Supporting Information

Ru(II)-Catalyzed Rearrangement of Allenic Sulfide Bearing Propargyl Moiety: Efficient Formation of Benzene Derivatives

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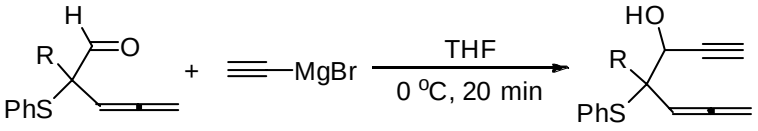
Contents

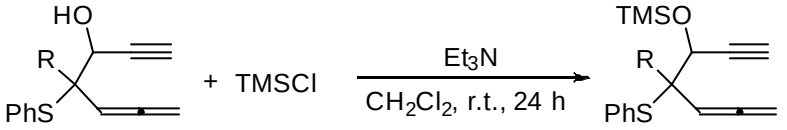
1. General

All reactions were performed under a nitrogen atmosphere in a flame-dried reaction flask. All solvents were distilled prior to use. Toluene and THF was distilled over sodium, DCE was distilled over NaH. For chromatography, 200-300 mesh silica gel (Yantai, China). ^{1}H and ^{13}C NMR spectra were recorded at 300 MHz (or 200 MHz) and 75 MHz (or 50 MHz) with Varian Mercury 300 spectrometer. Chemical shifts are reported in ppm using tetramethylsilane as internal standard. IR spectra were recorded with a Nicolet 5MX-S infrared spectrometer. Mass spectra were obtained on a VG ZAB-HS mass spectrometer.

2. Preparation of 1-ethynyl-2-phenylthio-3,4-pentadienyl trimethylsilyl ether 4a-j



(1)

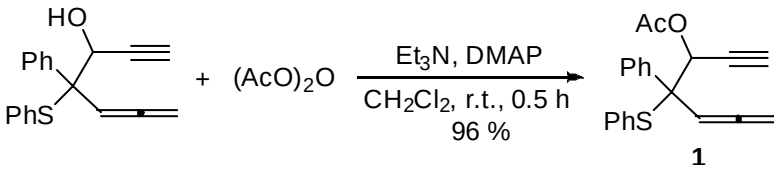


(2)

(1) Under a nitrogen atmosphere, 2-phenylthio-3,4-pentadienyl aldehyde (2.0 mmol) was dissolved in anhydrous THF (20 mL) in a 50 mL three necked-bottomed flask. To the solution was then added ethynylmagnesium bromide (0.5 mol/L in THF, 3.0 mmol) dropwise at 0 °C (ice-bath). The reaction was kept at the same temperature for about 20 min. Then saturated NH_4Cl was added, and the mixture was extracted with Et_2O. The combined organic layers were dried over $MgSO_4$ and evaporated; the residue was purified by a silica gel column. Elution with petroleum ether/ethyl acetate (15:1) afforded pure product of 1-Ethynyl-2-phenylthio-3,4-pentadienyl alcohol.

(2) Under a nitrogen atmosphere, 1-ethynyl-2-phenylthio-3,4-pentadienyl alcohol (2.0 mmol) and triethylamine (6.0 mmol) were mixed in anhydrous CH_2Cl_2 (20 mL) in a 50 mL round-bottomed flask. To the solution was then added TMSCl (4.0 mmol) at room temperature. The reaction was kept at the same temperature until completed as judged by TLC. Removal of the solvent in vacuo gave a crude residue, which was purified by silica gel column. Elution with petroleum ether/ethyl acetate (100:1) afforded pure product of **4a-i**.

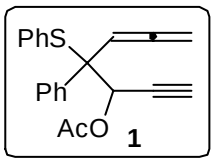
3. Preparation of 1-ethynyl-2-phenyl-2-phenylthio-3,4-pentadienyl acetate 1



Under a nitrogen atmosphere, 1-ethynyl-2-phenylthio-3,4-pentadienyl alcohol (2.0 mmol) was dissolved in anhydrous CH_2Cl_2 (20 mL) in a 50 mL round-bottomed flask. Triethylamine (10.0 mmol), Ac_2O (6.0 mmol) and DMAP (0.02 mmol) were then added to this solution in turn at 0 ^oC (ice- bath).The reaction was continued at room temperature for about 0.5 h. Removal of the solvent in *vacuo* gave a crude residue, which was purified by silica gel column. Elution with petroleum ether/ethyl acetate (20:1) afforded pure product of **1.**

4. Characterization data

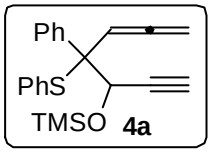
*1-Ethynyl-2-phenyl-2-phenylthio-3,4-pentadienyl acetate (**1**)*



Stereoisomer **1-A**: white solid; IR (film) 3285, 1954, 1745, 1370, 1225, 1025, 856, 751, 733, 694 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 2.09 (s, 3H), 2.45 (d, J = 2.1 Hz, 1H), 4.65 (dd, J = 6.9, 11.1 Hz,1H), 4.92 (dd, J = 6.9, 11.1 Hz,1H), 5.60-5.64 (m, 2H), 7.23-7.39 (m, 8H), 7.49-7.52 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 20.88, 60.34, 66.84, 75.65, 78.77, 79.55, 92.88, 127.62, 127.73, 128.48, 128.70, 129.42, 130.39, 137.90, 138.64, 169.47, 208.35. EI-MS (*m*/*z*, relative intensity): 334 (M^+, 0.36), 292 (4), 274 (3), 183 (15), 165 (100), 109 (9), 43(46). HRMS calcd for $C_{21}H_{18}O_2S$ [M^+] 334.1028; Found: 334.1036.

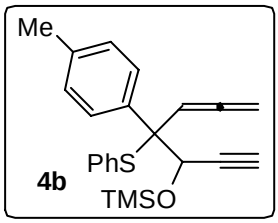
Stereoisomer **1-B**: ^1H NMR ($CDCl_3$, 300 MHz) δ 2.00 (s, 3H), 2.05 (s, 3H), 2.42 (d, J = 2.1 Hz, 1H), 2.54 (d, J = 2.1 Hz, 1H), 4.47 (dd, J = 6.6 Hz, 11.1Hz, 1H), 4.62 (dd, J = 6.6, 11.1 Hz, 1H), 4.69 (dd, J = 6.6, 11.1 Hz, 1H), 4.89 (dd, J = 6.6, 11.1 Hz, 1H), 5.54-5.62 (m, 4H), 7.20-7.40 (m, 12H), 7.43-7.52 (m, 5H), 7.66-7.69 (m, 3H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 20.62, 20.75, 60.31, 60.55, 66.78, 67.13, 75.64, 76.45, 78.70, 78.80, 78.88, 79.44, 92.83, 93.19, 127.54, 127.65, 127.81, 128.38, 128.42, 128.63, 128.97, 129.33, 129.38, 130.25, 130.36, 137.79, 138.14, 138.57, 169.08, 169.31, 207.44, 208.27.

*1-Ethynyl-2-phenyl-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4a**)*



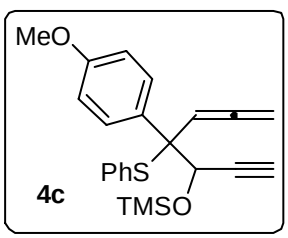
Mixture of two stereoisomers, yield-1: 96%, yield-2: 85%; IR (film) 3294, 2985, 1955, 1251, 1096, 842, 750, 693 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 0.037 (s, 9H), 0.092 (s, 9H), 2.44 (d, J = 2.1 Hz, 1H), 2.51 (d, J = 2.1 Hz, 1H), 4.52-4.77 (m, 6H), 5.56 (t, J = 6.9 Hz, 1H), 5.65 (t, J = 6.9 Hz, 1H), 7.15-7.39 (m, 16H), 7.58-7.61 (m, 2H), 7.70-7.72 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.032, 0.15, 62.76, 63.65, 68.01, 68.68, 75.56, 75.87, 78.26, 78.66, 82.57, 82.70, 93.05, 93.42, 127.15, 127.24, 127.30, 128.07, 128.46, 128.53, 129.66, 129.76, 131.88, 132.00, 136.84, 139.06, 139.21, 208.44, 208.85. EI-MS (*m*/*z*, relative intensity): 364 (M^+, 8), 255 (30), 237 (30), 165 (93), 128 (18), 91 (36), 73 (100). HRMS calcd for $C_{22}H_{24}OSSi$ [M^+] 364.1317; Found: 364.1316.

*1-Ethynyl-2-(4-methylphenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4b**)*



Mixture of two stereoisomers, yield-1: 99%, yield-2 84%; IR (film) 3298, 2958, 1955, 1251, 1097, 870, 843, 750, 692 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 0.088 (s, 9H), 0.15 (s, 9H), 2.36 (S, 6H), 2.44 (d, J = 2.1 Hz, 1H), 2.53 (d, J = 2.1 Hz, 1H), 4.54-4.81 (m, 6H), 5.59 (t, J = 6.9 Hz, 1H), 5.66 (t, J = 6.9 Hz, 1H), 7.11-7.44 (m, 14H), 7.55 (d, J = 8.4 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.056, 0.18, 21.03, 62.76, 63.46, 68.10, 68.73, 75.42, 75.76, 78.16, 78.52, 82.69, 82.85, 93.28, 93.59, 127.89, 127.99, 128.04, 128.38, 128.43, 129.60, 132.17, 136.02, 136.13, 136.77, 136.83, 208.40, 208.86. EI-MS (*m*/*z*, relative intensity): 378 (M^+, 5), 288 (5), 269 (56), 251 (24), 179 (94), 73 (100). HRMS calcd for $C_{23}H_{26}OSSi$ [M^+] 378.1474; Found: 378.1480.

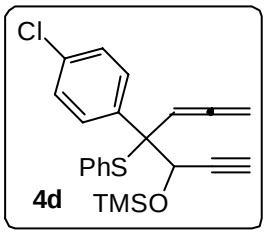
*1-Ethynyl-2-(4-methoxyphenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4c**)*



Mixture of two stereoisomers, yield-1: 99%, yield-2: 89%; IR (film) 3291, 2957, 1954, 1509, 1250, 1094, 870, 842, 750 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 0.052 (s, 9H), 0.11 (s, 9H), 2.41 (d, J = 2.1 Hz, 1H), 2.50 (d, J = 2.1 Hz, 1H), 3.80 (s, 6H), 4.53-4.63 (m, 4H), 4.72 (d, J = 6.9 Hz, 2H), 5.53 (t, J = 6.9 Hz, 1H), 5.60 (t, J = 6.9 Hz, 1H), 6.80-6.85 (m, 4H),

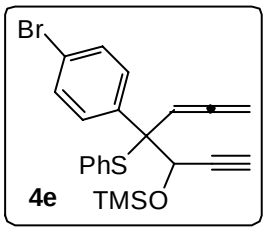
7.16-7.30 (m, 8H), 7.37-7.40 (m, 2H), 7.53-7.65 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.056, 0.18, 55.10, 62.57, 63.24, 68.14, 68.76, 75.42, 75.77, 78.19, 78.55, 82.67, 82.85, 93.35, 93.67, 112.43, 112.54, 128.07, 128.41, 128.46, 130.92, 131.06, 131.20, 132.15, 136.77, 136.81, 158.62, 158.68, 208.34, 208.83. EI-MS (*m*/*z*, relative intensity): 394 (M^+, 3), 379 (2), 285 (98), 267 (20), 195 (69), 73 (100). HRMS calcd for $C_{23}H_{26}O_2S_i\,S$ [M^+] 394.1423; Found: 394.1431.

*1-Ethynyl-2-(4-chlorophenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4d**)*



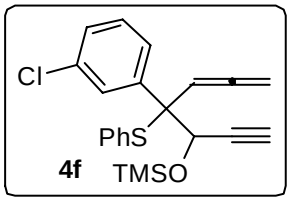
Mixture of two stereoisomers, yield-1: 90%, yield-2 82%; IR (film) 3296, 2959, 1955, 1490, 1252, 1094, 843, 750, 693 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.069 (s, 9H), 0.14 (s, 9H), 2.44 (d, J = 2.1 Hz, 1H), 2.54 (d, J = 2.1 Hz, 1H), 4.56-4.76 (m, 6H), 5.50 (t, J = 6.6 Hz, 1H), 5.57 (t, J = 6.6 Hz, 1H), 7.19-7.42 (m, 14H), 7.59 (d, J = 8.7 Hz, 2H), 7.69 (d, J = 8.7 Hz, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.040, 0.17, 62.59, 63.26, 68.05, 68.56, 75.72, 76.15, 78.47, 78.86, 82.31, 82.46, 92.90, 93.40, 127.23, 127.33, 128.24, 128.74, 128.78, 131.30, 131.36, 131.66, 133.13, 133.25, 136.88, 136.96, 137.63, 137.86. EI-MS (*m*/*z*, relative intensity): 398 (M^+, 4), 289 (26), 271 (19), 199 (39), 165 (10), 127 (9), 109 (10), 73 (100). HRMS calcd for $C_{22}H_{23}OSSi^{35}Cl$ [M^+] 398.0927; Found: 398.0921.

*1-Ethynyl-2-(4-bromophenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4e**)*



Mixture of two stereoisomers, yield-1: 73%, yield-2: 97%; IR (film) 3298, 2958, 1954, 1585, 1485, 1251, 1097, 1010, 843, 750, 692 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.047 (s, 9H), 0.12 (s, 9H), 2.42 (d, J = 2.1 Hz,1H), 2.53 (d, J = 2.1 Hz, 1H), 4.51-4.74 (m, 6H), 5.47 (t, J = 6.6 Hz, 1H), 5.53 (t, J = 6.6 Hz, 1H), 7.12-7.62 (m, 18H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.040, 0.17, 62.66, 63.30, 67.98, 68.47, 75.75, 76.19, 78.48, 78.87, 82.26, 82.42, 92.82, 93.32, 121.46, 121.57, 128.22, 128.74, 128.77, 130.16, 130.26, 131.44, 131.67, 131.71, 136.86, 136.96, 138.14, 138.38, 208.30, 208.74. EI-MS (*m*/*z*, relative intensity): 442 (M^+, 3), 333 (17), 315 (8), 236 (36), 165 (15), 127 (13), 109 (15), 73 (100). HRMS calcd for $C_{22}H_{23}OSSi^{79}Br$ [M^+] 442.0422; Found: 442.0425.

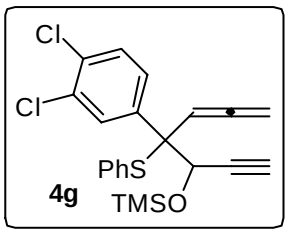
*1-Ethynyl-2-(3-chlorophenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4f**)*



4f

Mixture of two stereoisomers, yield-1: 99%, yield-2 69%; IR (film) 3301, 2959, 1955, 1252, 1098, 868, 843, 750, 693cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.047 (s, 9H), 0.11 (s, 9H), 2.45 (d, J = 2.1 Hz, 1H), 2.54 (d, J = 2.1 Hz, 1H), 4.58-4.78 (m, 6H), 5.49 (t, J = 6.6 Hz, 1H), 5.58 (t, J = 6.6 Hz, 1H), 7.18-7.71 (m, 18H), ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.024, 0.14, 62.45, 63.32, 67.92, 68.55, 75.81, 76.21, 78.52, 78.93, 82.22, 82.33, 92.64, 93.18, 127.27, 127.43, 127.93, 128.00, 128.23, 128.30, 128.39, 128.76, 128.87, 130.05, 130.28, 131.42, 131.52, 133.04, 133.15, 136.96, 137.00, 141.25, 141.45, 208.44, 208.80. EI-MS (*m*/*z*, relative intensity): 398 (M^+, 8), 289 (11), 271 (13), 199 (35), 127 (12), 109 (13), 73 (100). HRMS calcd for $C_{22}H_{23}OSSi^{35}Cl$ [M^+] 398.0927; Found: 398.0924.

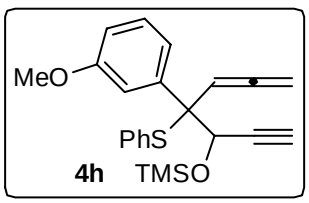
*1-Ethynyl-2-(3,4-dichlorophenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4g**)*



4g

Mixture of two stereoisomers, yield-1: 94%, yield-2 80%; IR (film) 3300, 2958, 1955, 1470, 1252, 1099, 867, 844, 750, 692 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.060 (s, 9H), 0.14 (s, 9H), 2.44 (d, J = 2.1 Hz, 1H), 2.55 (d, J = 2.1 Hz, 1H), 4.55-4.76 (m, 6H), 5.42 (t, J = 6.6 Hz, 1H), 5.49 (t, J = 6.6 Hz, 1H), 7.20-7.40 (m, 12H)，7.48-7.52 (m,1H), 7.58-7.61 (m, 1H), 7.69 (d, J = 2.1 Hz, 1H), 7.82 (d, J = 2.1 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.016, 0.14, 62.29, 62.96, 67.91, 68.41, 75.94, 76.45, 81.98, 82.08, 92.47, 93.13, 128.34, 128.36, 128.92, 128.99, 129.05, 129.19, 129.36, 131.10, 131.21, 131.37, 132.04, 132.24, 137.00, 137.10, 139.35, 139.64, 208.29, 208.71. EI-MS (*m*/*z*, relative intensity): 432 (M^+, 5), 323 (12), 307 (17), 233 (36), 163 (16), 127 (18), 109 (38), 73 (100), 45 (38). HRMS calcd for $C_{22}H_{22}OSSi^{35}Cl_2$ [M^+] 432.0538; Found: 432.0541.

*1-Ethynyl-2-(3-methoxyphenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4h**)*

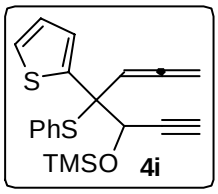


4h

Mixture of two stereoisomers; IR (film) 3292, 2956, 1954, 1251, 1097, 869, 842, 751, 693 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.092 (s, 9H), 0.15 (s, 9H), 2.47 (d, J = 2.1 Hz, 1H), 2.55 (d, J = 2.1 Hz,

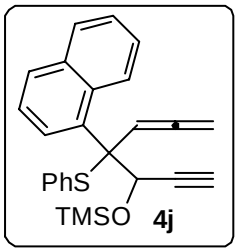
1H), 3.80 (s, 3H), 3.81 (s, 3H), 4.56-4.80 (m, 6H), 5.60 (t, J = 6.6 Hz, 1H), 5.68 (t, J = 6.6 Hz, 1H), 6.81-6.85 (m, 2H), 7.12-7.44 (m, 16H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.040, 0.15, 55.09, 55.13, 62.76, 63.62, 68.09, 68.71, 75.52, 75.85, 78.25, 78.63, 82.56, 82.73, 93.10, 93.45, 112.89, 115.62, 115.80, 122.10, 122.13, 127.95, 128.07, 128.45, 128.53, 131.96, 132.06, 136.74, 136.79, 140.70, 140.83, 158.57, 158.63, 208.42, 208.85. EI-MS (*m*/*z*, relative intensity): 394 (M^+, 18), 285 (26), 267 (20), 195 (70), 109 (14), 73 (100). HRMS calcd for $C_{23}H_{26}O_2SSi$ [M^+] 394.1423; Found: 394.1425.

*1-Ethynyl-2-(2- thiophenyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4i**)*



Mixture of two stereoisomers, yield-1: 98%, yield-2 94%; IR (film) 3295, 2958, 1954, 1251, 1098, 842, 749, 692 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.12 (s, 9H), 0.16 (s, 9H), 2.44 (d, J = 2.1 Hz, 1H), 2.53 (d, J = 2.1 Hz, 1H), 4.56-4.80 (m, 6H), 5.62 (t, J = 6.6 Hz, 1H), 5.67 (t, J = 6.6 Hz, 1H), 6.90-6.94 (m, 2H), 7.02-7.03 (m, 1H), 7.13-7.15 (m, 1H), 7.20-7.43 (m, 12H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 0.024, 0.11, 60.96, 61.45, 68.84, 69.83, 75.41, 75.77, 78.86, 79.16, 82.30, 82.42, 93.44, 93.83, 125.50, 125.66, 125.73 125.99, 127.63, 127.74, 128.14, 128.70, 128.79, 131.87, 136.82, 136.88, 144.22, 144.33. EI-MS (*m*/*z*, relative intensity): 370 (M^+, 3), 355 (1), 261 (64), 243 (18), 171 (52), 109 (11), 73 (100). HRMS calcd for $C_{20}H_{22}OSiS_2$ [M^+] 370.0881; Found: 370.0886.

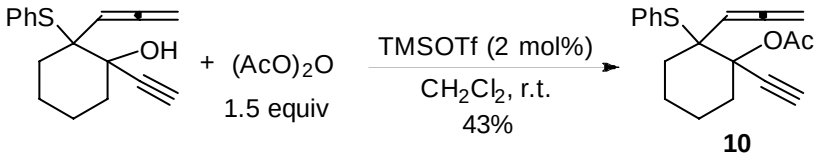
*1-Ethynyl-2-(1-naphthyl)-2-phenylthio-3,4-pentadienyl trimethylsilyl ether (**4j**)*



Mixture of two stereoisomers, yield-1: 90%, yield-2: 70%; IR (film) 3291, 2957, 1955, 1251,1092, 843, 775, 750, 692 cm^{-1}; ^{1}H NMR ($CDCl_3$, 300 MHz) δ 0.019 (s, 4.5H), 0.18 (s, 9H), 2.64 (d, J = 1.8 Hz, 0.5H), 2.67 (d, J = 2.1 Hz, 1H), 4.41-4.53 (m, 1H), 4.83-4.96 (m, 2H), 5.27(d, J = 2.1 Hz, 0.5H), 5.33 (d, J = 2.1 Hz, 1H), 5.98 (t, J = 6.3 Hz, 0.5H), 6.07 (t, J = 6.3 Hz, 1H), 7.03-7.60 (m, 12H), 7.71-7.89 (m, 4H), 8.33 (d, J = 7.2 Hz, 0.5H), 8.90 (d, J = 7.2 Hz, 0.5H), 9.12 (d, J = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ -0.15, 0.20, 62.61, 65.55, 68.63, 69.22, 75.87, 76.21, 78.21, 78.77, 83.08, 94.94, 123.86, 124.15, 124.50, 124.54, 124.72, 124.81, 127.73, 127.88, 128.18, 128.66, 128.88, 128.94, 129.15, 129.72, 131.62 131.82,

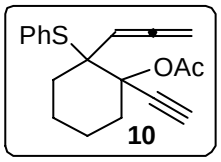
132.13, 132.90, 134.22, 134.63, 134.67, 136.08, 136.60, 209.01, 209.17. EI-MS (*m*/*z*, relative intensity): 414 (M^+, 81), 399 (14), 324 (23), 287 (44), 215 (22), 73 (100). HRMS calcd for $C_{26}H_{26}OSSi$ [M^+] 414.1474; Found: 414.1469.

