818500
N	-2.11876400	0.57092400	-0.50907700
H	-1.90199600	-0.00675500	-1.31838800
H	0.36959500	-2.24185300	-1.34457100
C	2.20280600	-1.75519400	-0.33822700
C	2.95970000	-1.81434600	-1.52511100
C	2.88826000	-1.78502900	0.88911400
C	4.34619600	-1.85777300	-1.48766800
H	2.44235700	-1.80909000	-2.47771700
C	4.27809100	-1.83653600	0.92456700
H	2.33481200	-1.80379000	1.81855100
C	5.01289500	-1.86298400	-0.26013400
H	4.91022000	-1.89469900	-2.41278900
H	4.78869300	-1.86674500	1.88039000
H	6.09577600	-1.90314100	-0.22837300
C	1.37869100	1.89137800	0.00449600
C	2.53940300	1.92418800	-0.78055700
C	1.34531700	2.66417400	1.17644400
C	3.62851700	2.70966200	-0.41297500
H	2.57342400	1.32522500	-1.68130100
C	2.43577500	3.44691600	1.54500600
H	0.47415200	2.64948900	1.82140900
C	3.58263700	3.47589300	0.75078700
H	4.51546800	2.72256100	-1.03681200
H	2.39158200	4.03117700	2.45752000
H	4.43114200	4.08588300	1.03948000
S	-3.71347500	1.07547800	-0.35747800
O	-4.53366000	-0.06744500	-0.74733600
O	-3.83220200	1.67627600	0.96901400
C	-3.93946000	2.37532100	-1.58503000
H	-3.23621300	3.17829400	-1.36997000
H	-3.77036700	1.94888200	-2.57228800
H	-4.96714700	2.72392600	-1.48470800

(Z) Boat 1 TS‡

Single Point Energy (A.U.): -1604.07044852

Sum of electronic and thermal Free Energies (A. U.) = -1603.756147

Imaginary Frequency (cm^{-1}) : -189.48

Cartesian Coordinates :

C	0.62929700	0.83906700	-0.78626100
C	-0.23633900	1.56567900	0.03670900
C	0.25570800	-0.55023500	1.67577200
C	0.74923900	-1.51734400	0.83061100
C	0.04269300	-1.99694700	-0.29591500
H	0.86682700	-0.15285400	2.47385200
H	-0.79065600	-0.29294000	1.67106100
O	0.15357400	-0.12581400	-1.48062800
C	2.08834900	1.15067000	-0.83850500
C	2.89841100	0.37294700	-1.67680200
C	2.68579800	2.19946600	-0.11968800
C	4.26355100	0.62750500	-1.78960500
H	2.44062600	-0.42838700	-2.24209500
C	4.04830500	2.45337000	-0.23267000
H	2.09523000	2.83150000	0.53259200
C	4.84524400	1.66790000	-1.06832600
H	4.87134100	0.01328500	-2.44477500
H	4.48964100	3.26890300	0.32950300
H	5.90669600	1.87035900	-1.15754900
C	2.18819700	-1.93732000	0.91127300
O	2.69907900	-2.75970900	0.18161200
O	2.84938400	-1.33488000	1.91528200
C	4.23498500	-1.70053300	2.07463900
H	4.32496200	-2.76816900	2.27794700
H	4.79610000	-1.45135900	1.17404700
H	4.59114700	-1.11794300	2.92090300
H	0.05758000	2.42704800	0.61607000
N	-1.60048900	1.33945800	-0.05752400
H	-1.87797600	0.69458100	-0.79709200
S	-2.75509900	2.51210800	0.33909200
O	-2.03278300	3.70544700	0.77492100
O	-3.71065800	2.56205900	-0.76394700
C	-3.59036400	1.80443600	1.76383900
H	-4.37532500	2.50736400	2.04220900
H	-4.01518500	0.84575500	1.47182100
H	-2.86699600	1.69601000	2.56980100
H	0.64861200	-2.50791700	-1.03344800
C	-1.39836800	-2.21972700	-0.40833900
C	-2.22010500	-2.43485100	0.71338000
C	-1.97707100	-2.31650200	-1.68826900
C	-3.57530600	-2.70928700	0.55883500
H	-1.78751900	-2.42233200	1.70602300
C	-3.33417800	-2.57628100	-1.83846800
H	-1.35274800	-2.16046400	-2.55973000
C	-4.14066700	-2.77069400	-0.71557800
H	-4.18932800	-2.89072600	1.43403200
H	-3.76404000	-2.63298200	-2.83201300
H	-5.19702700	-2.98341400	-0.83369000

(*Z*) Boat 2 TS‡

Single Point Energy (A.U.): -1604.06332308

Sum of electronic and thermal Free Energies (A. U.) = -1603.749459

Imaginary Frequency (cm^{-1}) : -200.17

Cartesian Coordinates :

