Supporting Information

For

Palladium-catalyzed allylic C–H amination of alkenes with *N*-fluorodibenzenesulfonimide: water plays an important role

Tao Xiong, Yan Li*, Lujia Mao, Qian Zhang and Qian Zhang*

Department of Chemistry, Northeast Normal University, Changchun, 130024, China
Email: liy078@nenu.edu.cn, zhangq651@nenu.edu.cn

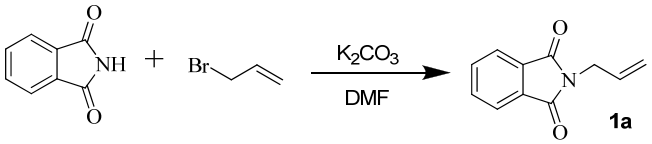
Table of Contents

I. General Remarks:

All reagents were purchased from commercial sources and used without further treatment, unless otherwise indicated. *N*-tosylcarbamates were synthesized using a literature procedure.[1] Anhydrous perchloromethane was dried with P_2O_5 at around 120 ^oC for 7hrs, distilled under vacuum, and kept with 4Å Molecular Seives. ^1H NMR and ^{13}C NMR spectra were recorded at 25 ºC on a Varian 500 MHz and 125 MHz, respectively, and TMS as internal standard. IR spectra (KBr) were recorded in the range of 400~4000 cm^{-1}. Melting points are uncorrected. All reactions were monitored by TLC with GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

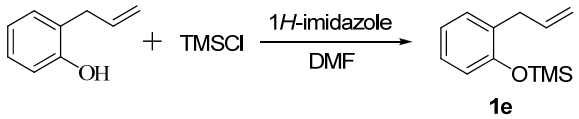
II. Synthesis procedure

General procedure for 2-alkylisoindoline-1,3-dione 1a, 1h and 1i (1a as an example):



To a solution of isoindoline-1,3-dione (735 mg, 5.0 mmol) in DMF (15 mL) was added 3-bromoprop-1-ene (780 mg, 6.5 mmol) and K_2CO_3 (897 mg, 6.5 mmol). The reaction mixture was stirred at room temperature for 6 h (monitored by TLC) before it was slowly poured into water (50 mL). Extracted with CH_2Cl_2 (8 mL×5), then the organic phase washed with water (20 mL×3), the solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (5% EtOAc/petro ether) to gain **1a** (889 mg, 95%) as white crystal.

Synthesis of substrate 1e:

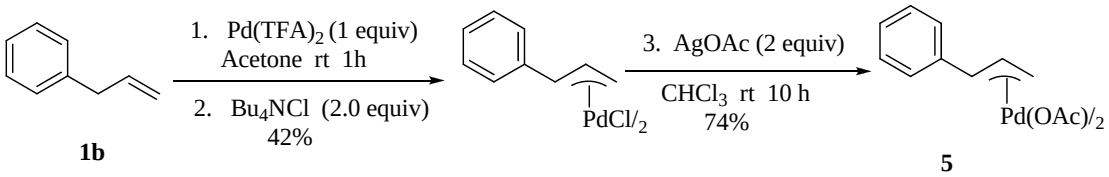


To a solution of 2-allylphenol (671 mg, 5.0 mmol) in anhydrous DMF (15 mL) was added imidazole (1.02 g, 15 mmol) in one portion under N_2. After the reaction mixture was stirred for 15 min, was added TMSCl (1.09 g, 10 mmol). The reaction mixture was then stirred at room temperature for 10 h (monitored by TLC) before it was slowly poured into water (50 mL). Extracted with CH_2Cl_2 (8 mL×5), then the organic phase washed with water (20 mL×3), the solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (2.5% ether/petro ether) to gain **1e** (999 mg, 97%) as colorless oil.

General procedure for the synthesis of 2 (with 2a as an example):

To a solution of substrate **1a** (225 mg, 1.2 mmol) in perchloromethane (5.0 mL) was added NFSI (315 mg, 1.0 mmol), $Pd(OAc)_2$ (22 mg, 0.1 mmol), KF (116 mg, 2.0 mmol) and H_2O (5.4 µl, 0.3 mmol). The mixture was stirred at 60 °C for 14 h (monitored by TLC), then poured into cold water (50 mL), extracted with dichloromethane (15 mL), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (25% ethyl ether/petro ether) to give compound **2a** (424 mg, 88%) as white crystal.

Synthesis of complexes 5:



1b **5**

bis[acetate(trihaptoallylbenzene)palladium(II)] and bis[chloro(trihaptoallylbenzene) palladium(II)] 5 were synthesized using a literature procedure. [2]

The compound **5**:

^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.05 (d, J = 12.0 Hz, 1H), 3.99 (d, J = 6.5 Hz, 1H), 4.66 (d, J = 11.5 Hz, 1H), 5.81 (dt, J_1 = 6.5 Hz, J_2 = 11.5 Hz, 1H), 7.27 (t, J = 7.5 Hz, 2H), 7.34 (t, J = 7.5 Hz, 1H), 7.49 (d, J = 7.5 Hz, 2H).

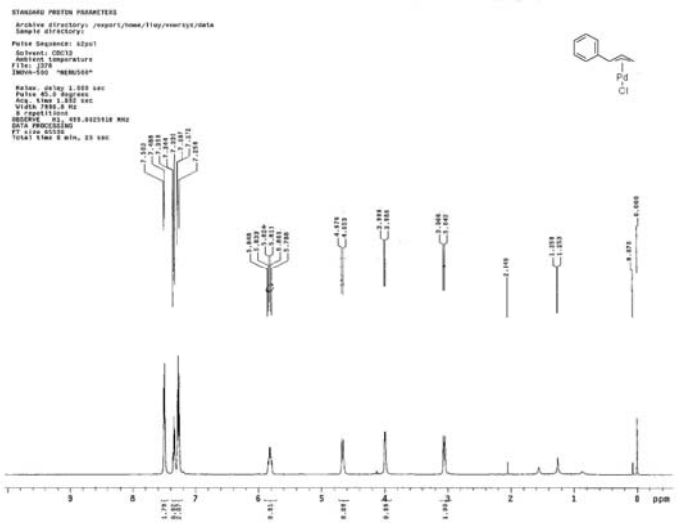


Figure S1. **^{1}H NMR of bis[acetate(trihaptoallylbenzene)palladium(II)]**

The compound **4**: ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.94 (broad, 1H), 3.88 (broad, 1H), 4.63 (broad, 1H), 5.87 (broad, 1H), 7.21 (d, J = 7.0 Hz, 2H), 7.35 (d, J = 7.0 Hz, 1H), 7.48 (broad, 2H).

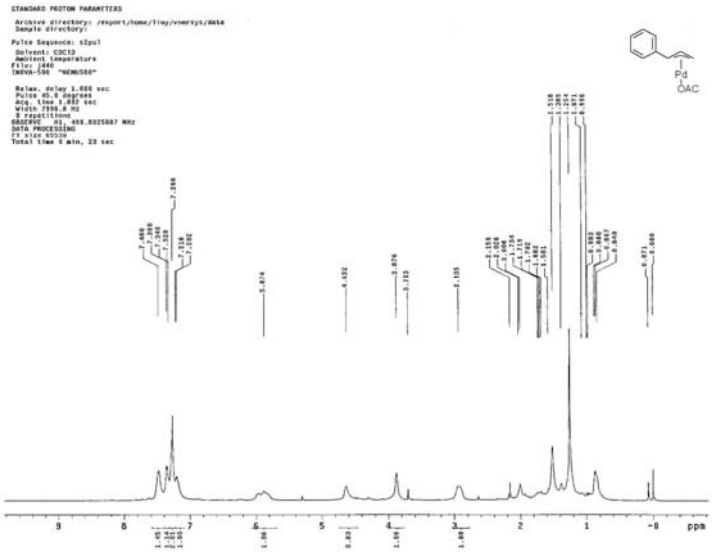
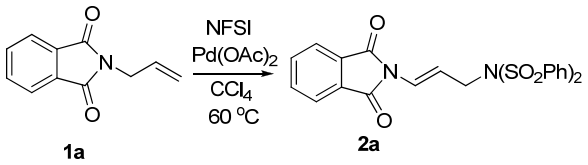


Figure S2. **^{1}H NMR of bis[chloro(trihaptoallylbenzene) palladium(II)] 5**

General procedure for the synthesis of 6 (with 6b1 as an example)

To a solution of Selectfluor (212.5 mg, 0.6 mmol) in water (1.5 mL) was added methyl tosylcarbamate (68.8 mg, 0.3 mmol) and allylbenzene (0.06 ml, 0.45 mmol) and $Pd(OAC)_2$ (6.7 mg, 0.03 mmol). The mixture was stirred at room temperature for 4 h (monitored by TLC), extracted with dichloromethane (5×3 mL), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by a shot flash silica gel column chromatography (10% ethyl ether/petro ether) to give compound **6b1** (85 mg, 82%).

Ⅲ. Allylic C–H amination of 1a with NFSI[a]



Entry	Catalyst (0.1 equiv)	Water (equiv)	Solvent	Additive (equiv)	Time (h)	Yield of **2a** (%)[b]
1	$Pd(OAc)_2$	None	CCl_4	None	5.5	0[c]
2	$Pd(OAc)_2$	0.1	CCl_4	None	5.5	57
3	$Pd(OAc)_2$	0.3	CCl_4	None	5.5	75
4	$Pd(OAc)_2$	0.5	CCl_4	None	5.5	75
5	**$Pd(OAc)_2$**	**0.3**	**CCl_4**	**KF (2.0)**	**14.0**	**88**
6	None	0.3	CCl_4	KF (2.0)	24.0	0
7	$Pd(OAc)_2$	0.3	CCl_4	KF (2.0)	24.0	0[d]
8	$Pd(OAc)_2$	0.3	CCl_4	KF (1.0)	3.5	48
9	$Pd(OAc)_2$	0.3	CCl_4	NaF (2.0)	22.5	47
10	$Pd(OAc)_2$	0.3	THF	KF (2.0)	8.5	15
11	$Pd(OAc)_2$	0.3	$C_6H_5CH_3$	KF (2.0)	2.0	64[e]
12	$Pd(TFA)_2$	0.3	CCl_4	KF (2.0)	1.5	52
13	$Pd(dba)_2$	0.3	CCl_4	KF (2.0)	2.5	72
14	$Pd(PPh_3)_4$	0.3	CCl_4	KF (2.0)	7.0	51
15	$PdCl_2$	0.3	CCl_4	KF (2.0)	24.0	0[f]

[a]Reactions were carried out with **1a** (1.2 mmol), NFSI (1.0 equiv) and Pd(II) catalyst (0.1 equiv) at 60 °C, unless specially mentioned. [b]Isolated yield. [c]Along with 44% **3a** obtained. [d] The reaction was carried out at room temperature. [e]The reaction was carried out at 100 °C. [f]80% **1a** was recovered.

1 S. A.Reed and M. C. White, *J. Am. Chem. Soc.* 2008, **130,** 3316.

2 B. M. Trost and P. J. Metzner, *J. Am. Chem. Soc.* 1980, **102**, 3572.

IV. Controlling Experiments

1). The stoichiometric reaction of $Pd(dba)_2$ with NFSI:

Under argon atmosphere, NFSI (0.10 mmol) and $Pd(dba)_2$ (0.025mmol) were added 1.0 mL $CDCl_3$ (dry with 4Å MS) at room temperature. After 5 minntes, the reaction was monitored by ^{19}F NMR, This stoichiometric reaction observed an two signals one at -37.7 ppm(NFSI) and another at -385.7 ppm, which characterized Pd–F bond and no signal appeared in $CDCl_3$ without pre-treatment with 4Å molecular seives.

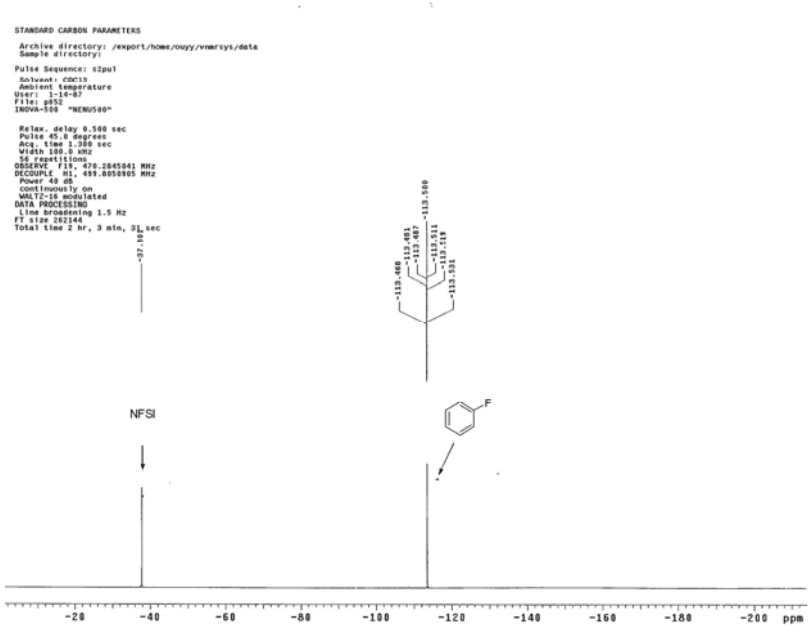


Figure S3. **The ^{19}F NMR spectroscopy of NFSI in $CDCl_3$(fluorobenzene as internal standard)**

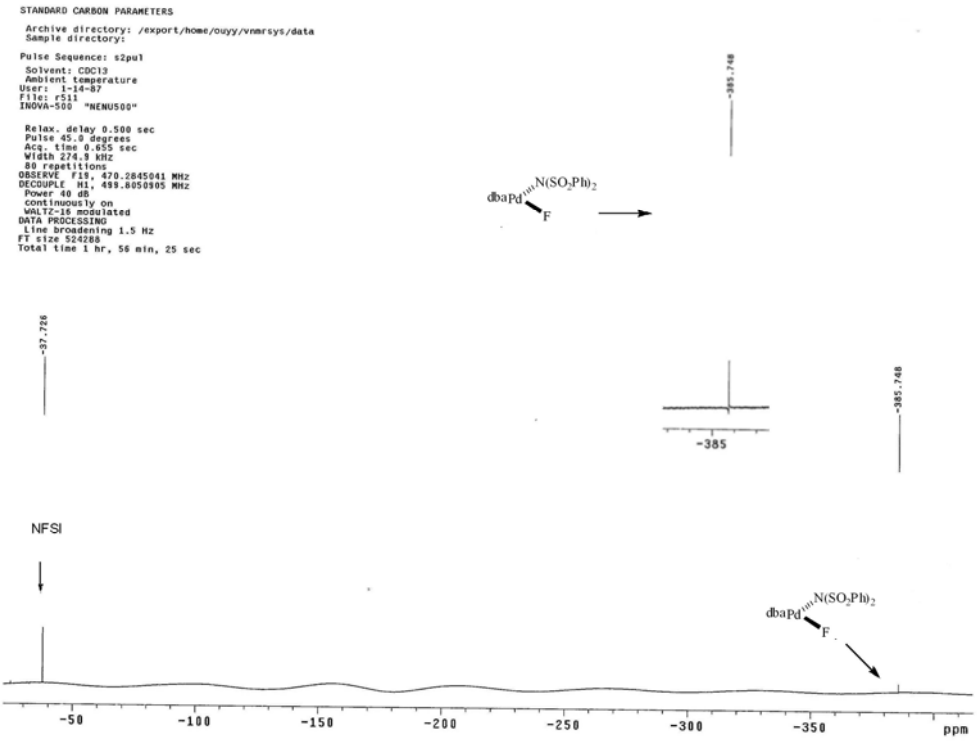


Figure S4. **The ^{19}F NMR spectroscopy of the reaction of $Pd(dba)_2$ with NFSI in $CDCl_3$**

2). The stoichiometric reaction of $Pd(dba)_2$, allylbenzene , NFSI and H_2O:

The mixture of allylbenzene (1.5 equiv), $Pd(dba)_2$ (0.025 mmol), water (4.0 equiv) and NFSI (4.0 equiv) in perchloromethane (1 ml, dry with P_2O_5) was reacted at room temperature for 30 min and 50 uL was used to perform the ESI in acetonitrile.

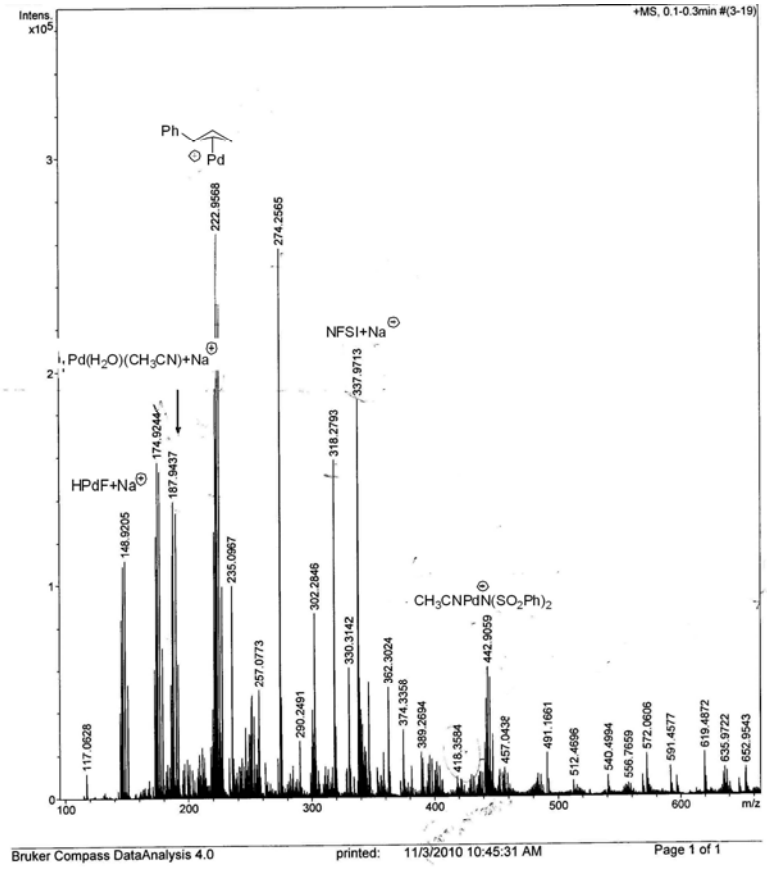
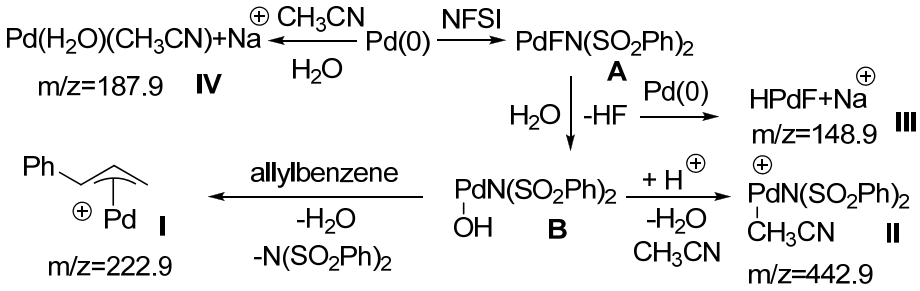


Figure S5. **The ESI(+)-MS of the reaction of allylbenzene, $Pd(dba)_2$, NFSI and H_2O**



Scheme S1. The proposed possible conversion procedure in ESI(+)-MS(Please note: The complexes A and B are in accord with scheme 2 of the paper and the other complexes use Roman numbers)

3). The stoichiometric reaction of $Pd(PPh_3)_4$, NFSI and H_2O:

The mixture of $Pd(PPh_3)_4$(0.025 mmol), water (4.0 equiv) and NFSI (4.0 equiv) in perchloromethane (1 ml, dry with P_2O_5) was reacted at room temperature for 30 min and 50 uL was used to perform the ESI in acetonitrile.

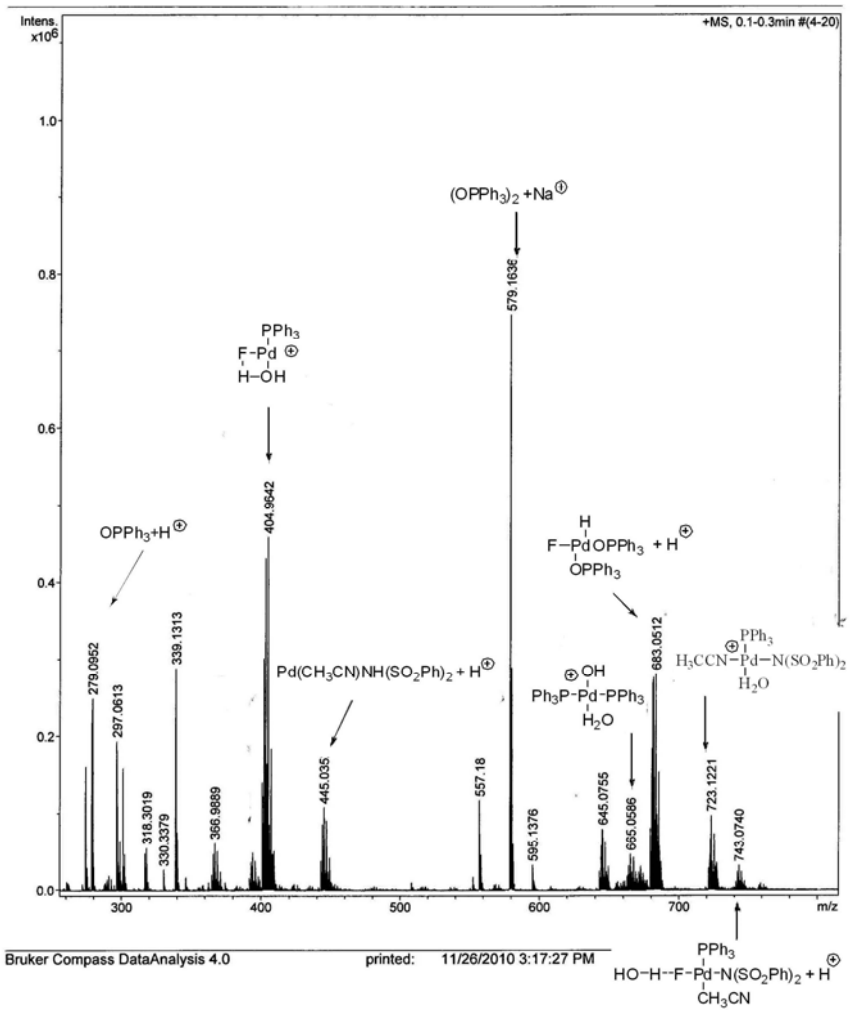
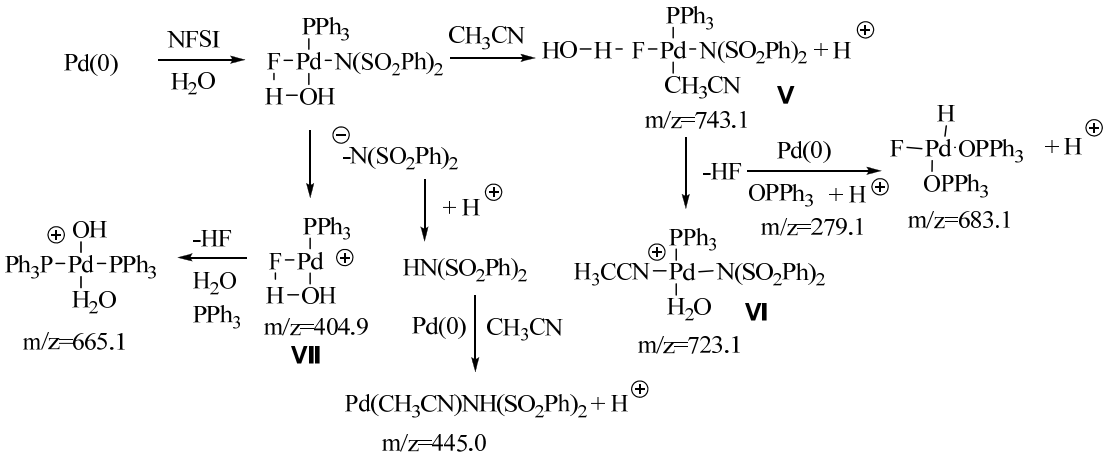
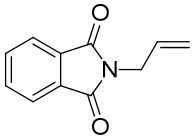


Figure S6. **The ESI(+)-MS of the reaction of $Pd(PPh_3)_4$, NFSI and H_2O**



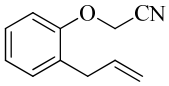
Scheme S2. **The proposed possible conversion procedure in ESI(+)-MS**

V. Analytical data of compounds 1, 2, 3, 4 and 6



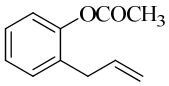
2-allylisoindoline-1,3-dione (1a)

White solid. Mp: 144 ^{o}C; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 4.30 (d, J = 6.0 Hz, 2H), 5.20 (d, J = 10.0 Hz, 1H), 5.26 (d, J = 17.5 Hz, 1H), 5.86-5.93 (m, 1H), 7.73 (dd, J_1 = 2.5 Hz, J_2 = 5.0 Hz, 2H), 7.86 (dd, J_1 = 6.0 Hz, J_2 = 5.0 Hz, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 39.9, 117.6, 123.2, 131.4, 131.9, 133.9, 167.8. IR (KBr, cm^{-1}): 3456, 1715, 1394, 946, 725. MS calcd *m/z* 187.1, found 188.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{11}H_9NO_2$: C, 70.58; H, 4.85; N, 7.48; Found: C, 70.56; H, 4.87; N, 7.49.