5. Preparation of 2-allenyl-1-ethynyl-2-phenylthio-cyclohexanyl acetate 10[1]



Under a nitrogen atmosphere, 2-allenyl-1-ethynyl-2-phenylthio-cyclohexanol (2.0 mmol) and Ac_2O (3.0 mmol) were mixed in anhydrous CH_2Cl_2 (20 mL) in a 50 mL round-bottomed flask. TMSOTf (0.04 mmol) was then added to this solution at room temperature. The reaction was kept at the same temperature until completion as judged by TLC. Then saturated $NaHCO_3$ was then added, and the mixture was extracted with CH_2Cl_2. The combined organic layers were dried over $NaSO_4$ and evaporated, Removal of the solvent in *vacuo* gave a crude residue, which was purified by silica gel column. Elution with petroleum ether/ethyl acetate (20:1) afforded pure product of **10.**

*2-Allenyl-1-ethynyl-2-phenylthio-cyclohexanyl acetate (**10**)*

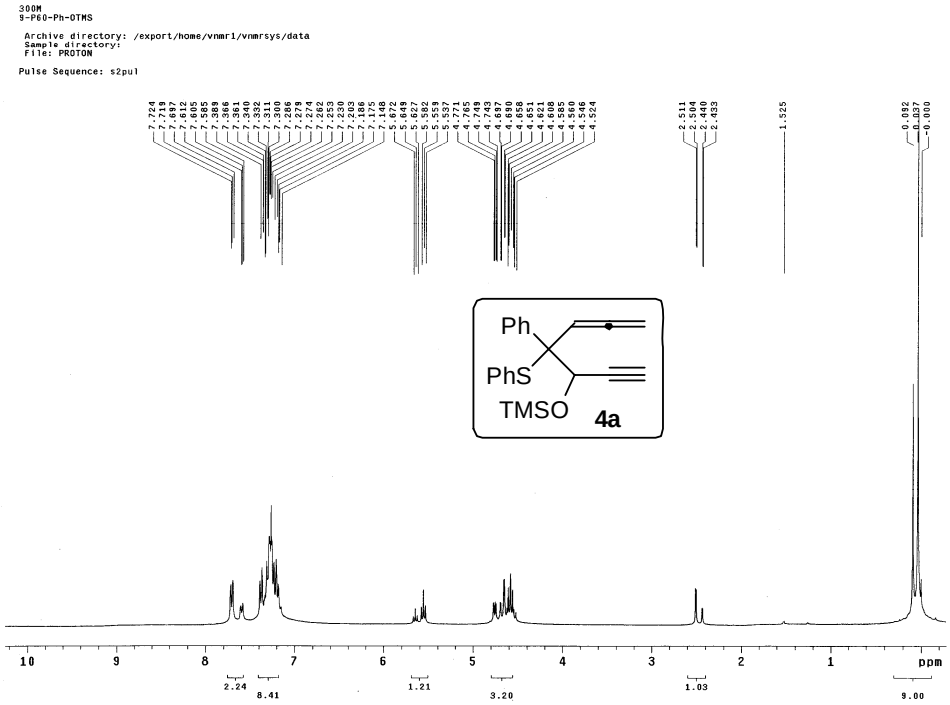


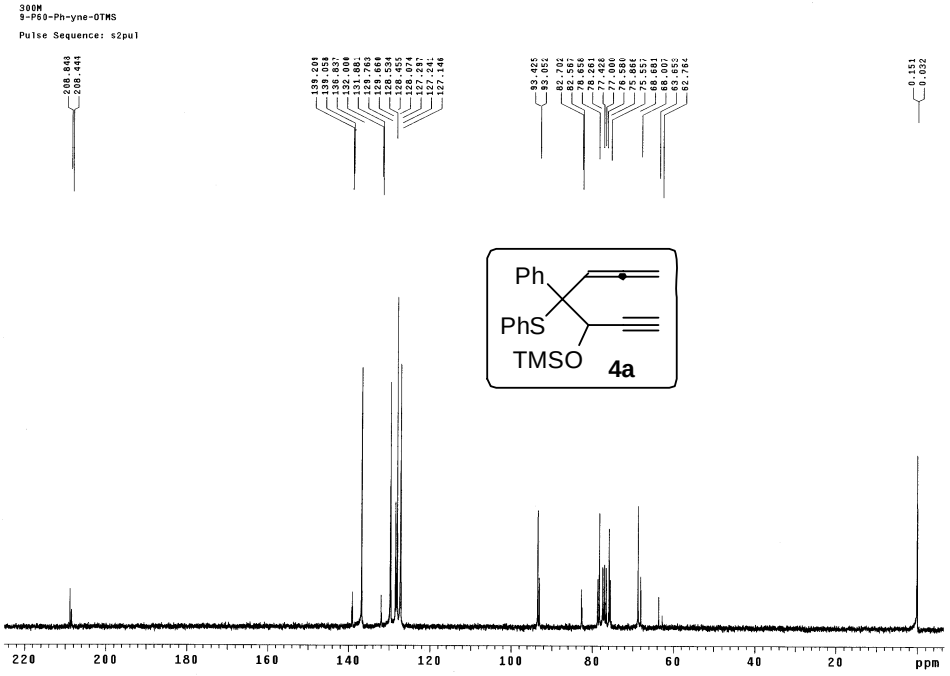
IR (film) 3284, 2940, 2863, 1953, 1748, 1229, 1216, 1016, 1003, 750, 693 cm^{-1}; ^1H NMR ($CDCl_3$, 300 MHz) δ 1.39-1.47 (m,1H), 1.59-1.88 (m, 5H), 2.09 (s, 3H), 2.26-2.42 (m, 1H), 2.54-2.66 (m, 1H), 2.75 (s, 1H), 4.32 (dd, J = 6.6, 10.8 Hz, 1H), 4.71 (dd, J = 6.6, 10.8 Hz, 1H), 5.65 (t, J = 6.6 Hz, 1H), 7.28-7.41 (m, 3H), 7.51-7.55 (m, 2H); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 21.19, 21.58, 21.73, 31.23, 31.99, 60.20, 76.58, 77.62, 80.41, 80.94, 93.41, 128.08, 128.87, 131.37, 138.38, 168.82, 208.72. EI-MS (*m*/*z*, relative intensity): 312 (M^+, 0.33), 270 (25), 252 (37), 161 (77), 143 (23), 128 (32), 110 (31), 91 (48), 43 (100). HRMS calcd for $C_{19}H_{20}O_2S$ [M^+] 312.1184; Found: 312.1192.

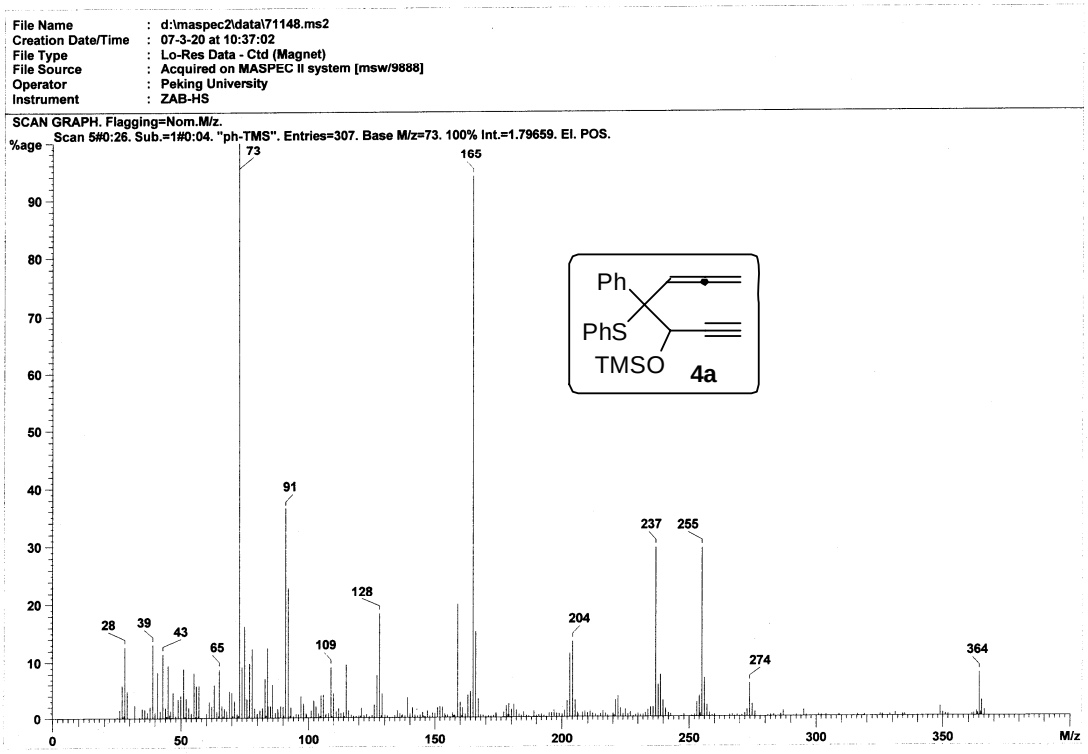
6. Reference

1 P. A. Procopiou, S. P. D. Baugh, S. S. Flack, G. G. A. Inglis, *J. Org. Chem.* 1998, **63**, 2342.

7. Spectra (^{1}H, ^{13}C NMR; MS, IR)



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Operator : Peking University
Instrument : ZAB-HS
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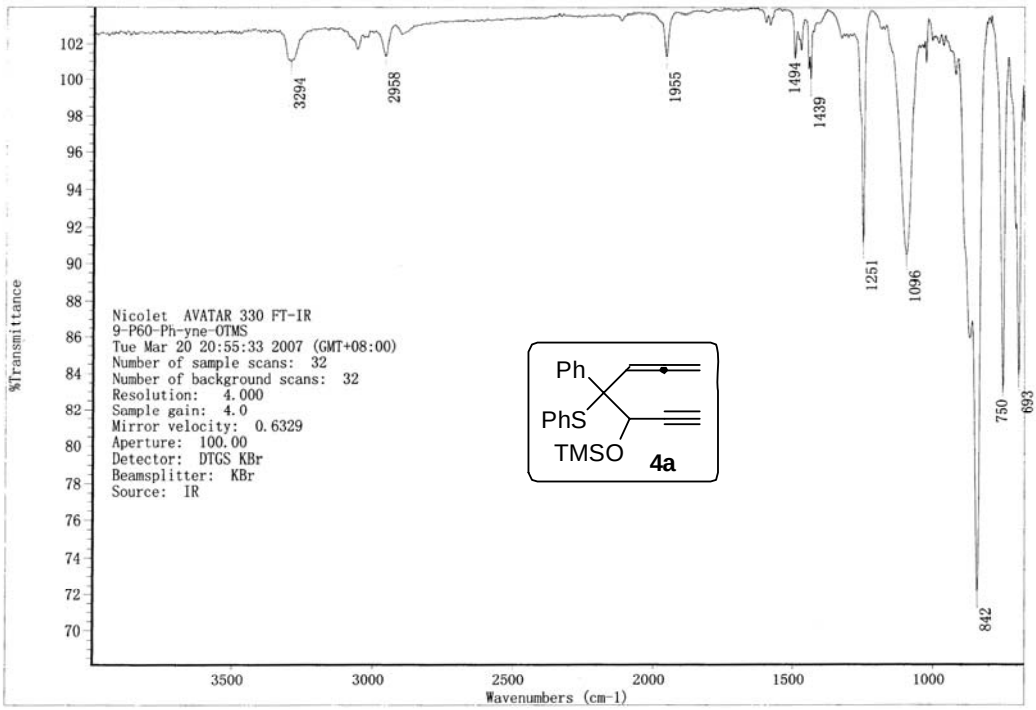
Ph
PhS
TMSO
4a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Wavenumbers (cm-1)
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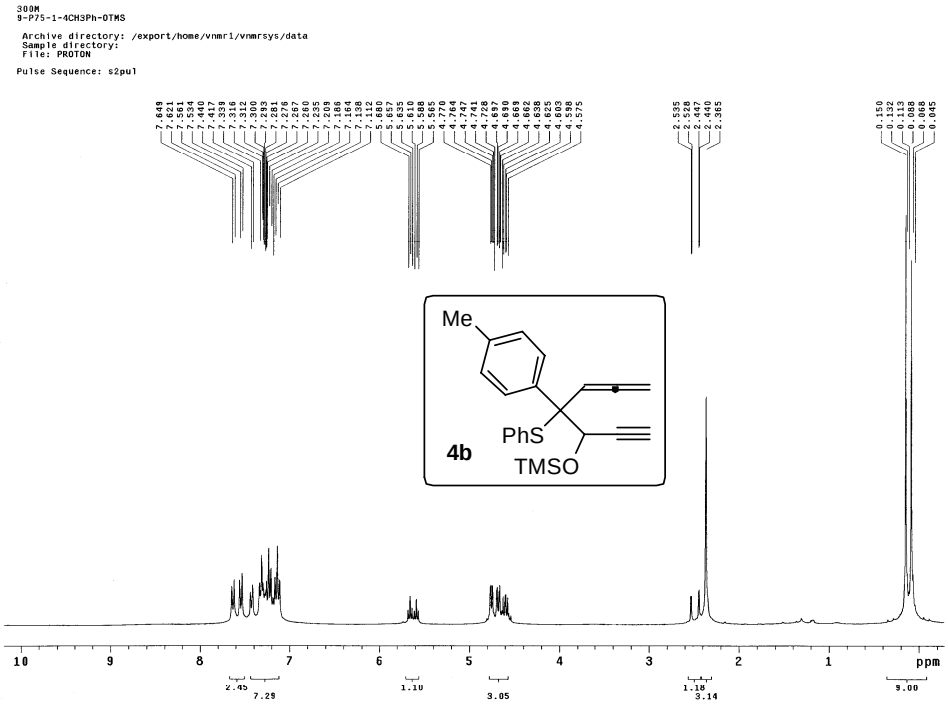
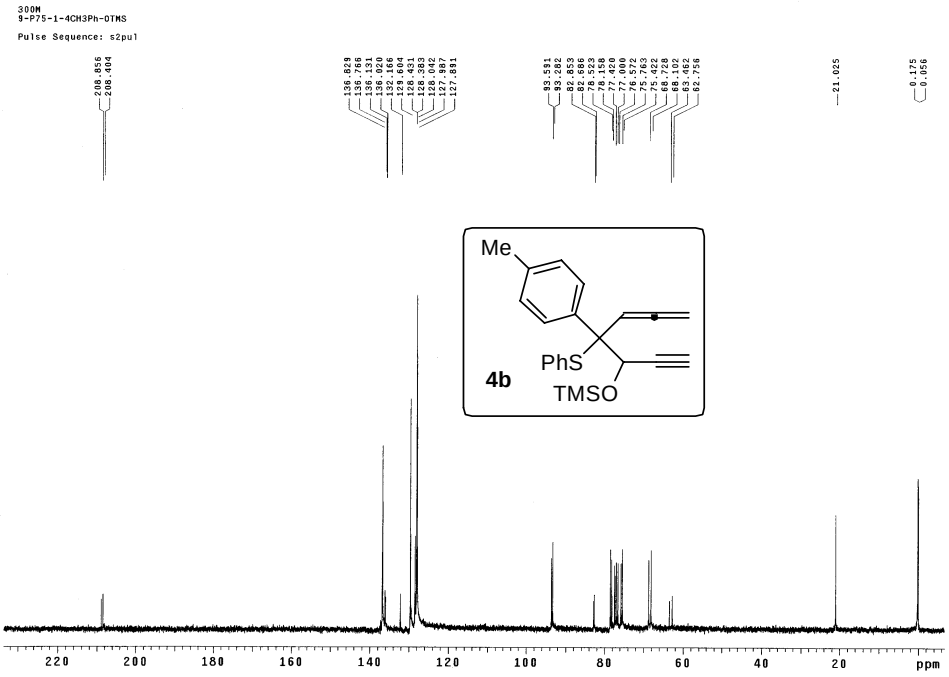
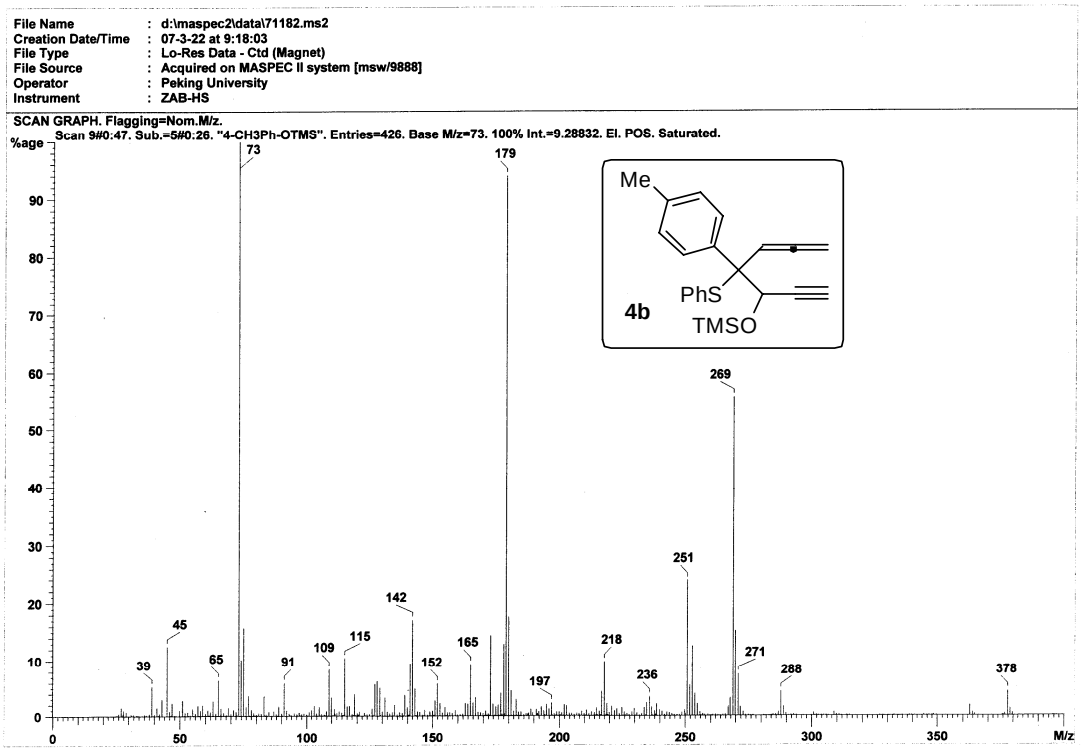
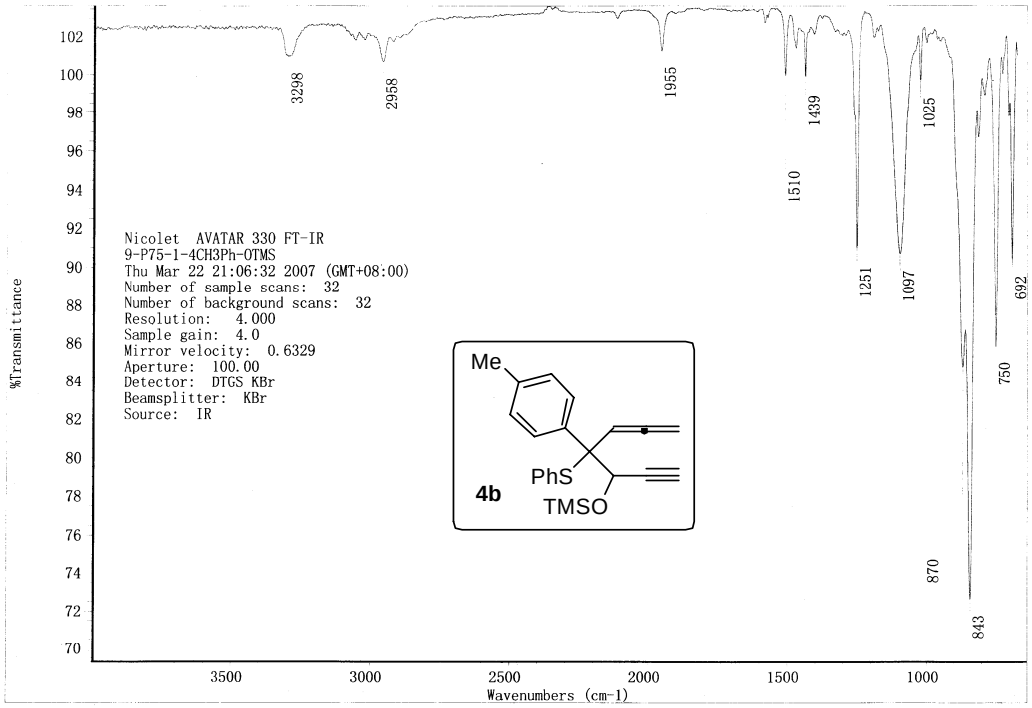
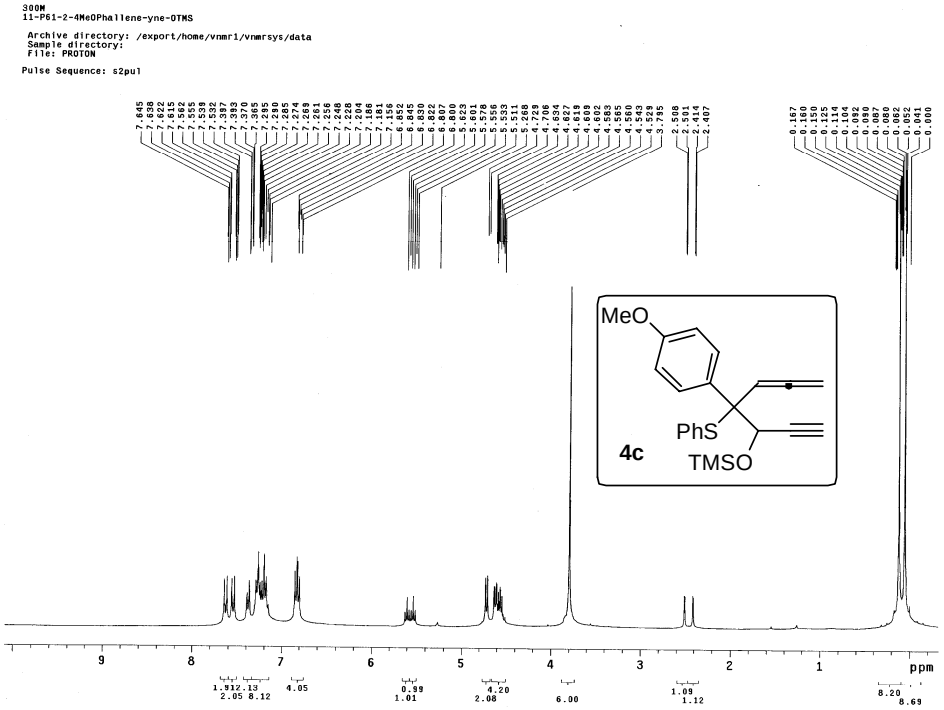
9-P60-Ph-yne-OTMS
Tue Mar 20 20:55:33 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
Ph
PhS
TMSO
4a