C	-0.80056500	0.64835000	-0.67737600
C	-2.07382900	0.51115900	-0.14149700
C	-0.47143500	-0.06416100	2.13202800
C	0.74085600	-0.35585500	1.56164300

C	0.79528200	-1.38926400	0.58904200
H	-0.57014800	0.76298000	2.82272100
H	-1.31155900	-0.73236600	2.01645200
O	-0.15840900	-0.40520400	-1.05722100
C	-0.17802700	1.99484500	-0.84097900
C	0.88932800	2.12120700	-1.74049200
C	-0.62582900	3.14293800	-0.16955000
C	1.48213000	3.35919500	-1.97396600
H	1.24161200	1.23452300	-2.25199800
C	-0.02950900	4.37939400	-0.39920200
H	-1.43246100	3.07849300	0.55145600
C	1.02568600	4.49452400	-1.30543000
H	2.30077400	3.43783100	-2.68113400
H	-0.38570200	5.25373400	0.13420500
H	1.48724100	5.45904100	-1.48526700
C	1.84819000	0.61352500	1.87278300
O	1.94115100	1.19270100	2.93414300
O	2.69194900	0.79822200	0.85255900
C	3.76034300	1.74342100	1.06505300
H	3.35147200	2.73712600	1.24769400
H	4.37452600	1.43912100	1.91340700
H	4.34042600	1.73157300	0.14587500
C	1.95585300	-2.03894400	-0.02562600
C	1.77532700	-2.72601900	-1.24010800
C	3.21453400	-2.10170300	0.59558100
C	2.82630300	-3.41676400	-1.83105000
H	0.80979000	-2.68310800	-1.72835700
C	4.25891600	-2.81244100	0.01240200
H	3.37324200	-1.62312300	1.55287500
C	4.07382100	-3.46324400	-1.20706100
H	2.67179000	-3.92448100	-2.77640300
H	5.21858100	-2.86164200	0.51446400
H	4.89157300	-4.01050600	-1.66214700
H	-0.09777500	-1.99952400	0.56711400
H	-2.70243900	1.34181300	0.14011200
N	-2.67755400	-0.74377400	-0.13480700
H	-2.20224600	-1.43910900	-0.70718500
S	-4.36227300	-0.93826400	-0.10078800
O	-4.97347400	0.38641900	-0.17733900
O	-4.67297700	-1.98041000	-1.07649900
C	-4.67113800	-1.59906900	1.54157400
H	-5.74759000	-1.75350600	1.61390900
H	-4.13734700	-2.54233000	1.64055700
H	-4.33785200	-0.86827700	2.27615300

(*E*) Chair 1 TS‡

Single Point Energy (A.U.): -1604.06497176

Sum of electronic and thermal Free Energies (A. U.) = -1603.750639

Imaginary Frequency (cm^{-1}) : -287.25

Cartesian Coordinates :

C	-0.15181900	-0.69081600	1.75423100
C	-1.41088500	-0.13460000	-0.37363700
C	1.86630300	0.15208000	0.75984400
C	1.07576200	-0.94786600	1.18828800
H	-1.09940700	-1.11136400	-0.71339600
H	-0.36800600	0.28728600	2.16327300
H	-0.81726900	-1.49542400	2.03491200
H	1.65370400	1.07970800	1.28040800
O	0.71409800	0.62485800	-0.81985000

C	1.44849000	-2.36684000	0.89429400
O	2.55645700	-2.83570400	1.01397100
O	0.37507300	-3.09918200	0.52065600
C	0.61209200	-4.50336800	0.28763700
H	0.96325300	-4.98560200	1.20077200
H	-0.34821200	-4.91127300	-0.01863900
H	1.35260500	-4.63752900	-0.50103900
C	3.18903100	0.13269100	0.12158900
C	4.16649600	1.02538200	0.58731900
C	3.49880600	-0.69349900	-0.96858900
C	5.43362500	1.06083800	0.01152800
H	3.93261400	1.68839300	1.41381500
C	4.75812700	-0.64579100	-1.55423800
H	2.74355700	-1.35315300	-1.37435400
C	5.73327800	0.22388000	-1.06181000
H	6.18094200	1.74696200	0.39382100
H	4.98031100	-1.28517400	-2.40116100
H	6.71571500	0.25490800	-1.51941500
C	-0.80941500	2.32568900	-0.09693400
C	-0.12273900	3.34832400	-0.77091600
C	-1.72414300	2.68490700	0.90602600
C	-0.36217100	4.68493000	-0.47067000
H	0.59817300	3.07531300	-1.53152600
C	-1.95804000	4.02562300	1.21118700
H	-2.23290600	1.92178500	1.48397000
C	-1.28380800	5.02956900	0.51964100
H	0.17020500	5.46073600	-1.00954600
H	-2.66007400	4.28308400	1.99635600
H	-1.46889600	6.07167600	0.75413700
N	-2.78818700	0.00969700	-0.17796900
H	-3.19150800	0.93931200	-0.22685500
S	-3.89610300	-1.18120700	-0.65625200
O	-5.08788400	-0.45143300	-1.08420000
O	-3.21951200	-2.12500500	-1.54157200
C	-4.27886700	-2.03847500	0.87656900
H	-3.36109000	-2.47599800	1.26544900
H	-4.70922200	-1.32143100	1.57275500
H	-4.99889900	-2.81667100	0.62446900
C	-0.49453400	0.91194800	-0.46376700