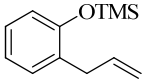
2-(2-allylphenoxy)acetonitrile (1c)

Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 3.39 (d, J = 7.0 Hz, 2H), 4.73 (s, 2H), 5.02-5.07 (m, 2H), 5.95 (dd, J_1 = 10.0 Hz, J_2 = 16.5 Hz, 1H), 6.90 (d, J = 8.5 Hz, 1H), 7.02-7.05 (m, 1H), 7.19-7.25 (m, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 34.1, 53.8, 111.9, 115.4, 115.9, 123.1, 127.6, 129.6, 130.7, 136.3, 154.3. IR (KBr, cm^{-1}): 1592, 1491, 1451, 1221, 1049, 917, 755. MS calcd *m/z* 173.1, found 174.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{11}H_{11}NO$: C, 76.28; H, 6.40; N, 8.09; Found: C, 76.32; H, 6.38; N, 8.10.



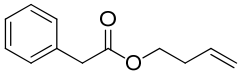
2-allylphenyl acetate (1d)

Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.27 (s, 3H), 3.30 (d, J = 6.5Hz, 2H), 5.04-5.07 (m, 2H), 5.85-5.93 (m, 1H), 7.02 (dd, J_1 = 1.5 Hz, J_2 = 6.5 Hz, 1H), 7.16 (dd, J_1 = 1.5 Hz, J_2 = 7.5 Hz, 1H), 7.18-7.24 (m, 2H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 20.8, 34.6, 116.1, 122.3, 126.1, 127.3, 130.3, 131.8, 135.8, 148.8, 169.2. IR (KBr, cm^{-1}): 1726, 1372, 1169, 746, 579, 549. MS calcd *m/z* 176.1, found 177.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{11}H_{12}O_2$: C, 74.98; H, 6.86; Found: C, 74.96; H, 6.87.



(2-allylphenoxy)trimethylsilane (1e)

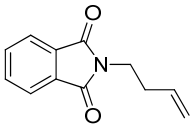
Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 0.26 (s, 9H), 3.34 (d, J = 6.5 Hz, 2H), 5.02-5.07 (m, 2H), 5.94 (m, 1H), 6.78 (dd, J_1 = 1.0 Hz, J_2 = 8.0 Hz, 1H), 6.90 (dt, J_1 = 1.0 Hz, J_2 = 7.5 Hz, 1H), 7.06-7.13 (m, 1H), 7.13 (dd, J_1 = 1.5 Hz, J_2 = 7.5 Hz, 1H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 0.5, 34.6, 115.5, 118.8, 121.4, 127.1, 130.2, 130.8, 137.1, 153.2. IR (KBr, cm^{-1}): 1490, 1257, 929, 844, 758. MS calcd *m/z* 206.1, found 207.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{12}H_{18}OSi$: C, 69.84; H, 8.79; Found: C, 69.84; H, 8.78.



But-3-enyl 2-phenylacetate (1g)

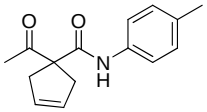
Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.22-2.26 (m, 2H), 3.50 (s, 2H), 4.03 (t, J = 7.0 Hz,

2H), 4.92-4.97 (m, 2H), 5.63 (dd, J_1 = 10.5 Hz, J_2 = 17.0 Hz, 1H), 7.13-7.21 (m, 5H). ^{13}C NMR(125 MHz; $CDCl_3$): δ = 32.8, 41.1, 63.6, 117.0, 126.8, 128.3, 129.1, 133.7, 133.9, 171.3. IR (KBr, cm^{-1}): 3066, 3031, 2958, 1737, 1249, 1147, 990, 918. MS calcd *m/z* 190.10, found 191.10 $[(M + 1)]^+$; Anal. Calcd for: $C_{12}H_{14}O_2$: C, 75.76; H, 7.42; Found: C, 75.73; H, 7.45.



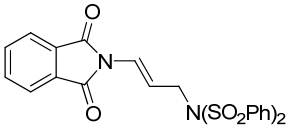
2-(but-3-enyl)isoindoline-1,3-dione (1h)

White solid. Mp: 92 °C; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.46 (dd, J_1 = 6.5 Hz, J_2 = 13.5 Hz, 2H), 3.77 (t, J = 7.0 Hz, 2H), 5.02 (d, J = 10.5 Hz, 1H), 5.07 (d, J = 17.0 Hz, 1H), 5.75-5.83 (m, 1H), 7.70-7.73 (m, 2H), 7.82-7.84 (m, 2H). ^{13}C NMR(125 MHz; $CDCl_3$): δ = 32.7, 37.2, 117.4, 123.1, 131.9, 133.8, 134.4, 168.2. IR (KBr, cm^{-1}): 3062, 2975, 2942, 1701, 1398, 1057, 936, 866, 723. MS calcd *m/z* 201.1, found 202.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{12}H_{11}NO_2$: C, 71.63; H, 5.51; N, 6.96; Found: C, 71.61; H, 5.53; N, 6.97.



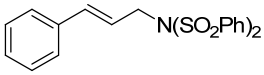
1-acetyl-*N*-p-tolylcyclopent-3-enecarboxamide (1k)

White solid. Mp: 122 °C; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.28 (s, 3H), 2.31 (s, 3H), 3.02 (d, J = 15.5 Hz, 2H), 3.12(d, J = 16.0 Hz, 2H), 5.68 (s, 2H), 7.12 (d, J = 8.0 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.61 (s, 1H). ^{13}C NMR(125 MHz; $CDCl_3$): δ = 20.7, 26.5, 39.4, 67.0, 119.9, 128.2, 129.4, 134.1, 135.0, 169.3, 207.0. IR (KBr, cm^{-1}): 3248, 3119, 3056, 2923, 2859, 1717, 1699, 1601, 1529, 1514, 1316, 814. MS calcd *m/z* 243.1, found 244.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{15}H_{17}NO_2$: C, 74.05; H, 7.04; N, 5.76; Found: C, 74.07; H, 7.02; N, 5.75.



(*E*)-*N*-(3-(1,3-dioxoisoindolin-2-yl)allyl)-*N*-(phenylsulfonyl)benzenesulfonamide (2a)

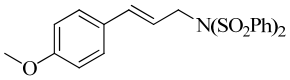
White solid. Mp: 192℃; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.46 (d, J = 7.0 Hz, 2H), 6.58-6.64 (m, 1H), 6,85 (d, J = 15.0 Hz, 1H), 7.55-7.64 (m, 4H), 7.71 (t, J = 6.5 Hz, 2H), 7.70 (dd, J_1 = 3.0 Hz, J_2 = 5.5 Hz, 2H), 7.88 (dd, J_1 = 3.0 Hz, J_2 = 5.5 Hz, 2H), 8.07-8.13 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 49.8, 114.3, 122.5, 123.8, 128.3, 129.1, 131.4, 133.8, 134.7, 139.8, 165.9. IR (KBr, cm^{-1}): 1720, 1369, 1164, 717, 579, 545. MS calcd *m/z* 482.1, found 483.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{23}H_{18}N_2O_6S_2$: C, 57.25; H, 3.76; N, 5.81. Found: C, 57.23; H, 3.74; N, 5.82.



***N*-cinnamyl-*N*-(phenylsulfonyl)benzenesulfonamide (2b)**

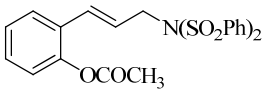
Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.50 (d, J = 7.0 Hz, 2H), 6.05-6.10 (m, 1H), 6.59 (d, J = 16.0 Hz, 1H), 7.24-7.33 (m, 6H), 7.41-7.51 (m, 4H), 7.60 (m, 2H), 8.05 (dd, J_1 = 1.5 Hz, J_2 = 8.5 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 51.3, 123.3, 126.6, 128.2, 128.3, 128.6, 128.9, 133.8, 135.3, 139.9. IR (KBr, cm^{-1}): 1374, 1182, 912, 747, 579, 547. MS calcd *m/z* 413.1, found 414.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{21}H_{19}NO_4S_2$: C, 61.00; H, 4.63; N, 3.39. Found: C, 61.03; H,

4.64; N, 3.37.



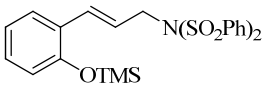
(*E*)-*N*-(3-(4-methoxyphenyl)allyl)-*N*-(phenylsulfonyl)benzenesulfonamide (2c)

White solid. Mp: 187 ^{o}C; ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.83 (s, 3H), 4.48 (d, J = 6.5 Hz, 2H), 5.93 (dt, J_1 = 6.5 Hz, J_2 = 14.0 Hz, 1H), 6.55 (d, J = 15.5 Hz, 1H), 6.85 (d, J = 9.0 Hz, 2H), 7.21 (d, J = 8.5 Hz, 2H), 7.50 (t, J = 8.0 Hz, 4H), 7.61 (t, J = 7.0 Hz, 2H), 8.04 (d, J = 8.0 Hz, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 51.5, 55.3, 113.9, 120.9, 127.9, 128.3, 128.6, 128.9, 133.7, 134.9, 140.0, 159.6. IR (KBr, cm^{-1}): 1375, 1227, 1057, 917, 745, 550. MS calcd *m/z* 443.1, found 444.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{22}H_{21}NO_5S_2$; C, 59.57; H, 4.77; N, 3.16. Found: C, 59.58; H, 4.75; N, 3.15.



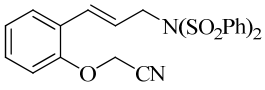
(*E*)-2-(3-(*N*-(phenylsulfonyl)phenylsulfonamido)prop-1-enyl)phenyl acetate (2d)

White solid. Mp: 165 ^{o}C; ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.31 (s, 3H), 4.48 (d, J = 6.5 Hz, 2H), 6.12 (dt, J_1 = 6.5 Hz, J_2 = 16.0 Hz, 1H), 6.68 (d, J = 16.0 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 7.19 (t, J = 7.5 Hz, 1H), 7.29-7.35 (m, 2H), 7.51 (t, J = 8.0 Hz, 4H), 7.62 (t, J = 7.5 Hz, 2H), 8.02 (t, J = 7.5 Hz, 4H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 20.9, 51.1, 122.7, 125.9, 126.2, 127.1, 128.3, 128.5, 129.0, 129.1, 129.1, 133.8, 139.8, 148.1, 169.4. IR (KBr, cm^{-1}): 1764, 1374, 1172, 912, 745,581, 550. MS calcd *m/z* 471.1, found 472.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{23}H_{21}NO_6S_2$: C, 58.58; H, 4.49; N, 2.97; Found: C, 58.59; H, 4.46; N, 2.95.



(*E*)-*N*-(phenylsulfonyl)-*N*-(3-(2-(trimethylsilyloxy)phenyl)allyl)benzenesulfonamide (2e)

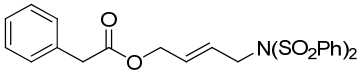
Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 0.16-0.22 (m, 9H), 4.43 (d, J = 6.0 Hz, 2H), 6.02 (dt, J_1 = 6.0 Hz, J_2 = 16.0 Hz, 1H), 6.72 (d, J = 8.0 Hz, 1H), 6.83 (t, J = 7.5 Hz, 2H), 7.06-7.09 (m, 1H), 7.15-7.17 (m, 1H), 7.41 (t, J = 7.5 Hz, 4H), 7.51 (t, J = 7.5 Hz, 2H), 7.97 (t, J = 7.0 Hz, 4H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 0.36, 51.8, 119.6, 121.5, 123.4, 127.0, 127.2, 128.3, 128.9, 129.1, 130.9, 133.7, 140.0, 152.9. IR (KBr, cm^{-1}): 1484, 1375, 1254, 1169, 846, 578, 550. MS calcd *m/z* 501.1, found 502.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{24}H_{27}NO_5S_2Si$: C, 57.46; H, 5.42; N, 2.79; Found: C, 57.49; H, 5.44; N, 2.76.



(*E*)-*N*-(3-(2-(cyanomethoxy)phenyl)allyl)-*N*-(phenylsulfonyl)benzenesulfonamide (2f)

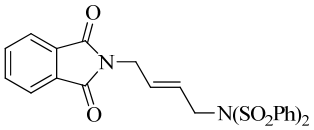
Yellow oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 4.51 (dd, J_1 = 1.0 Hz, J_2 = 7.0 Hz, 2H), 4.77 (s, 2H), 6.09 (dt, J_1 = 6.5 Hz, J_2 = 16.0 Hz, 1H), 6.88 (d, J =16.0 Hz, 1H), 6.95 (d, J = 8.0 Hz, 1H), 7.03 (t, J = 7.0 Hz, 1H), 7.25-7.31 (m, 2H), 7.49 (t, J = 8.0 Hz, 4H), 7.59-7.62 (m, 2H), 8.04 (t, J = 8.0 Hz, 4H). ^{13}C NMR (125 MHz; $CDCl_3$): δ = 51.5, 53.8, 112.5, 115.0, 123.2, 125.2, 125.9, 127.5, 128.2, 128.9, 129.0, 129.4, 133.8, 139.8, 153.5. IR (KBr, cm^{-1}): 1374, 1168, 911, 747, 580, 551. MS calcd *m/z* 468.1, found 469.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{23}H_{20}N_2O_5S_2$: C, 58.96; H, 4.30; N,

5.98; Found: C, 58.99; H, 4.28; N, 5.97.



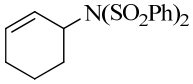
(*E*)-4-(*N*-(phenylsulfonyl)phenylsulfonamido)but-2-enyl 2- phenylacetate (2g)

Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.64 (s, 2H), 4.32 (d, J = 6.5 Hz, 2H), 4.50 (d, J = 5.5 Hz, 2H), 5.65-5.69 (m, 1H), 5.78 (dd, J_1 = 5.5 Hz, J_2 = 15.5 Hz, 1H), 7.25-7.34 (m, 5H), 7.51 (t, J = 8.0 Hz, 4H), 7.67 (t, J = 7.0 Hz, 2H), 8.01 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 41.2, 50.1, 63.8, 127.2, 127.8, 128.2, 128.6, 129.0, 129.2, 129.7, 133.7, 133.9, 139.8, 171.1. IR (KBr, cm^{-1}): 1738, 1735, 1168, 745, 582, 550. MS calcd *m/z* 485.1, found 486.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{24}H_{23}NO_6S_2$: C, 59.36; H, 4.77; N, 2.88. Found: C, 59.34; H, 4.79; N, 2.87..



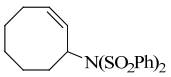
(*E*)-*N*-(4-(1,3-dioxoisoindolin-2-yl)but-2-enyl)-*N*-(phenylsulfonyl)benzenesulfonamide (2h)

Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 4.23 (d, J = 5.0 Hz, 2H), 4.29 (d, J = 6.0 Hz, 2H), 5.65 (dd, J_1 = 7.5 Hz, J_2 = 15.0 Hz, 1H), 5.77 (dd, J_1 = 7.5 Hz, J_2 = 15.5 Hz, 1H), 7.50-7.59 (m, 6H), 7.74-7.78 (m, 2H), 7.83-7.88 (m, 2H), 7.89-8.02 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 38.5, 49.8, 123.3, 126.9, 128.1, 128.2, 129.0, 129.8, 131.9, 133.8, 134.1, 139.6, 167.7. IR (KBr, cm^{-1}): 1715, 1374, 1169, 720, 583, 550. MS calcd *m/z* 496.1, found 497.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{24}H_{20}N_2O_6S_2$: C, 58.05; H, 4.06; N, 5.64. Found: C, 58.03; H, 4.07; N, 5.66.



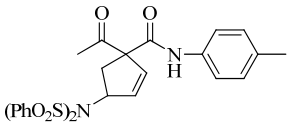
***N*-(cyclohex-2-enyl)-*N*-(phenylsulfonyl)benzenesulfonamide (2j)**

White solid. Mp: 154 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 1.57-1.59 (m, 1H), 1.85-1.86 (m, 2H), 1.92-1.96 (m, 1H), 2.07-2.09 (m, 1H), 2.39-2.42 (m, 1H), 4.83 (t, J = 3.5 Hz, 1H), 5.37 (d, J = 10.5 Hz, 1H), 5.72-5.74 (m, 1H), 7.56 (t, J = 7.5 Hz, 4H), 7.65 (t, J = 7.5 Hz, 2H), 8.02-8.07 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 22.8, 23.9, 28.5, 60.8, 126.9, 128.2, 128.9, 129.0, 129.8, 133.7. IR (KBr, cm^{-1}): 1336, 1170, 721. MS calcd *m/z* 377.1, found 378.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{18}H_{19}NO_4S_2$: C, 57.27; H, 5.07; N, 3.71. Found: C, 57.25; H, 5.07; N, 3.70.



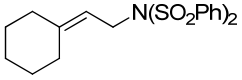
(*Z*)-*N*-(cyclooct-2-enyl)-*N*-(phenylsulfonyl)benzenesulfonamide (2k)

White solid. Mp: 187 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 1.25-1.37 (m, 2H), 1.43-1.49 (m, 2H), 1.57-1.77 (m, 3H), 1.99-2.09 (m, 2H), 2.36-2.42 (m, 1H), 5.08-5.14 (m, 1H), 5.59-5.65 (m, 1H), 5.96-6.00 (m, 1H), 7.52-7.58 (m, 4H), 7.61-7.66 (m, 2H), 8.01-8.06 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 25.0, 25.8, 25.9, 28.9, 35.1, 61.2, 128.3, 128.8, 128.9, 131.2, 133.5, 133.6. IR (KBr, cm^{-1}): 1335, 720, 722. MS calcd *m/z* 405.1, found 406.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{20}H_{23}NO_4S_2$: C, 59.23; H, 5.72; N, 3.45. Found: C, 59.26; H, 5.73; N, 3.43.



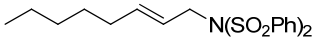
1-acetyl-4-(*N*-(phenylsulfonyl)phenylsulfonamido)-*N*-p-tolylcyclopent-2-enecarboxamide (2l)

White soild. Mp: 183 ^{o}C. (Major isomer/minor isomer = 5/4) ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.26 (s, 6H), 2.28-2.36 (m, 7H), 2.78 (dd, J_1 = 5.0 Hz, J_2 = 14.0 Hz, 1H), 2.94 (dd, J_1 = 9.5 Hz, J_2 = 14.5 Hz, 1H), 3.28 (dd, J_1 = 9.0 Hz, J_2 = 14.5 Hz, 1H), 5.45 (dd, J_1 = 7.0 Hz, J_2 = 9.0 Hz, 1H), 5.51-5.54 (m, 1H), 5.75 (dd, J_1 = 2.0 Hz, J_2 = 5.5 Hz, 1H), 5.96 (dd, J_1 = 1.5 Hz, J_2 = 5.5 Hz, 1H), 6.11 (dd, J_1 = 2.5 Hz, J_2 = 6.0 Hz, 1H), 6.29 (dd, J_1 = 2.0 Hz, J_2 = 5.5 Hz, 1H), 7.06(d, J = 8.0 Hz, 2H), 7.12 (t, J = 8.0 Hz, 3H), 7.31-7.39 (m, 4H), 7.50-7.54 (m, 8H), 7.57-7.71 (m, 4H), 7.79 (s, 1H), 8.02-8.06 (m, 7H), 8.10 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 20.8, 27.8, 27.9, 36.1, 37.1, 66.1, 66.4, 73.4, 73.9, 119.4, 119.8, 120.0, 126.4, 128.2, 129.2, 129.3, 129.4, 129.5, 129.9, 132.3, 132.9, 134.0, 134.1, 134.3, 134.5, 134.6, 135.2, 135.9, 139.8, 140.1, 166.3, 169.6, 201.3, 208.7. IR (KBr, cm^{-1}): 1718, 1654, 1529, 1316, 814. MS calcd *m/z* 538.1, found 539.1 [(M + 1)]$^{+}$; Anal. Calcd for: $C_{27}H_{26}N_2O_6S_2$: C, 60.21; H, 4.87; N, 5.20; Found: C, 60.23; H, 4.86; N, 5.18.

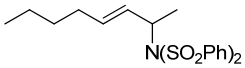


_N_-(2-cyclohexylideneethyl)-_N_-(phenylsulfonyl)benzenesulfonamide (2m)

White soild. Mp: 121 ^{o}C. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.54 (s, 6H), 2.02 (*d*, J = 6.0 Hz, 2H), 2.20 (s, 2H), 4.37 (d, J = 7.0 Hz, 2H), 5.12 (t, J = 7.0 Hz, 1H), 7.53-5.58 (m, 4H), 7.62-7.66 (m, 2H), 8.02-8.11 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 27.3, 28.0, 36.8, 46.8, 116.1, 128.1, 128.5, 128.9, 133.6, 145.4. IR (KBr, cm^{-1}): 1333, 1171, 724. MS calcd *m/z* 405.1, found 406.1 [(M + 1)]$^{+}$; Anal. Calcd for: C, 59.23; H, 5.72; N, 3.45; Found: C, 59.203; H, 5.74; N, 3.48.

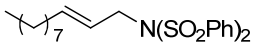


(*E*)-_N_-(oct-2-enyl)-_N_-(phenylsulfonyl)benzenesulfonamide (2n)

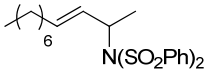


(*E*)-_N_-(oct-3-en-2-yl)-_N_-(phenylsulfonyl)benzenesulfonamide (2n')

Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.75-0.79 (m, 1H), 0.82-0.91 (m, 3H), 1.15-1.32 (m, 3H), 1.40 (*d*, J = 6.5 Hz, 2H), 1.89-1.95 (m, 2H), 4.29 (dd, J_1 = 4.0 Hz, J_2 = 6.5 Hz, 0.5H), 4.74 (t, J = 7.0 Hz, 0.5H), 5.34 (dd, J_1 = 7.0 Hz, J_2 = 15.0 Hz, 1H), 5.73-5.78 (m, 1H), 7.52-7.57 (m, 4H), 7.61-7.66 (m, 2H), 7.99-8.05 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.9, 14.0, 17.6, 20.5, 22.1, 30.9, 31.4, 31.7, 32.0, 51.2, 66.4, 128.3, 128.6, 128.7, 128.8, 128.8, 128.9, 129.0, 129.0, 131.4, 133.5, 133.7, 135.2. IR (KBr, cm^{-1}): 1333, 724. MS calcd *m/z* 407.1, found 408.1 [(M + 1)]$^{+}$; Anal. Calcd for: C, 58.94; H, 6.18; N, 3.44; Found: C, 58.90; H, 6.14; N, 3.47.



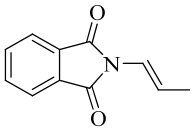
(*E*)-_N_-(phenylsulfonyl)-_N_-(undec-2-enyl)benzenesulfonamide (2o)



(*E*)-_N_-(phenylsulfonyl)-_N_-(undec-3-en-2-yl)benzenesulfonamide (2o')

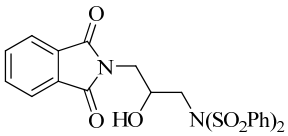
Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 0.85-0.90 (m, 5H), 1.21-1.26 (m, 14H), 1.48 (d, J = 7.0 Hz, 2H), 1.59 (dd, J_1 = 1.5 Hz, J_2 = 6.5 Hz, 1H), 1.88-1.95 (m, 2H), 4.30 (t, J = 5.5 Hz, 0.5H), 4.74 (t, J = 7.0 Hz, 0.5H), 5.33-5.39 (m, 1H), 5.72-5.77 (m, 1H), 7.54 (d, J = 7.5 Hz, 5H), 7.61-7.65 (m, 2H), 7.99-8.04 (m, 5H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 13.7, 13.9, 14.0, 19.1, 22.5, 28.4, 30.5, 31.4, 32.0, 51.2, 65.5, 128.1, 128.1, 128.2, 128.3, 128.3, 128.8, 128.8, 128.9, 128.9, 129.0, 130.9, 133.7, 133.8, 137.3. IR (KBr, cm^{-1}): 1336, 1169, 724. MS calcd *m/z* 449.2, found 45.0.2 [(M + 1)]$^{+}$; Anal. Calcd for: C, 61.44; H, 6.95; N, 3.12; Found: C, 61.47; H, 6.93; N,

3.15.