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Sample directory:
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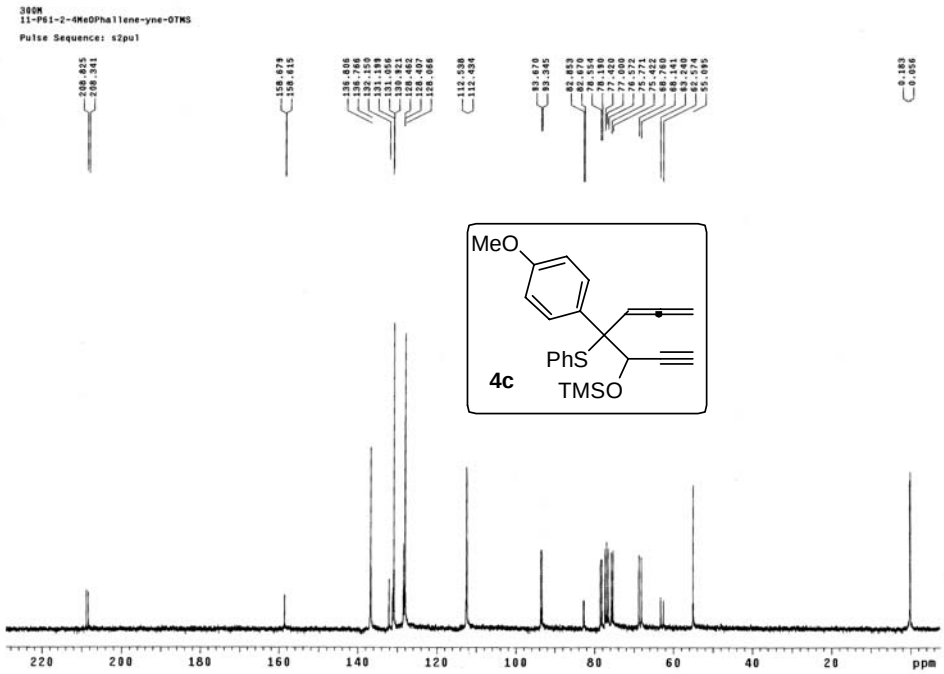
PhS
TMSO
4c
ppm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Pulse Sequence: s2pul
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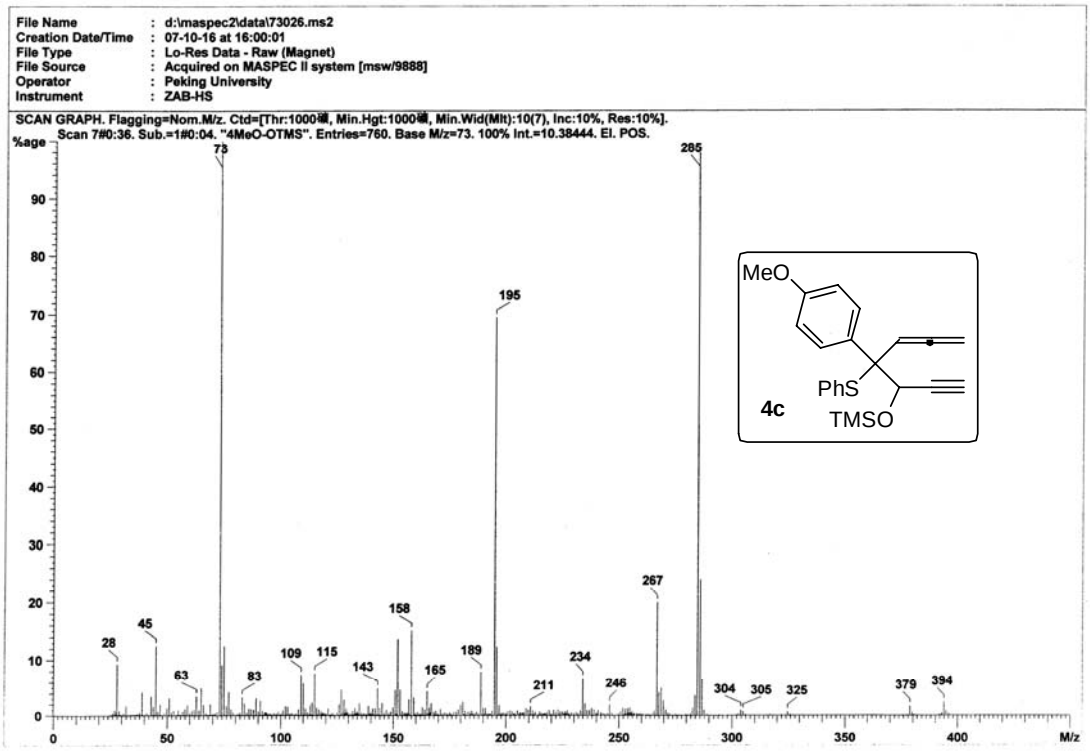
TMSO
4c
ppm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Operator : Peking University
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195
267
158
45
28
109
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143
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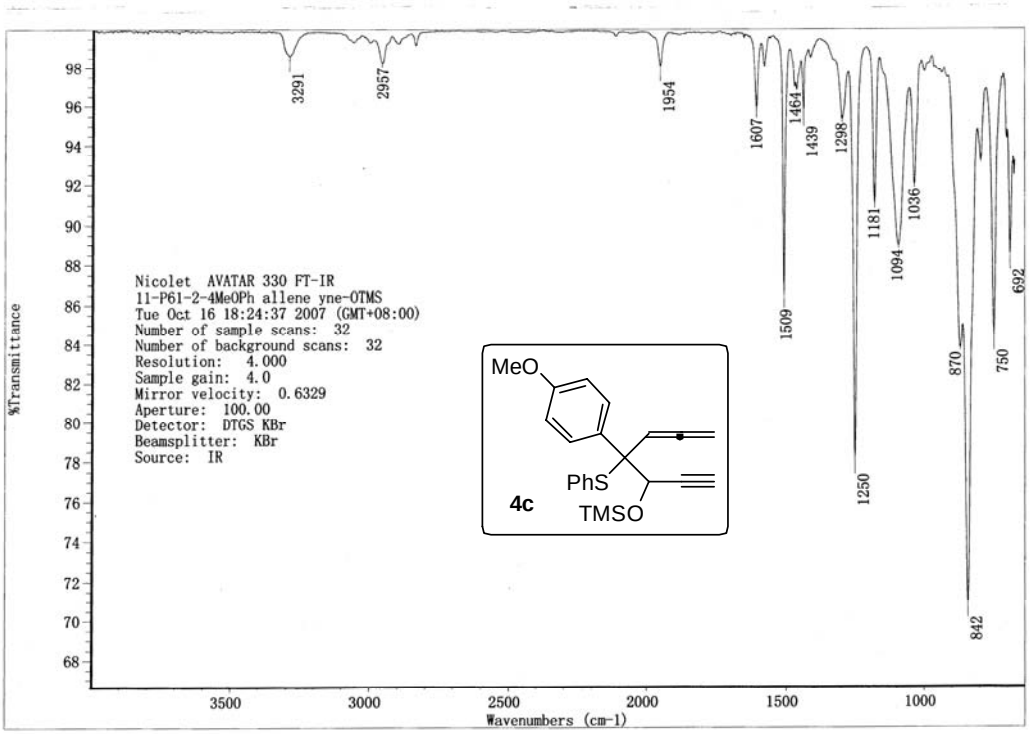
63
83
211
234
246
304
305
325
379
394
M/z
MeO
PhS
TMSO
4c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1464
1439
1298
1181
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1036
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1250
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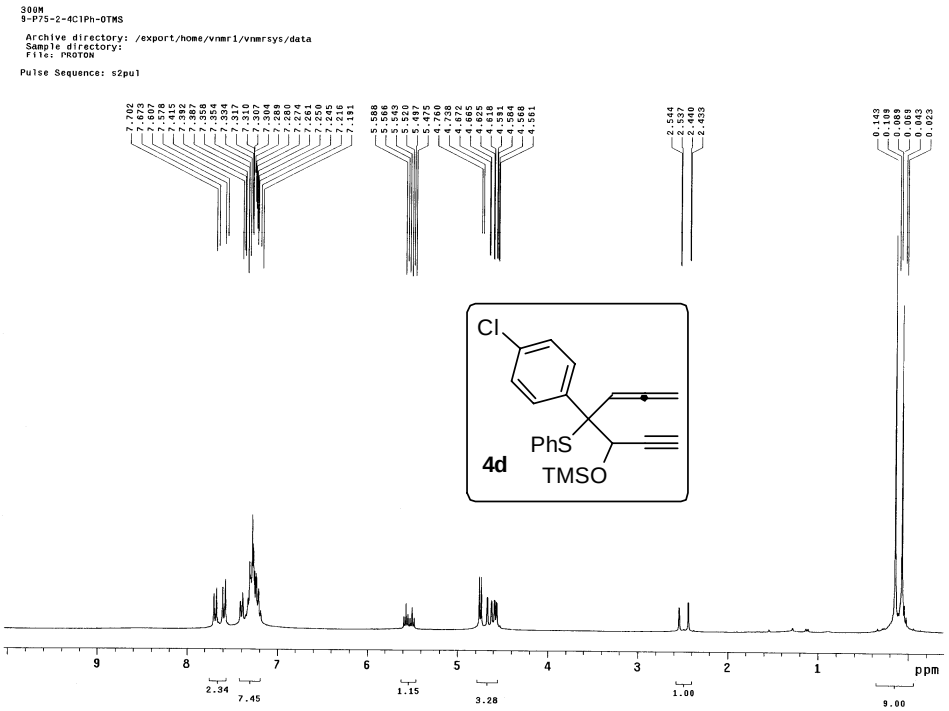
842
750
692
Nicolet AVATAR 330 FT-IR
11-P61-2-4MeOPh allene yne-OTMS
Tue Oct 16 18:24:37 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
Wavenumbers (cm-1)
MeO
PhS
TMSO
4c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File: PROTON
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Cl
PhS
TMSO
4d
ppm
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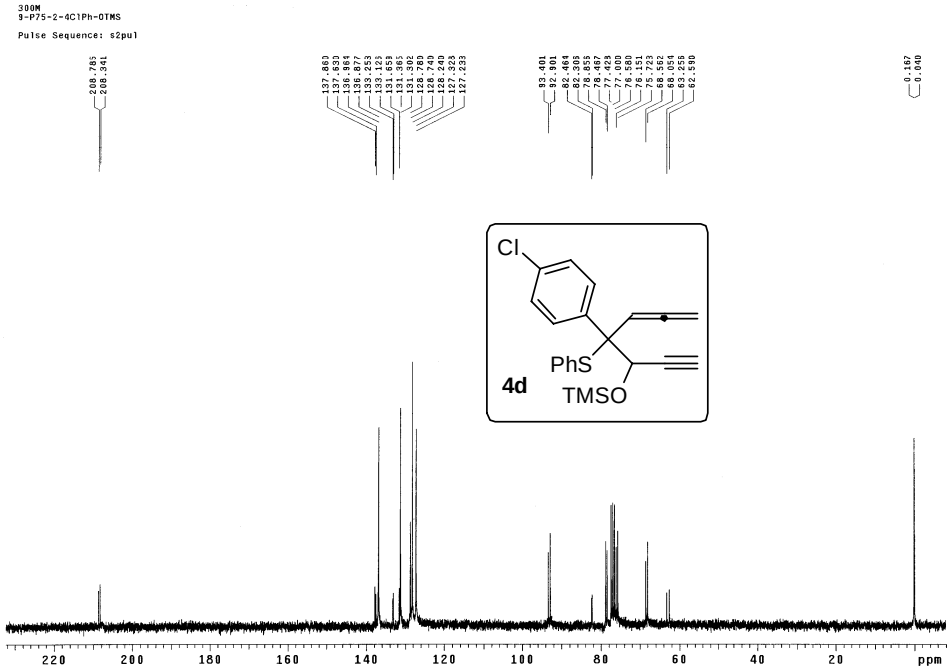
7.45
1.15
3.28
1.00
9.00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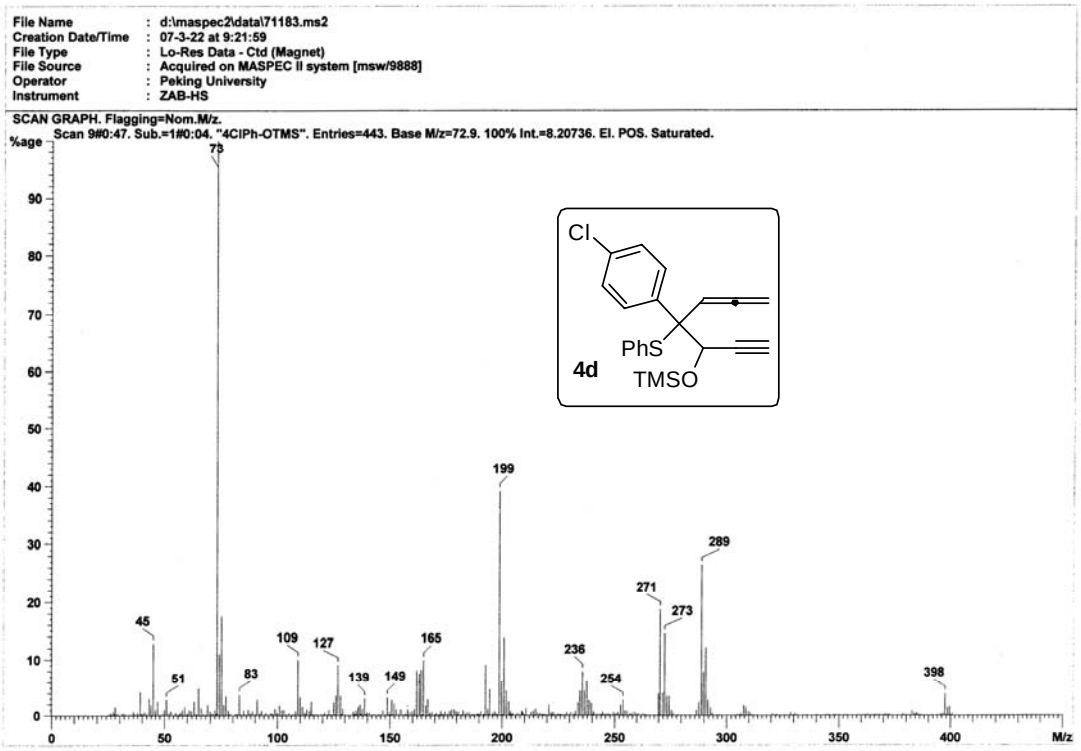
Pulse Sequence: s2pul
Cl
PhS
TMSO
4d
ppm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Operator : Peking University
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M/z
Cl
PhS
TMSO
4d
73
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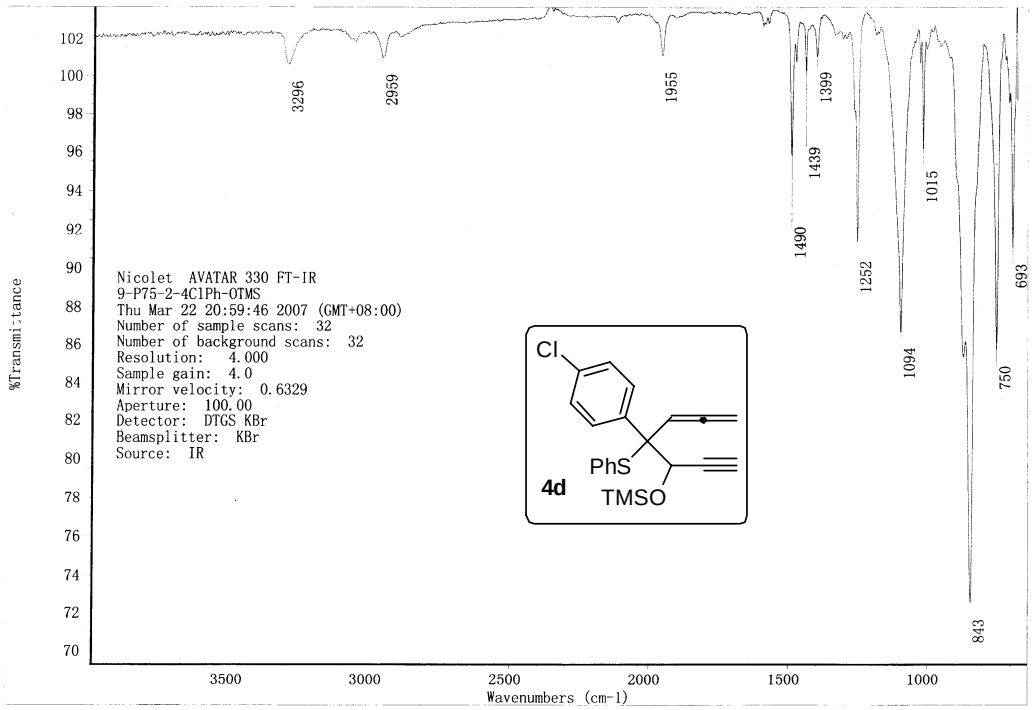
289
271
273
45
109
127
165
236
254
51
83
139
149
398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Thu Mar 22 20:59:46 2007 (GMT+08:00)
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Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
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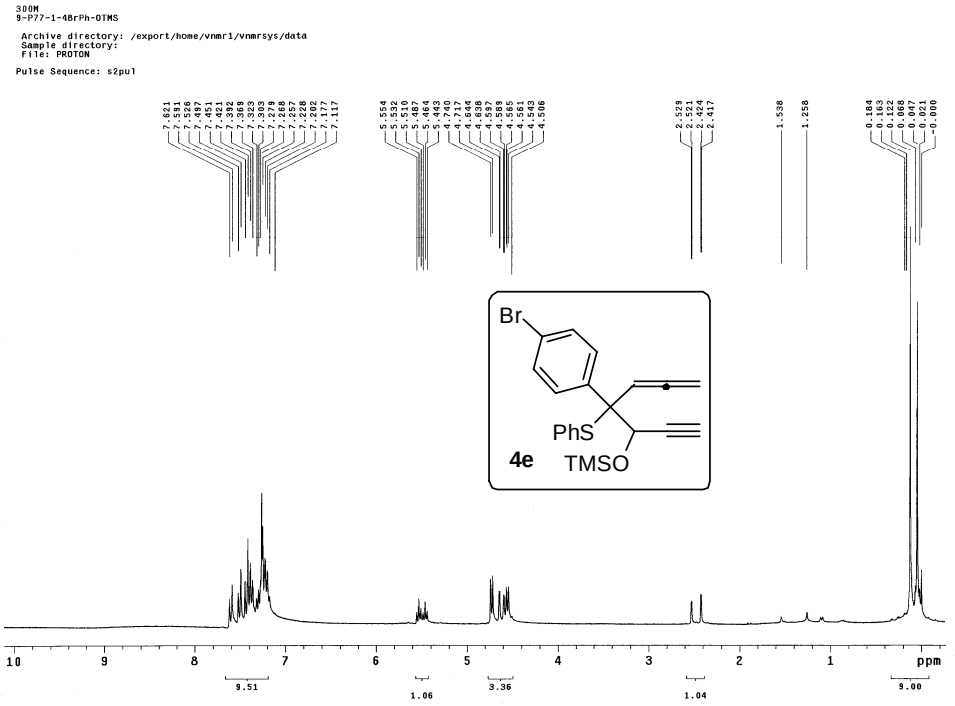
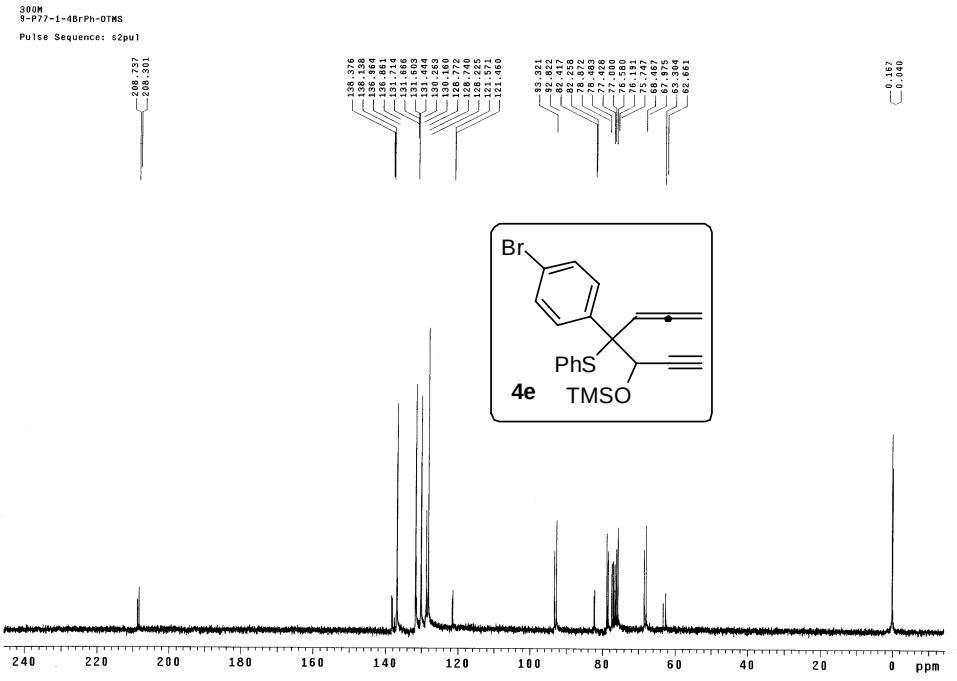
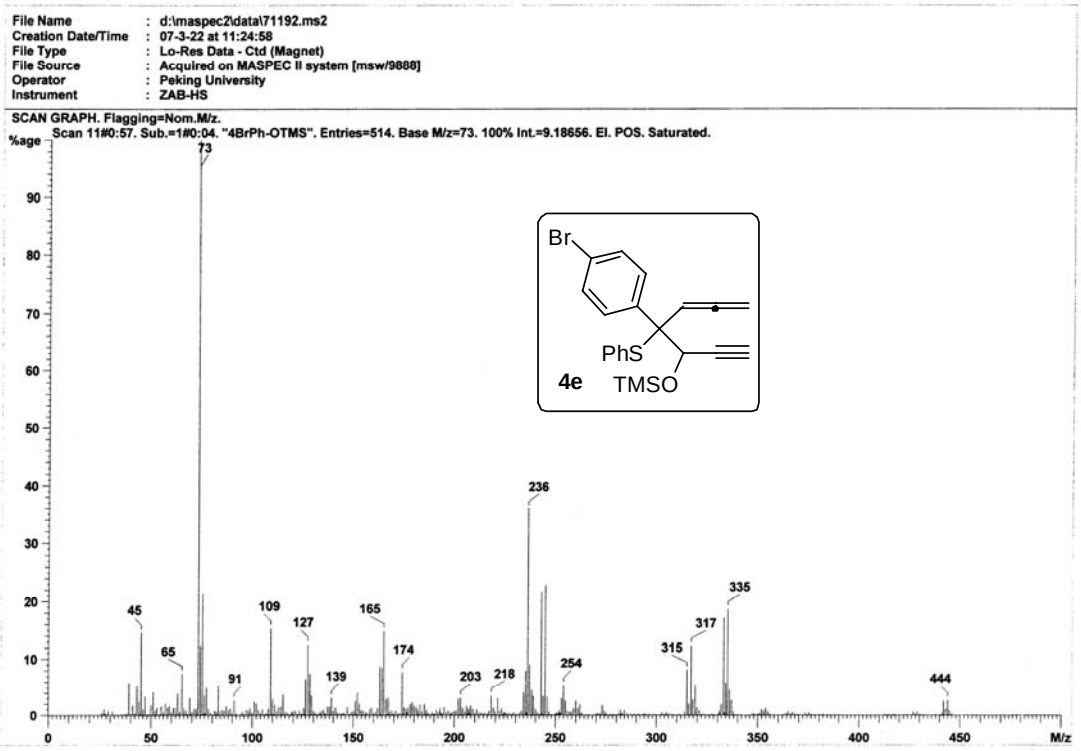
PhS
TMSO
4d
3296
2959
1955
1439
1399
1490
1252
1094
1015
750
693
843



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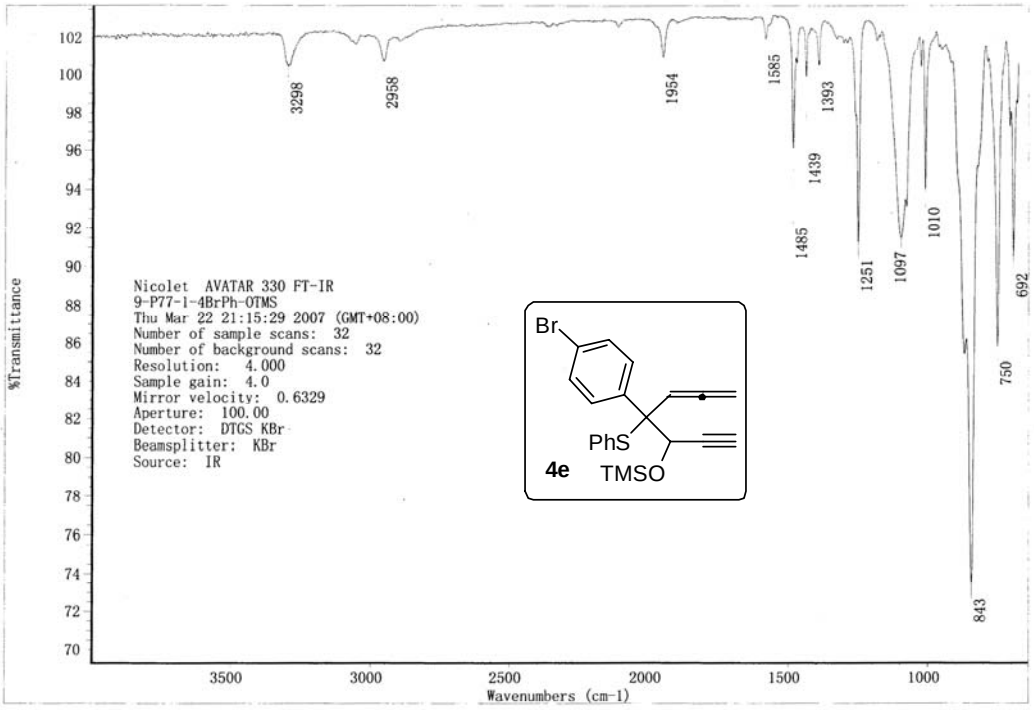
M/z
Br
PhS
TMSO
4e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Aperture: 100.00
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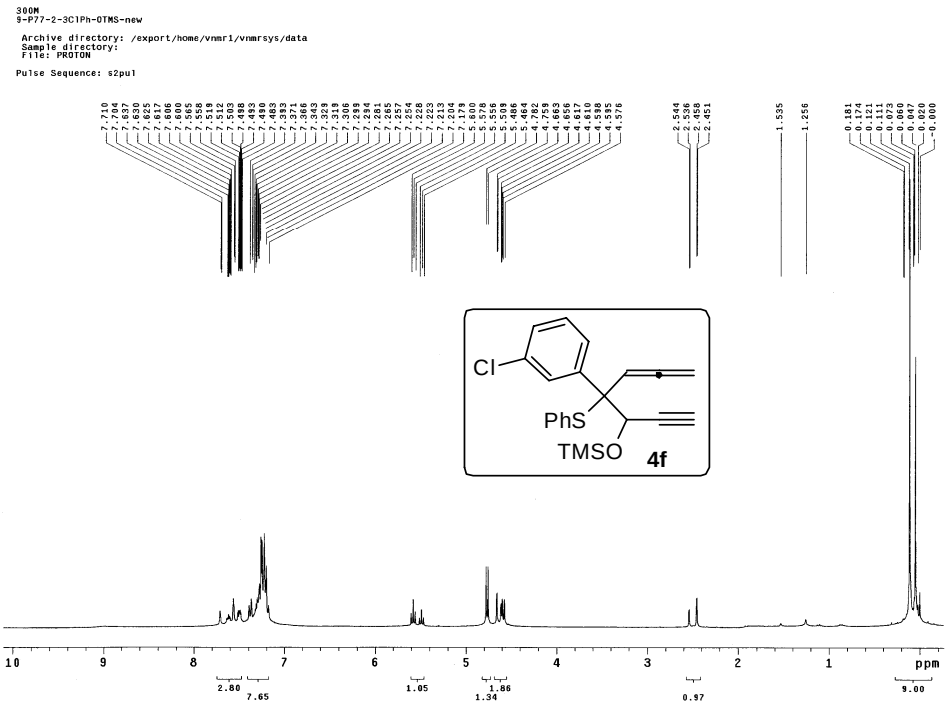
Beamsplitter: KBr
Source: IR
Br
PhS
TMSO
4e