(*E*) Chair 2 TS‡

Single Point Energy (A.U.): -1604.06678404
Sum of electronic and thermal Free Energies (A. U.) = -1603.752548
Imaginary Frequency (cm^{-1}) : -273.73
Cartesian Coordinates :

C	0.43052300	1.22807800	1.21154800
C	1.28336100	-0.45262900	-0.48168500
C	-0.04737700	-0.54032900	-0.89142200
C	-1.25169500	1.94827000	-0.42573500
C	-0.04524500	2.14121600	0.30160200
H	-0.21371700	0.47948000	1.64639300
H	1.40069400	1.36234300	1.66778800
O	-0.54038500	0.44171900	-1.57088700
C	0.85614400	3.20529100	-0.23789900
O	0.53212600	4.01966400	-1.07569600
O	2.08588000	3.18021500	0.31792400
C	3.01308800	4.18242500	-0.14560400
H	2.62600000	5.18144200	0.05738800
H	3.93070600	4.00675400	0.41101100

H	3.18815200	4.07047400	-1.21577100
H	-1.34744500	2.58248500	-1.29775200
H	1.88279100	0.36122300	-0.86010600
C	-2.53270500	1.45308300	0.09901400
C	-3.56963300	1.18651200	-0.81373200
C	-2.80695000	1.32568700	1.47018800
C	-4.82054200	0.77429200	-0.37486500
H	-3.37493500	1.29449200	-1.87449000
C	-4.06396000	0.91738500	1.90994700
H	-2.05038500	1.58333900	2.19989100
C	-5.07226300	0.63240200	0.99164700
H	-5.60341300	0.56757700	-1.09581400
H	-4.25844500	0.83467700	2.97343000
H	-6.05027600	0.31585700	1.33607000
C	-0.91815400	-1.71049100	-0.55957600
C	-1.82839400	-2.15373400	-1.53103800
C	-0.86760300	-2.38924300	0.66723600
C	-2.64818200	-3.25064700	-1.29016600
H	-1.87972000	-1.62664000	-2.47582400
C	-1.69704100	-3.48353000	0.91200000
H	-0.20624100	-2.04656400	1.45529800
C	-2.58482000	-3.92168400	-0.06765400
H	-3.33833300	-3.58492300	-2.05680000
H	-1.65301800	-3.98739400	1.87112800
H	-3.22580000	-4.77559100	0.12004600
N	2.01015100	-1.48897200	0.11303100
H	1.59434800	-2.41372500	0.15657600
S	3.70141500	-1.54494500	0.08115300
O	4.04531600	-2.96025300	-0.03880800
O	4.18073500	-0.55705600	-0.88165600
C	4.17621400	-0.99077200	1.72427300
H	3.81269500	0.02560300	1.86528100
H	3.74945500	-1.67563500	2.45451400
H	5.26522600	-1.01713900	1.75660800

(*E*) Boat 1 TS‡

Single Point Energy (A.U.): -1604.06459975

Sum of electronic and thermal Free Energies (A. U.) = -1603.749551

Imaginary Frequency (cm^{-1}) : -240.59

Cartesian Coordinates :

C	0.46337900	-0.14659700	-1.11552300
C	0.49056900	1.12161200	-0.53674900
C	-0.72795000	0.23615600	1.59719900
C	-1.07200200	-1.03428800	1.21138200
C	-1.92612400	-1.29882500	0.10903000
H	0.03263800	0.39632500	2.34853000
H	-1.90028900	-2.32013400	-0.24869000
H	-1.30654900	1.09646900	1.30441800
O	-0.68712100	-0.64719500	-1.41994800
H	-0.41201000	1.71186200	-0.58432300
C	1.68145700	-0.99112400	-1.31687500
C	1.56266500	-2.38615200	-1.22288500
C	2.92713000	-0.45320900	-1.68121900
C	2.66118400	-3.21242400	-1.43966000
H	0.60027100	-2.81902300	-0.98565200
C	4.02264400	-1.28277000	-1.91343500
H	3.03720900	0.61355400	-1.83089100
C	3.89790500	-2.66471000	-1.78177100
H	2.54890900	-4.28728300	-1.35058400