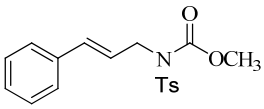
(*E*)-2-(prop-1-enyl)isoindoline-1,3-dione (3a)

White solid. Mp: 203 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 1.85 (d, J = 5.5 Hz, 3H), 6.55-6.63 (m, 2H), 7.73 (dd, J_1 = 3.0 Hz, J_2 = 5.5 Hz, 2H), 7.86 (dd, J_1 = 3.5 Hz, J_2 = 6.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 16.3, 118.1, 118.3, 123.4, 131.7, 134.2, 166.7. IR (KBr, cm^{-1}): 1716, 1394, 943, 728. MS calcd *m/z* 187.1, found 188.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{11}H_9NO_2$: C, 70.58; H, 4.85; N, 7.48. Found: C, 70.57; H, 4.88; N, 7.44.



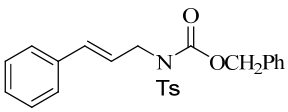
***N*-(3-(1,3-dioxoisoindolin-2-yl)-2-hydroxypropyl)-*N*-(phenylsulfonyl)benzenesulfonamide (4a)**

Yellow solid. Mp: 165 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 3.03 (d, J = 5.5 Hz, 1H), 3.77-3.87 (m, 4H), 4.32-4.33 (m, 1H), 7.55 (dd, J_1 = 2.0 Hz, J_2 = 7.5 Hz, 4H), 7.64-7.68 (m, 2H), 7.71-7.74 (m, 2H), 7.83-7.86 (m, 2H), 8.05-8.07 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 41.6, 52.1, 69.2, 123.4, 128.5, 129.1, 131.8, 134.1, 134.2, 139.0, 168.5. IR (KBr, cm^{-1}): 1718, 1398, 1170, 720, 580. MS calcd *m/z* 500.1, found 501.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{23}H_{20}N_2O_7S_2$: C, 55.19; H, 4.03; N, 5.60; Found: C, 55.21; H, 4.07; N, 5.63.



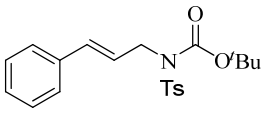
Methyl cinnamyl(tosyl)carbamate (6b1)

Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.42 (s, 3H), 3.72 (s, 3H), 4.63 (t, J = 3.5 Hz, 2H), 6.22-6.27 (m, 1H), 6.67 (d, J = 16.0 Hz, 1H), 7.27 (d, J = 8.5 Hz, 3H), 7.33 (t, J = 8.0 Hz, 2H), 7.37 (d, J = 7.0 Hz, 2H), 7.84 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.6, 48.8, 53.9, 123.8, 126.6, 127.9, 128.5, 128.6, 129.3, 134.1, 136.3, 136.5, 144.6, 152.7. IR (KBr, cm^{-1}): 1735, 1359, 1168, 674, 576, 544. MS calcd *m/z* 345.1, found 346.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{18}H_{19}NO_4S$: C, 62.59; H, 5.54; N, 4.06; Found: C, 62.55; H, 5.55; N, 4.09.



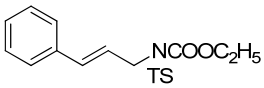
Benzyl cinnamyl(tosyl)carbamate (6b2)

White solid. Mp: 106 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 2.37 (s, 3H), 4.63 (d, J = 6.0 Hz, 2H), 5.10 (s, 2H), 6.22-6.27 (m, 1H), 6.62 (d, J = 16.0 Hz, 1H), 7.14 (d, J = 8.0 Hz, 2H), 7.20 (d, J = 6.5 Hz, 2H), 7.24-7.33 (m, 8H), 7.73 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.5, 48.8, 69.0, 123.7, 126.6, 127.9, 128.4, 128.5, 128.5, 128.5, 129.2, 134.2, 134.5, 136.3, 136.5, 144.4, 152.1. IR (KBr, cm^{-1}): 1728, 1357, 1153, 720, 673. MS calcd *m/z* 421.1, found 422.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{24}H_{23}NO_4S$: C, 68.39; H, 5.50; N, 3.32; Found: C, 68.41; H, 5.53; N, 3.31.



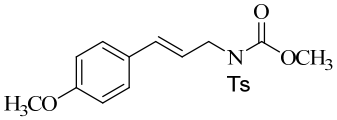
Tert-butyl cinnamyl(tosyl)carbamate (6b3)

Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.36 (s, 9H), 2.42 (s, 3H), 4.61 (t, J = 3.5 Hz, 2H), 6.25-6.31 (m, 1H), 6.66 (d, J = 16.0 Hz, 1H), 7.26 (d, J = 8.0 Hz, 3H), 7.33 (t, J = 7.5 Hz, 2H), 7.38 (d, J = 7.5 Hz, 2H), 7.80 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.6, 27.9, 48.5, 84.3, 124.3, 126.6, 127.8, 128.1, 128.6, 129.2, 133.9, 136.5, 137.3, 144.1, 150.8. IR (KBr, cm^{-1}):1731, 1356, 1169, 743, 545. MS calcd *m/z* 387.1, found 388.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{21}H_{25}NO_4S$: C, 65.09; H, 6.50; N, 3.61; Found: C, 65.07; H, 6.52; N, 3.64.



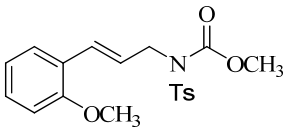
Ethyl cinnamyl(tosyl)carbamate (6b4)

Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 1.19 (d, J = 7.0 Hz, 3H), 2.42 (s, 3H), 4.15 (dd, J_1 = 7.0 Hz, J_2 = 14.0 Hz, 2H), 4.63 (dd, J_1 = 1.0 Hz, J_2 = 6.5 Hz, 2H), 6.22-6.28 (m, 1H), 6.58 (d, J = 15.5 Hz, 1H), 7.26 (d, J = 9.0 Hz, 3H), 7.33 (t, J = 7.5 Hz, 2H), 7.38 (d, J = 7.5 Hz, 2H), 7.83 (d, J = 8.5 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ =13.9, 21.6, 48.6, 63.4, 123.8, 126.5, 127.9, 128.5, 128.5, 129.2, 134.1, 136.3, 136.6, 144.5, 152.1. IR (KBr, cm^{-1}):1731, 1357, 1153, 721, 673. MS calcd *m/z* 359.1, found 360.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{19}H_{21}NO_4S$: C, 63.49; H, 5.89; N, 3.90; Found: C, 63.47; H, 5.87; N, 3.92.



(*E*)-tert-butyl 3-(4-methoxyphenyl)allyl(tosyl)carbamate (6f)

Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.41 (s, 3H), 3.71 (s, 3H), 3.82 (s, 3H), 4.60 (d, J = 7.5 Hz, 2H), 6.09 (d, J = 16.0 Hz, 1H), 6.62 (d, J = 16.0 Hz, 1H), 6.86 (d, J = 9.0 Hz, 3H), 7.28 (d, J = 7.5 Hz, 1H), 7.31 (d, J = 9.0 Hz, 2H), 7.83 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.6, 48.9, 53.8, 55.3, 113.9, 121.5, 127.8, 128.5, 129.0, 129.3, 131.0, 133.7, 136.5, 144.5, 152.7, 159.5. IR (KBr, cm^{-1}): 1734, 1511, 1249, 1170, 1033, 579. MS calcd *m/z* 375.1, found 376.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{19}H_{21}NO_5S$: C, 60.78; H, 5.64; N, 3.73; Found: C, 60.75; H, 5.62; N, 3.76.

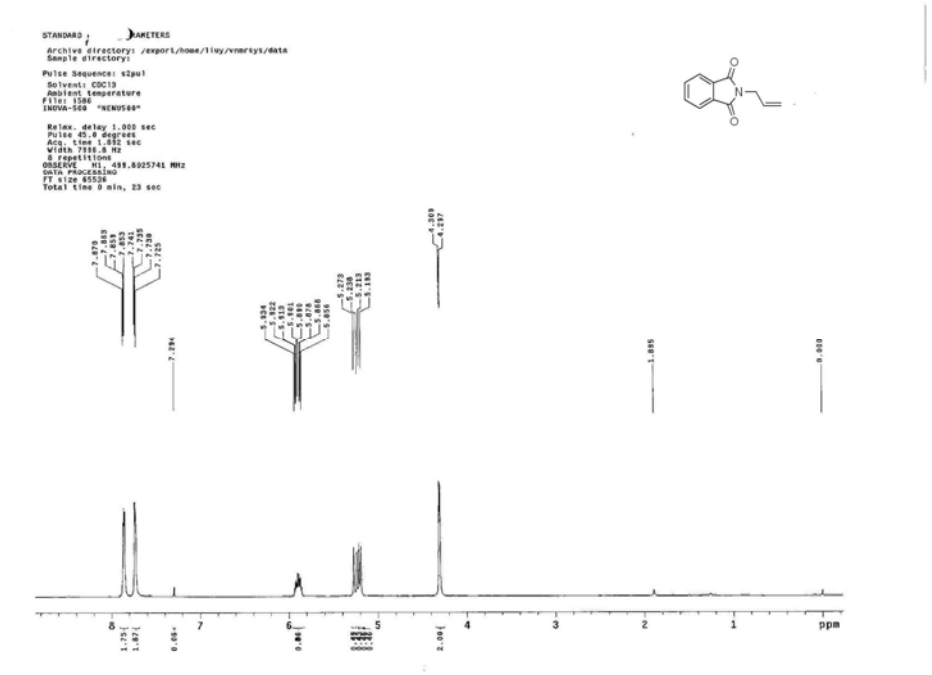


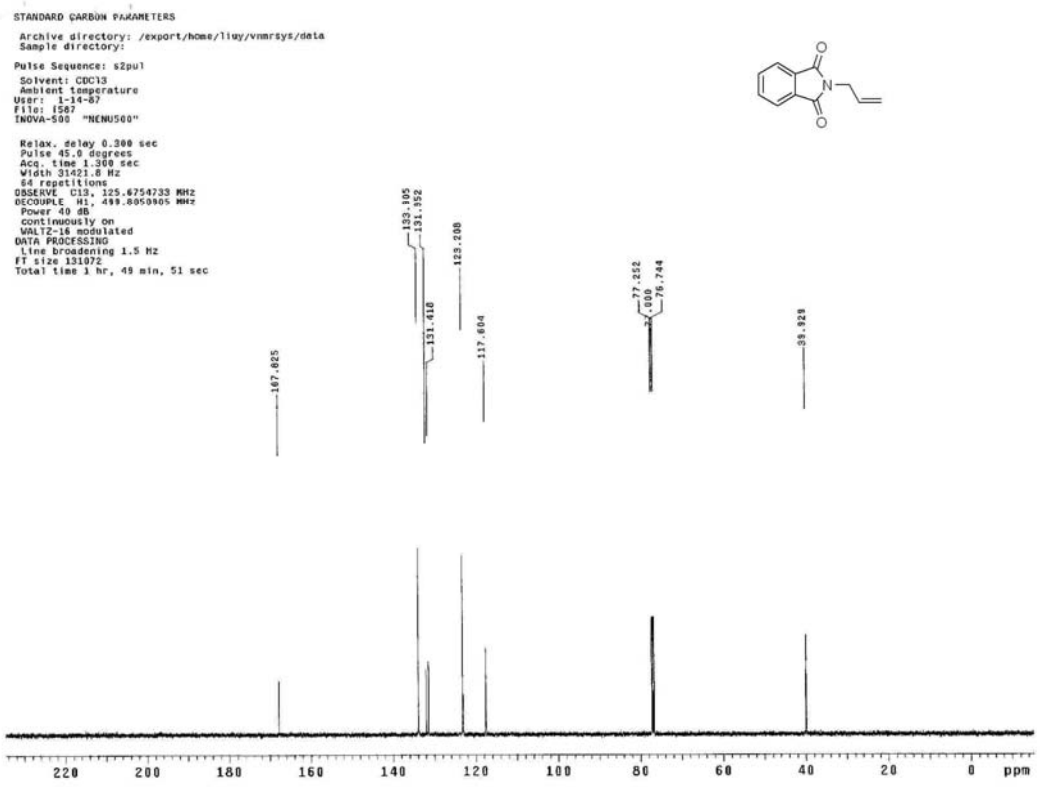
(*E*)-methyl 3-(2-methoxyphenyl)allyl(tosyl)carbamate (6l)

Colorless oil. ^{1}H NMR (500 MHz; $CDCl_3$): δ = 2.41 (s, 3H), 3.71 (s, 3H), 3.85 (s, 3H), 4.63 (d, J = 6.5 Hz, 2H), 6.21-6.27 9 (m, 1H), 6.87-6.93 (m, 2H), 7.01 (d, J = 15.5 Hz, 1H), 7.23-7.26 (m, 3H), 7.39 (t, J = 6.5 Hz, 1H), 7.86 (d, J = 8.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 21.4, 49.1, 53.6, 55.3, 110.7, 120.5, 124.2, 125.2, 126.9, 128.5, 128.9, 129.1, 129.2, 136.4, 144.3, 152.6, 156.8. IR (KBr, cm^{-1}): 1735, 1360, 1245, 1170, 1027, 756. MS calcd *m/z* 375.1, found 376.1 $[(M + 1)]^+$; Anal. Calcd for: $C_{19}H_{21}NO_5S$: C, 60.78; H, 5.64; N, 3.73; Found: C, 60.78; H, 5.61; N, 3.76.

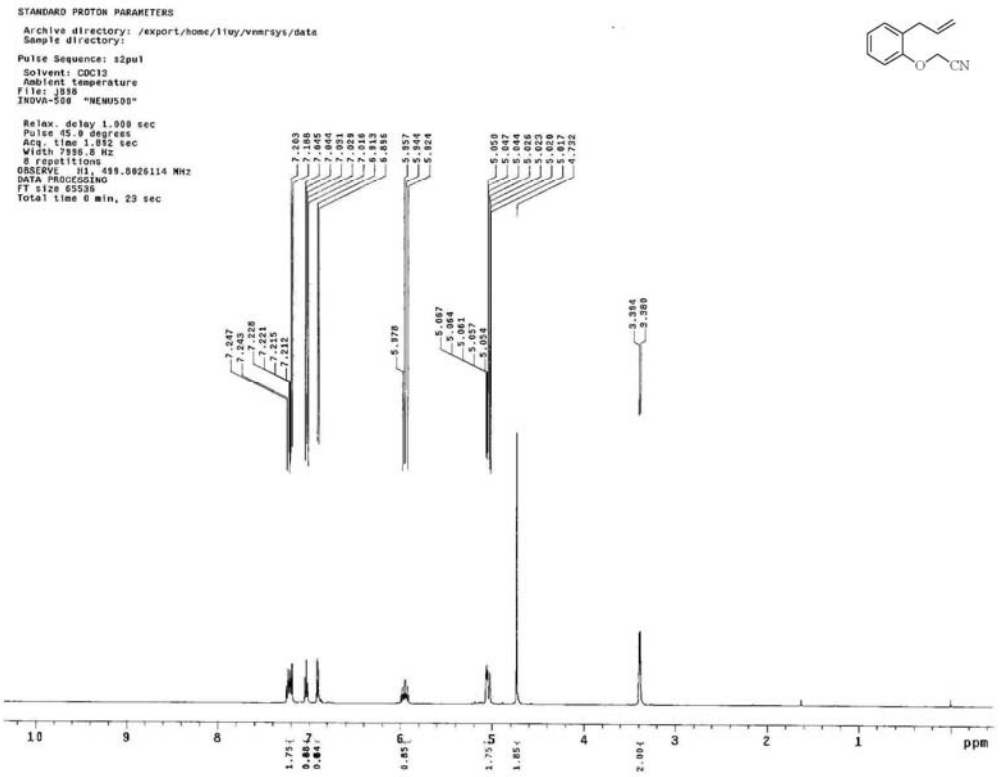
VI. ^{1}H NMR and ^{13}C NMR spectra copies

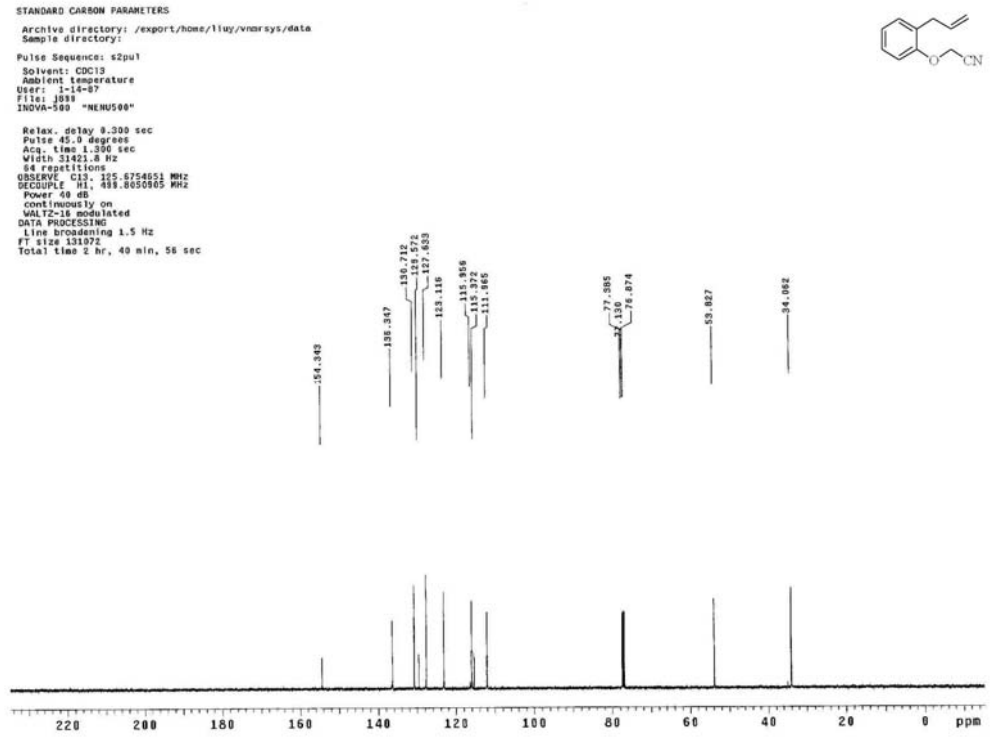
Compound **1a**



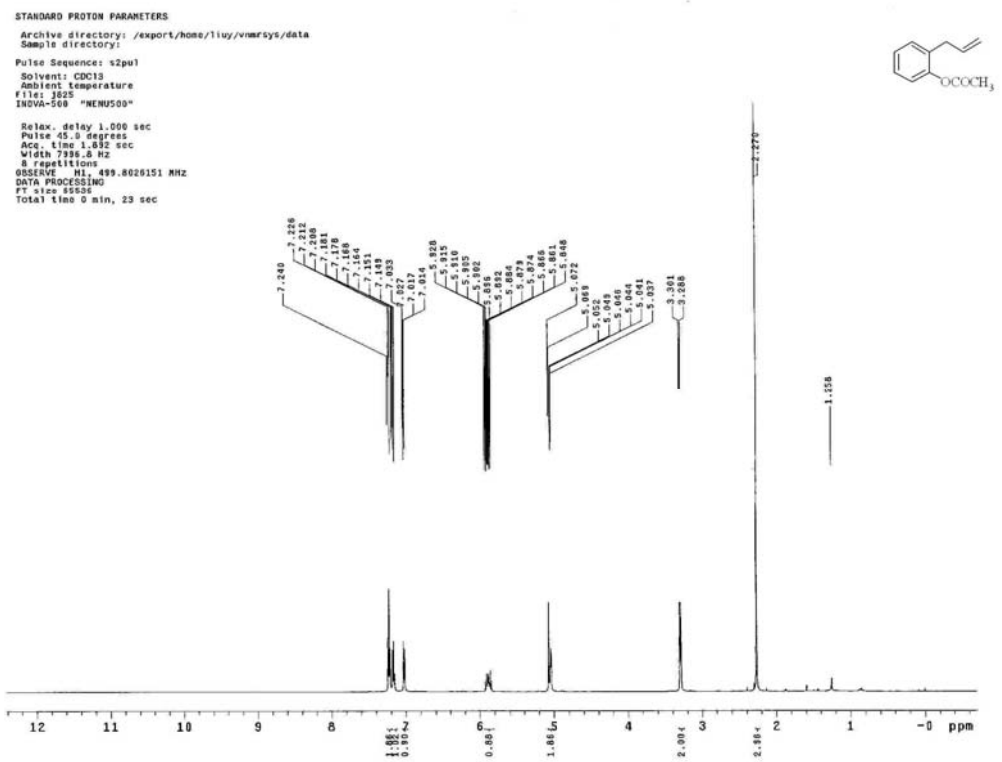


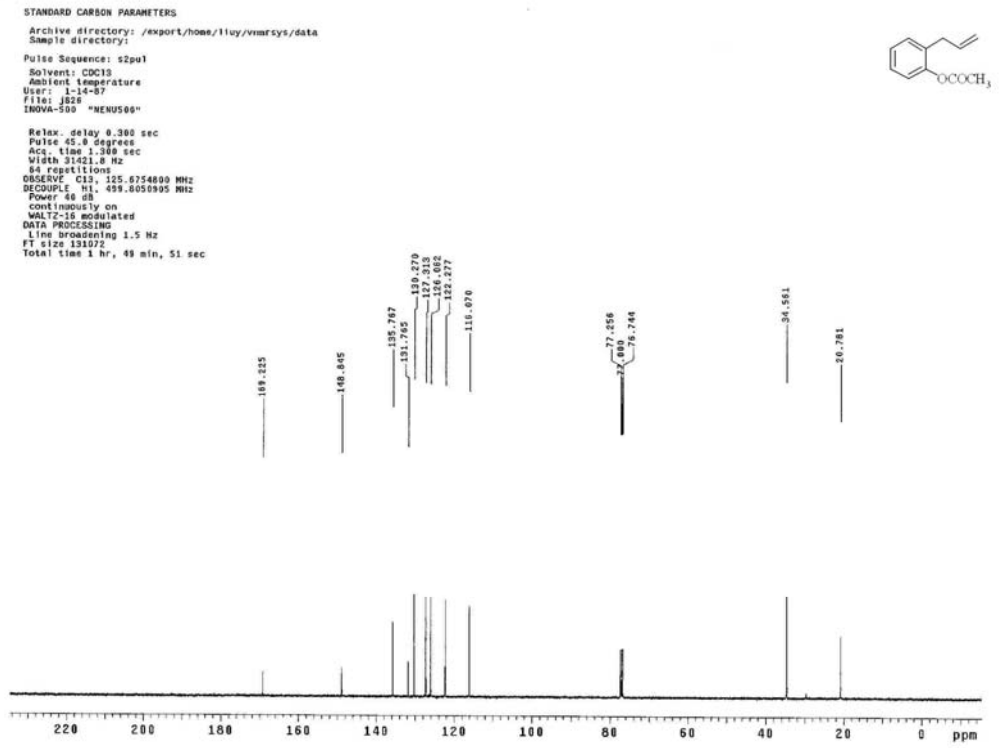
Compound **1c**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j088
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7998.8 Hz
8 repetitions
OBSERVE H1, 499.8826114 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
CN
ppm

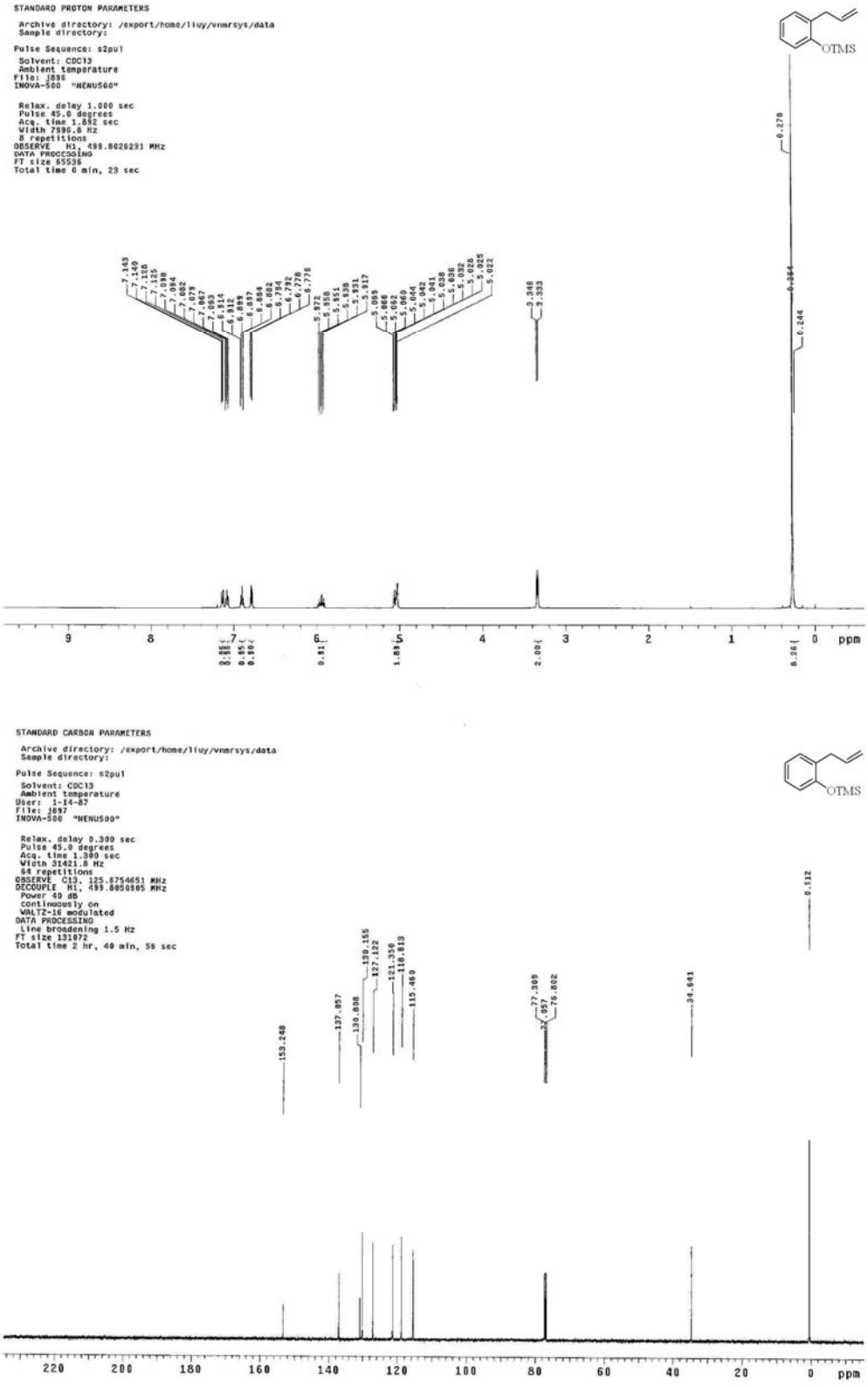

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: j088
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754651 MHz
DECOUPLE H1, 499.8050985 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
CN
ppm