V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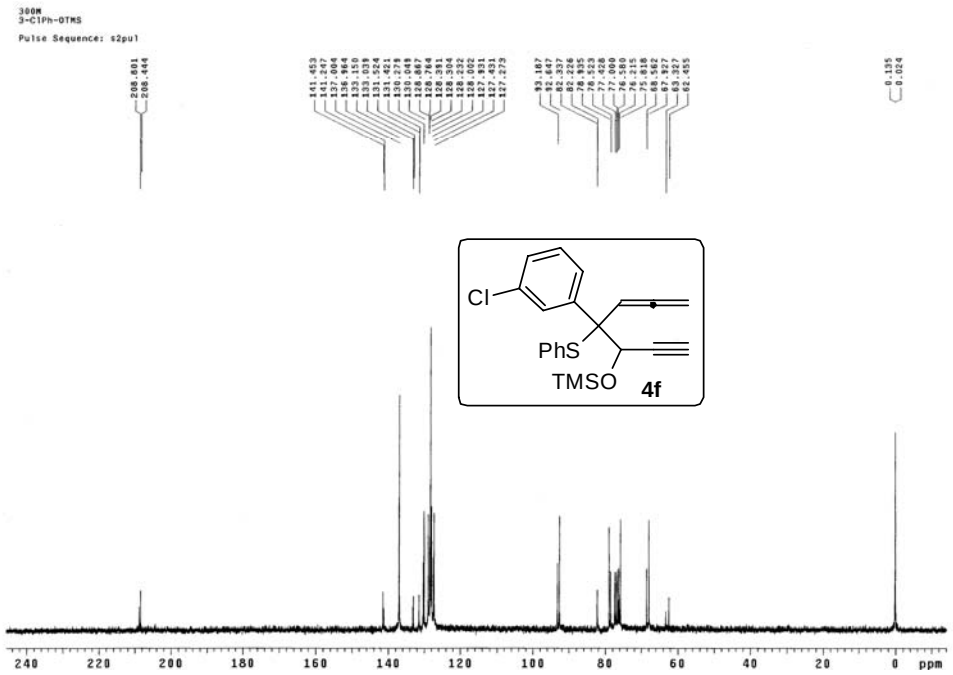
TMSO
4f
ppm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Pulse Sequence: s2pul
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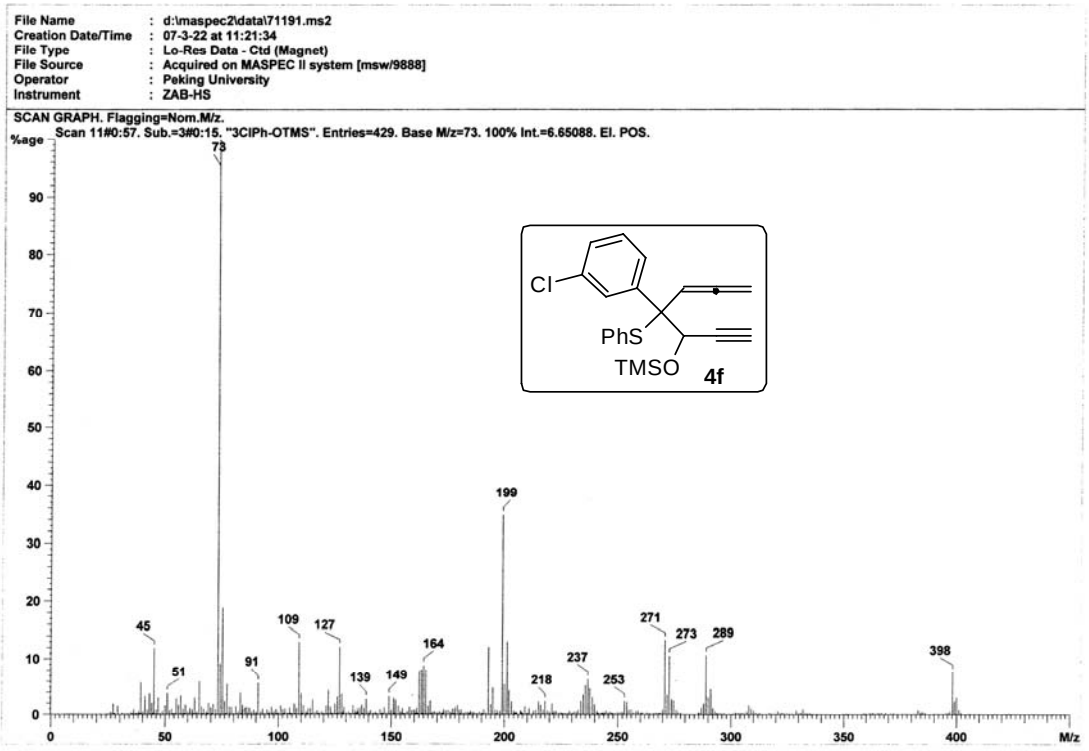
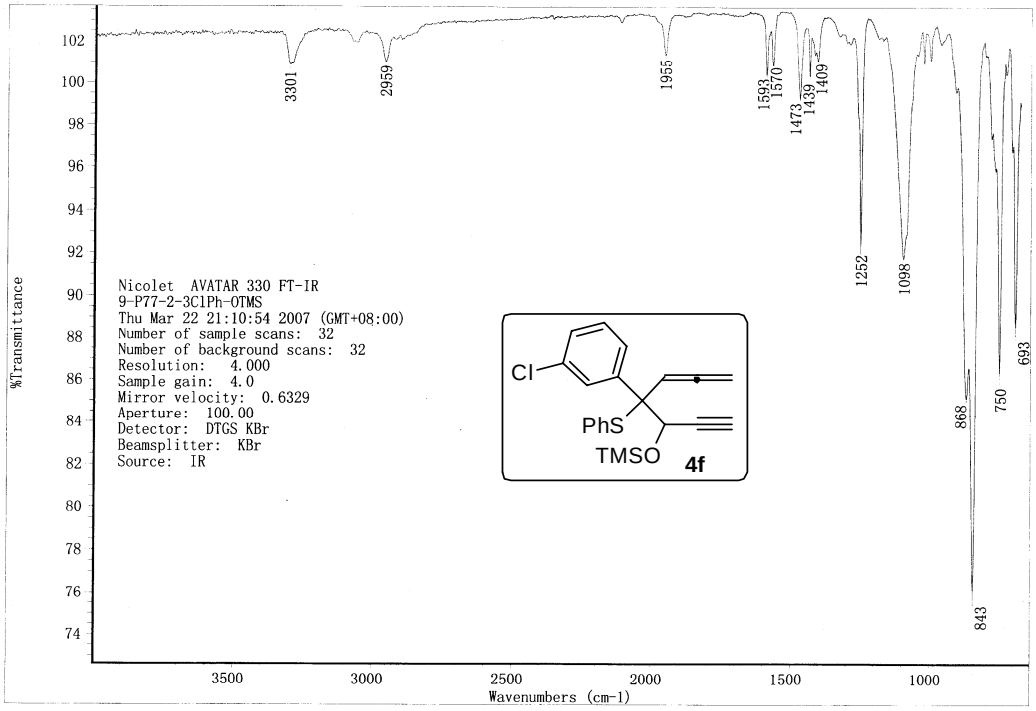
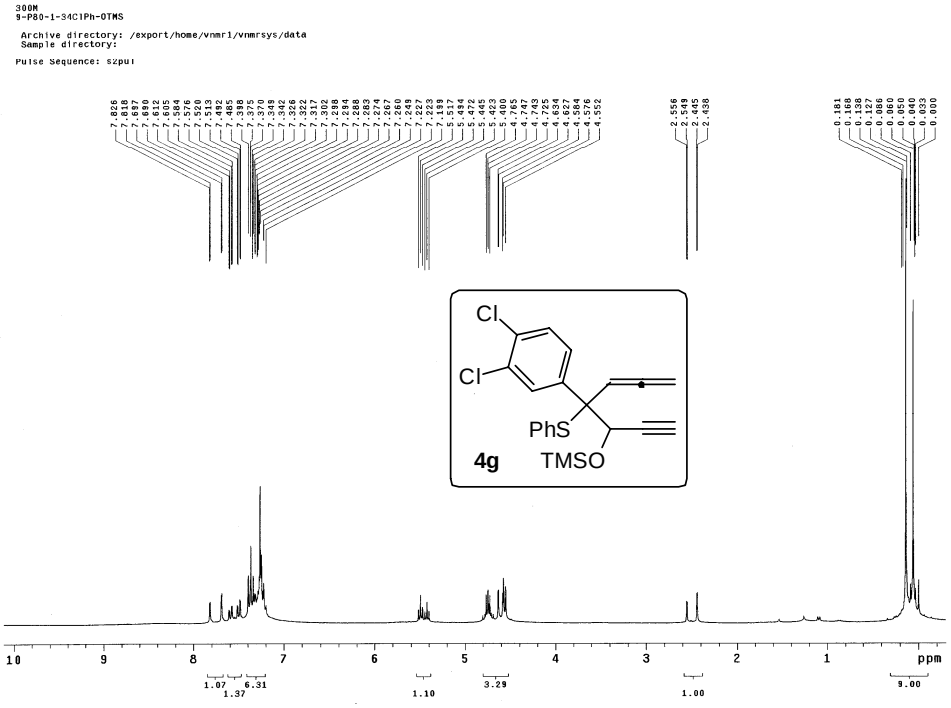
TMSO
4f
ppm



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Sample directory:
Pulse Sequence: s2pul
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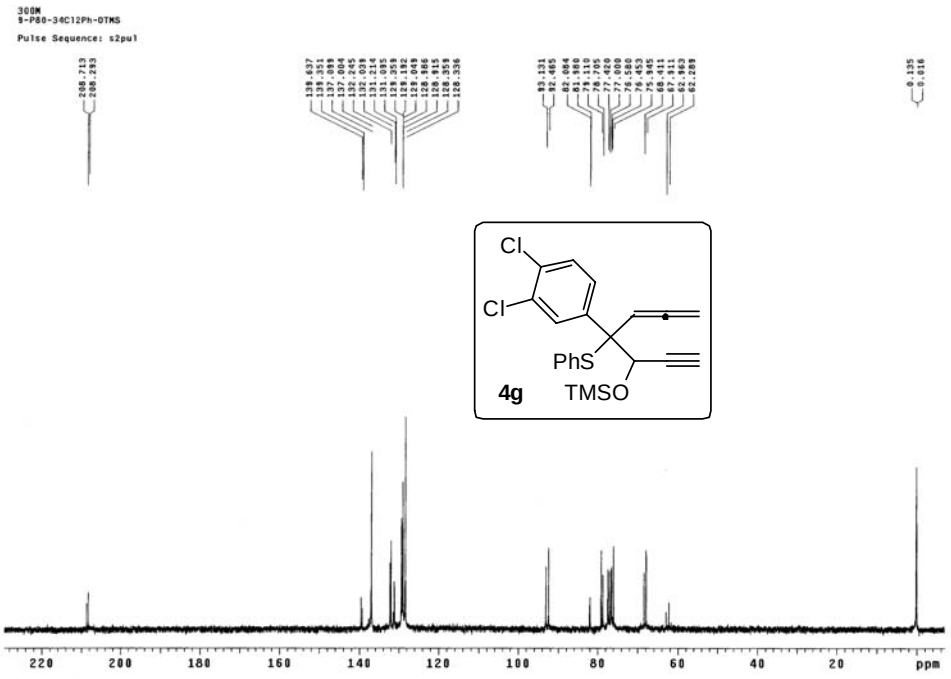
Cl
PhS
TMSO
4g
ppm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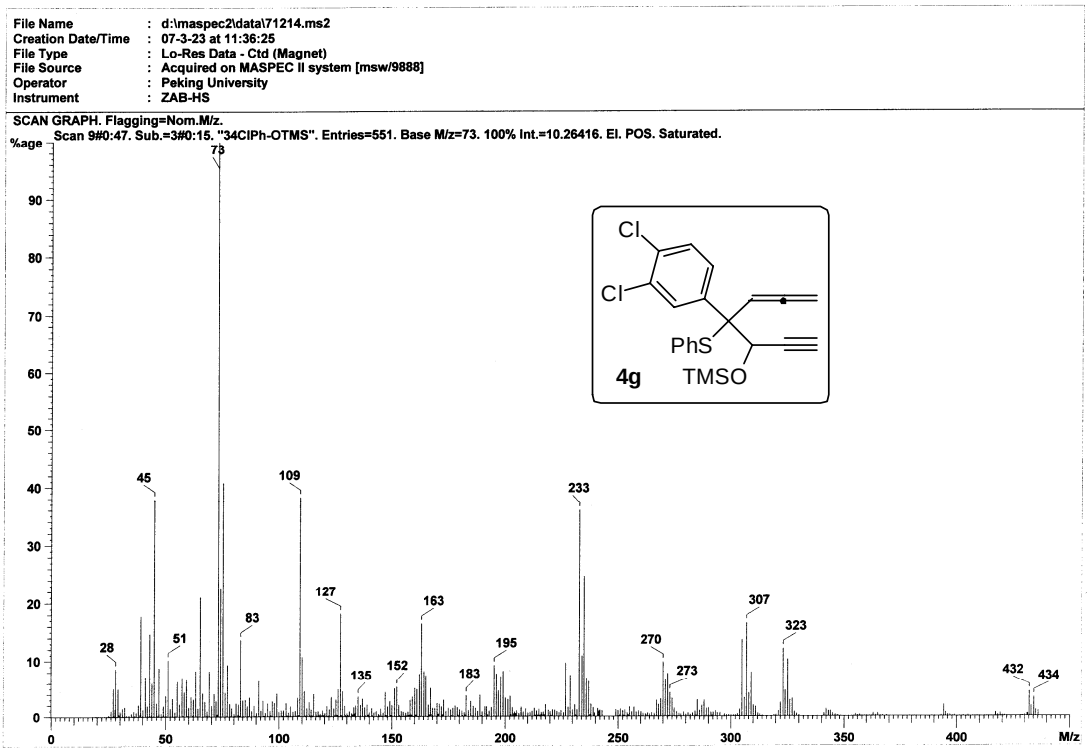
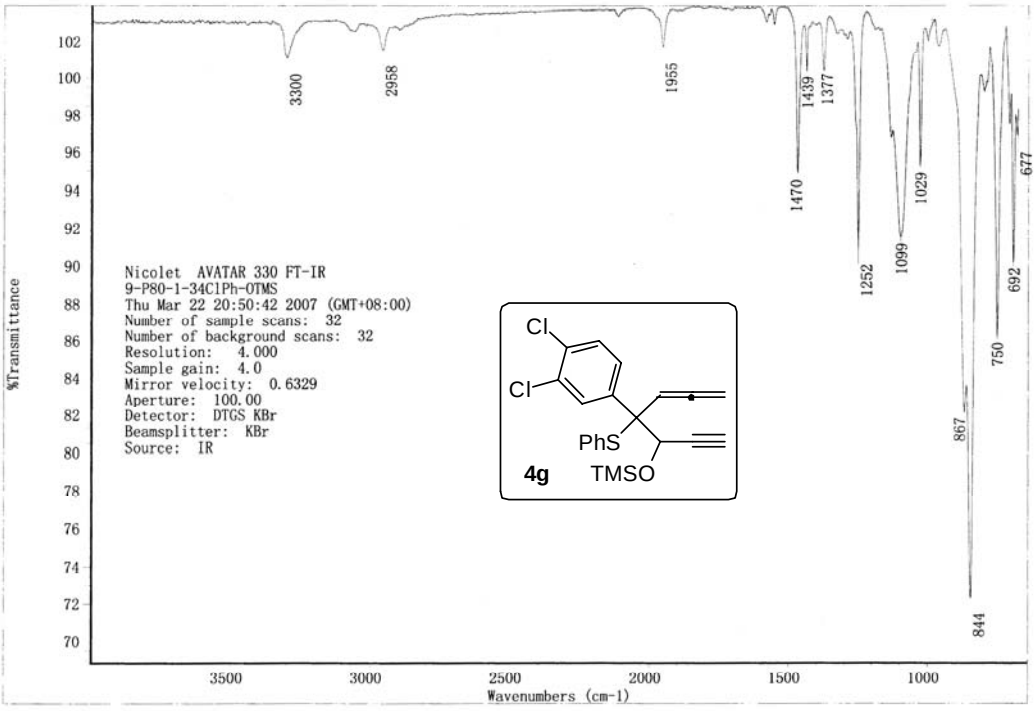
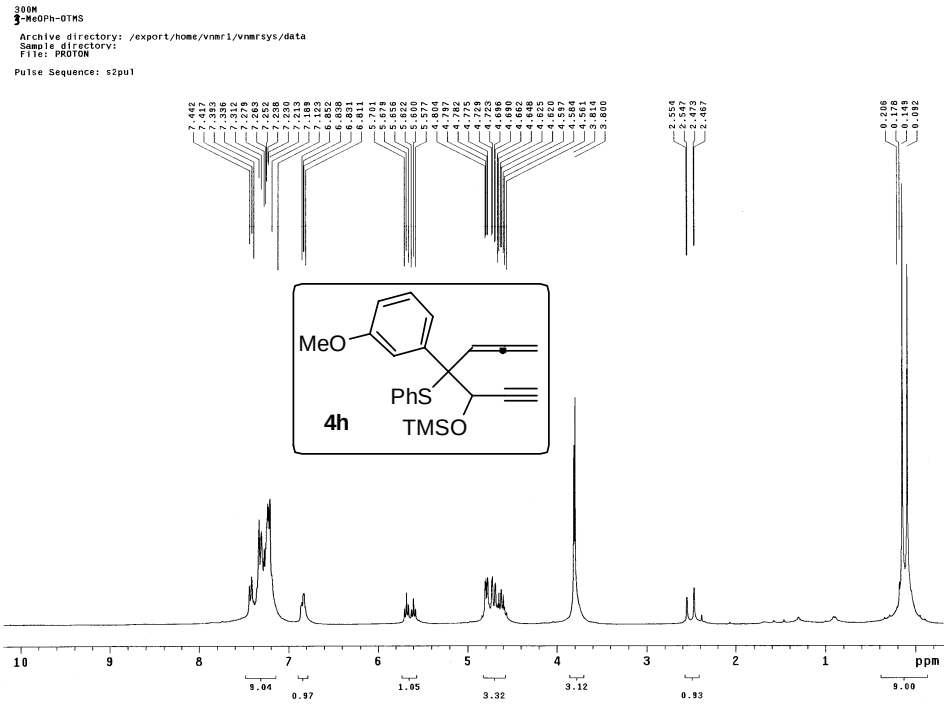
TMSO
4g
ppm



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File: PROTON
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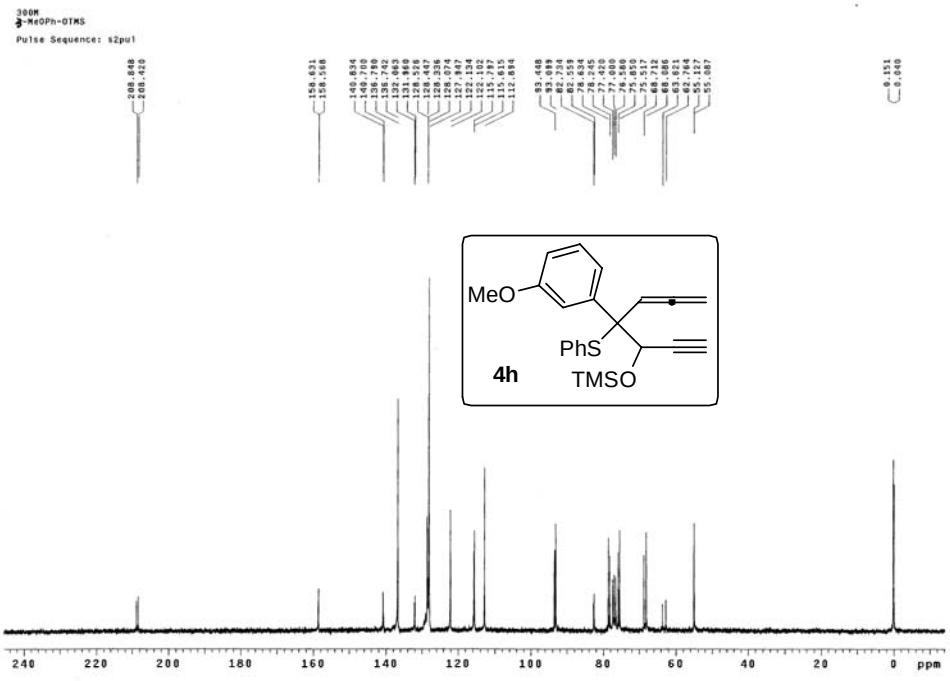
TMSO
4h
ppm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Pulse Sequence: s2pul
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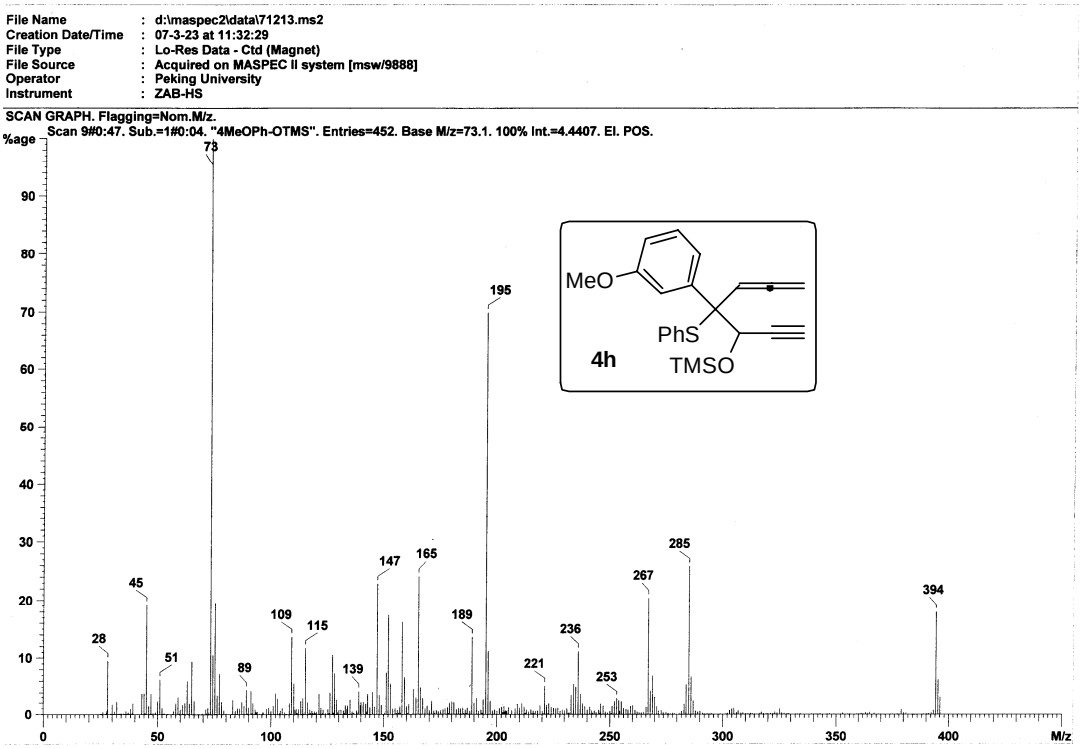
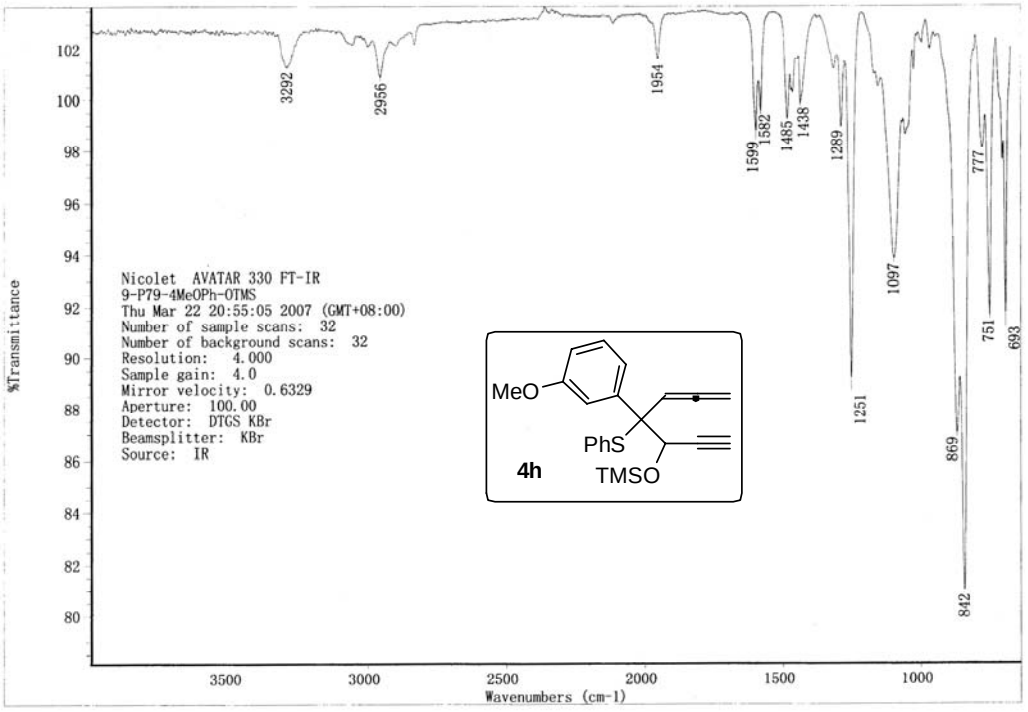
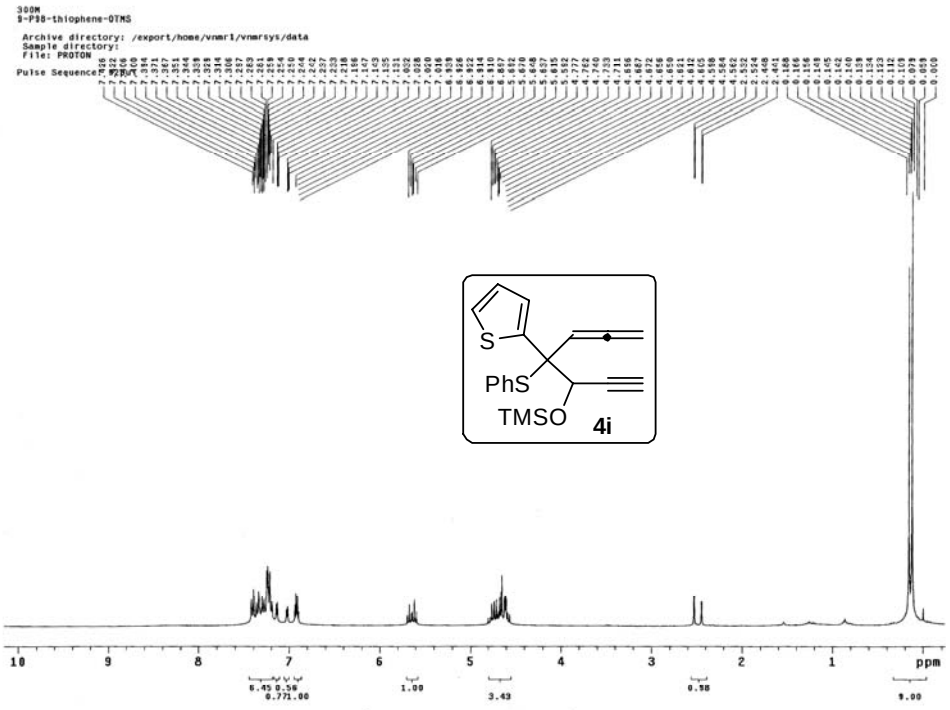
4h
ppm