H	4.97151300	-0.84787700	-2.20740800
H	4.75168200	-3.30923600	-1.95802000
N	1.63473200	1.82751800	-0.13868900
H	2.43324400	1.30656600	0.20818000
C	-0.33327700	-2.21884400	1.75409000
O	-0.56442900	-3.36892200	1.44278900
O	0.60082500	-1.88128400	2.66194500
C	1.33287500	-2.97005600	3.25900700
H	1.87969600	-3.52260000	2.49453500
H	2.02091400	-2.50422600	3.96044700
H	0.65221300	-3.64467700	3.77918900
S	1.52784500	3.35638300	0.57474800
O	0.16821300	3.55415500	1.07563800
O	2.68268900	3.44594900	1.46678300
C	1.77356800	4.48031900	-0.80566500
H	2.76628900	4.30670900	-1.21593600
H	0.99680100	4.29164800	-1.54500300
H	1.68586800	5.48967300	-0.40431000
C	-3.12469700	-0.54602800	-0.27541000
C	-3.67167300	-0.76286500	-1.55364400
C	-3.79522500	0.32560700	0.59818300
C	-4.82655800	-0.10416000	-1.95542300
H	-3.16586300	-1.43781200	-2.23348300
C	-4.95875600	0.97728400	0.19681600
H	-3.42883100	0.46944500	1.60639900
C	-5.47375300	0.77272600	-1.08214400
H	-5.22724500	-0.27658600	-2.94798600
H	-5.46765300	1.63886700	0.88871700
H	-6.37904900	1.28203900	-1.39275000

(*E*) Boat 2 TS‡

Single Point Energy (A.U.): -1604.05734095

Sum of electronic and thermal Free Energies (A. U.) = -1603.743379

Imaginary Frequency (cm^{-1}) : -241.31

Cartesian Coordinates :

C	-0.52685000	0.23414800	-1.09209900
C	-1.59018000	-0.62307200	-0.83074200
C	-0.29765800	-1.62776500	1.29547600
C	0.95056000	-1.08007400	1.12840200
C	1.64167100	-1.41737800	-0.07204600
H	-0.94261000	-1.32433800	2.10772700
H	-0.60554600	-2.49310400	0.72786400
O	0.61246900	-0.27833100	-1.43618700
H	-1.49696700	-1.65831000	-1.12040900
C	-0.60778100	1.72048400	-0.93801200
C	0.53544200	2.43016600	-0.54092600
C	-1.76274200	2.44890500	-1.26955100
C	0.50870900	3.81709300	-0.43150800
H	1.44242600	1.88608300	-0.31620500
C	-1.78272900	3.83929100	-1.17299600
H	-2.63869300	1.93807800	-1.64996000
C	-0.65087400	4.52856400	-0.74190000
H	1.39972100	4.34482400	-0.10970500
H	-2.68035500	4.38305500	-1.44620500
H	-0.66724300	5.60980100	-0.66260400
N	-2.88643200	-0.24301100	-0.44189600
H	-2.99199900	0.61189100	0.09462800
C	1.37258200	0.02951200	2.04143500
O	2.21954000	0.86241700	1.80674900

O	0.68074900	0.00620500	3.19974000
C	0.97111900	1.06365200	4.13519000
H	0.32222000	0.87915400	4.98801800
H	2.01870700	1.02796700	4.43578200
H	0.75415100	2.03503600	3.68983900
S	-4.04312800	-1.39544600	0.00044900
O	-3.37882700	-2.68678300	0.17669700
O	-4.81382400	-0.78703900	1.08421600
C	-5.09334500	-1.50858900	-1.45297500
H	-4.47930300	-1.81644300	-2.29764100
H	-5.85122600	-2.25979100	-1.23191900
H	-5.54676800	-0.53422900	-1.62372100
C	3.03316600	-1.21527100	-0.49469600
C	4.09261700	-0.89531300	0.36966700
C	3.33078800	-1.46676500	-1.84830900
C	5.39775800	-0.81958700	-0.10835100
H	3.90604300	-0.71505900	1.41710400
C	4.63101700	-1.36851500	-2.32692900
H	2.52228400	-1.71812700	-2.52402900
C	5.67265700	-1.04468000	-1.45641100
H	6.20316800	-0.58176700	0.57741700
H	4.83427500	-1.55142100	-3.37603800
H	6.69027100	-0.97615900	-1.82437400
H	1.18609800	-2.25951200	-0.57551000