Compound **1d**

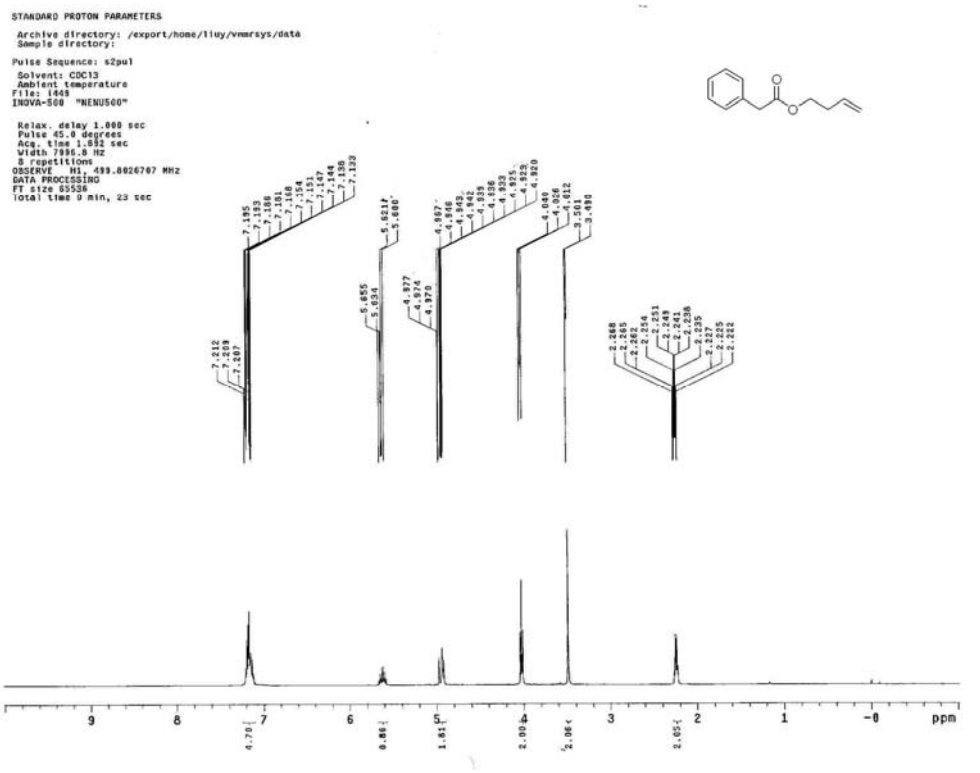

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j025
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8026151 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
OCOCH3
ppm

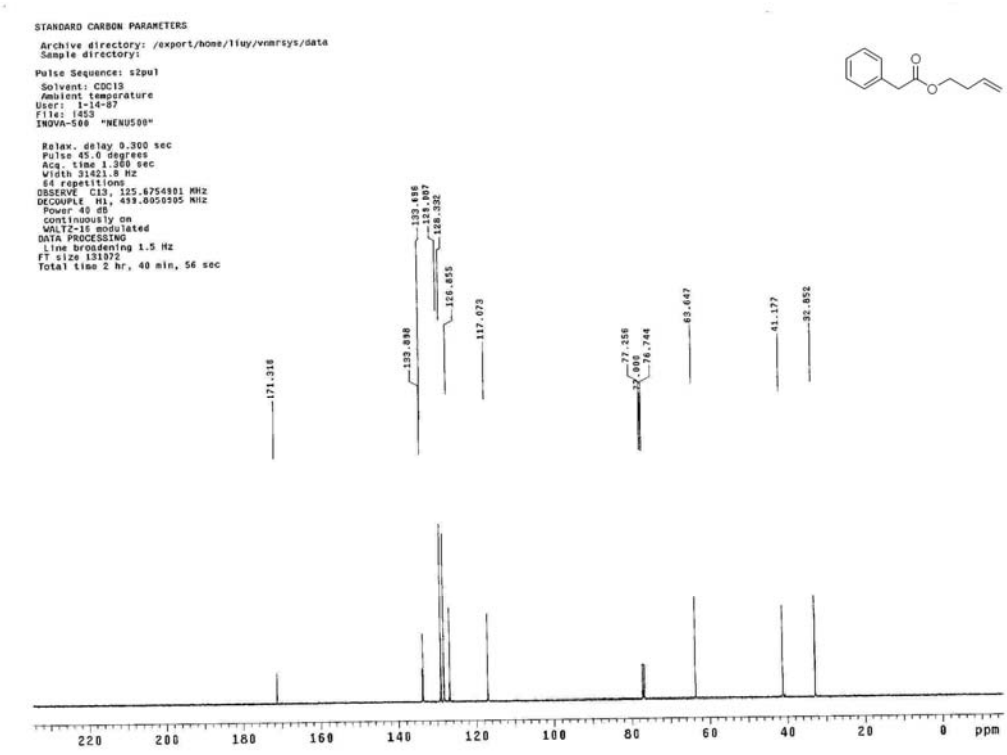

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: j026
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754800 MHz
DECOUPLE H1, 499.8050995 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
OCOCH3
ppm

Compound **1e**

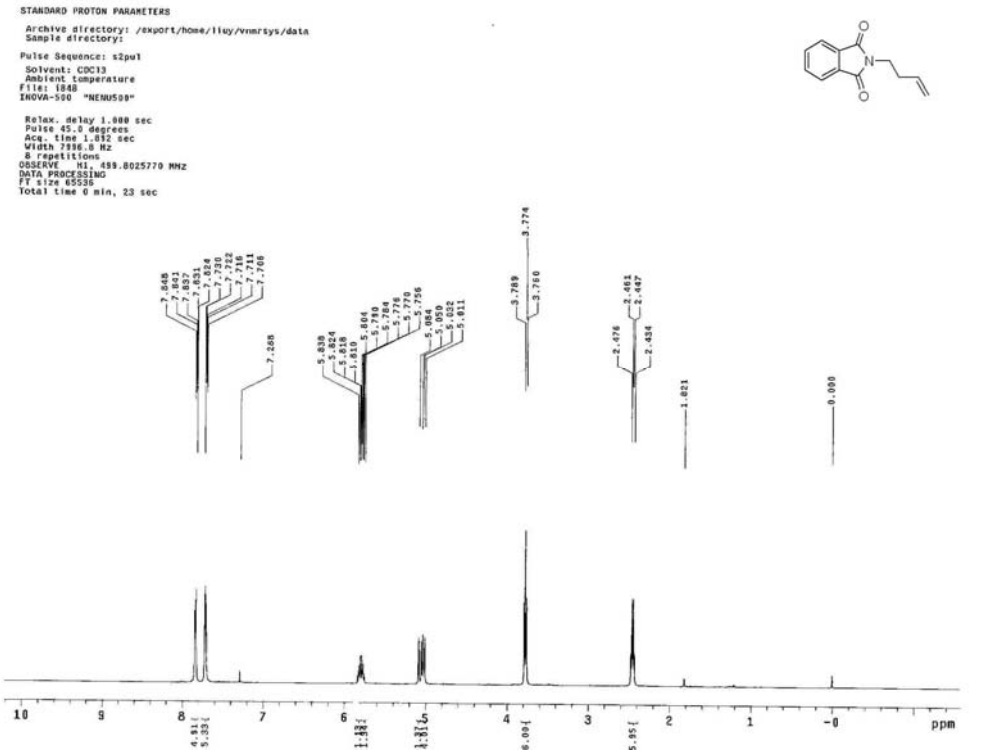

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j895
INOVA-500 "MENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7396.8 Hz
8 repetitions
OBSERVE H1, 499.8026231 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
OTMS
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: j897
INOVA-500 "MENUS00"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754651 MHz
DECOUPLE H1, 499.8050305 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
OTMS
ppm

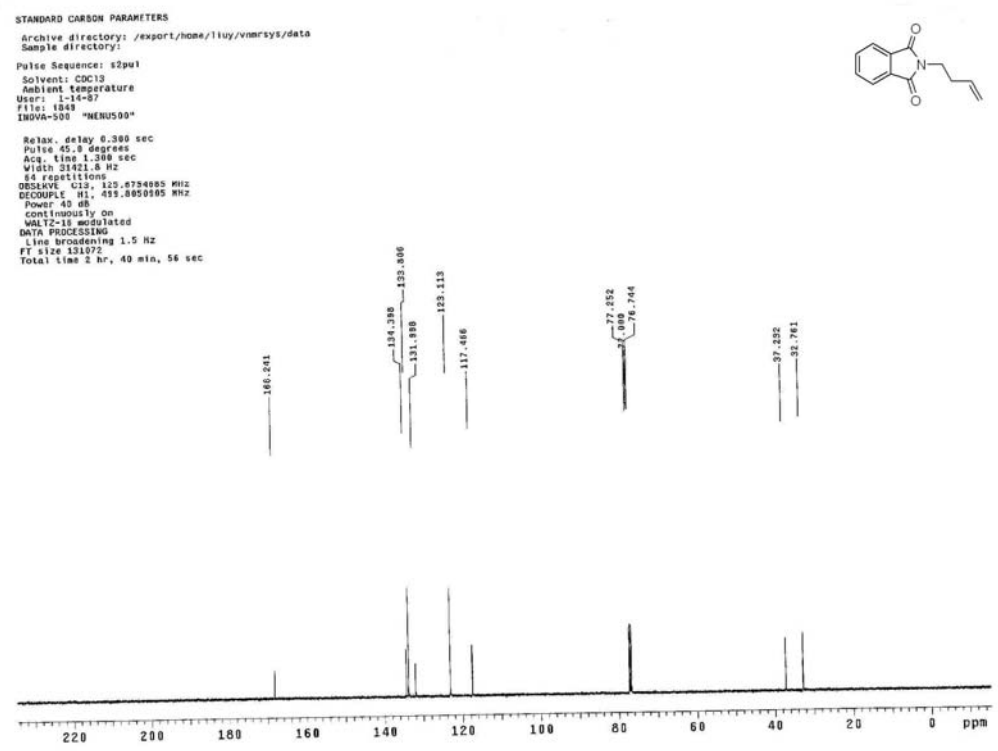
Compound **1g**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1469
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8026707 MHz
DATA PROCESSING
FT size 65536
Total time 9 min, 23 sec
ppm

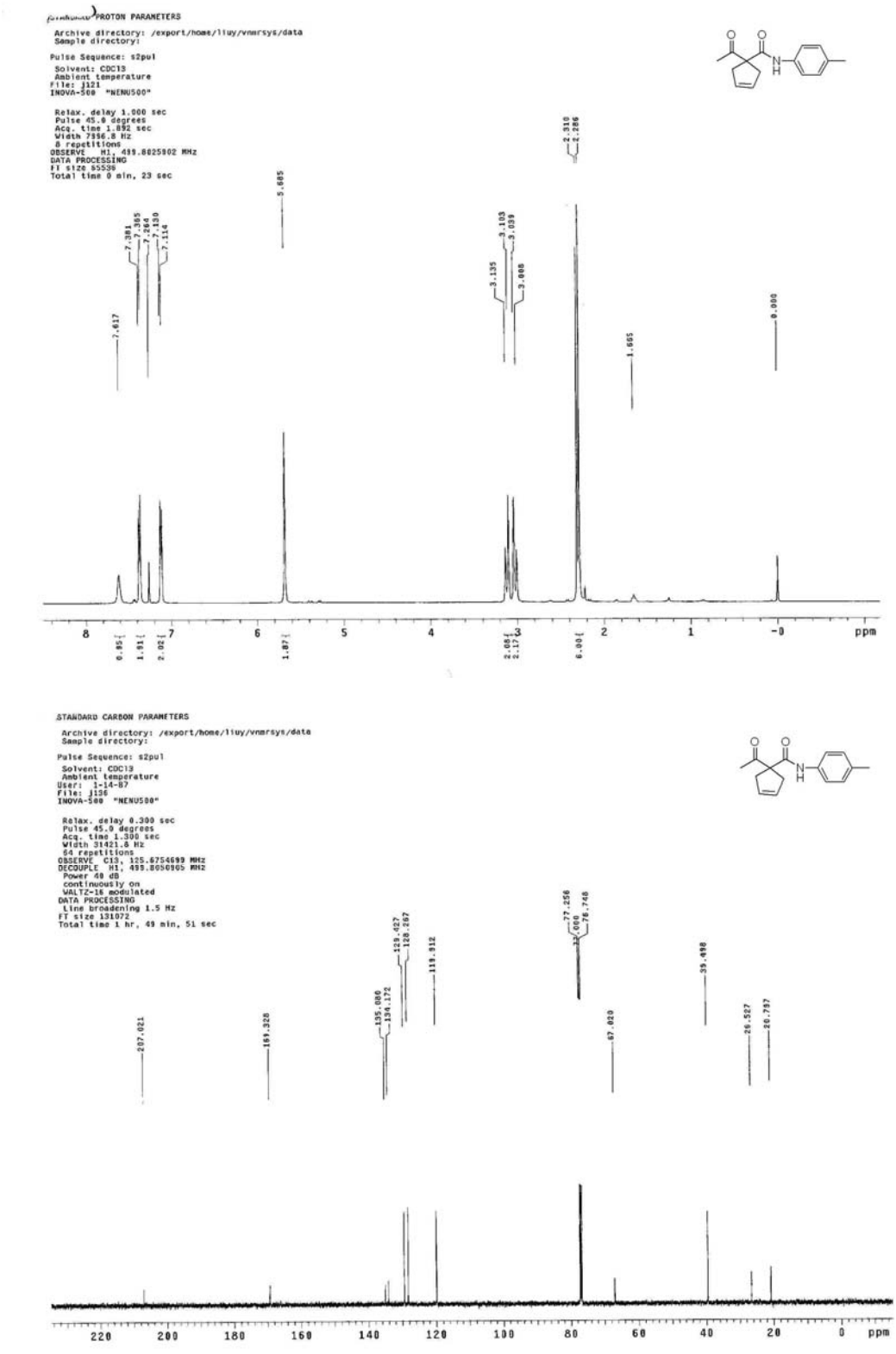

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: 1453
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.360 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754981 MHz
DECOUPLE H1, 499.8050305 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
ppm

Compound **1h**

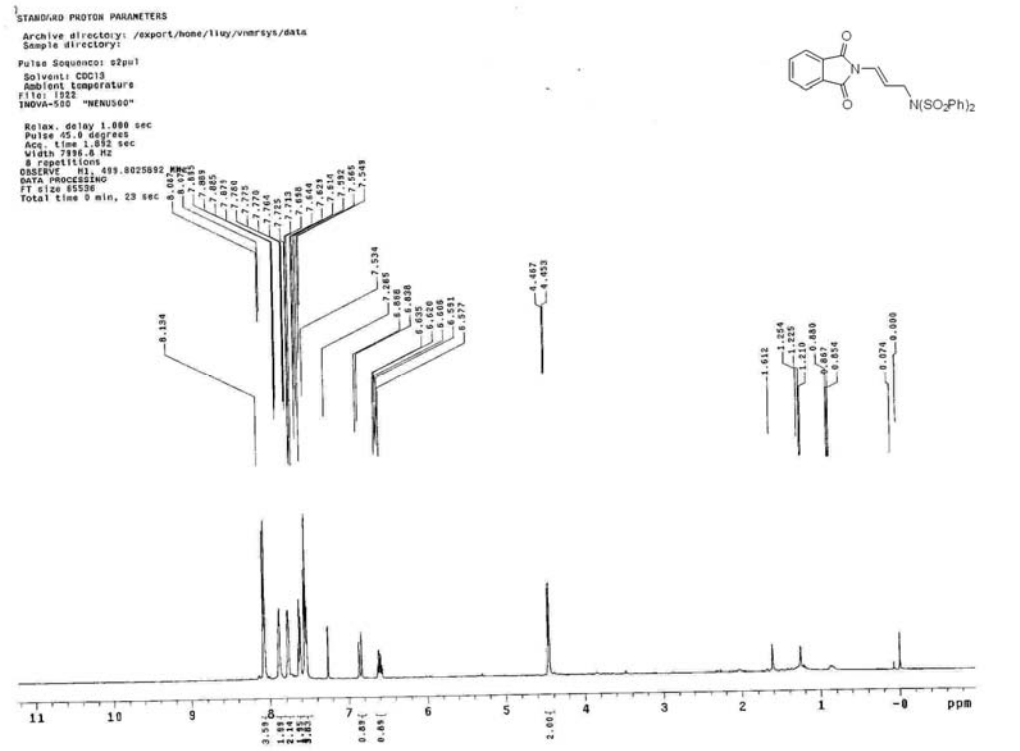

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1848
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.852 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8025770 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

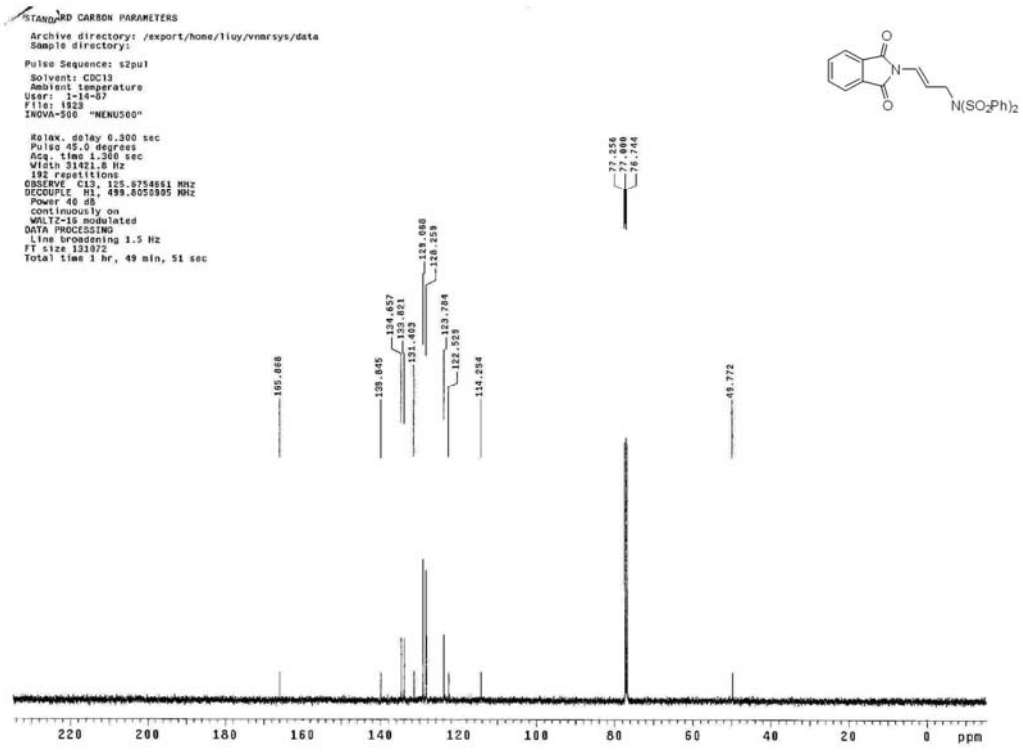

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: 1849
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754885 MHz
DECOUPLE H1, 499.8050505 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
ppm

Compound **1k**

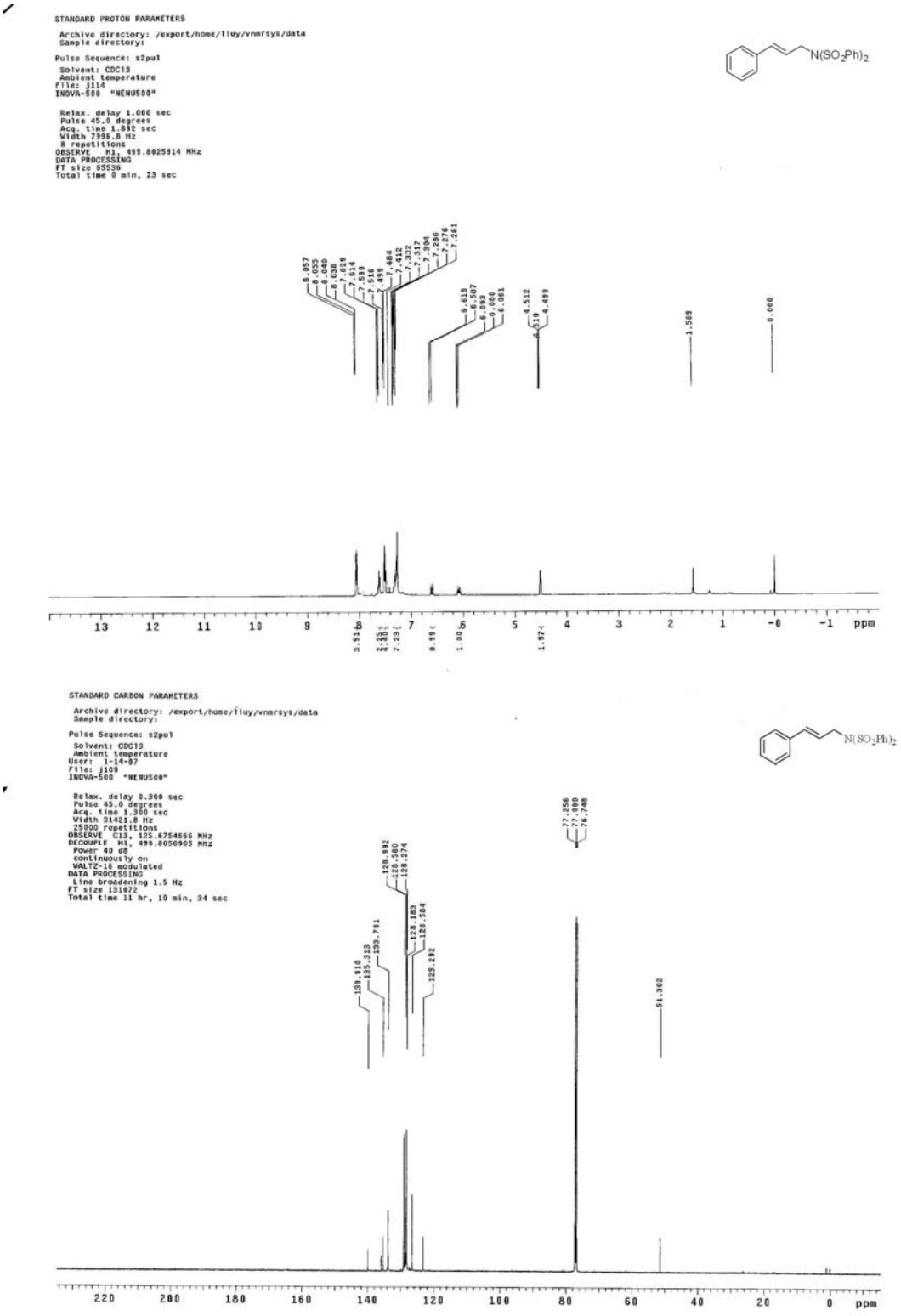

PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: jl21
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7936.8 Hz
8 repetitions
OBSERVE H1, 499.8825802 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.617
7.381
7.365
7.264
7.130
7.114
5.685
3.135
3.103
3.059
3.008
2.310
2.286
1.665
0.900
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: jl36
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754699 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
207.021
169.328
135.080
134.172
129.027
128.267
111.912
77.256
77.000
76.748
67.020
55.498
26.527
26.797
ppm