S
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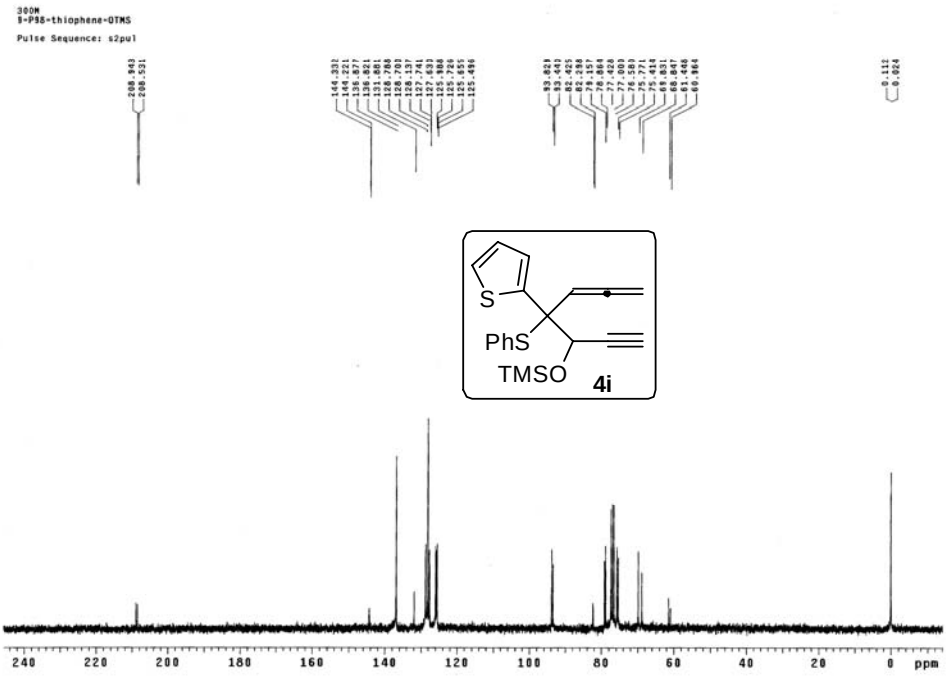
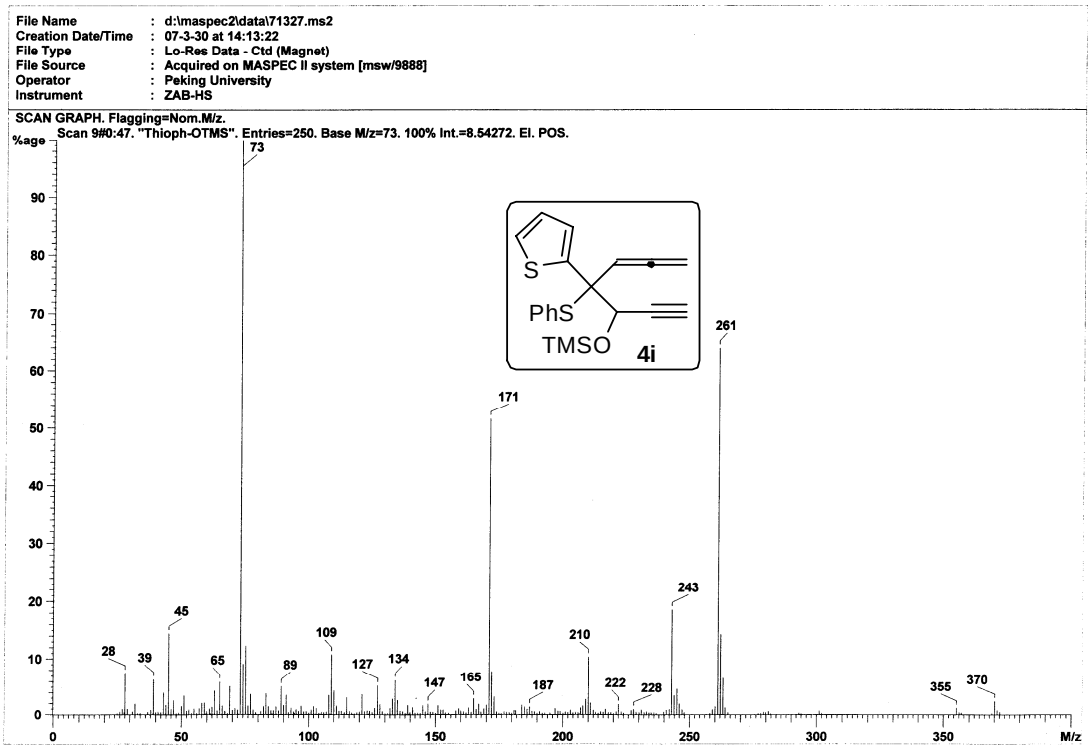
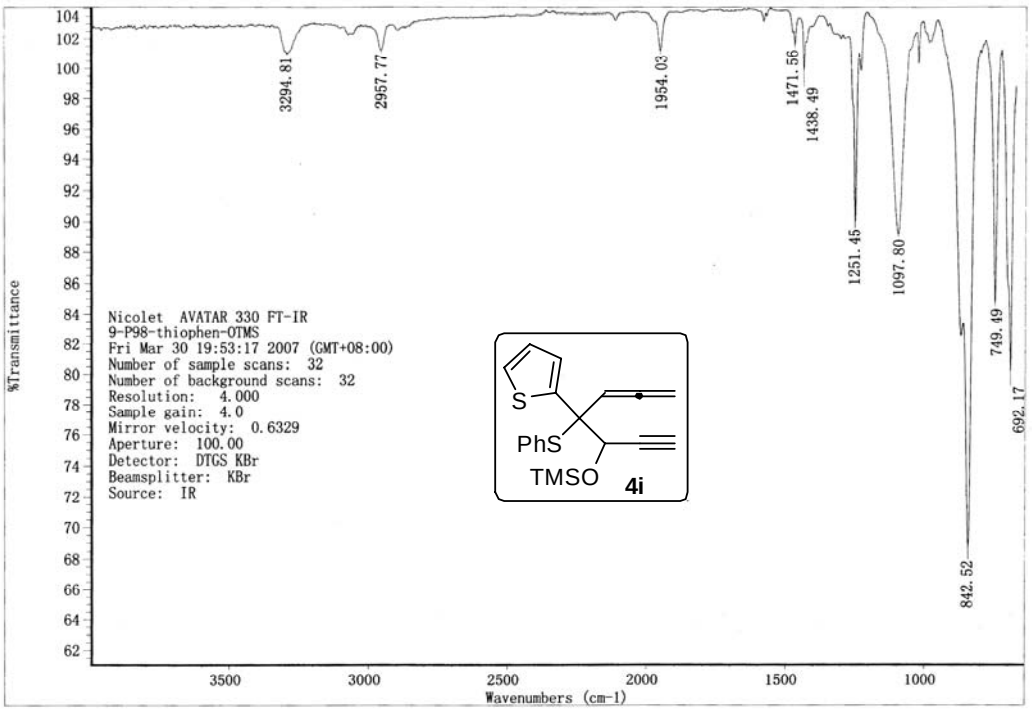
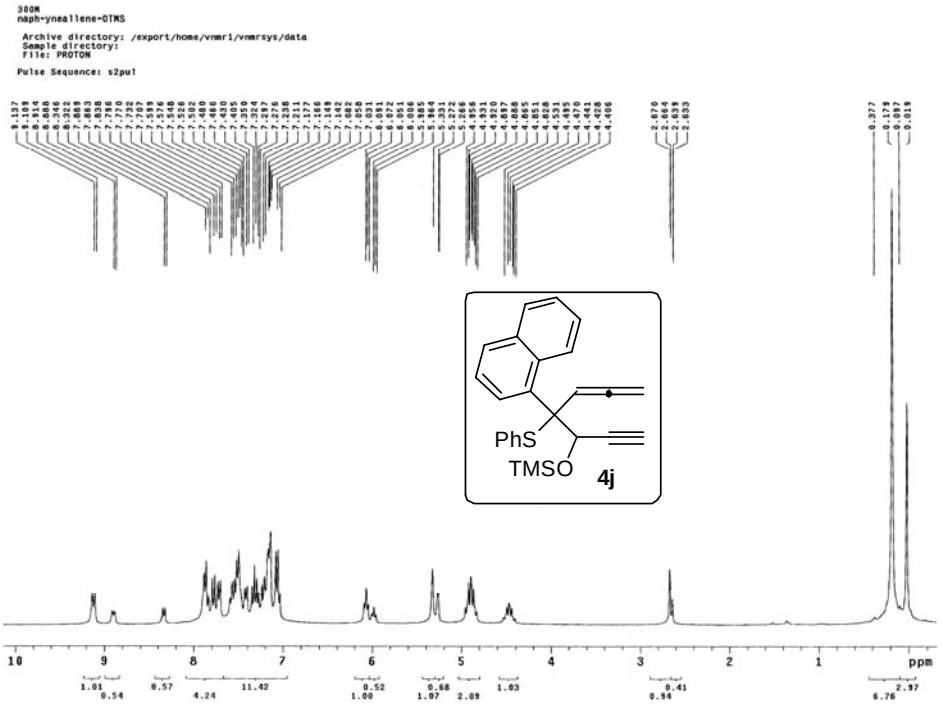
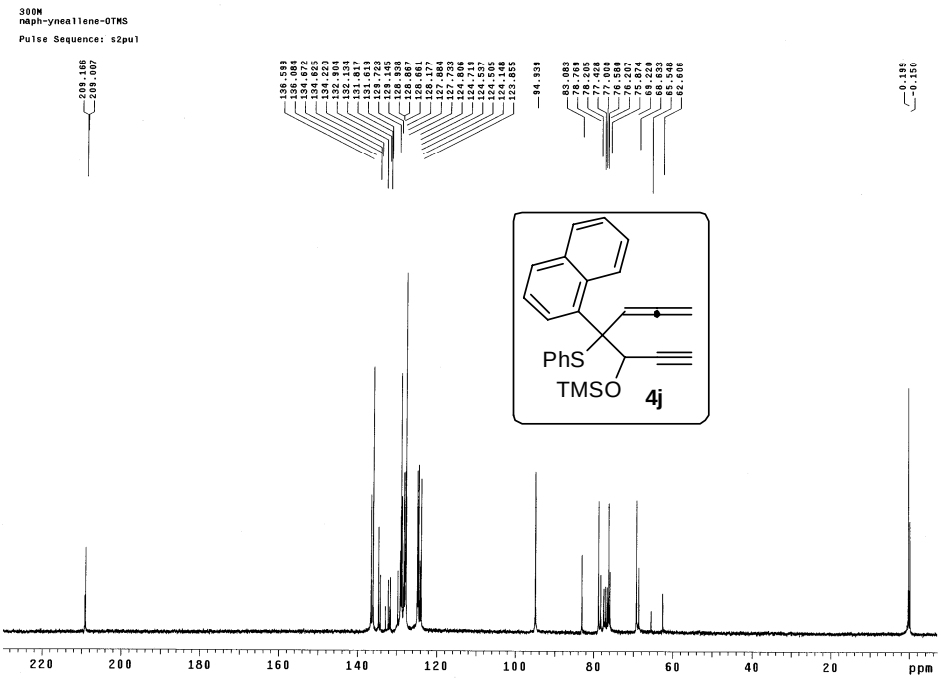
TMSO
4i
ppm

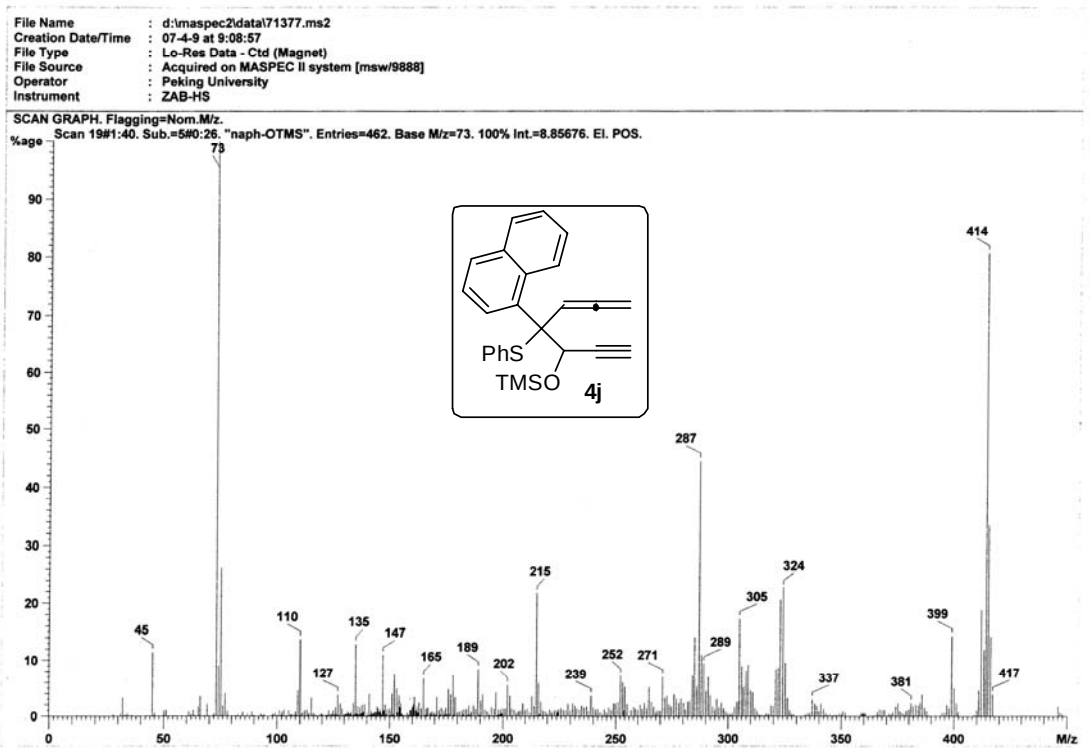

S
PhS
TMSO
4i
ppm

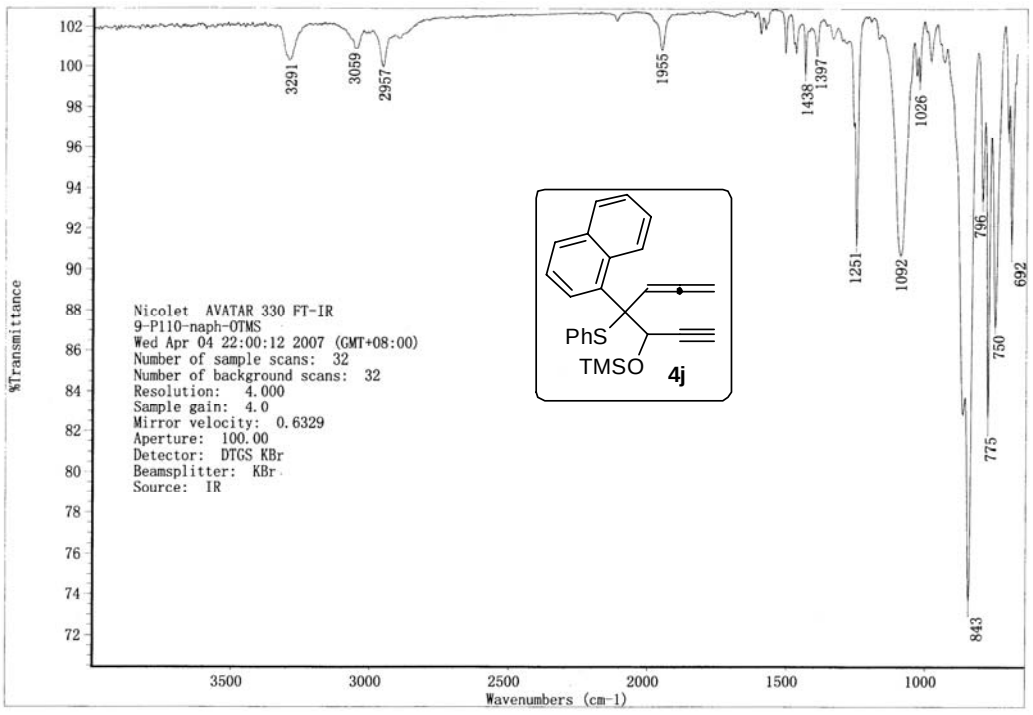

File Name : d:\maspec2\data\71327.ms2
Creation Date/Time : 07-3-30 at 14:13:22
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [msw/9888]
Operator : Peking University
Instrument : ZAB-HS
SCAN GRAPH. Flagging=Nom.M/z.
Scan 9#0:47. "Thioph-OTMS". Entries=250. Base M/z=73. 100% Int.=8.54272. EI. POS.
%age
M/z
S
PhS
TMSO
4i

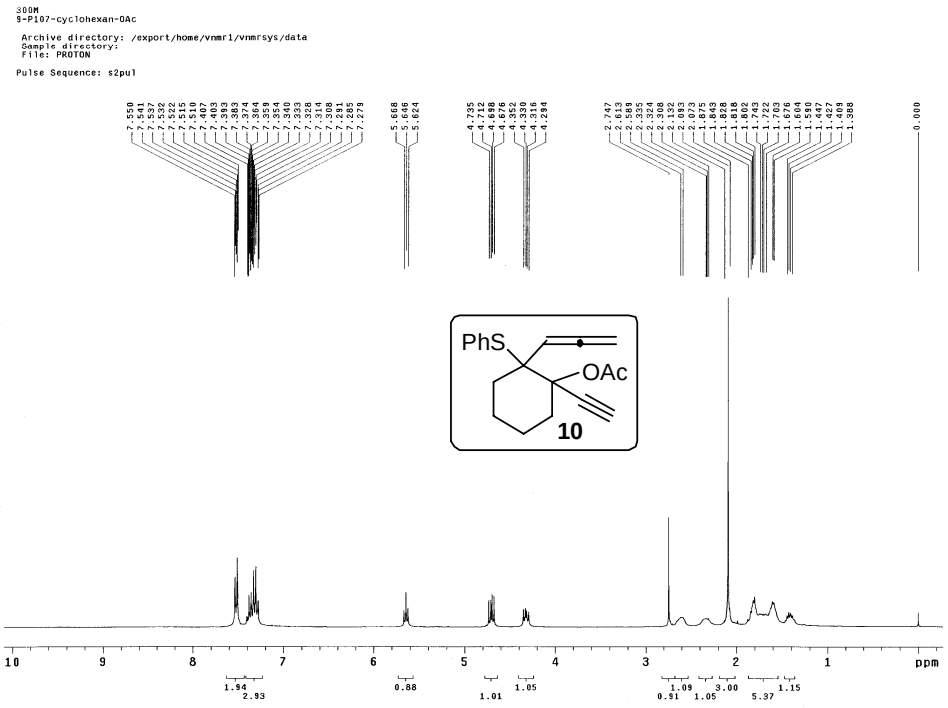

%Transmittance
Wavenumbers (cm-1)
Nicolet AVATAR 330 FT-IR
9-P98-thiophen-OTMS
Fri Mar 30 19:53:17 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
S
PhS
TMSO
4i

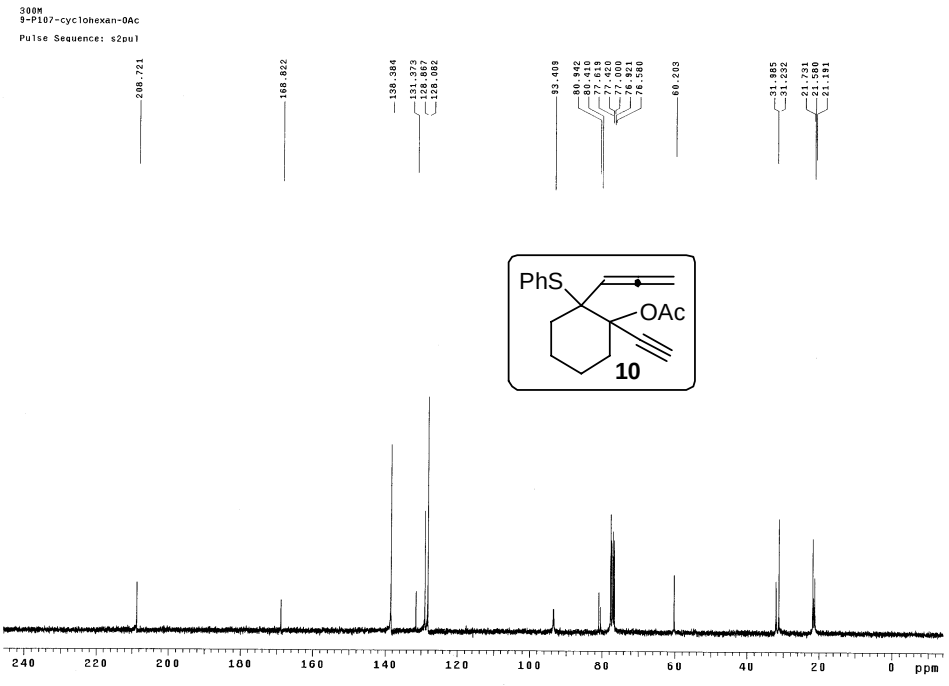

300M
naph-yneallene-OTMS
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
PhS
TMSO
4j
ppm

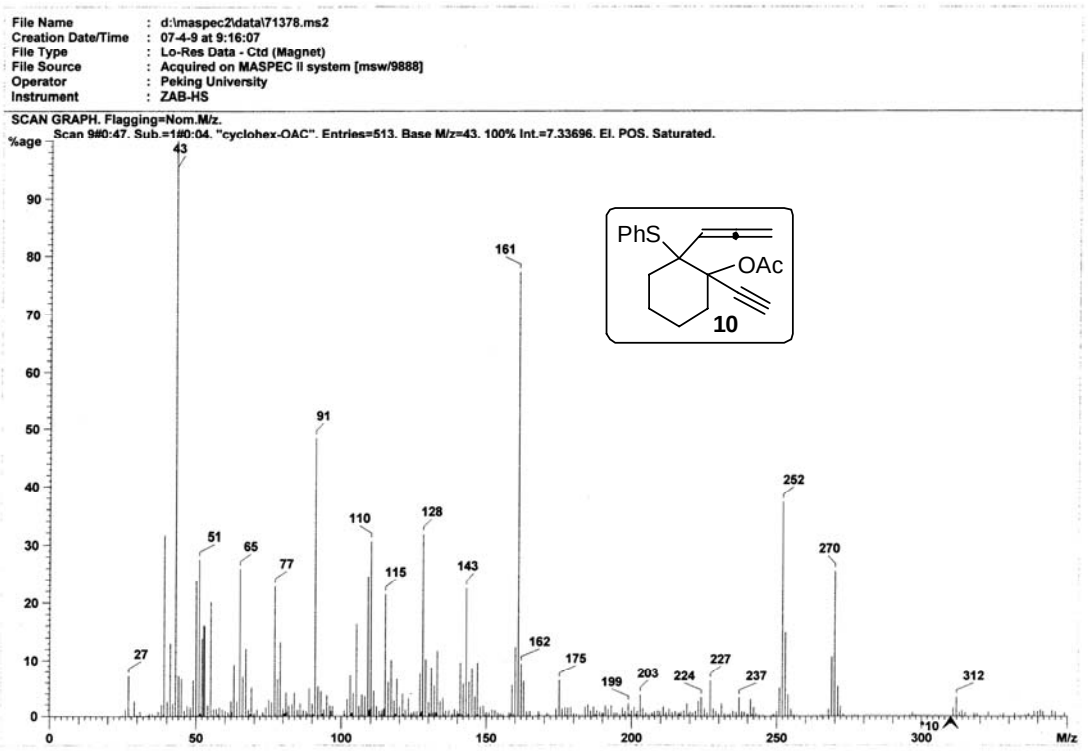

300M
naph-yneallene-OTMS
Pulse Sequence: s2pul
PhS
TMSO
4j
ppm

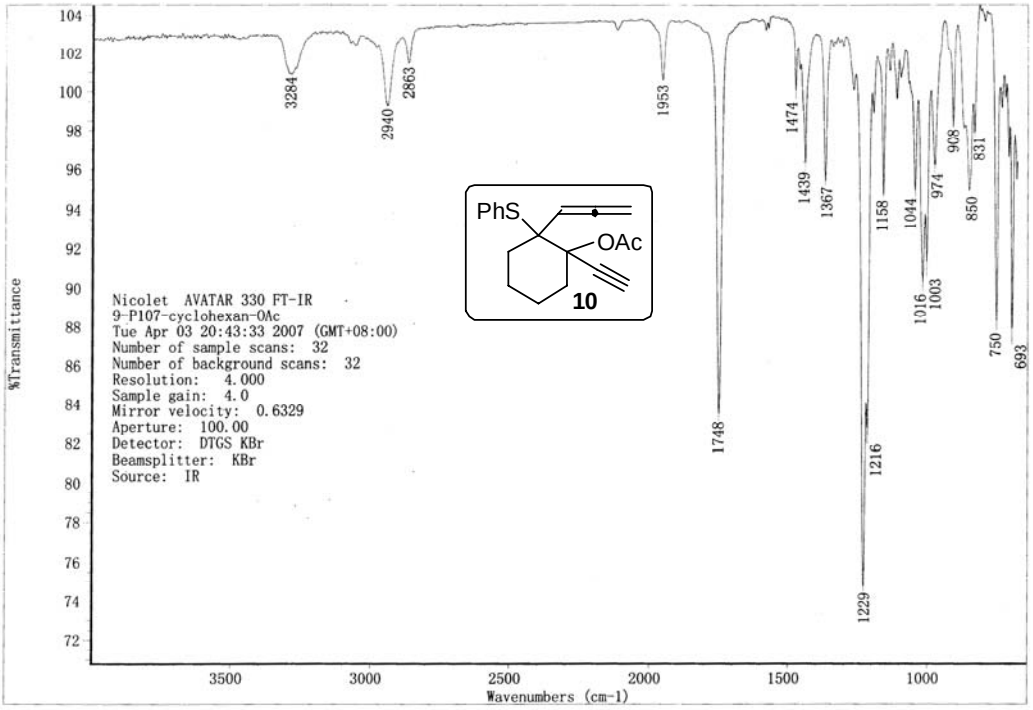

File Name : d:\maspec2\data\71377.ms2
Creation Date/Time : 07-4-9 at 9:08:57
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [msw/9888]
Operator : Peking University
Instrument : ZAB-HS
SCAN GRAPH. Flagging=Nom.M/z.
Scan 19#1:40. Sub.=5#0:26. "naph-OTMS". Entries=462. Base M/z=73. 100% Int.=8.85676. EI. POS.
%age
M/z
PhS
TMSO
4j

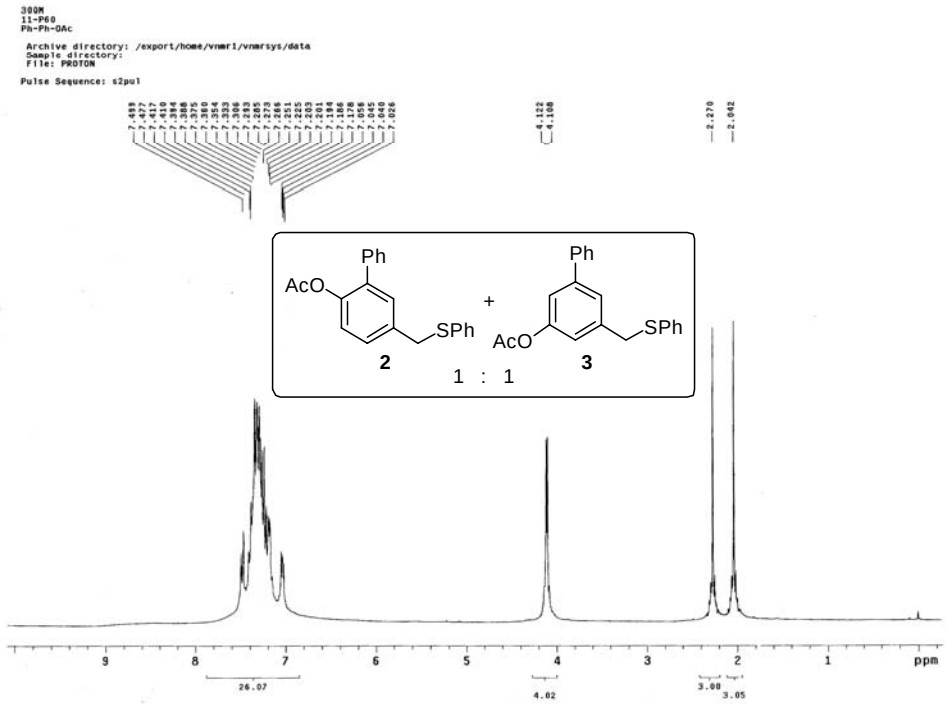

%Transmittance
Wavenumbers (cm-1)
Nicolet AVATAR 330 FT-IR
9-P110-naph-OTMS
Wed Apr 04 22:00:12 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
PhS
TMSO
4j

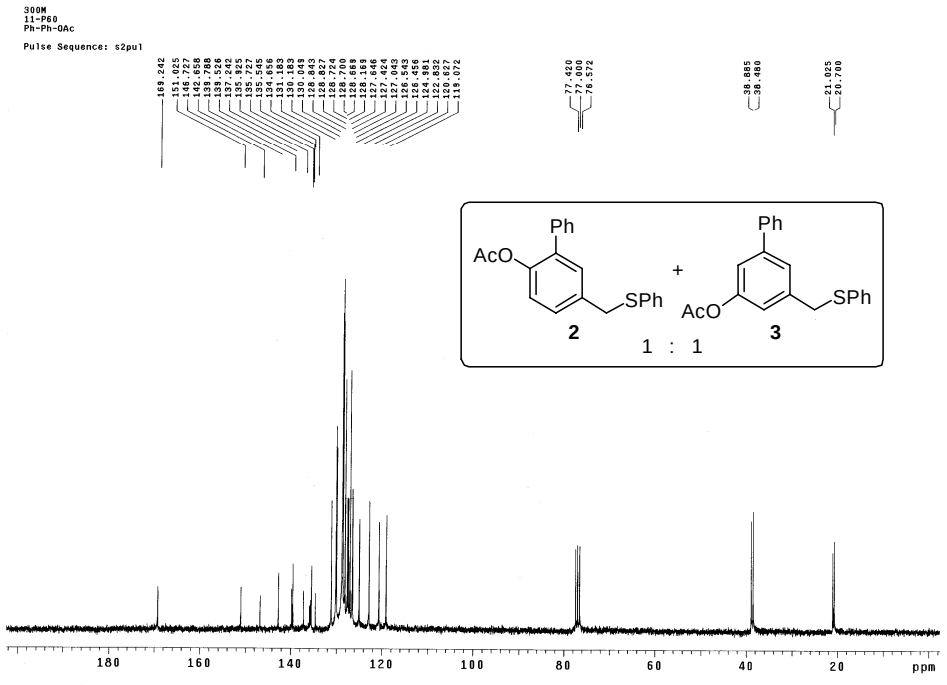

300M
9-P107-cyclohexan-OAc
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
PhS
OAc
10
ppm

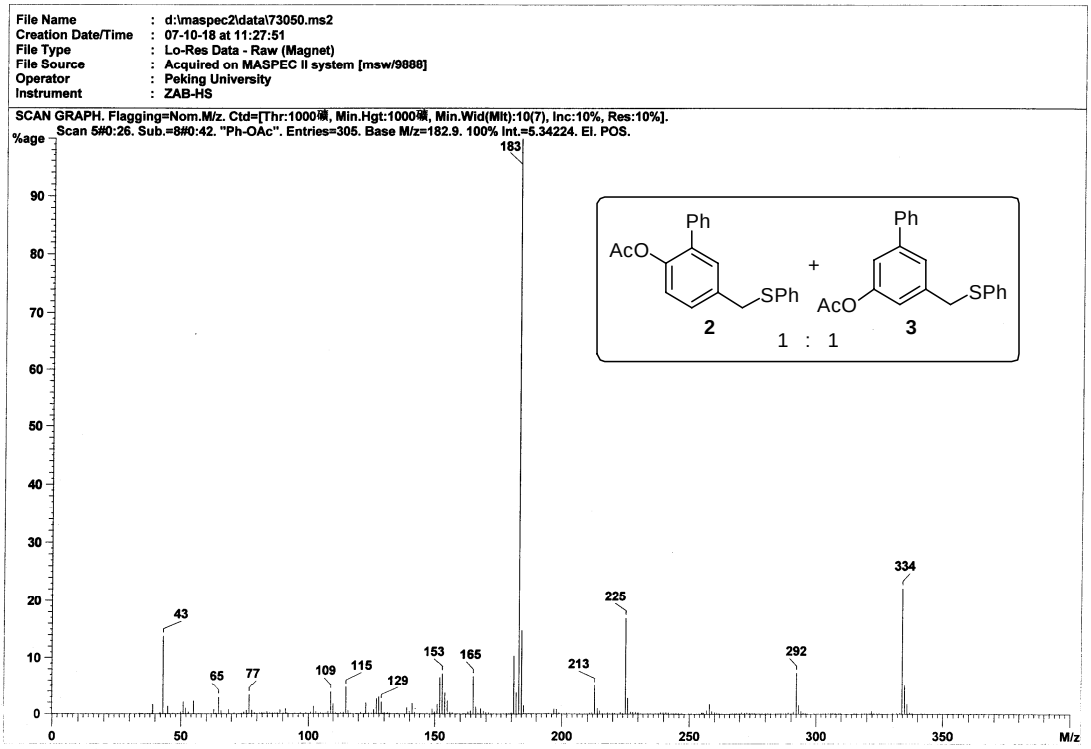

300M
9-P107-cyclohexan-OAc
Pulse Sequence: s2pul
PhS
OAc
10
ppm

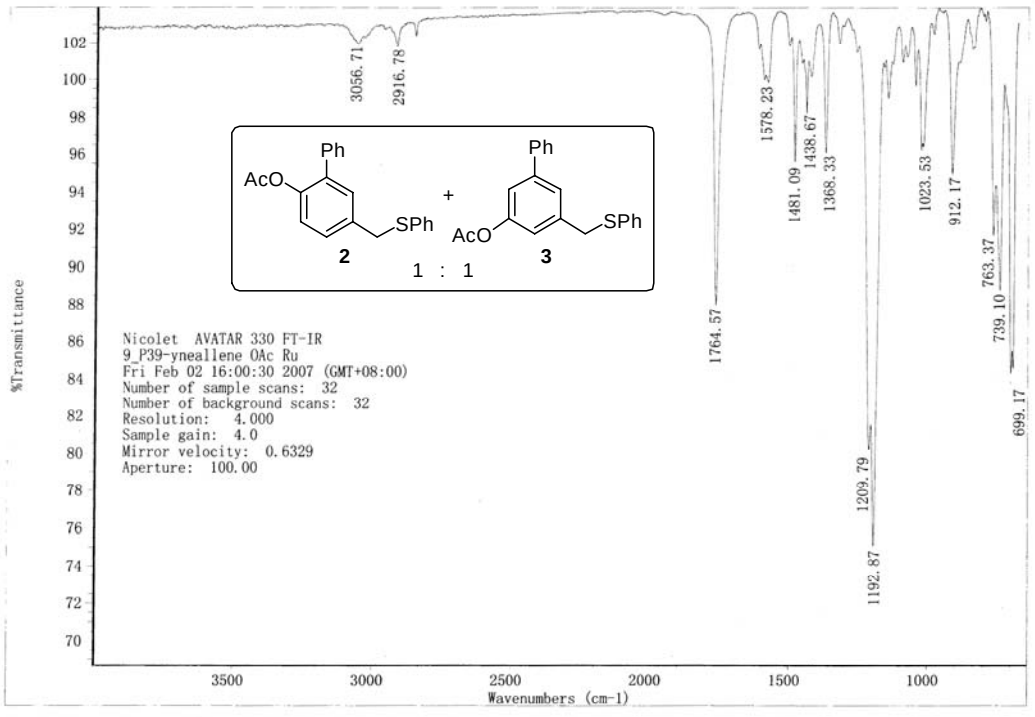


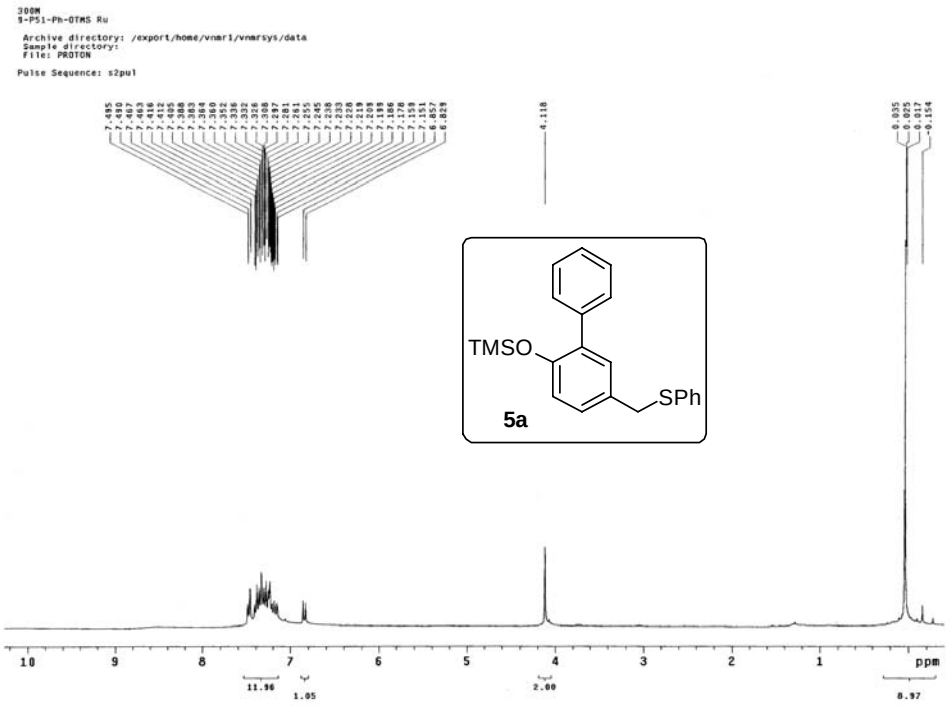


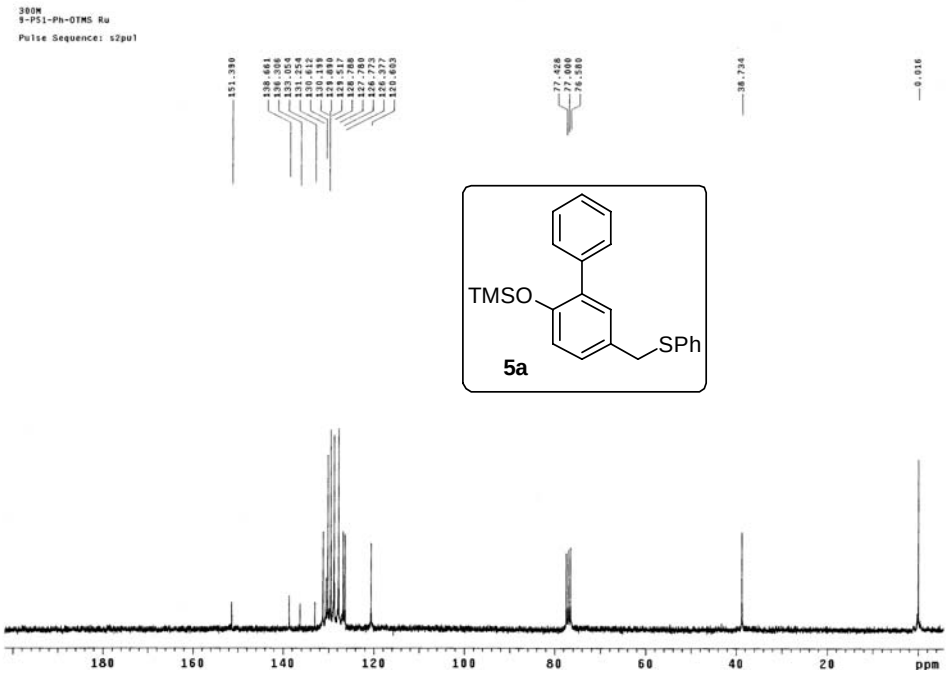

300M
11-P60
Ph-Ph-OAc
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
Ph
AcO
SPh
2
+
Ph
AcO
SPh
3
1 : 1
ppm
26.07
4.02
3.00
3.05

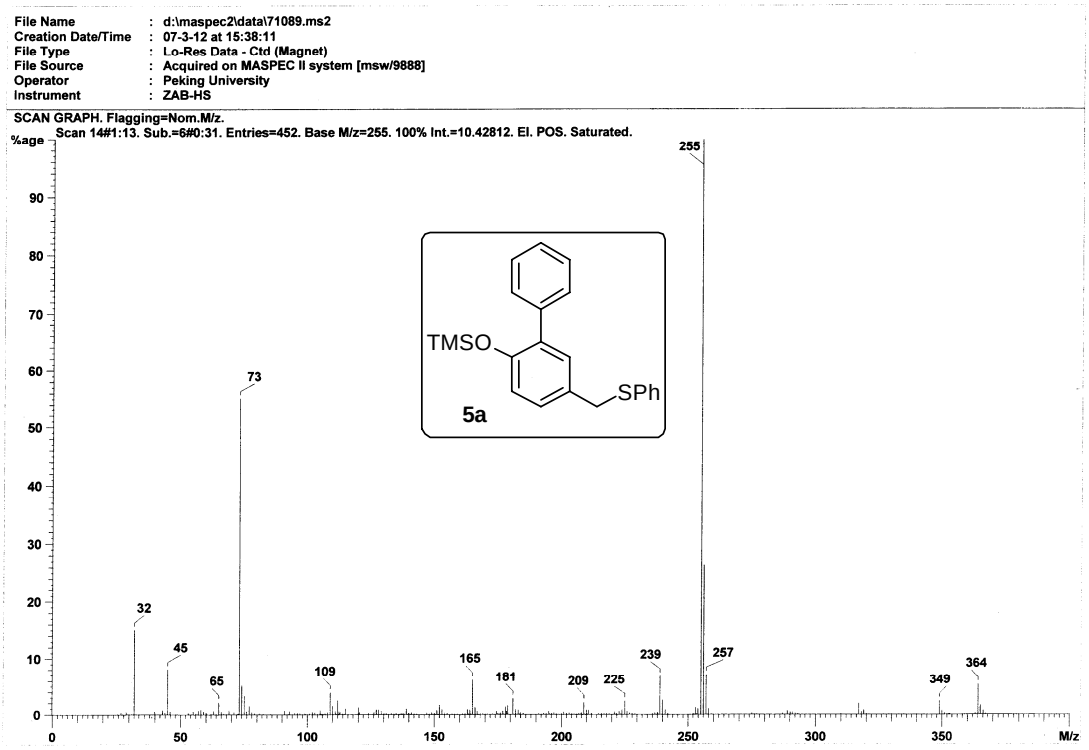

300M
11-P60
Ph-Ph-OAc
Pulse Sequence: s2pul
Ph
AcO
SPh
2
+
Ph
AcO
SPh
3
1 : 1
ppm

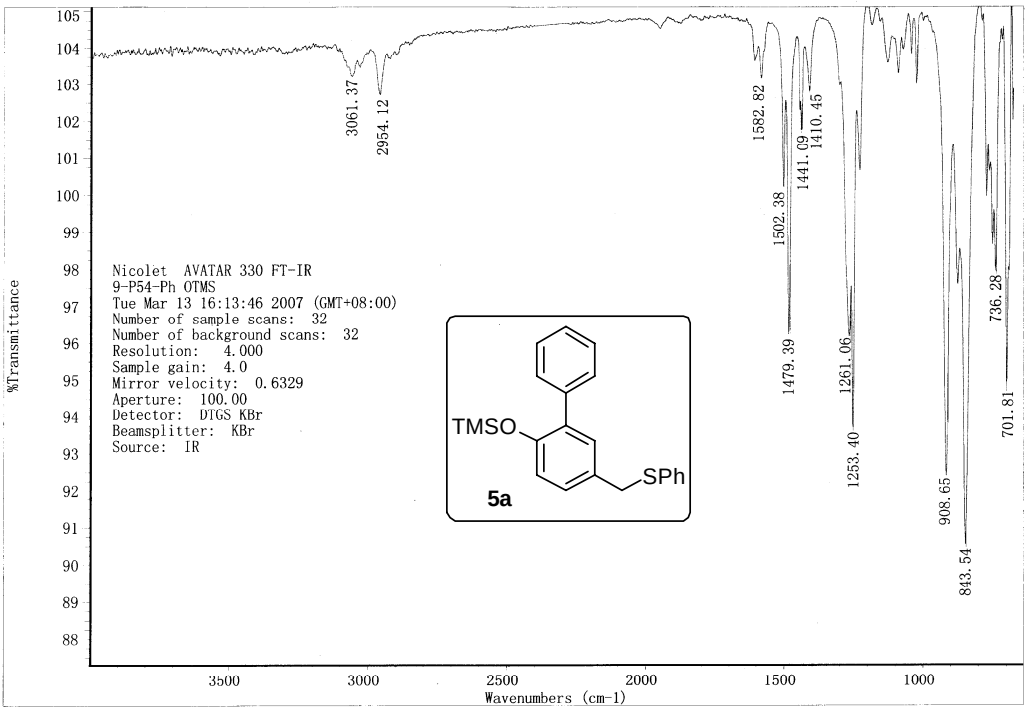

File Name : d:\maspec2\data\73050.ms2
Creation Date/Time : 07-10-18 at 11:27:51
File Type : Lo-Res Data - Raw (Magnet)
File Source : Acquired on MASPEC II system [msw/9888]
Operator : Peking University
Instrument : ZAB-HS
SCAN GRAPH. Flagging=Nom.M/z. Ctd=[Thr:1000嶂, Min.Hgt:1000嶂, Min.Wid(Mlt):10(7), Inc:10%, Res:10%].
Scan 5#0:26. Sub.=8#0:42. "Ph-OAc". Entries=305. Base M/z=182.9. 100% Int.=5.34224. El. POS.
%age
M/z
183
334
225
43
292
153
165
213
65
77
109
115
129
Ph
AcO
SPh
2
1 : 1
3

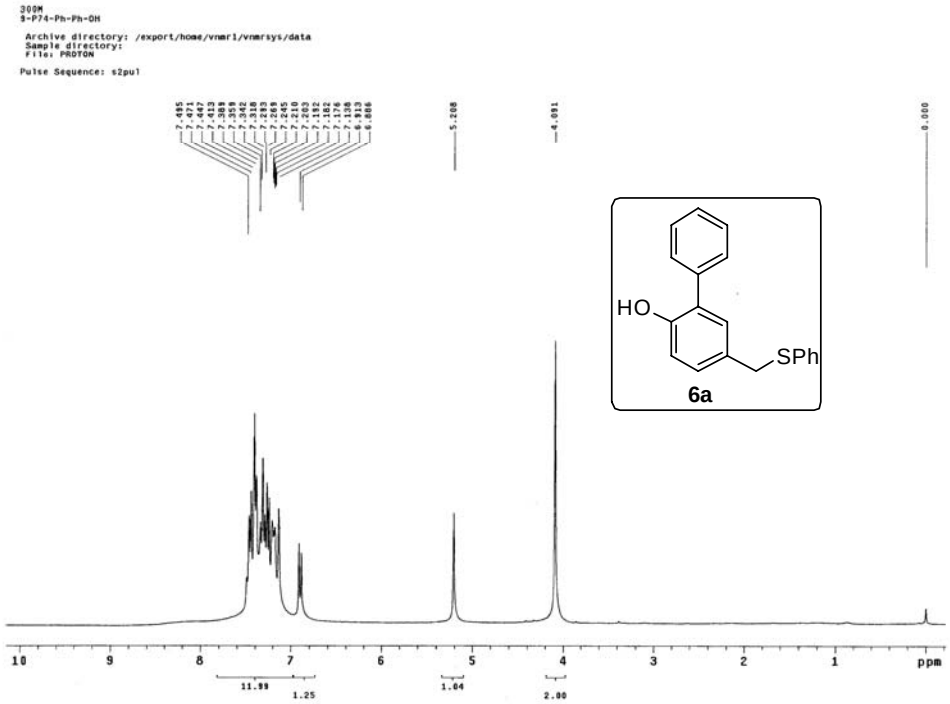

%Transmittance
Wavenumbers (cm-1)
3056.71
2916.78
1764.57
1578.23
1481.09
1438.67
1368.33
1209.79
1192.87
1023.53
912.17
763.37
739.10
699.17
Nicolet AVATAR 330 FT-IR
9_P39-yneallene OAc Ru
Fri Feb 02 16:00:30 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Ph
AcO
SPh
2
1 : 1
3

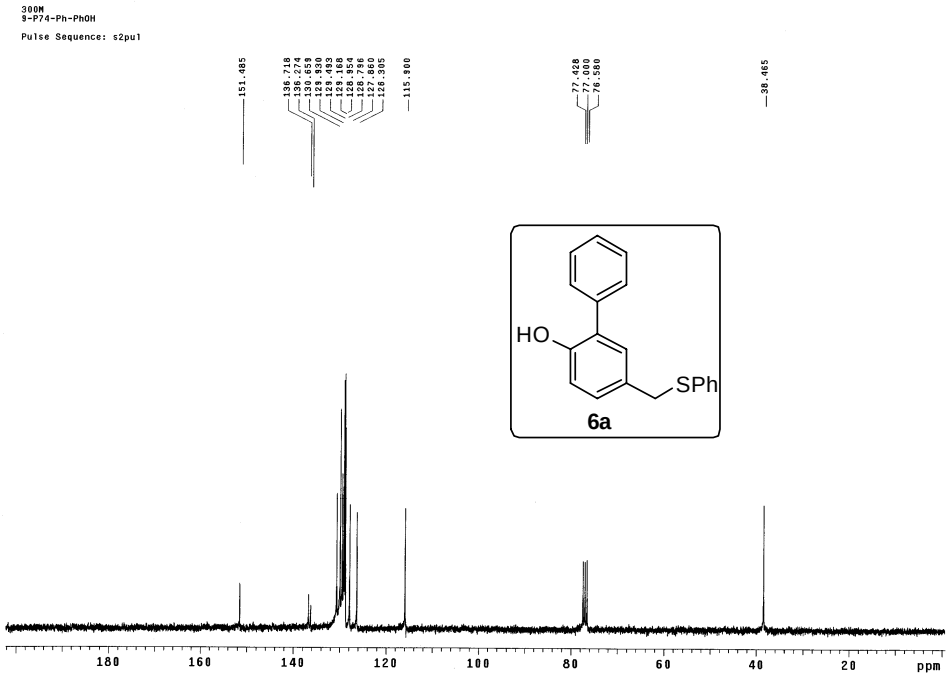

300M
9-P51-Ph-OTMS Ru
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
TMSO
SPh
5a
ppm
11.96
1.05
2.00
8.97