Product **2a**

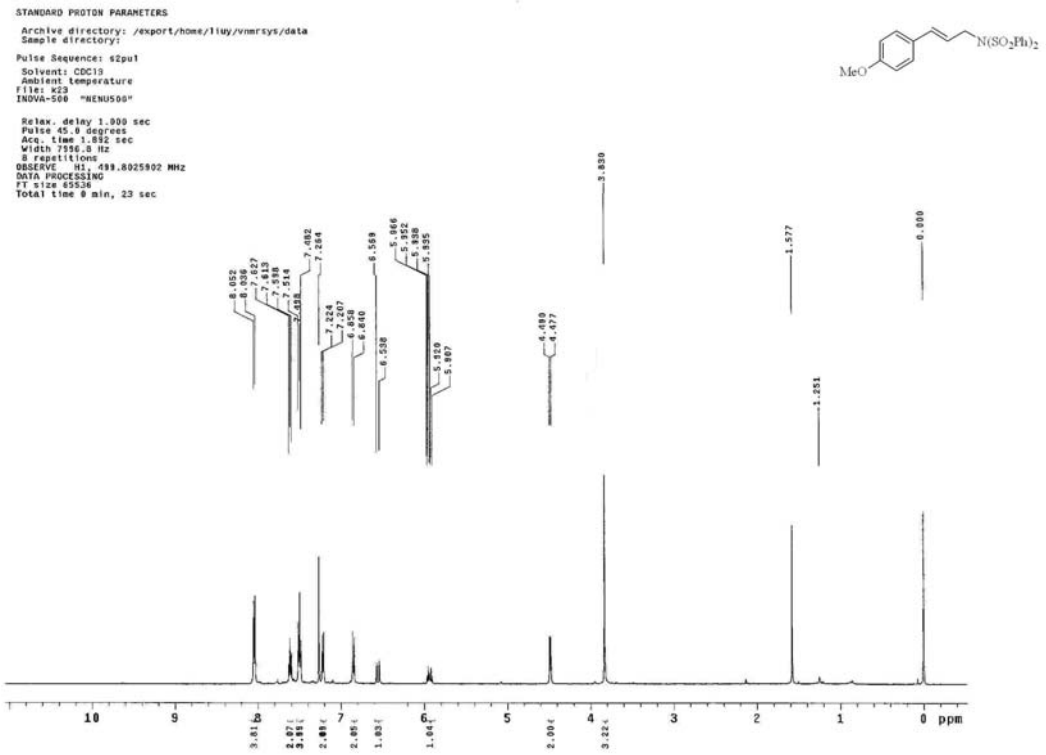

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1922
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7986.8 Hz
8 repetitions
OBSERVE H1, 499.8025892 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
N(SO2Ph)2
ppm

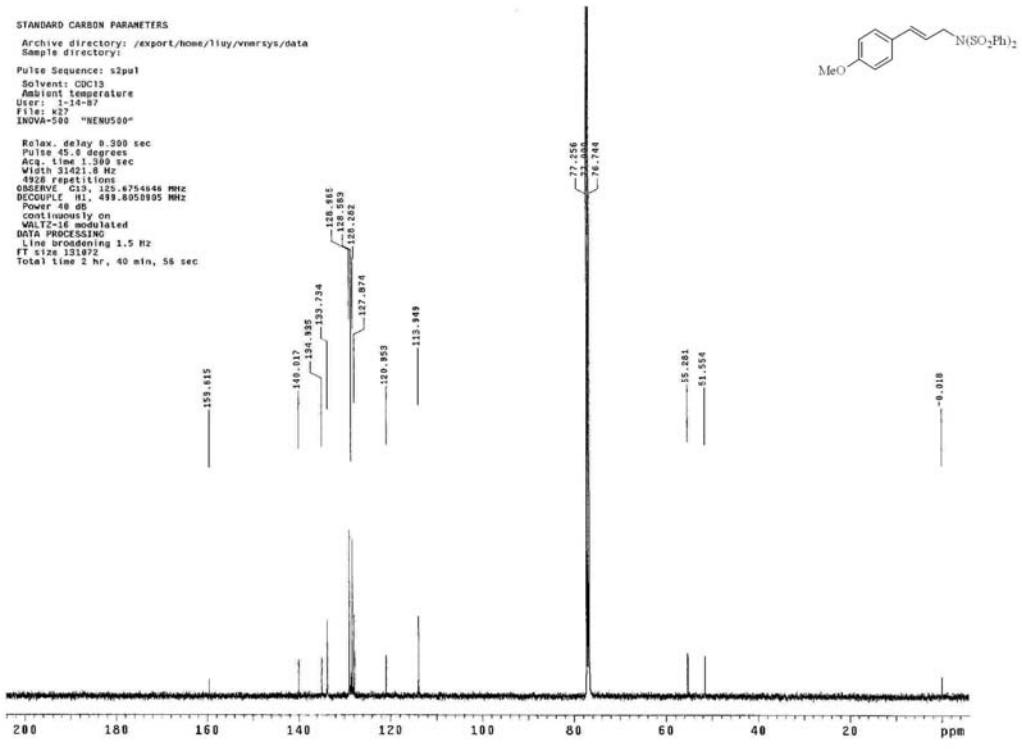

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: 1923
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.8754651 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
N(SO2Ph)2
ppm

Product **2b**

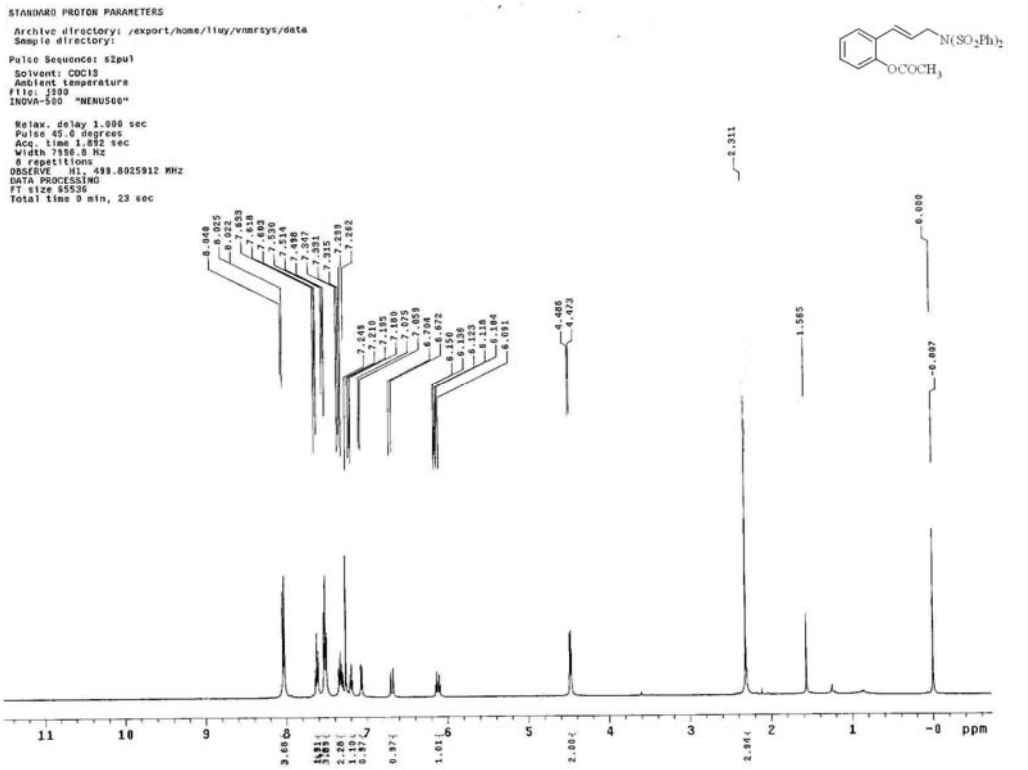

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: jj14
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7398.8 Hz
8 repetitions
OBSERVE H1, 499.8025914 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
N(SO2Ph)2
8.057
8.055
8.048
8.046
7.628
7.614
7.559
7.555
7.484
7.412
7.332
7.327
7.304
7.286
7.270
7.261
6.613
6.587
6.089
6.080
6.061
4.512
4.510
4.493
1.569
0.000
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: jj09
INOVA-500 "NENUS00"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
25000 repetitions
OBSERVE C13, 125.6754656 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 11 hr, 10 min, 34 sec
N(SO2Ph)2
139.910
135.313
133.781
129.892
129.450
128.274
128.183
126.584
125.292
77.256
77.000
76.744
51.302
220 200 180 160 140 120 100 80 60 40 20 0 ppm

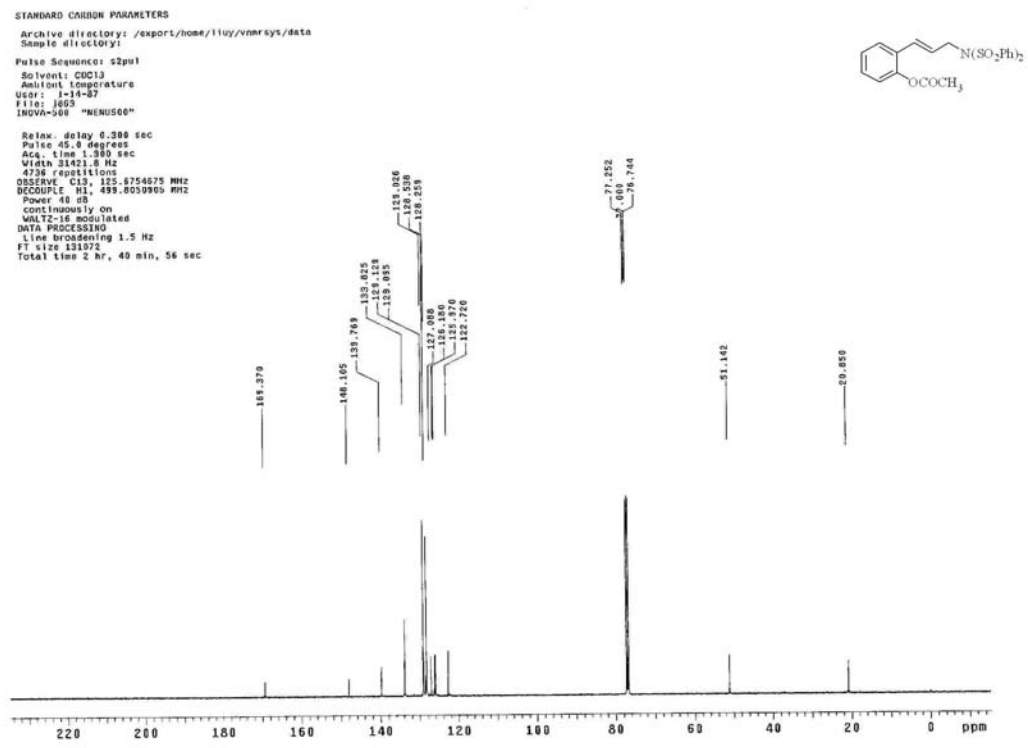
Product **2c**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: k23
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7556.8 Hz
8 repetitions
OBSERVE H1, 499.8025902 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
MeO
N(SO2Ph)2
ppm

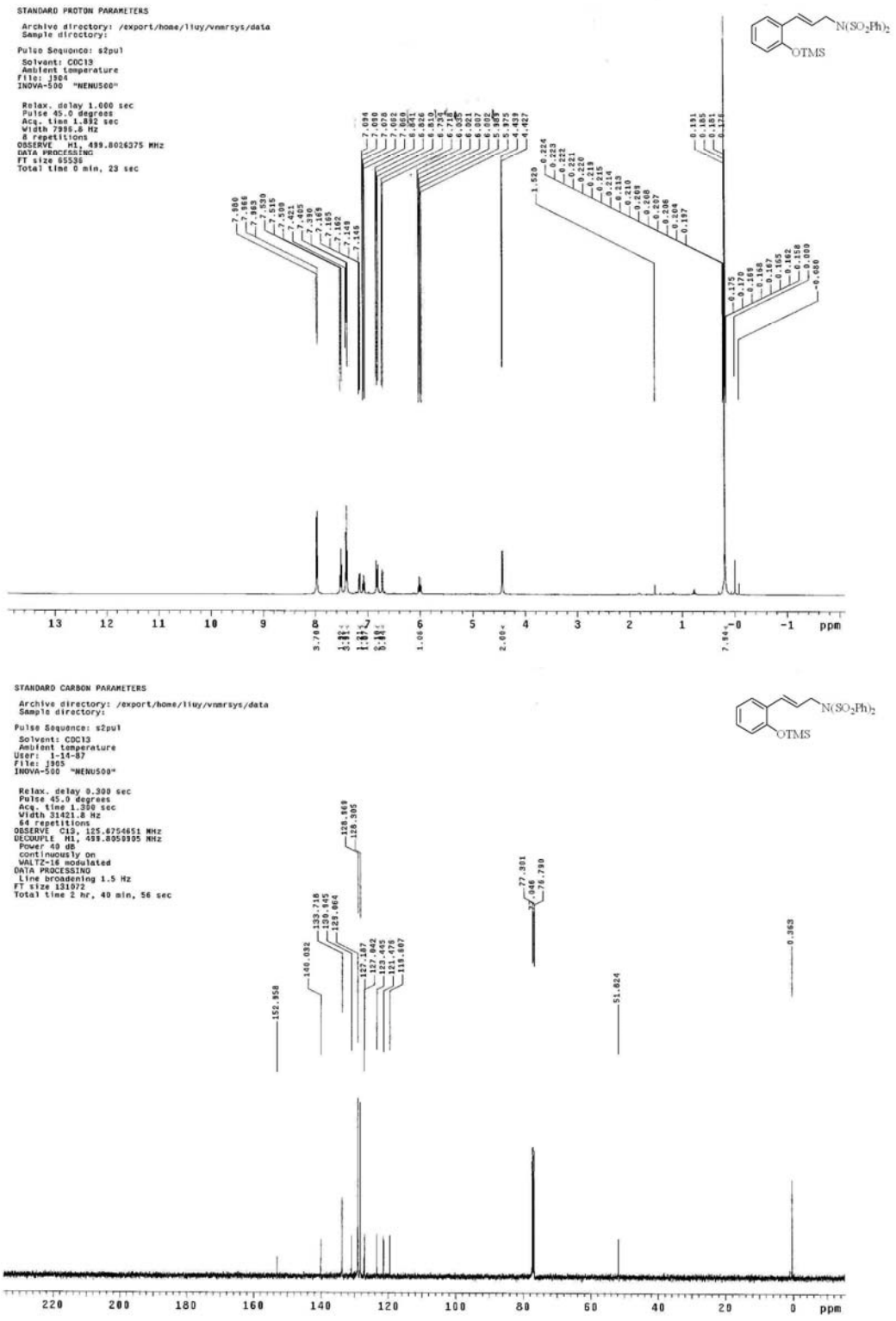

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: k27
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4928 repetitions
OBSERVE C13, 125.6754646 MHz
DECOUPLE H1, 499.8050805 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
MeO
N(SO2Ph)2
ppm

Product **2d**

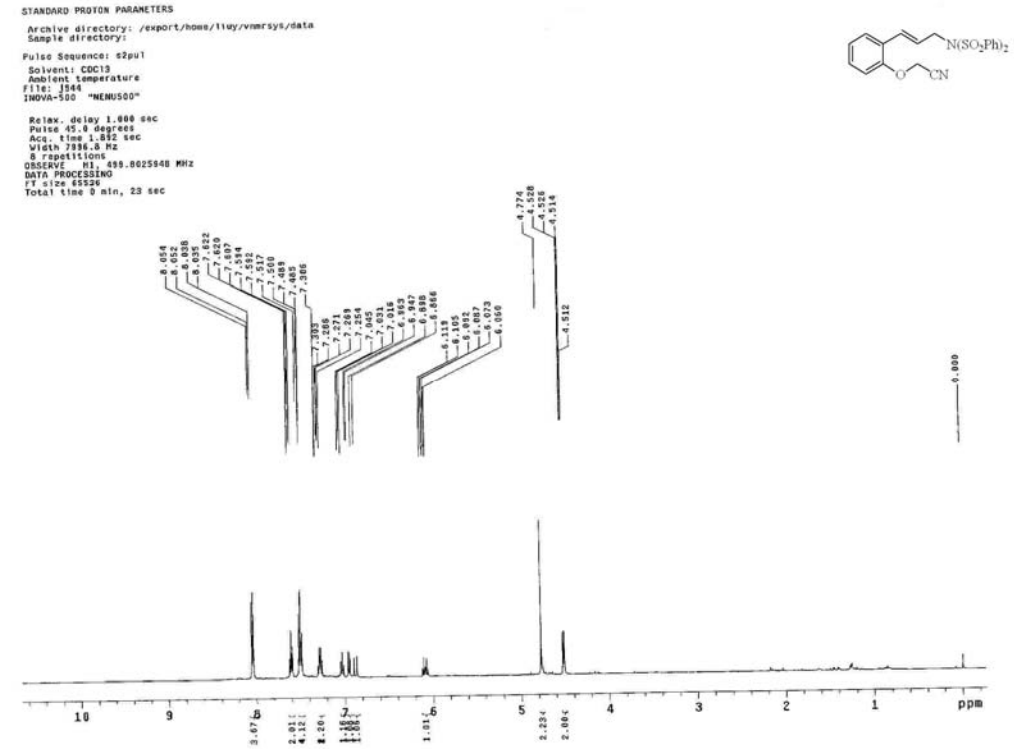

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j300
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7556.8 Hz
8 repetitions
OBSERVE H1, 499.8025912 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
N(SO2Ph)2
OCOCH3
ppm

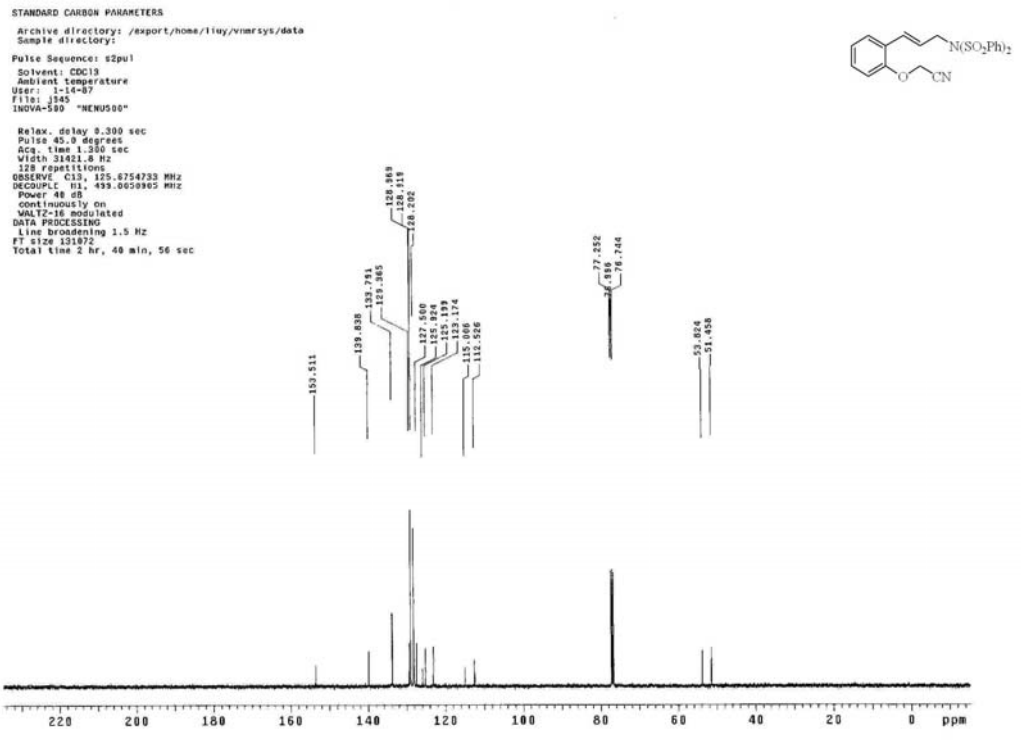

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: j003
INOVA-500 "NENUS00"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4736 repetitions
OBSERVE C13, 125.6754675 MHz
DECOUPLE H1, 499.8059905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
N(SO2Ph)2
OCOCH3
ppm

Product **2e**

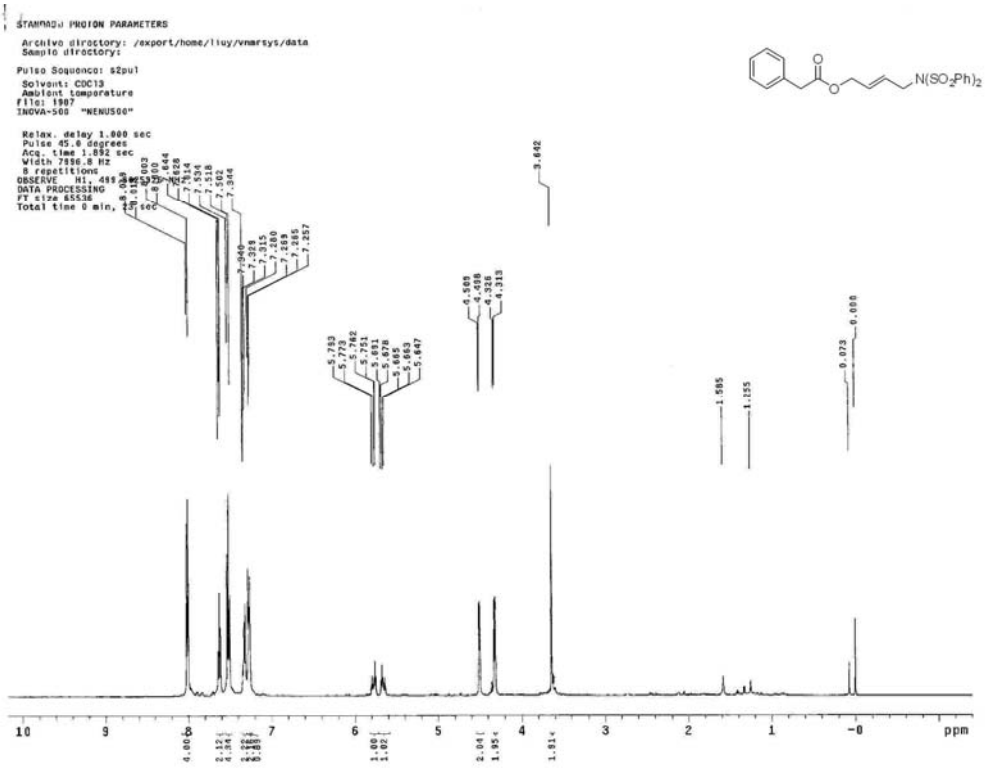

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j304
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7986.8 Hz
8 repetitions
OBSERVE H1, 499.8026375 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
N(SO2Ph)2
OTMS
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: j305
INOVA-500 "NENUS00"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
64 repetitions
OBSERVE C13, 125.6754651 MHz
DECOUPLE H1, 499.8958905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
N(SO2Ph)2
OTMS
ppm

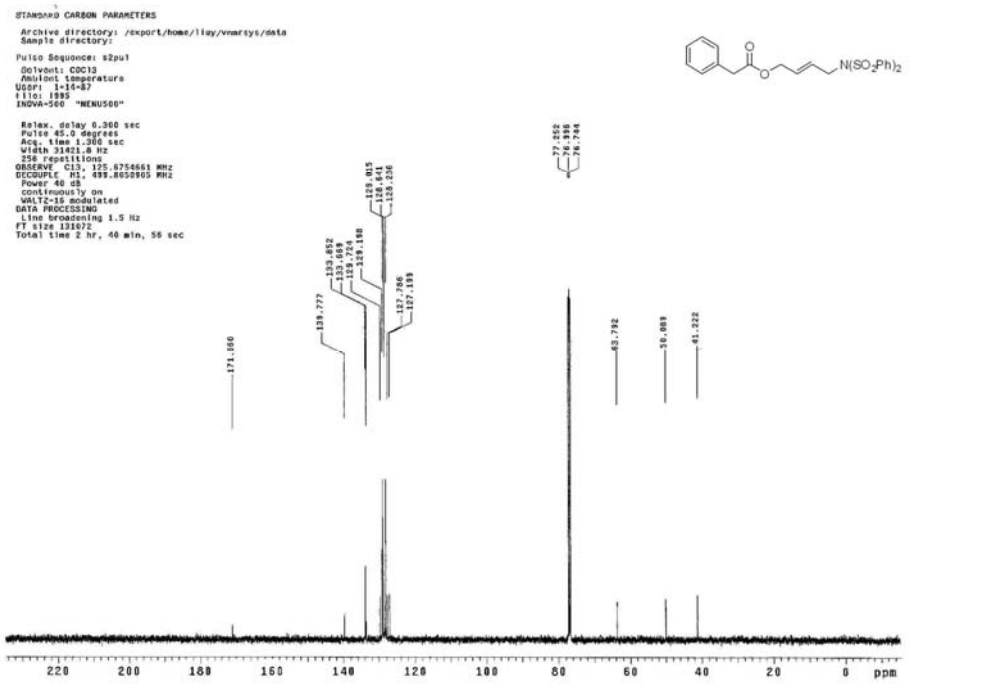
Product **2f**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: j344
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7936.8 Hz
8 repetitions
OBSERVE H1, 499.8025948 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
N(SO2Ph)2
O
CN
ppm

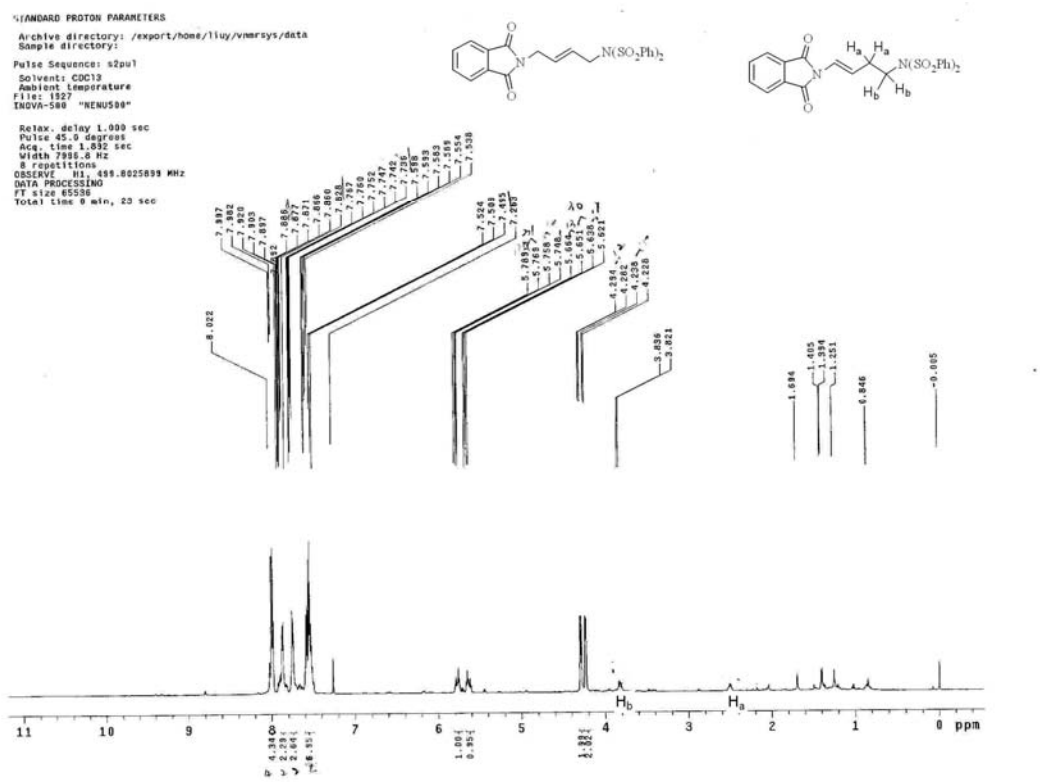

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: j345
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754733 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
N(SO2Ph)2
O
CN
ppm

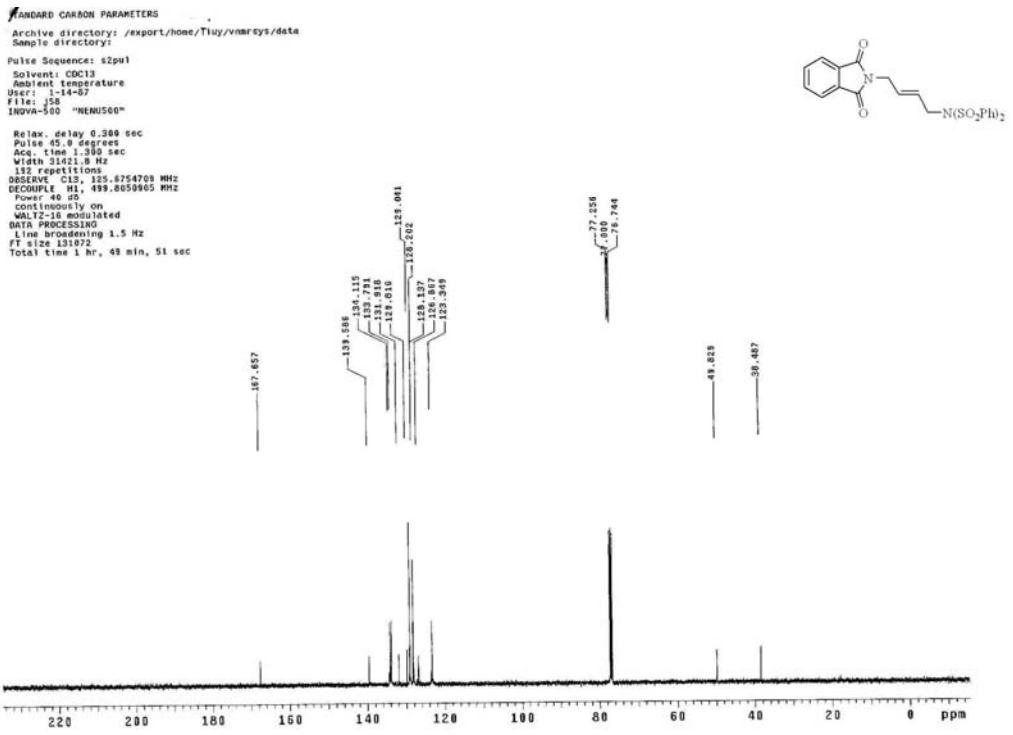
Product **2g**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1907
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7986.8 Hz
8 repetitions
OBSERVE H1, 499.8650905 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 15 sec
N(SO2Ph)2
ppm

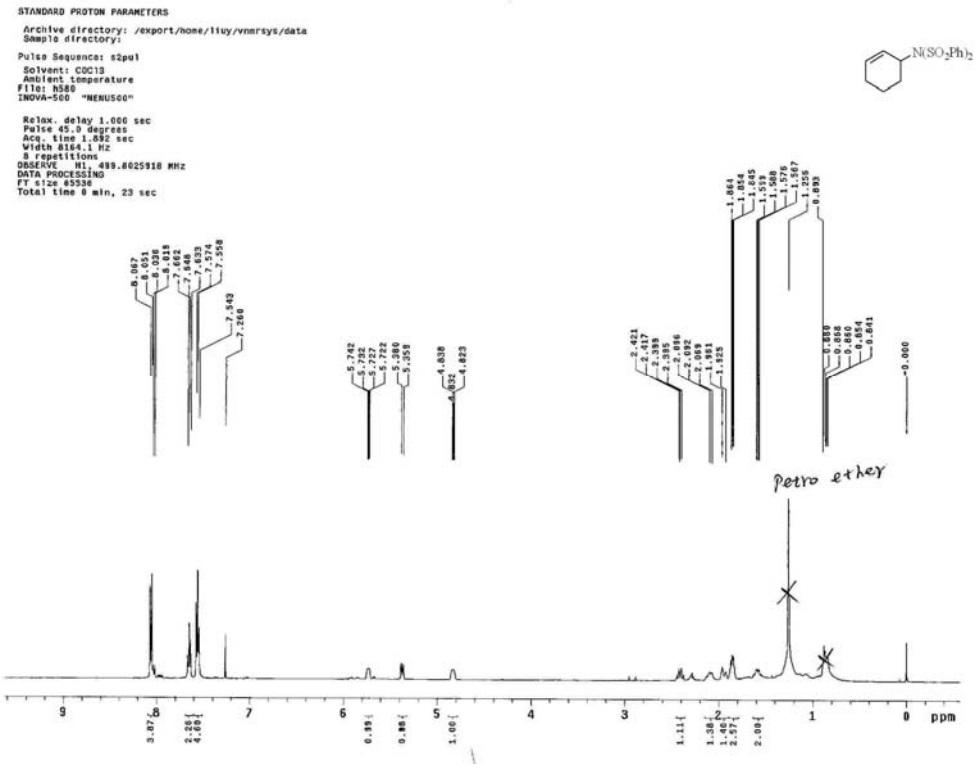

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: 1995
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754661 MHz
DECOUPLE H1, 499.8650905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
N(SO2Ph)2
ppm

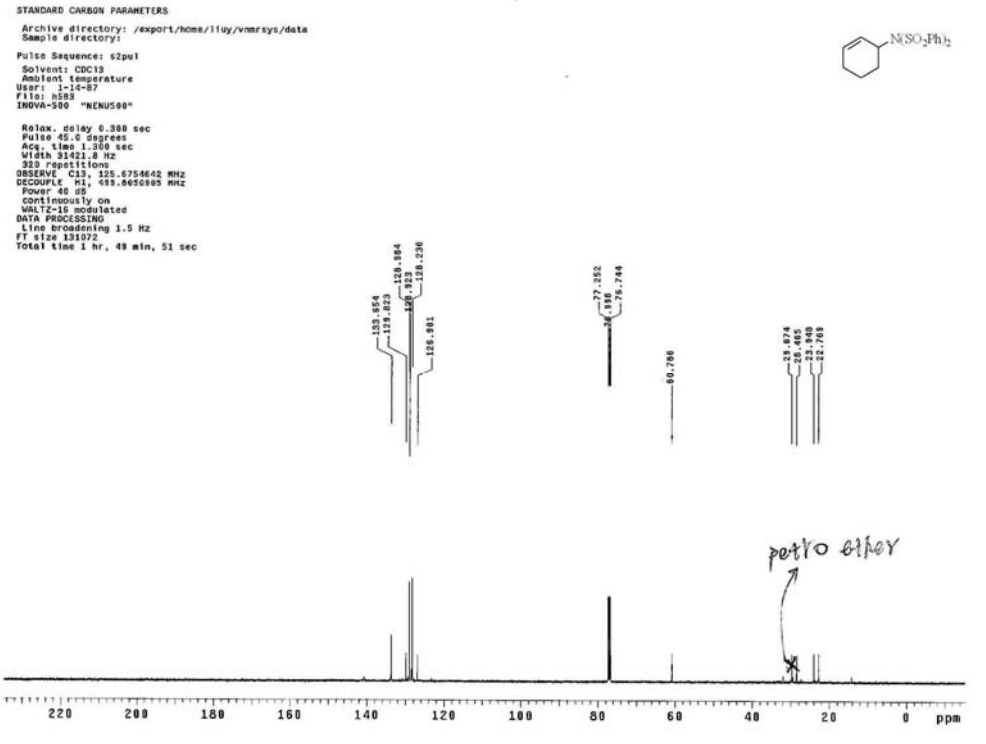
Product **2h**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1927
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7995.8 Hz
8 repetitions
OBSERVE H1, 499.8025899 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
N(SO2Ph)2
Ha Ha
Hb Hb
Hb
Ha
11 10 9 8 7 6 5 4 3 2 1 0 ppm

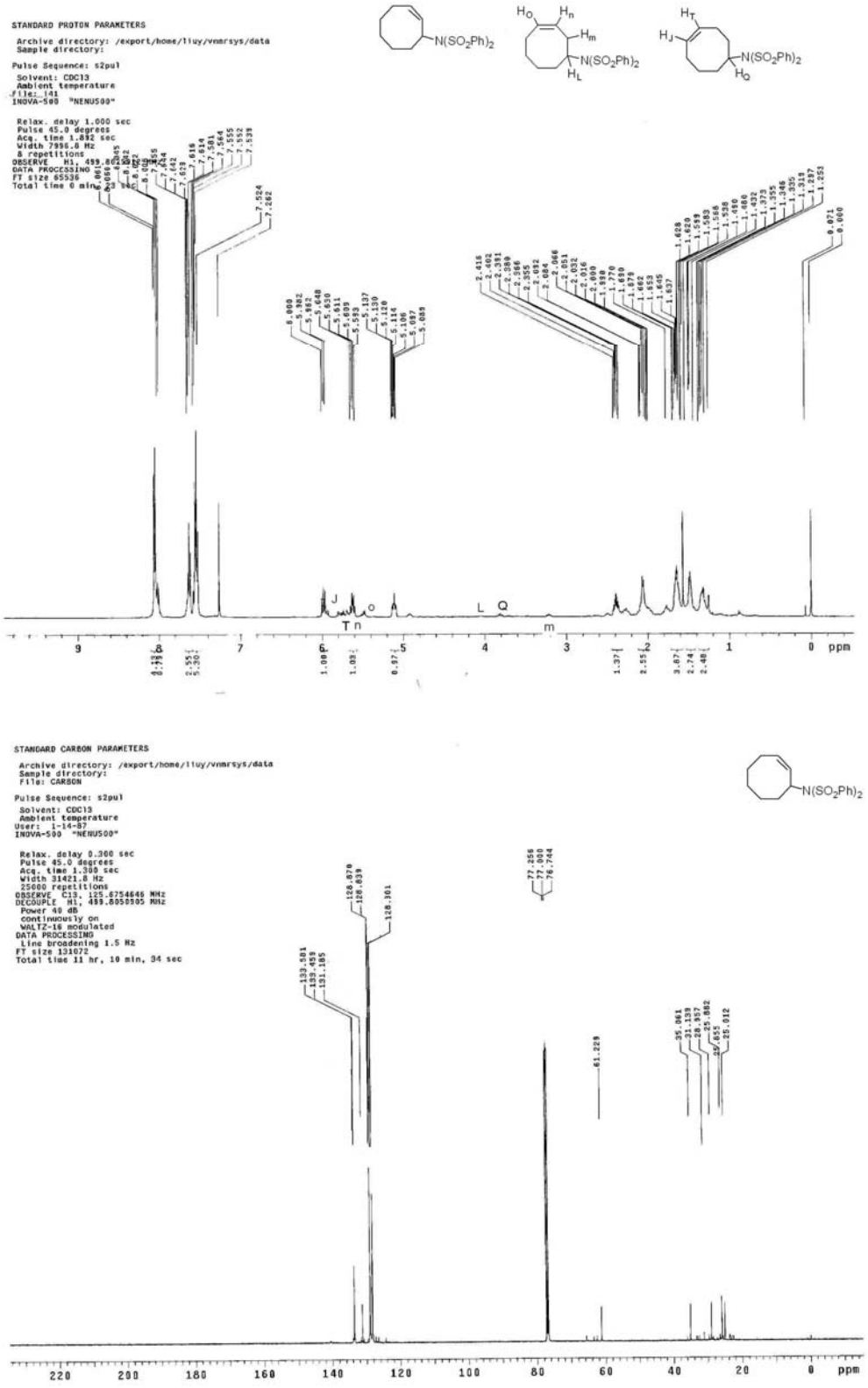

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: 15B
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754709 MHz
DECOUPLE H1, 499.8059965 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
N(SO2Ph)2
220 200 180 160 140 120 100 80 60 40 20 0 ppm

Product **2j**

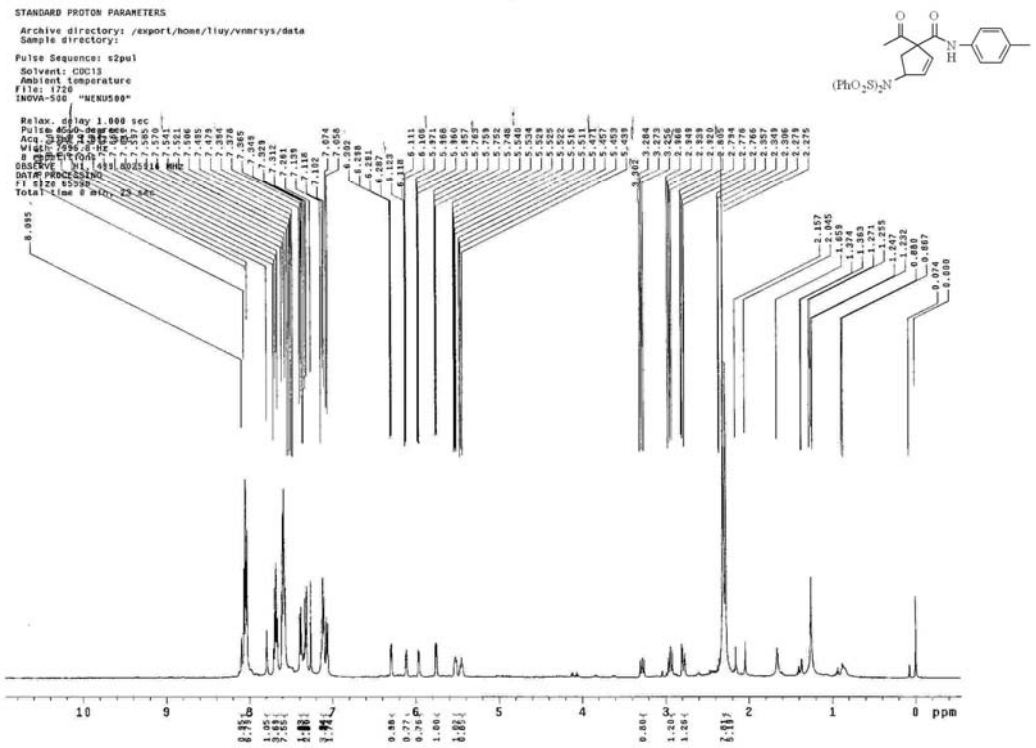

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: h580
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8164.1 Hz
8 repetitions
OBSERVE H1, 499.8025918 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
N(SO2Ph)2
petro ether
ppm

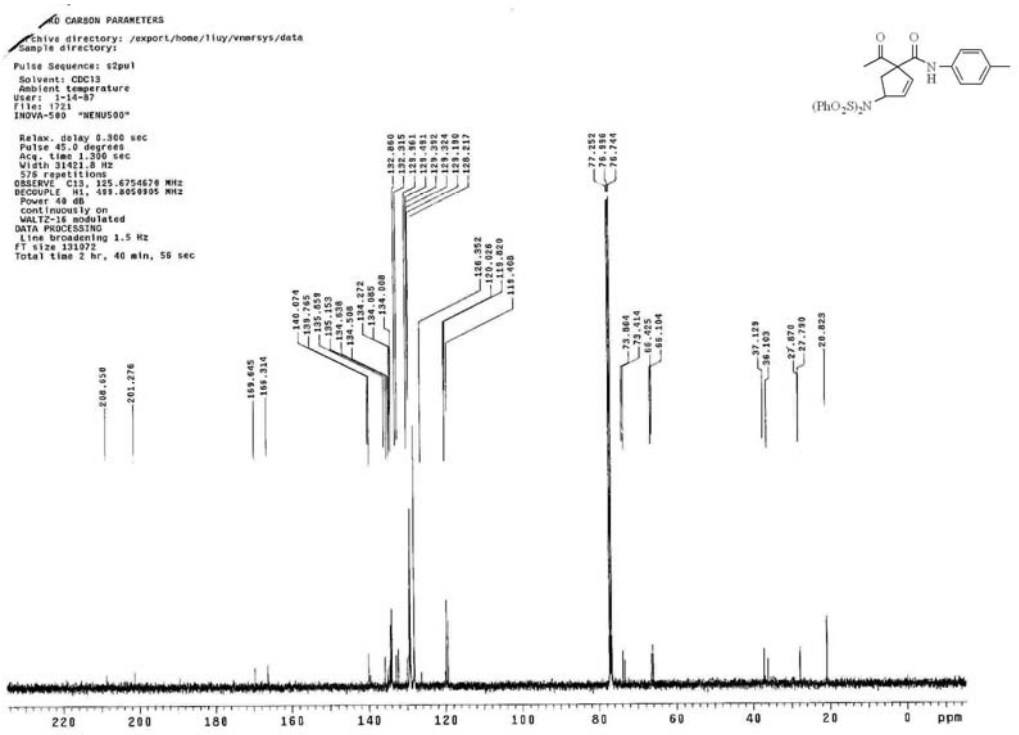

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: h583
INOVA-500 "NENUS00"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
320 repetitions
OBSERVE C13, 125.6754642 MHz
DECOUPLE H1, 499.8650305 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 1 hr, 49 min, 51 sec
N(SO2Ph)2
petro ether
ppm

Product **2k**

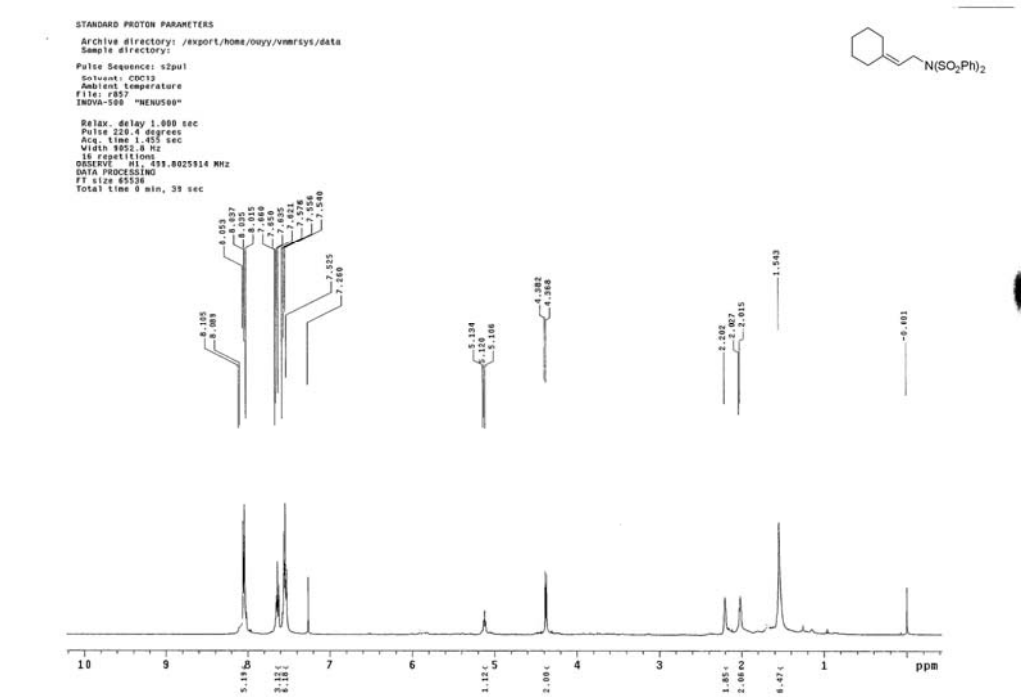

STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 141
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 7996.8 Hz
8 repetitions
OBSERVE H1, 499.8
DATA PROCESSING
FT size 65536
Total time 0 min, 34 sec
N(SO2Ph)2
Ho Hn Hm HL
HT HJ HQ
ppm
STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
File: CARBON
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
INOVA-500 "NENUS00"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.309 sec
Width 31421.8 Hz
25000 repetitions
OBSERVE C13, 125.8754646 MHz
DECOUPLE H1, 499.8959595 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 11 hr, 10 min, 34 sec
ppm

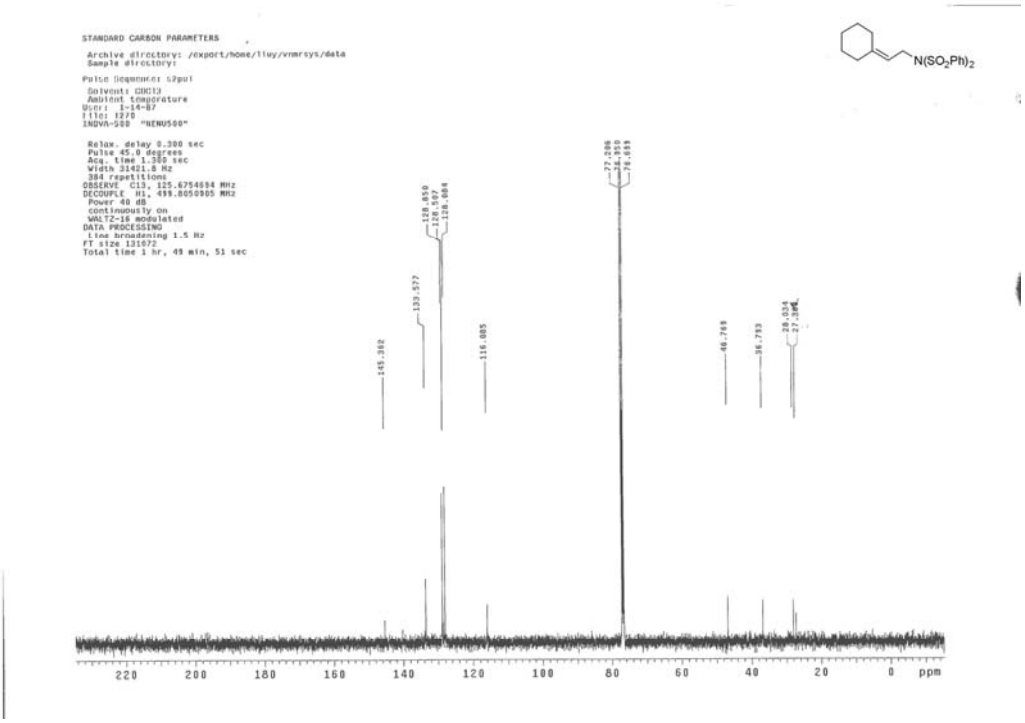
Product **2l**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1720
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Total time 8 min, 25 sec
ppm