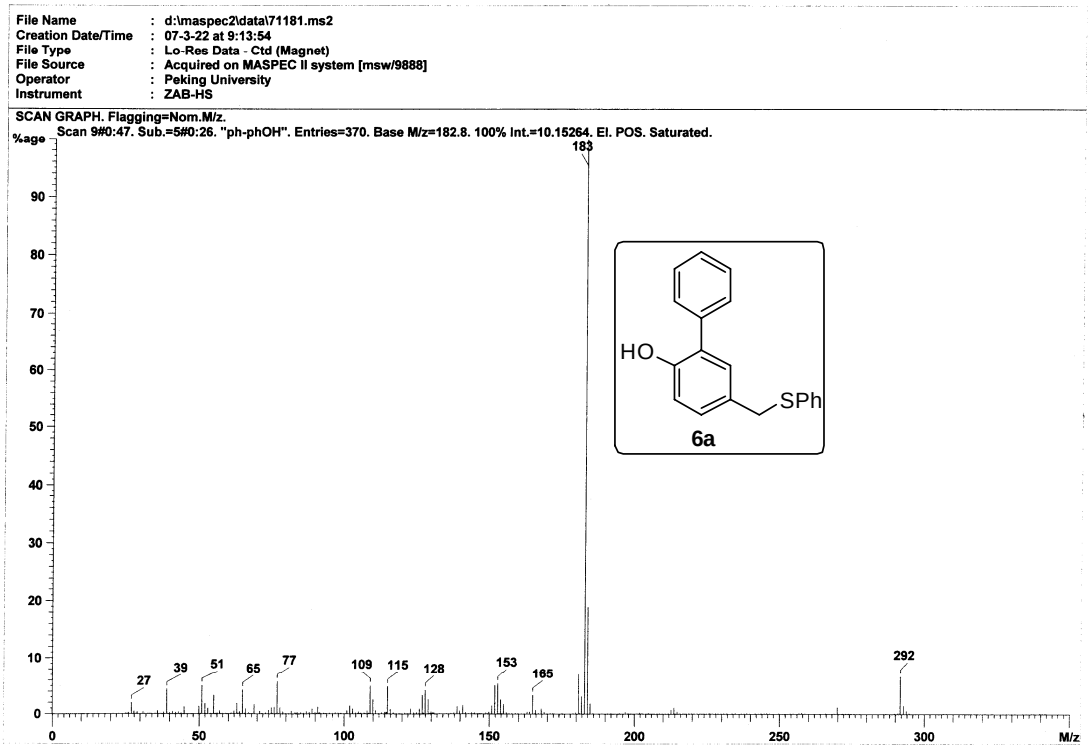

300M
9-P51-Ph-OTMS Ru
Pulse Sequence: s2pul
TMSO
SPh
5a
ppm

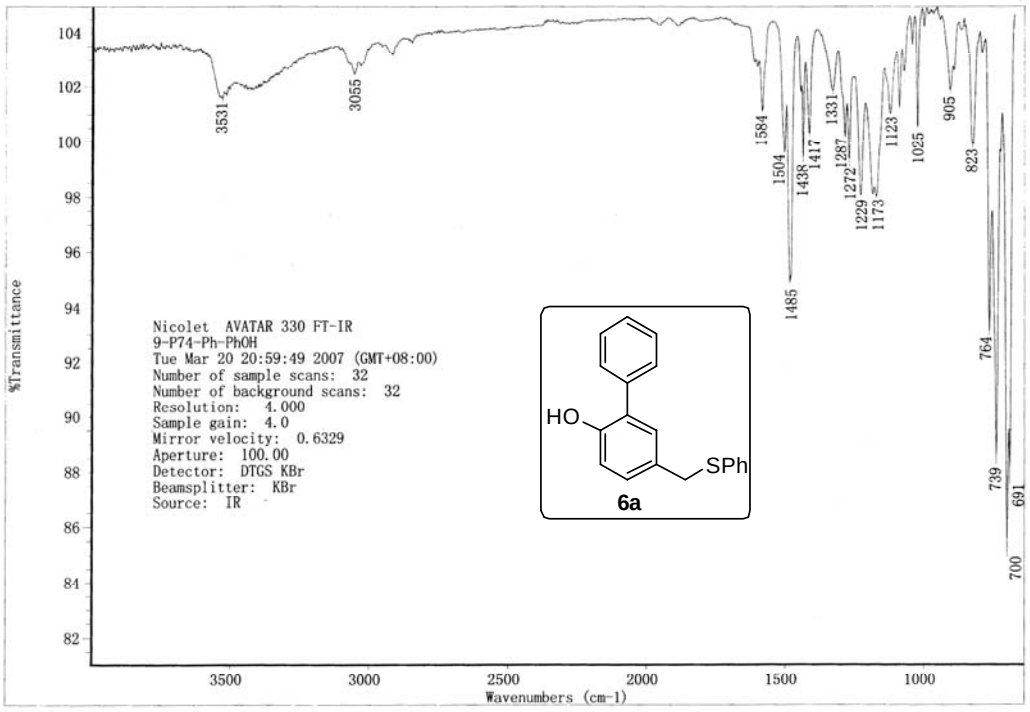


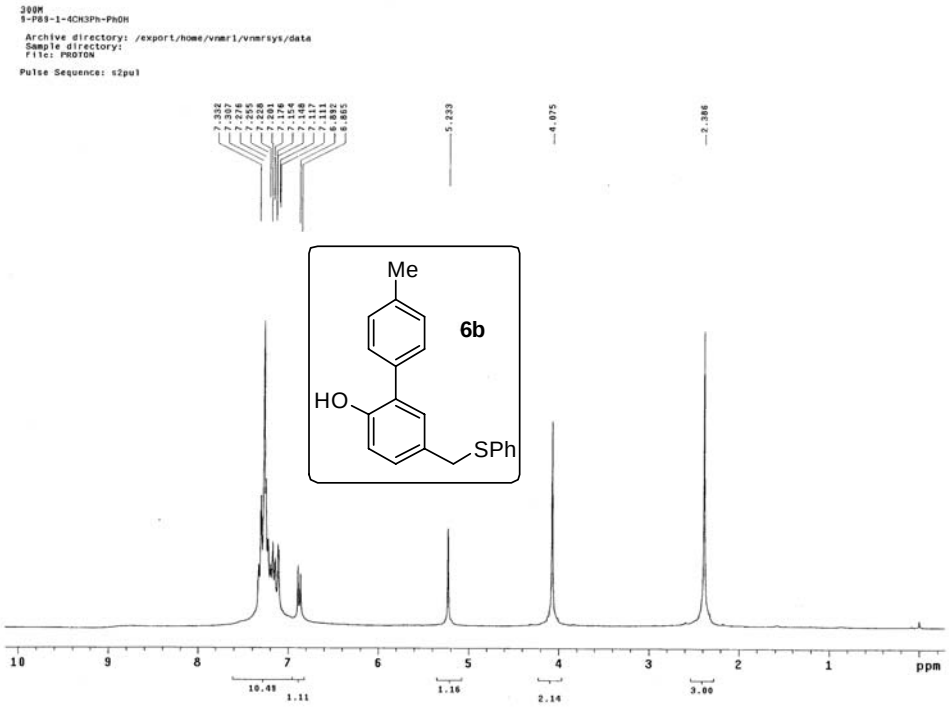


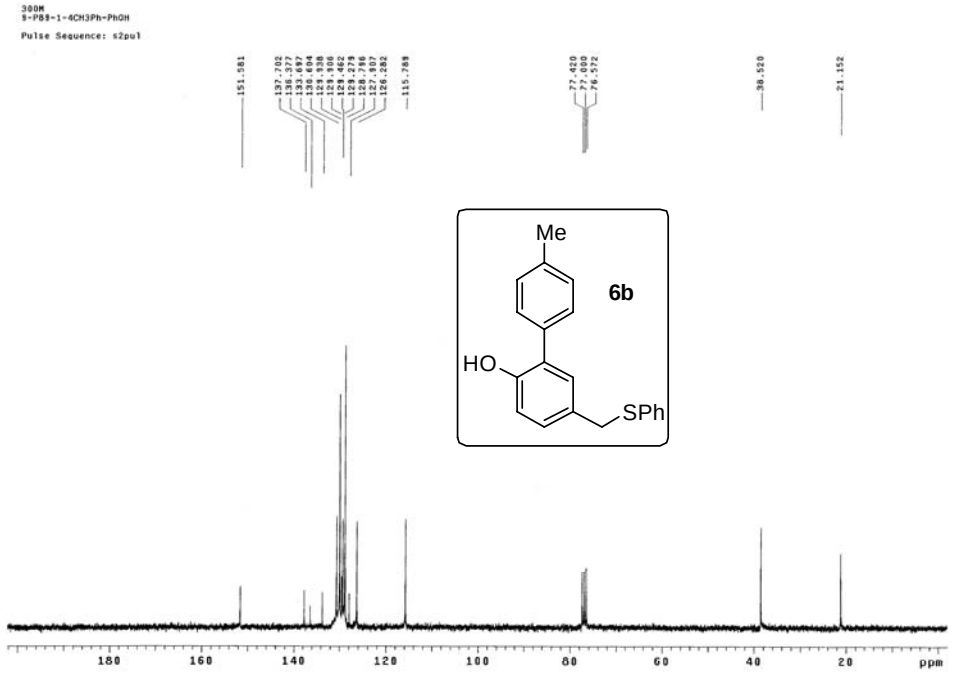

300M
S-P74-Ph-Ph-OH
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
7.495
7.471
7.447
7.413
7.384
7.359
7.342
7.318
7.293
7.269
7.245
7.210
7.183
7.162
7.136
7.116
6.913
6.886
5.208
4.091
0.000
HO
SPh
6a
10
9
8
7
6
5
4
3
2
1
ppm
11.99
1.25
1.04
2.00

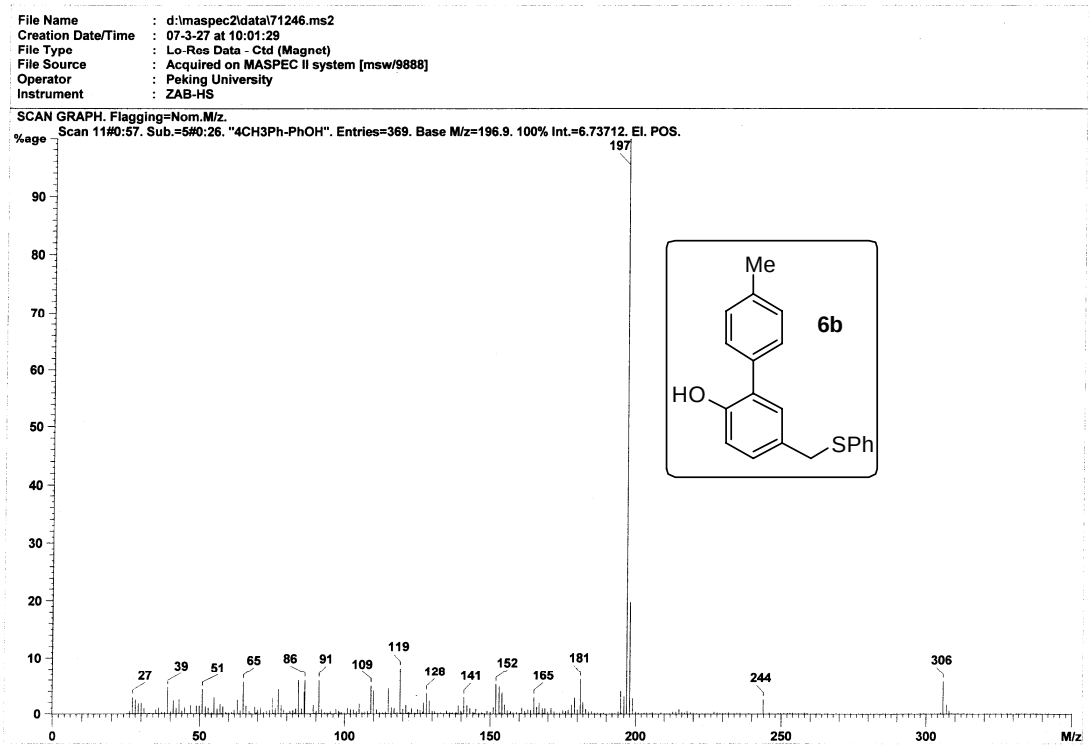

300M
S-P74-Ph-PhOH
Pulse Sequence: s2pul
151.485
136.718
136.274
130.459
130.030
129.493
129.168
128.754
128.396
127.860
126.305
115.900
77.428
77.000
76.580
38.465
HO
SPh
6a
180
160
140
120
100
80
60
40
20
ppm

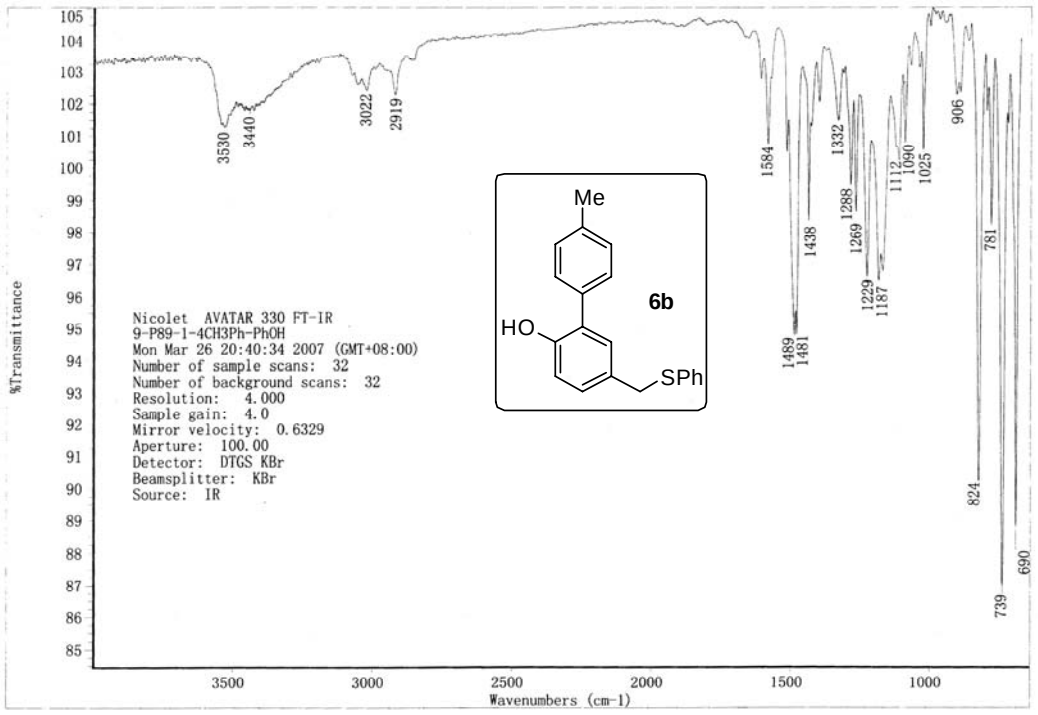

File Name : d:\maspec2\data\71181.ms2
Creation Date/Time : 07-3-22 at 9:13:54
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [msw/9888]
Operator : Peking University
Instrument : ZAB-HS
SCAN GRAPH. Flagging=Nom.M/z.
Scan 9#0:47. Sub.=5#0:26. "ph-phOH". Entries=370. Base M/z=182.8. 100% Int.=10.15264. EI. POS. Saturated.
%age
M/z
183
292
27
39
51
65
77
109
115
128
153
165
HO
SPh
6a

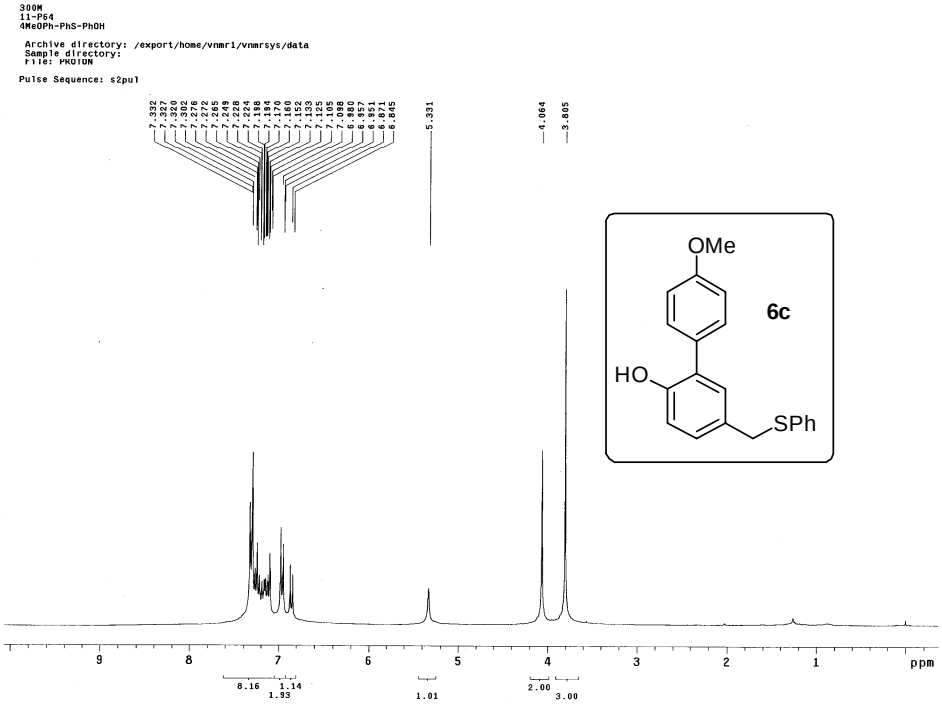

%Transmittance
Wavenumbers (cm-1)
3531
3055
1584
1504
1485
1438
1417
1331
1287
1272
1229
1173
1123
1025
905
823
764
739
700
691
Nicolet AVATAR 330 FT-IR
9-P74-Ph-PhOH
Tue Mar 20 20:59:49 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
HO
SPh
6a

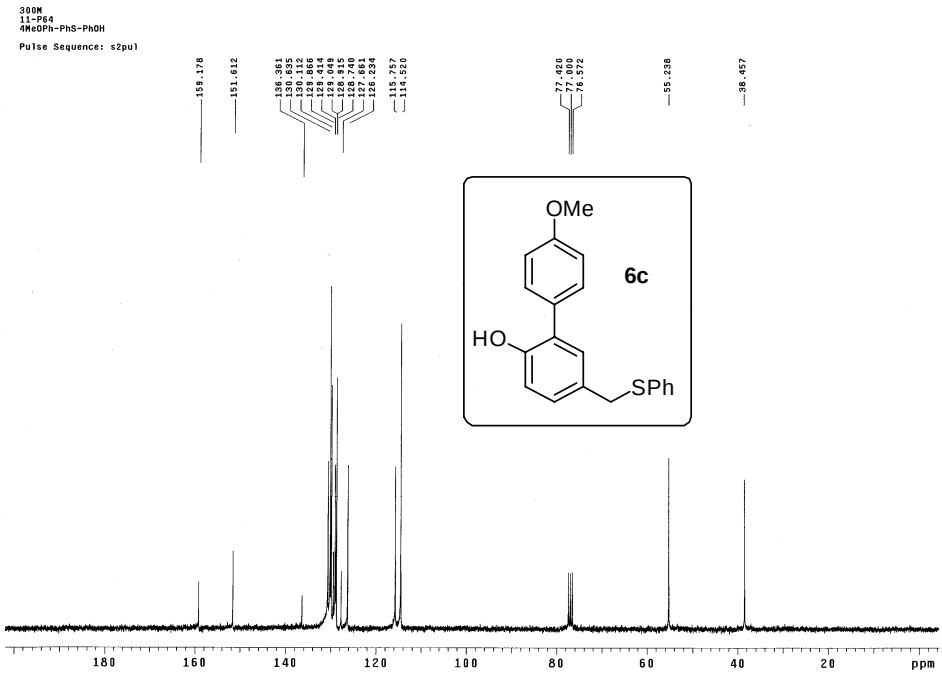


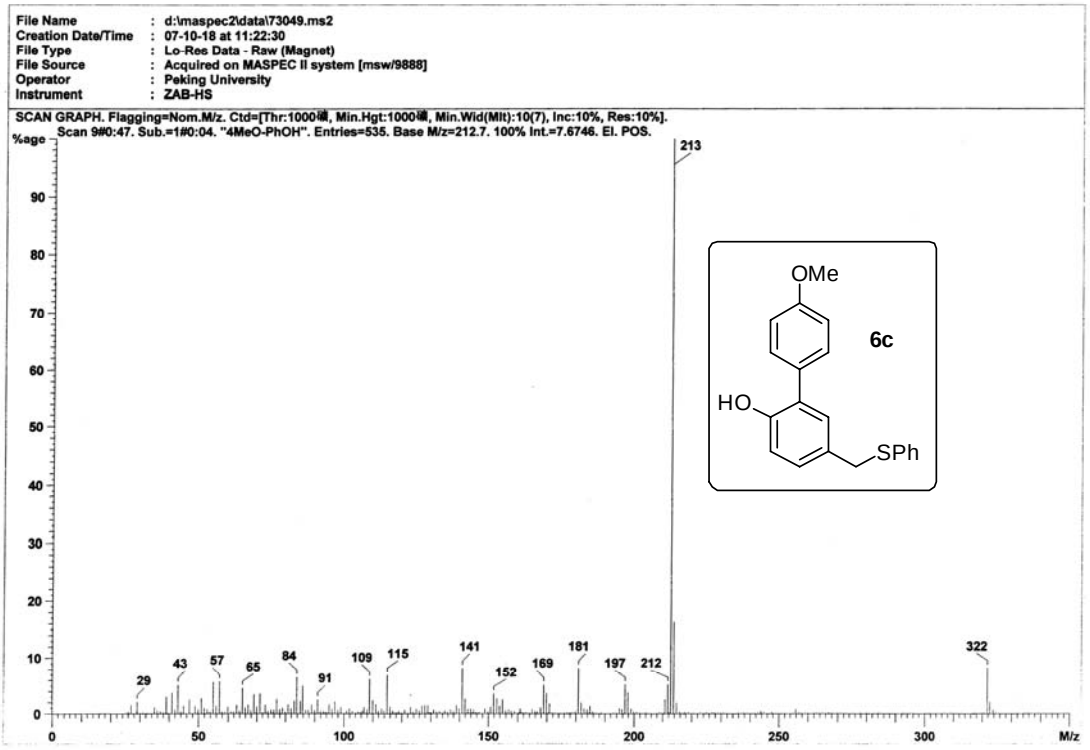


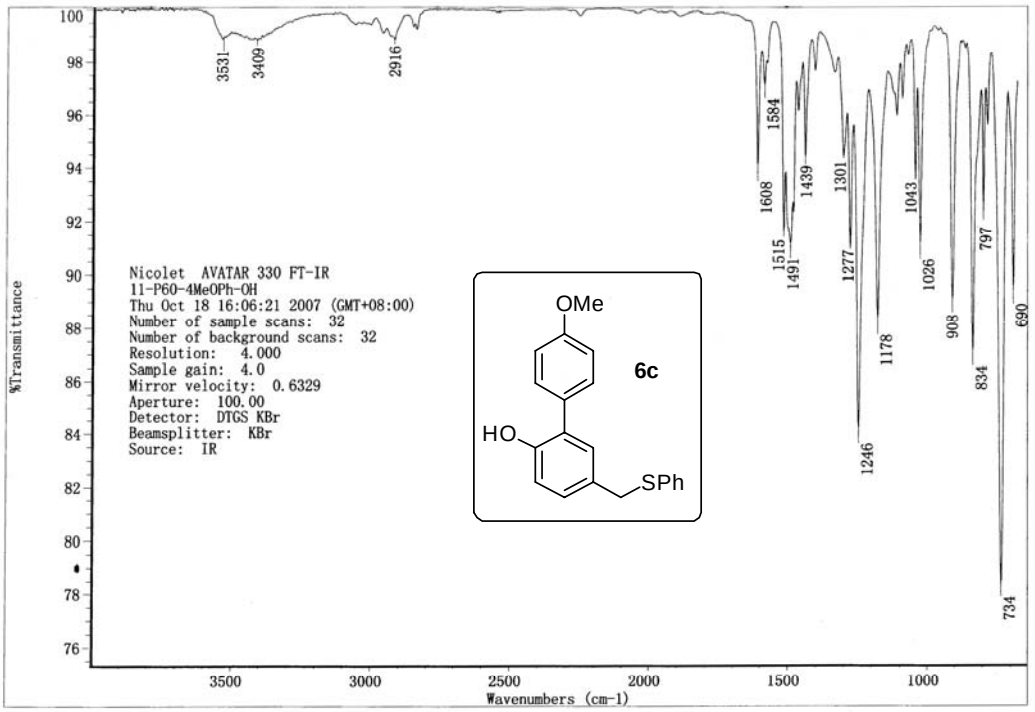

File Name : d:\maspec2\data\71246.ms2
Creation Date/Time : 07-3-27 at 10:01:29
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [msw/9888]
Operator : Peking University
Instrument : ZAB-HS
SCAN GRAPH. Flagging=Nom.M/z.
Scan 11#0:57. Sub.=5#0:26. "4CH3Ph-PhOH". Entries=369. Base M/z=196.9. 100% Int.=6.73712. EI. POS.
%age
M/z
Me
6b
HO
SPh