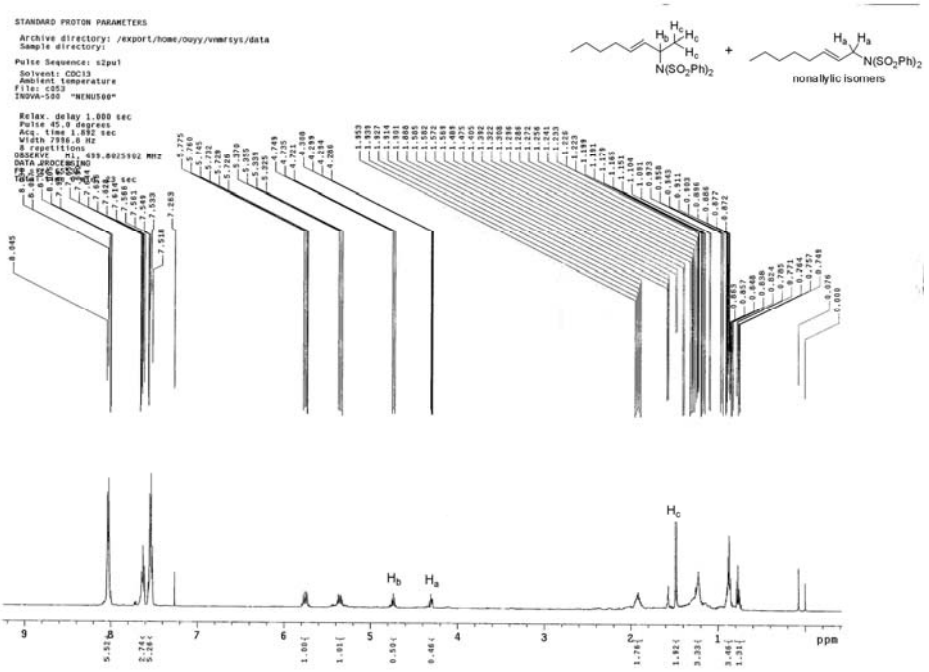

CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
576 repetitions
OBSERVE C13, 125.6754670 MHz
DECOUPLE H1, 499.8059895 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
ppm

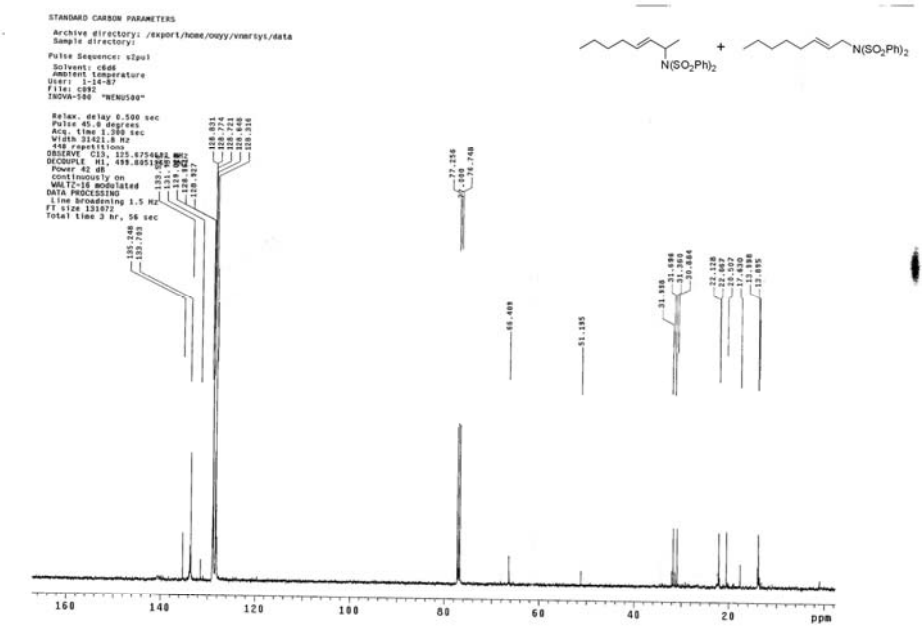
Product **2m**



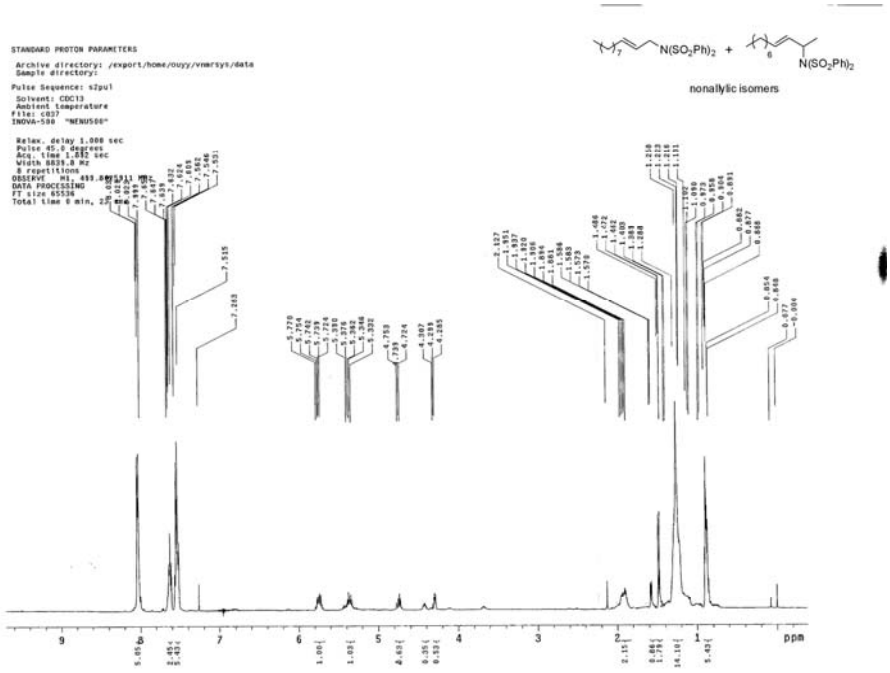


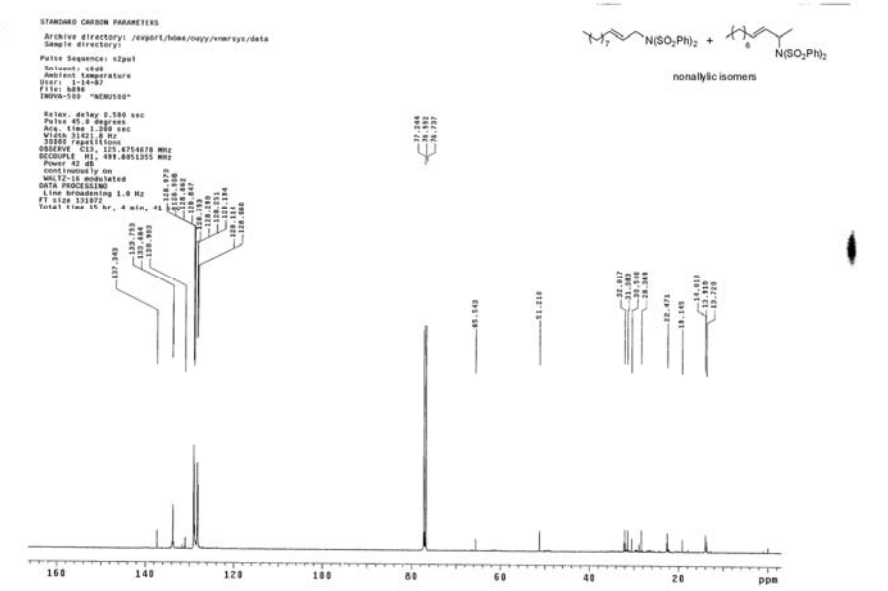
Product **2n**



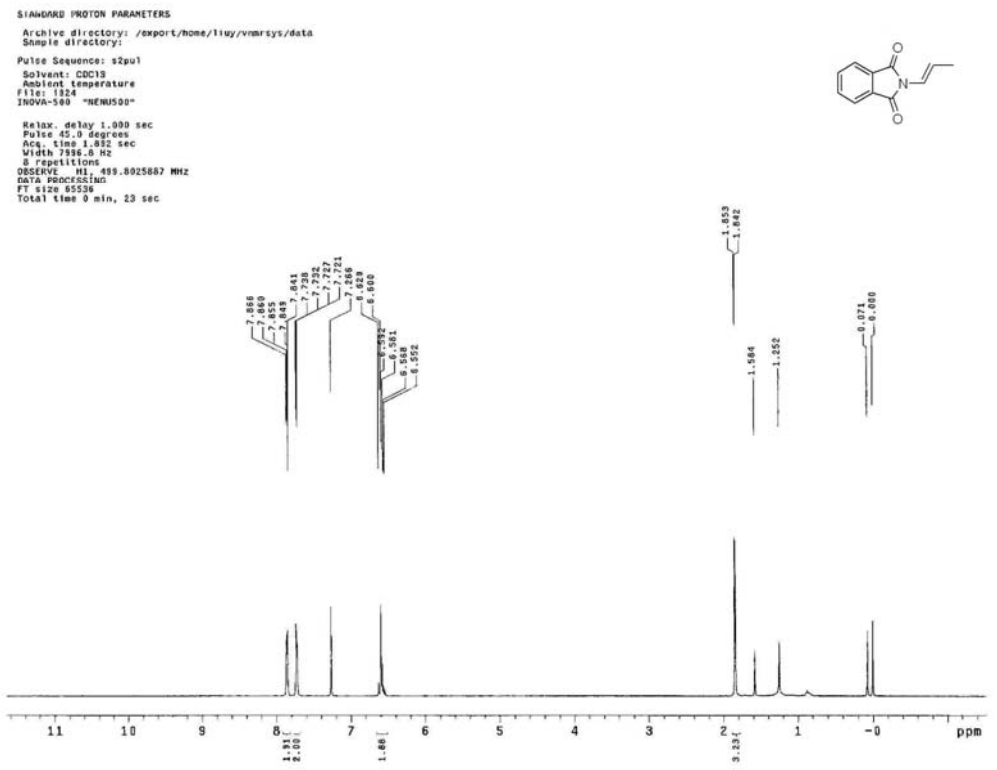


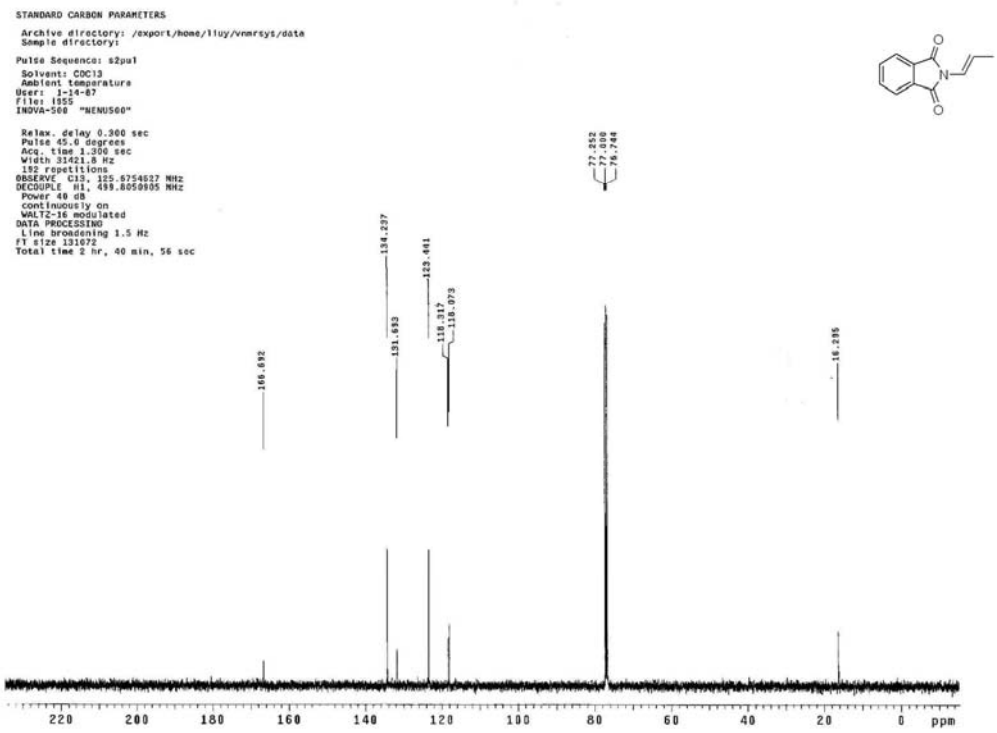
Product **2o**



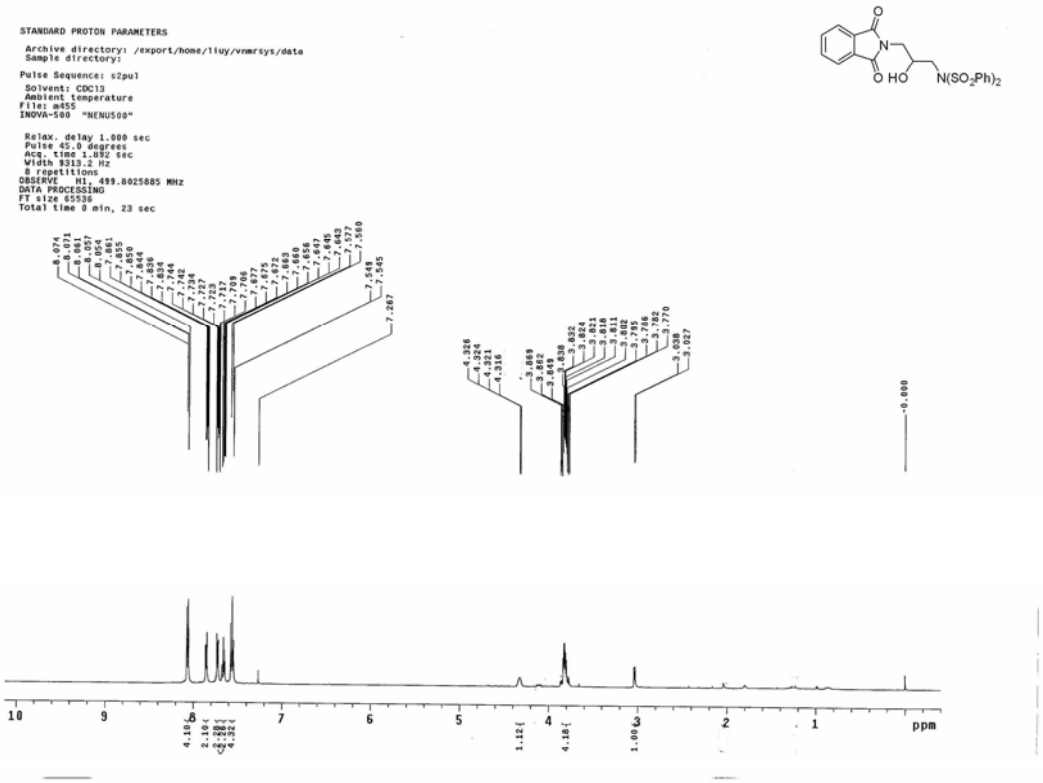


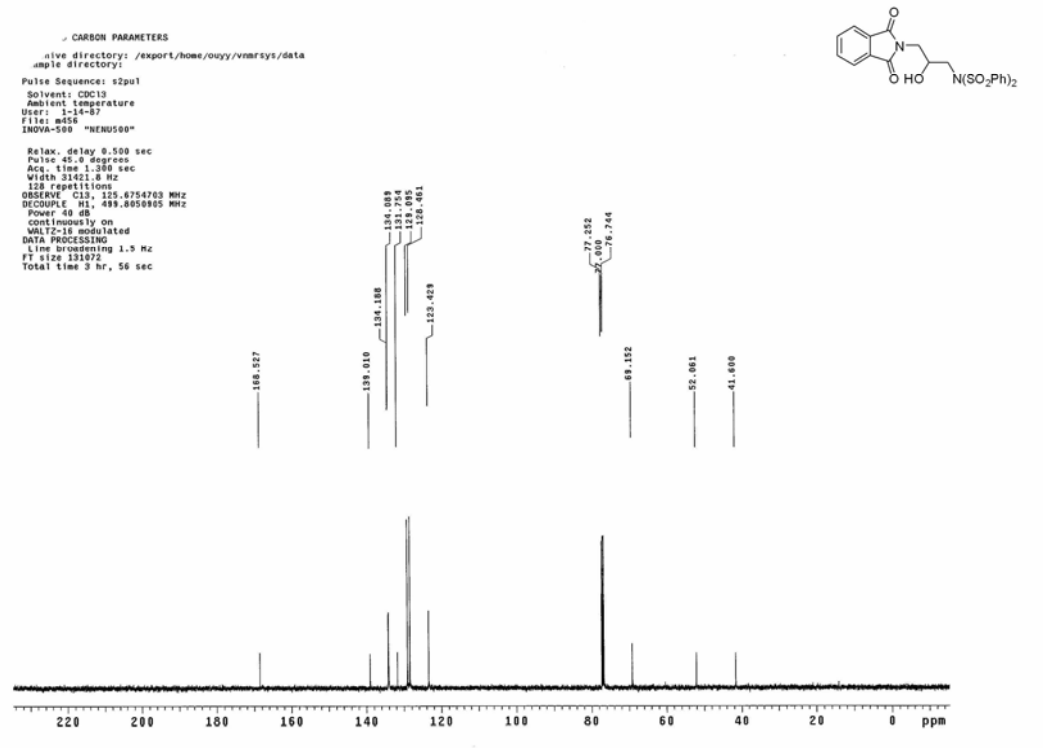
Product **3a**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: 1824
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 7986.8 Hz
8 repetitions
OBSERVE H1, 499.8025887 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

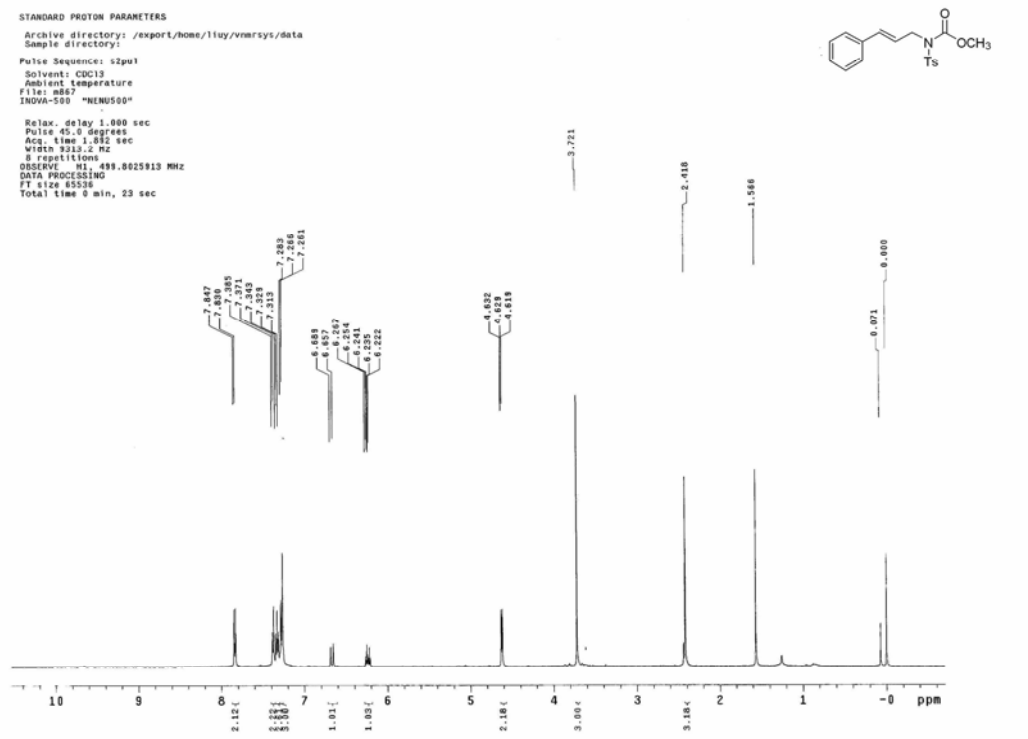

STANDARD CARBON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: 1955
INOVA-500 "NENU500"
Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
192 repetitions
OBSERVE C13, 125.6754622 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 40 min, 56 sec
ppm

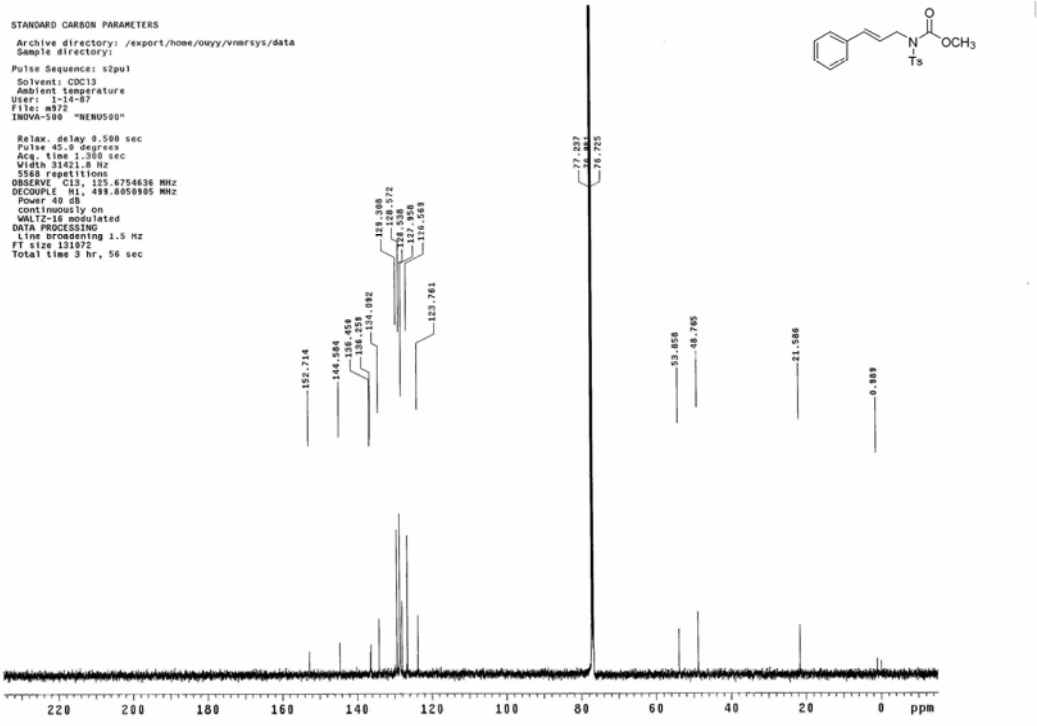
Product **4a**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: a455
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8313.2 Hz
8 repetitions
OBSERVE H1, 499.8025885 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
ppm

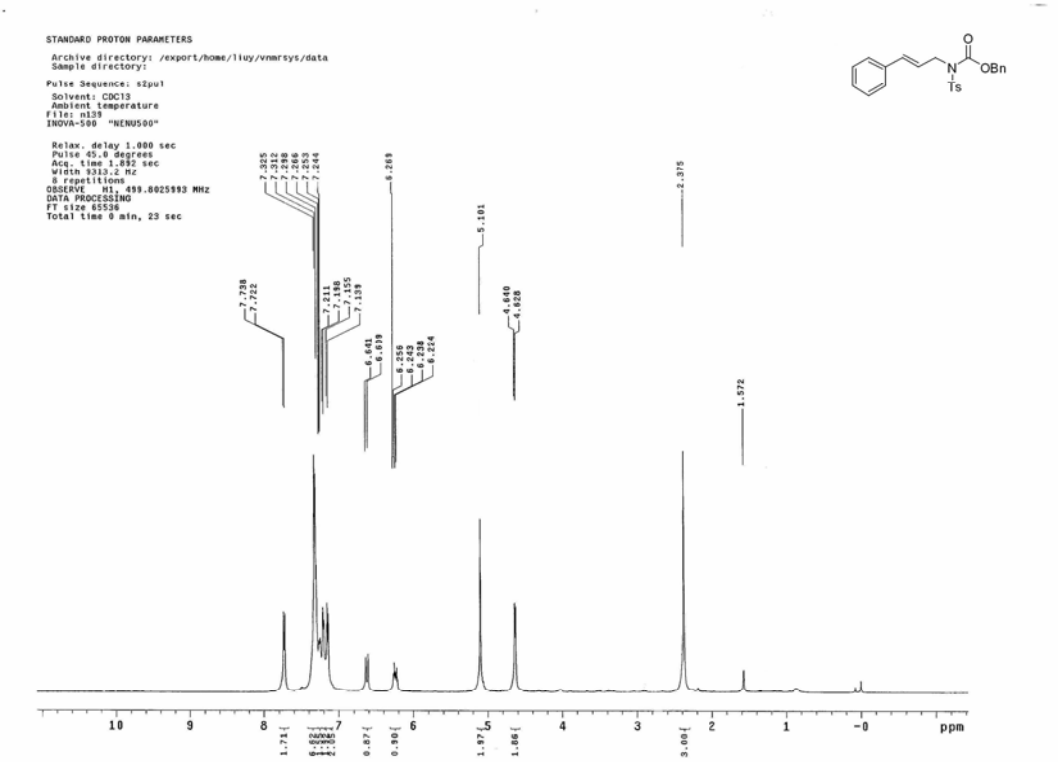

CARBON PARAMETERS
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: a456
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
128 repetitions
OBSERVE C13, 125.6754703 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
ppm

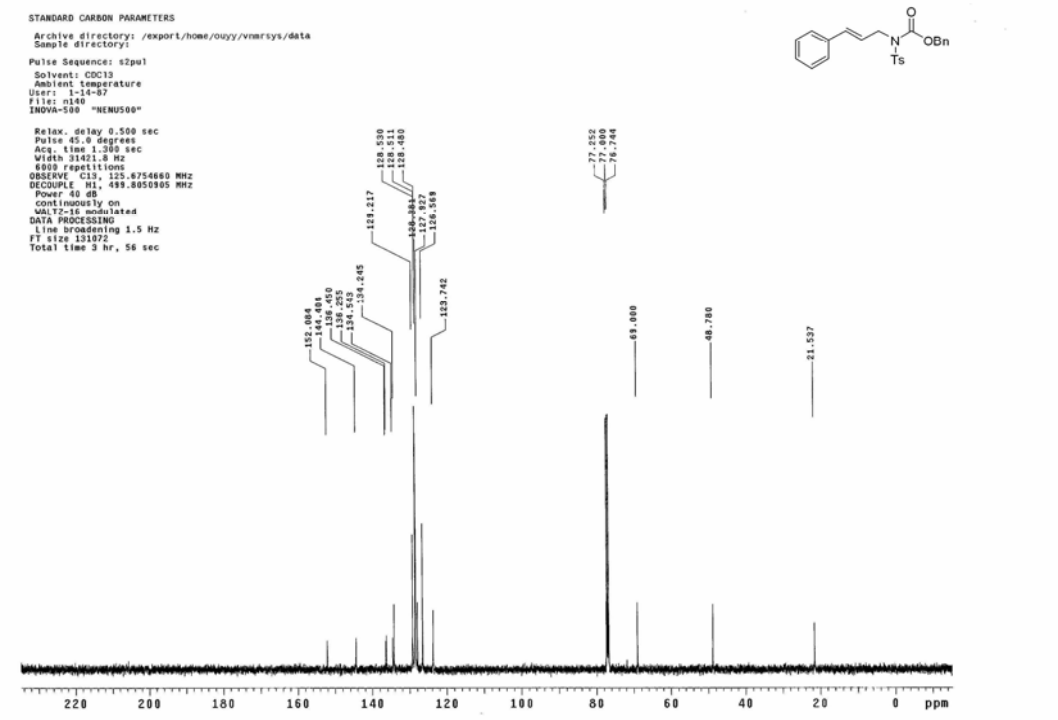
Product 6**b1**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: m867
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.882 sec
Width 9313.2 Hz
8 repetitions
OBSERVE H1, 499.8025913 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
OCH3
Ts
ppm

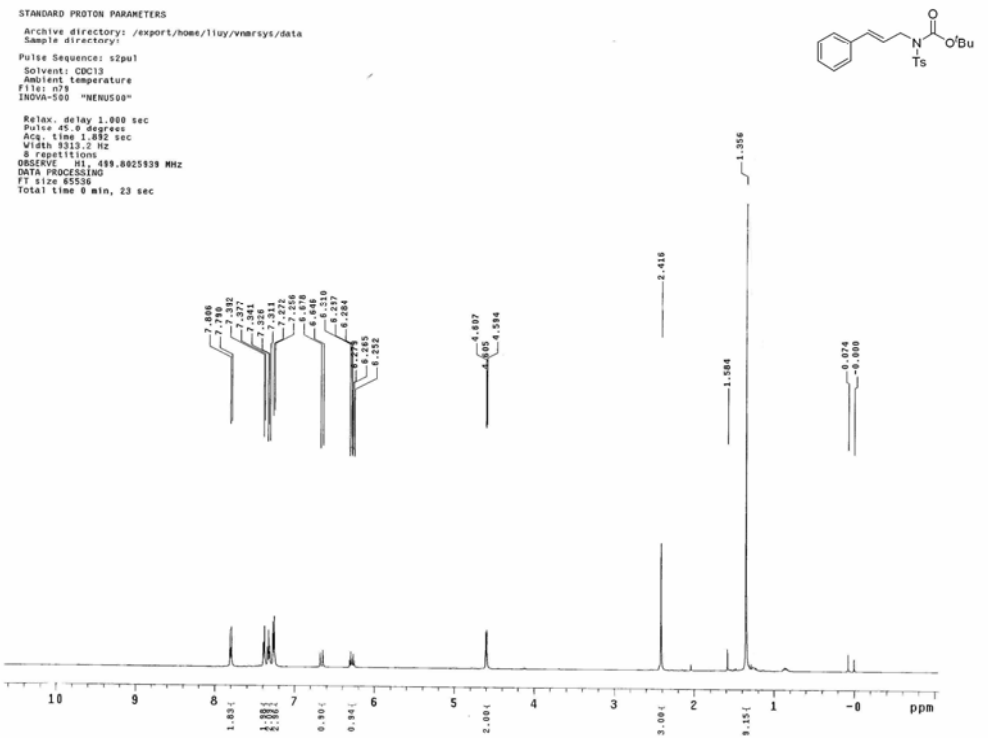

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: m972
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
5568 repetitions
OBSERVE C13, 125.6754636 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
OCH3
Ts
ppm

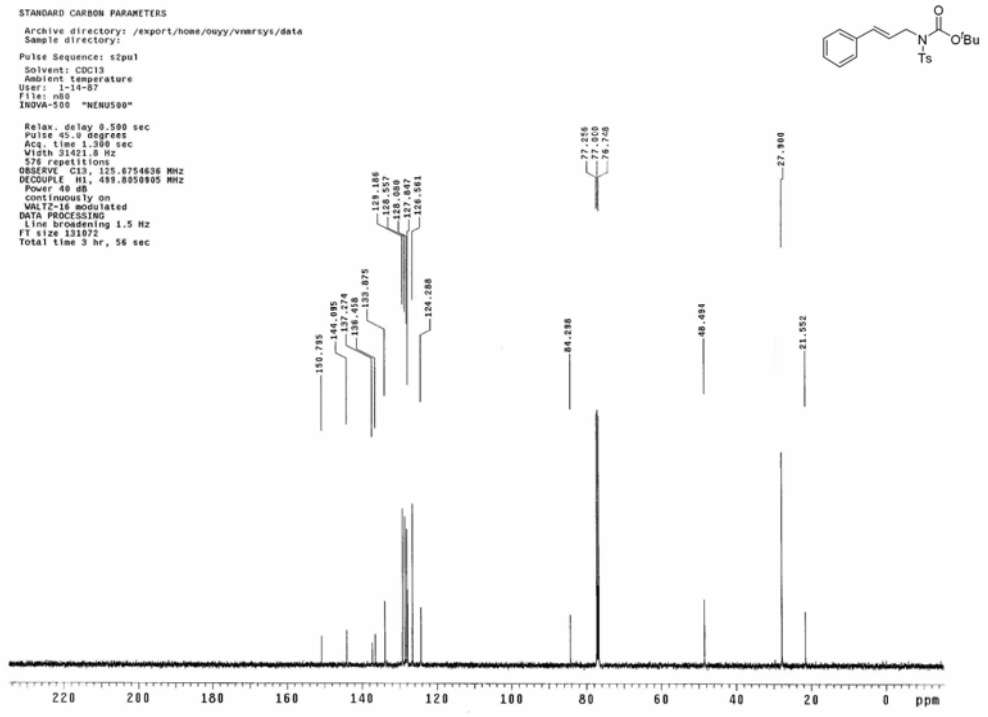
Product 6**b2**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: n139
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9313.2 Hz
8 repetitions
OBSERVE H1, 499.8025993 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
OBn
Ts
ppm

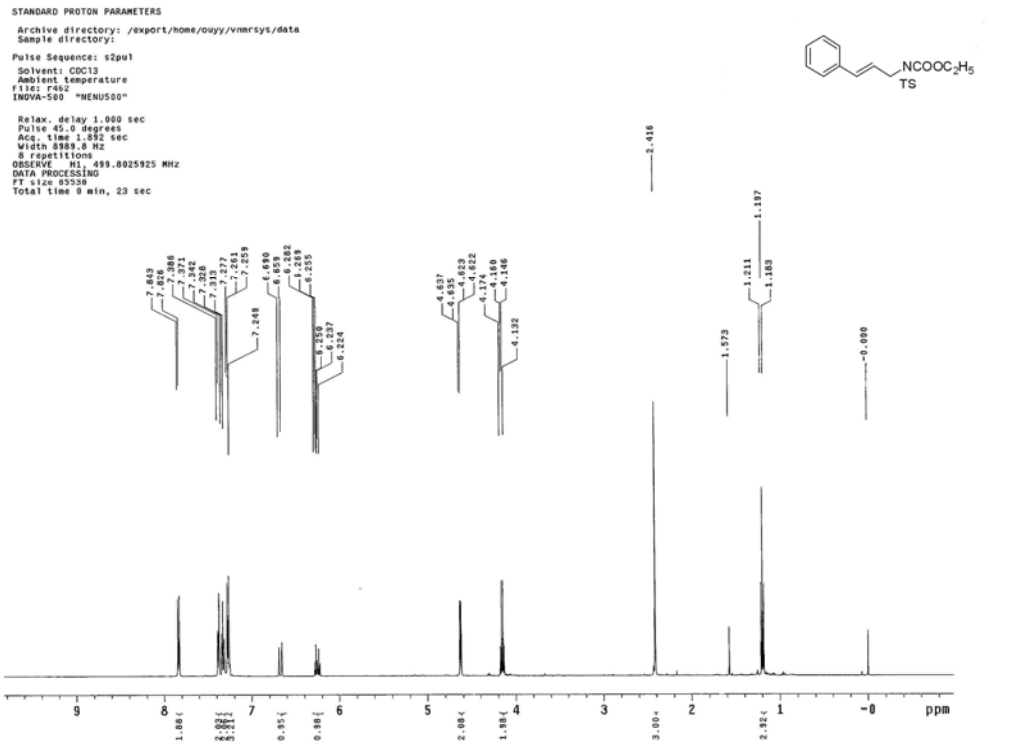

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: n140
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
6000 repetitions
OBSERVE C13, 125.6754660 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
OBn
Ts
ppm

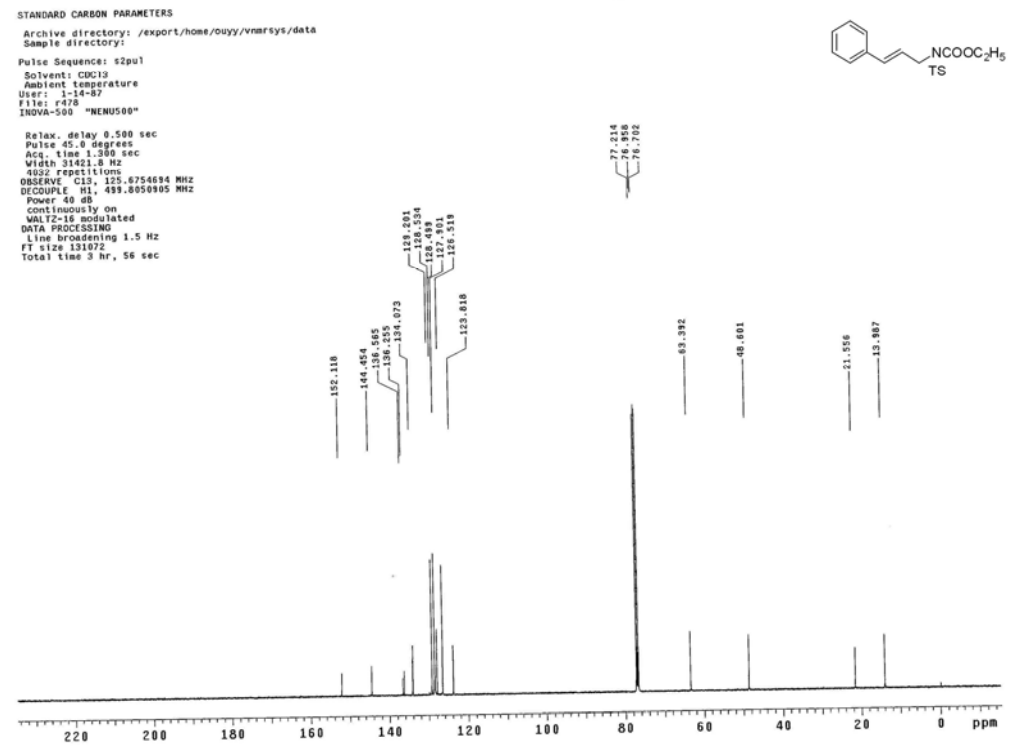
Product 6**b3**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: n79
INOVA-500 "NENUS00"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 9313.2 Hz
8 repetitions
OBSERVE H1, 499.8025939 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
O
N
Ts
O'Bu
7.806
7.790
7.332
7.327
7.321
7.311
7.256
6.678
6.646
6.633
6.237
6.284
6.265
6.252
4.607
4.605
4.594
2.416
1.584
1.356
0.074
0.000
10
9
8
7
6
5
4
3
2
1
-0
ppm

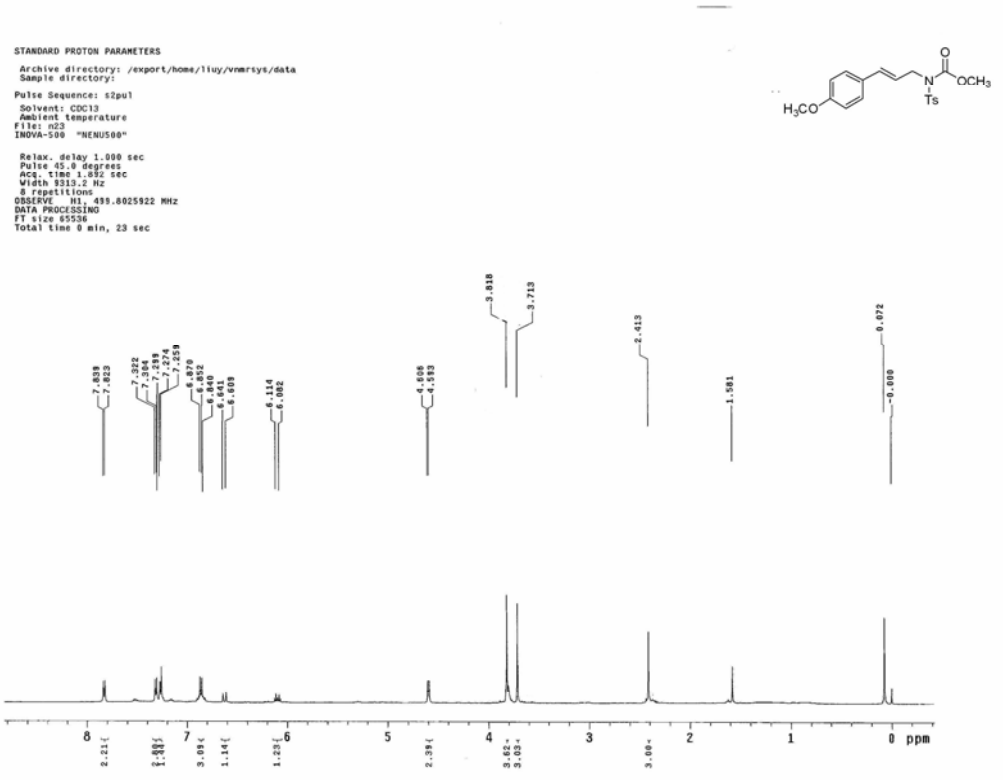

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: n80
INOVA-500 "NENUS00"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
576 repetitions
OBSERVE C13, 125.6754636 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
O
N
Ts
O'Bu
150.795
144.095
137.274
136.458
130.875
129.186
128.557
128.089
127.607
126.581
124.288
77.256
77.000
76.748
64.288
48.484
27.300
21.552
220
200
180
160
140
120
100
80
60
40
20
0
ppm

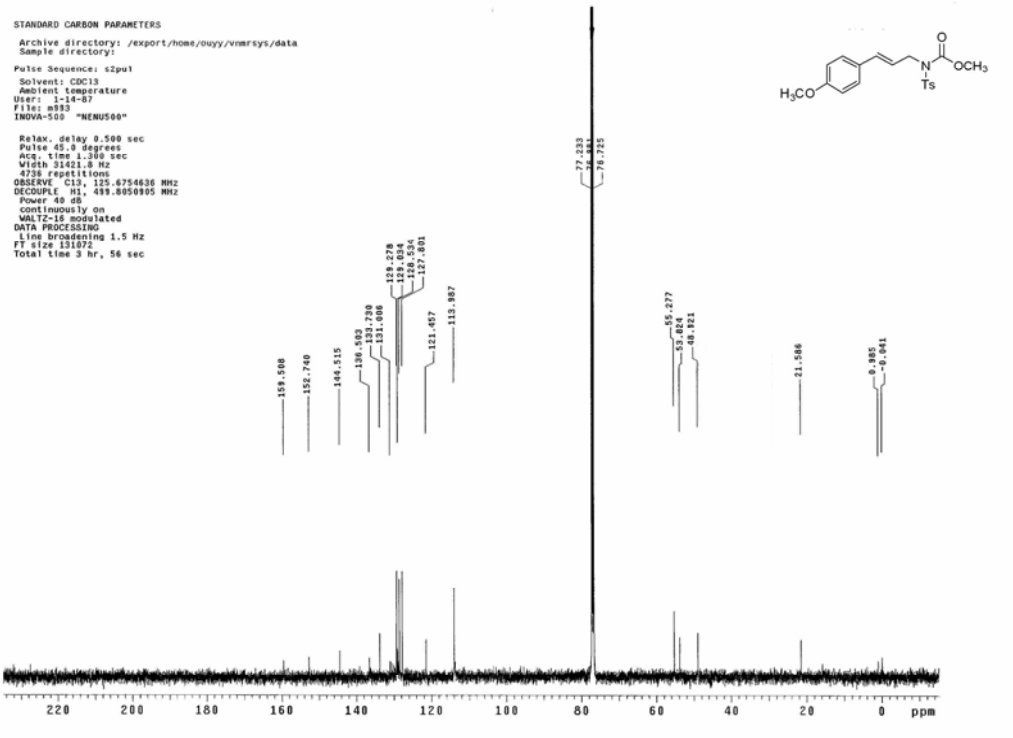
Product 6b4


STANDARD PROTON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: r462
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8989.8 Hz
8 repetitions
OBSERVE H1, 499.8025925 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
NCOOC2H5
TS
ppm

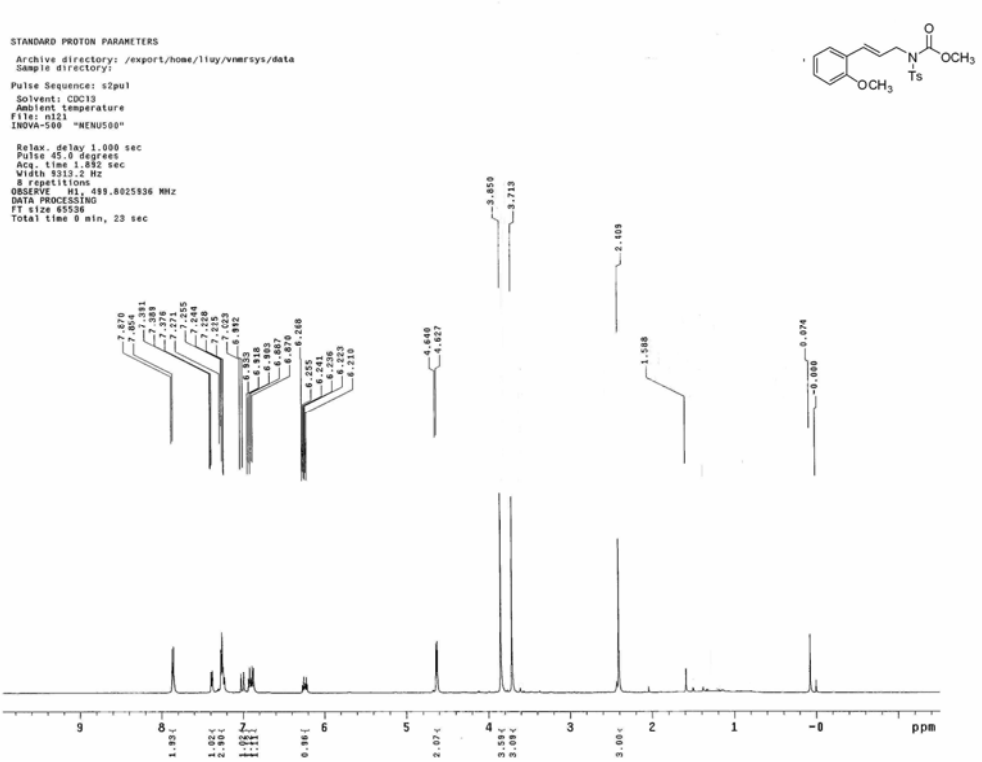

STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: r478
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4032 repetitions
OBSERVE C13, 125.6754694 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
NCOOC2H5
TS
ppm

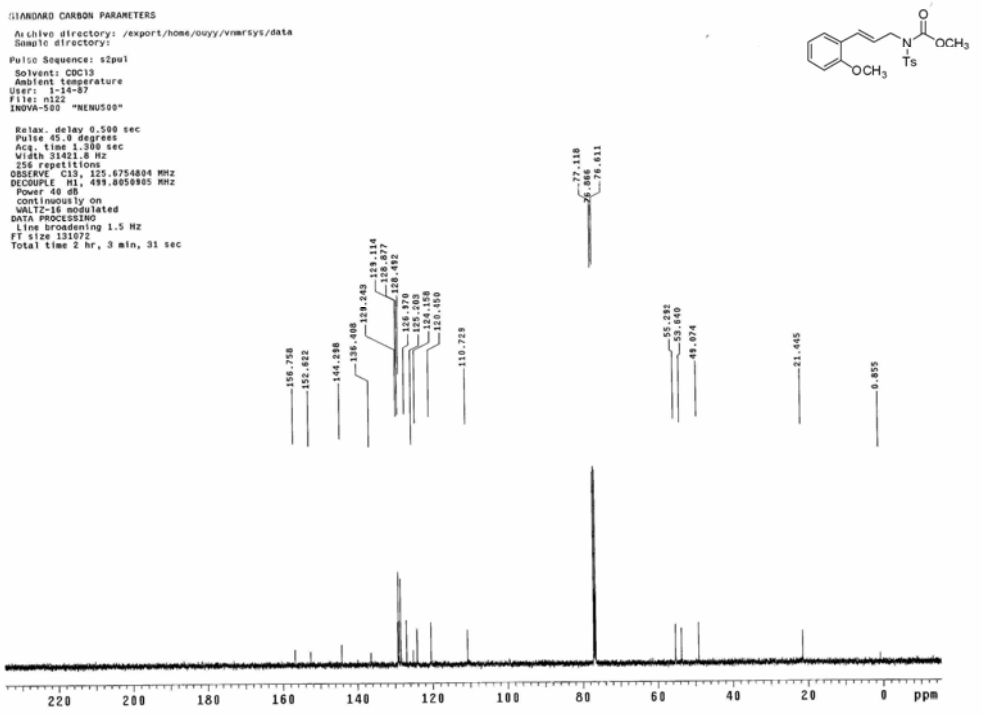
Product 6**f**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: n23
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.032 sec
Width 8313.2 Hz
8 repetitions
OBSERVE H1, 499.8025922 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
7.839
7.823
7.322
7.304
7.288
7.274
7.259
6.670
6.652
6.645
6.641
6.609
6.114
6.092
4.606
4.593
3.818
3.713
2.413
1.581
0.072
-0.000
8
7
6
5
4
3
2
1
0 ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-07
File: m993
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
4736 repetitions
OBSERVE C13, 125.6754636 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 3 hr, 56 sec
159.508
152.740
144.515
136.503
133.730
131.006
129.278
129.034
128.534
127.801
121.457
113.987
77.233
76.725
55.277
53.824
48.921
21.586
0.985
-0.041
220
200
180
160
140
120
100
80
60
40
20
0 ppm

Product 6**l**


STANDARD PROTON PARAMETERS
Archive directory: /export/home/liuy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: n121
INOVA-500 "NENU500"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.892 sec
Width 5313.2 Hz
8 repetitions
OBSERVE H1, 499.8025936 MHz
DATA PROCESSING
FT size 65536
Total time 0 min, 23 sec
OCH3
N
Ts
ppm


STANDARD CARBON PARAMETERS
Archive directory: /export/home/ouyy/vnmrsys/data
Sample directory:
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: 1-14-87
File: n122
INOVA-500 "NENU500"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 31421.8 Hz
256 repetitions
OBSERVE C13, 125.6754804 MHz
DECOUPLE H1, 499.8050905 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.5 Hz
FT size 131072
Total time 2 hr, 3 min, 31 sec
OCH3
N
Ts
ppm