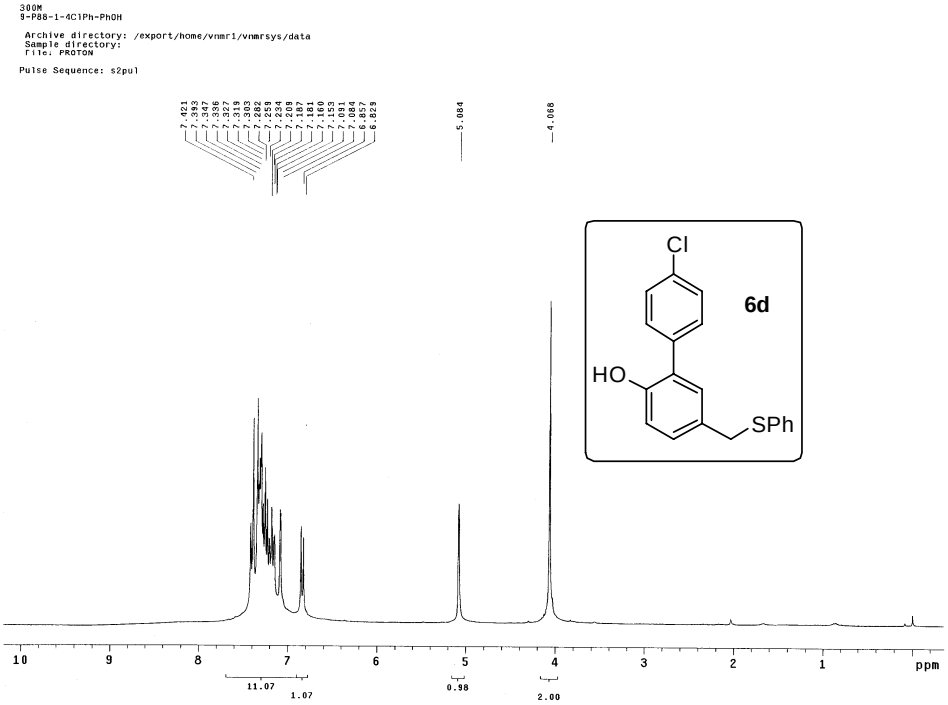

%Transmittance
Wavenumbers (cm-1)
Nicolet AVATAR 330 FT-IR
9-P89-1-4CH3Ph-PhOH
Mon Mar 26 20:40:34 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
Me
6b
HO
SPh

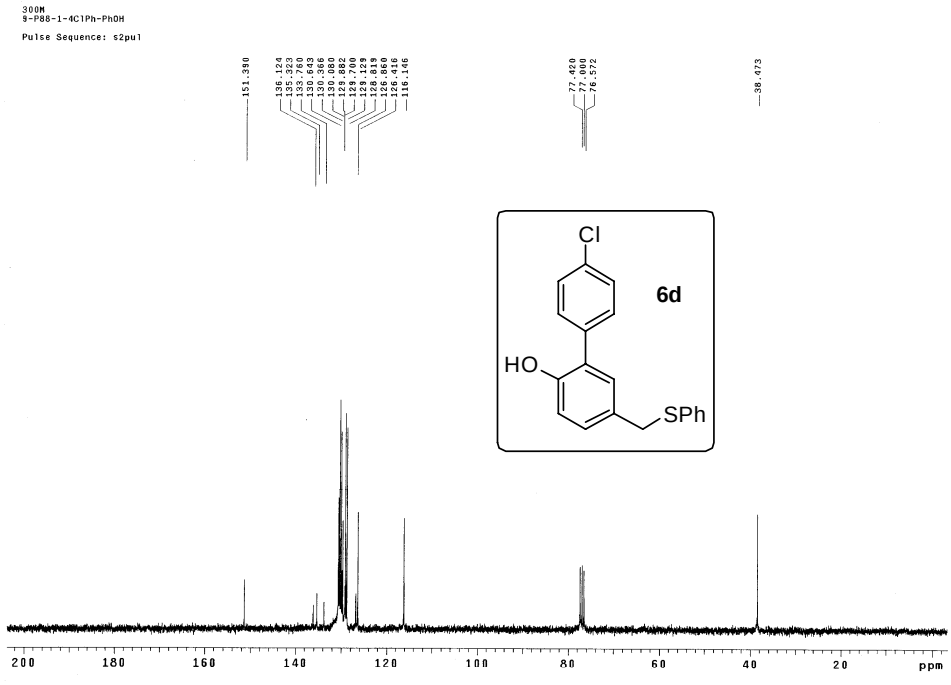

300M
11-P64
4MeOPh-PhS-PhOH
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
7.332
7.327
7.320
7.302
7.276
7.272
7.265
7.248
7.230
7.224
7.198
7.194
7.170
7.160
7.152
7.130
7.125
7.105
7.088
6.960
6.957
6.951
6.871
6.845
5.331
4.064
3.805
OMe
6c
HO
SPh
9
8
7
6
5
4
3
2
1
ppm
8.16
1.14
1.93
1.01
2.00
3.00

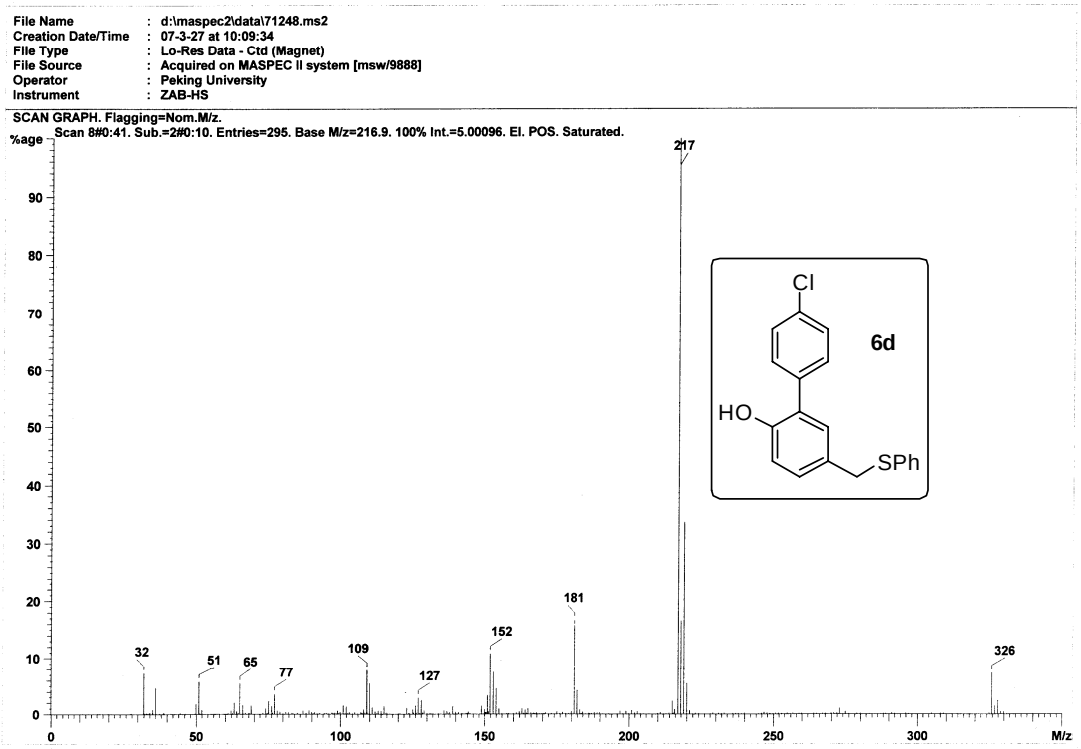

300M
11-P64
4MeOPh-PhS-PhOH
Pulse Sequence: s2pul
159.178
151.612
136.361
130.635
130.112
129.886
129.644
129.049
128.915
127.740
127.248
126.234
115.757
114.520
77.420
77.000
76.572
55.238
38.457
OMe
6c
HO
SPh
180
160
140
120
100
80
60
40
20
ppm

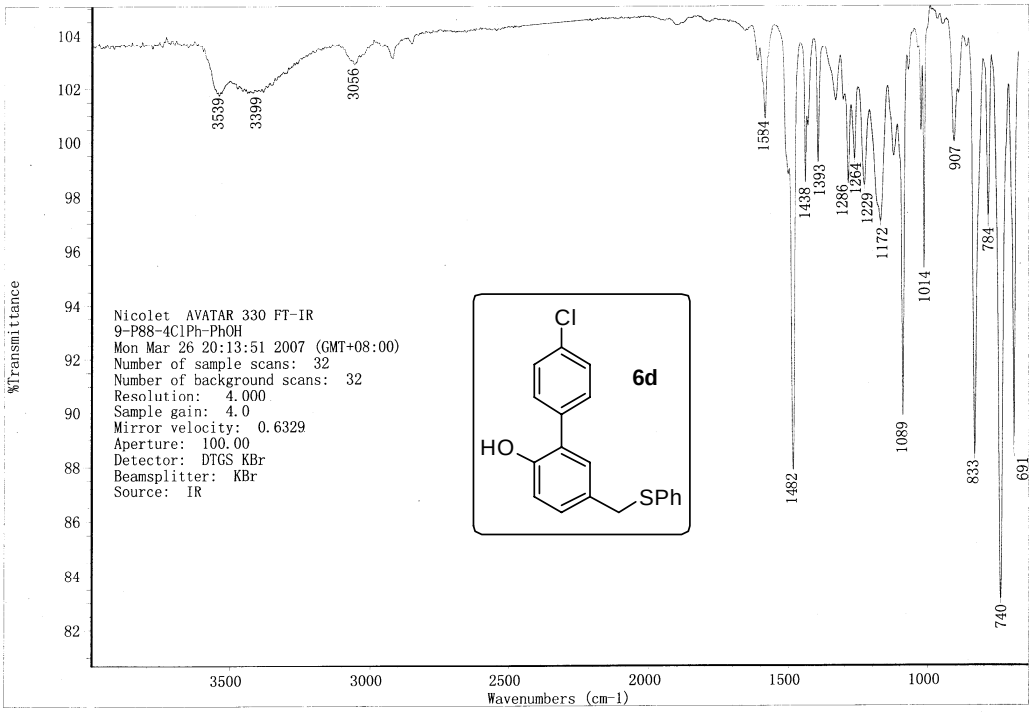


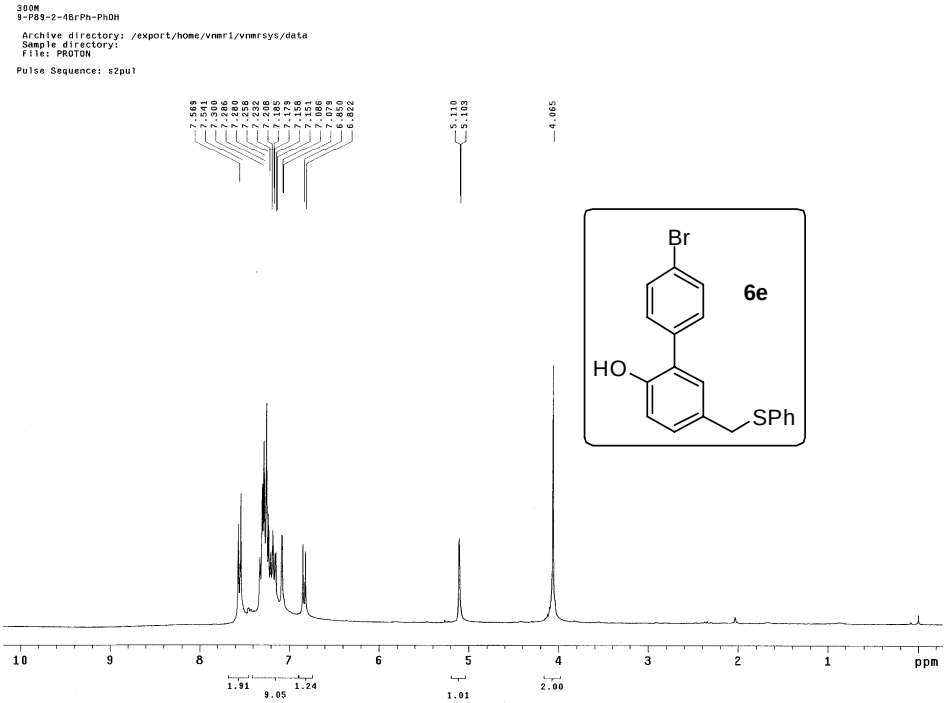


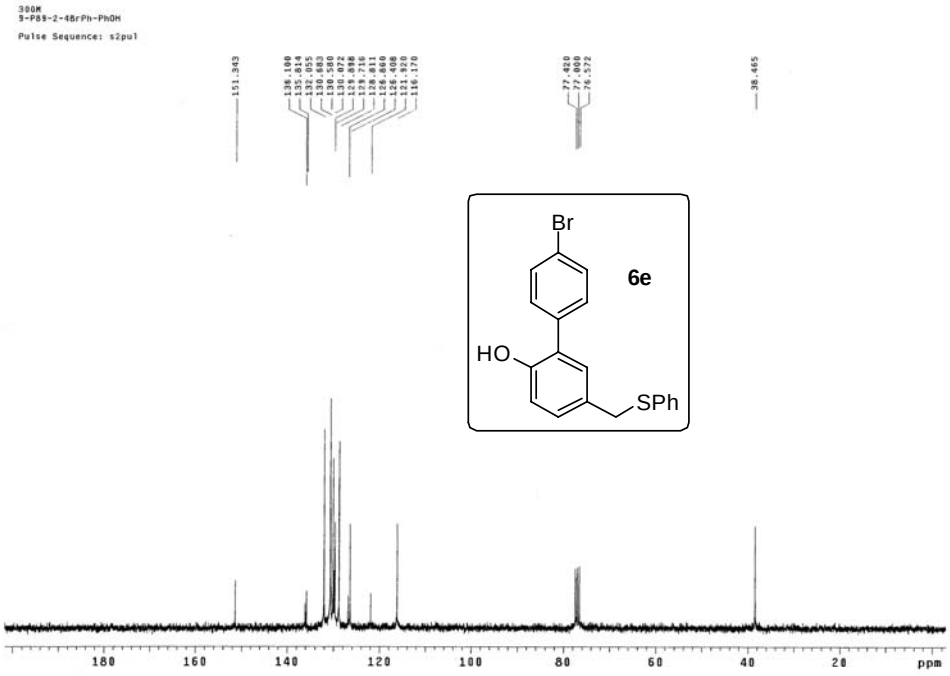

300M
9-P88-1-4ClPh-PhOH
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
7.421
7.408
7.347
7.336
7.327
7.313
7.303
7.282
7.259
7.234
7.209
7.187
7.181
7.160
7.153
7.091
7.084
6.857
6.829
5.084
4.068
Cl
6d
HO
SPh
10
9
8
7
6
5
4
3
2
1
ppm
11.07
1.07
0.98
2.00

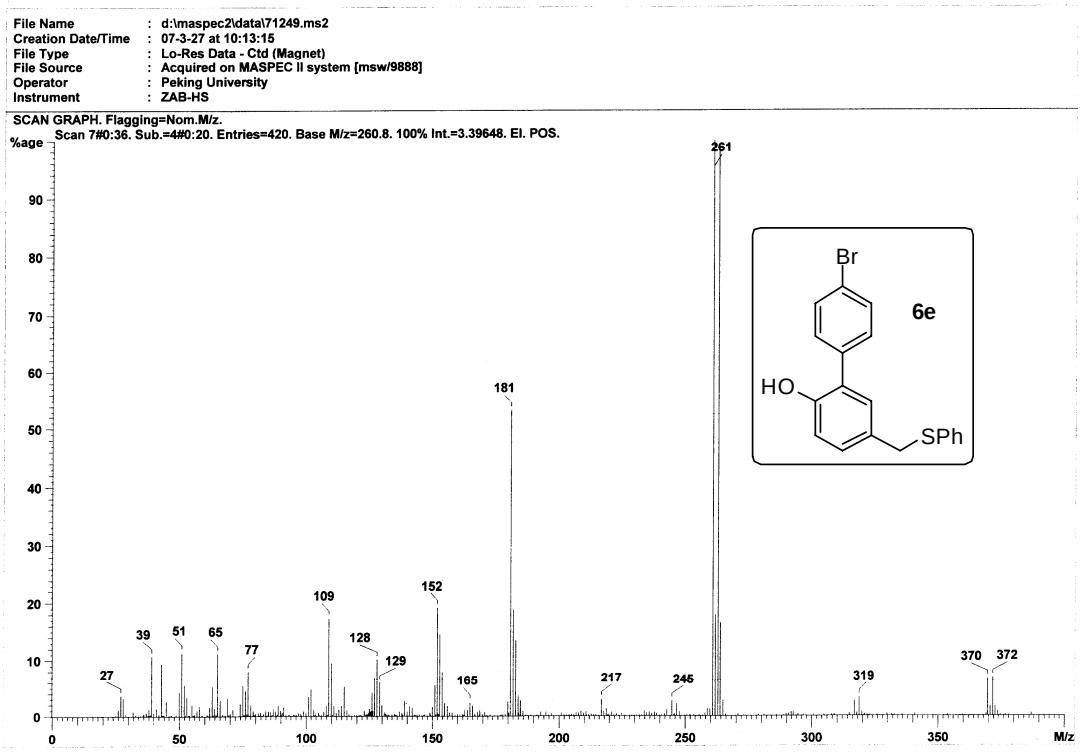

300M
9-P88-1-4ClPh-PhOH
Pulse Sequence: s2pul
151.390
136.124
135.323
133.760
130.643
130.086
130.080
129.882
129.700
129.129
128.819
126.860
126.416
116.146
77.420
77.000
76.572
38.473
Cl
6d
HO
SPh
200
180
160
140
120
100
80
60
40
20
ppm

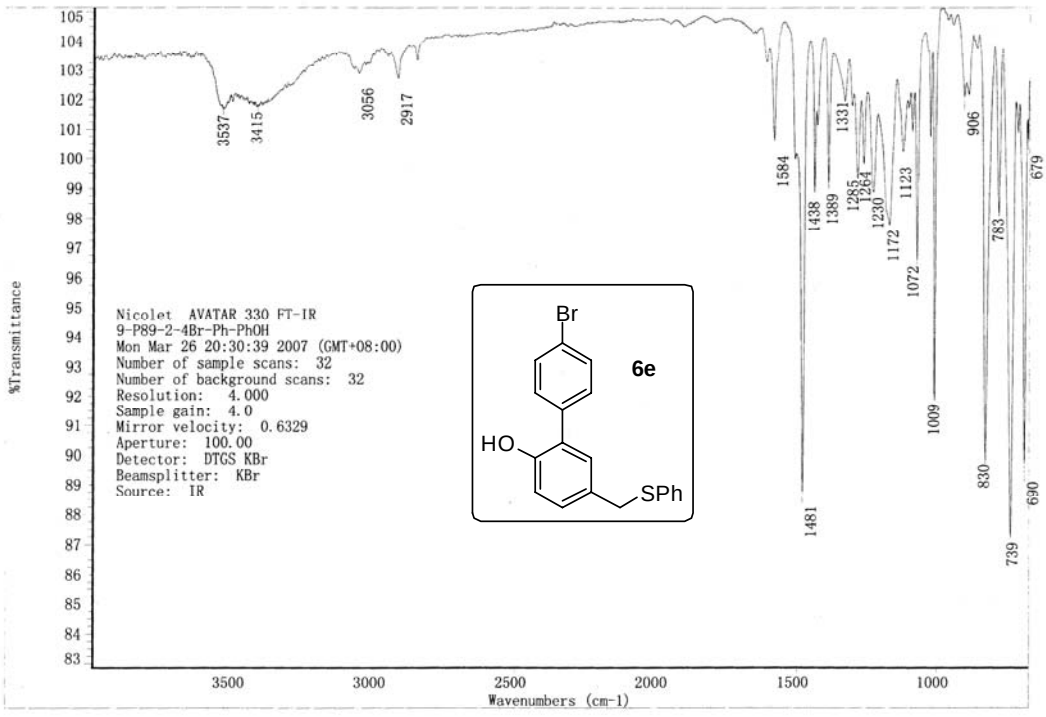

File Name : d:\maspec2\data\71248.ms2
Creation Date/Time : 07-3-27 at 10:09:34
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [msw/9888]
Operator : Peking University
Instrument : ZAB-HS
SCAN GRAPH. Flagging=Nom.M/z.
Scan 8#0:41. Sub.=2#0:10. Entries=295. Base M/z=216.9. 100% Int.=5.00096. EI. POS. Saturated.
%age
M/z
217
181
152
109
326
32
51
65
77
127
Cl
6d
HO
SPh

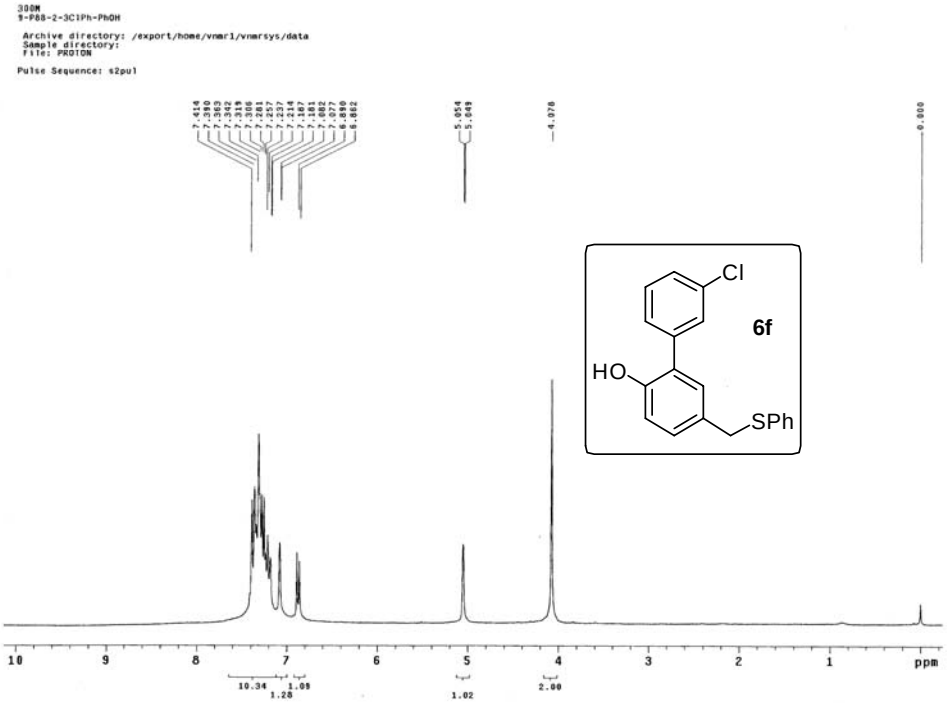

%Transmittance
Wavenumbers (cm-1)
3539
3399
3056
1584
1482
1438
1393
1286
1264
1229
1172
1089
1014
907
833
784
740
691
Nicolet AVATAR 330 FT-IR
9-P88-4ClPh-PhOH
Mon Mar 26 20:13:51 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
Cl
6d
HO
SPh

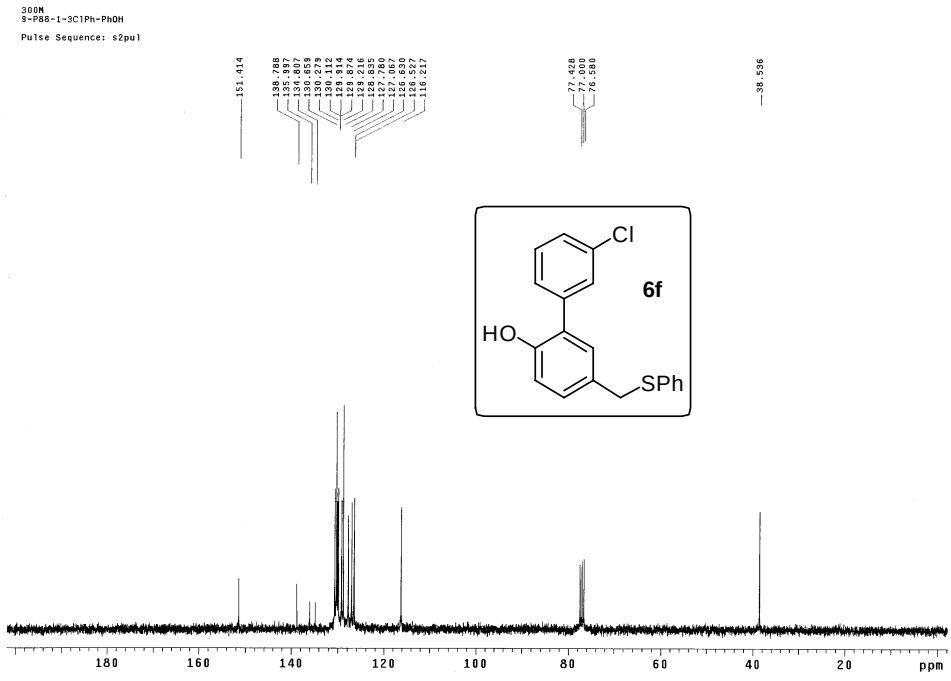


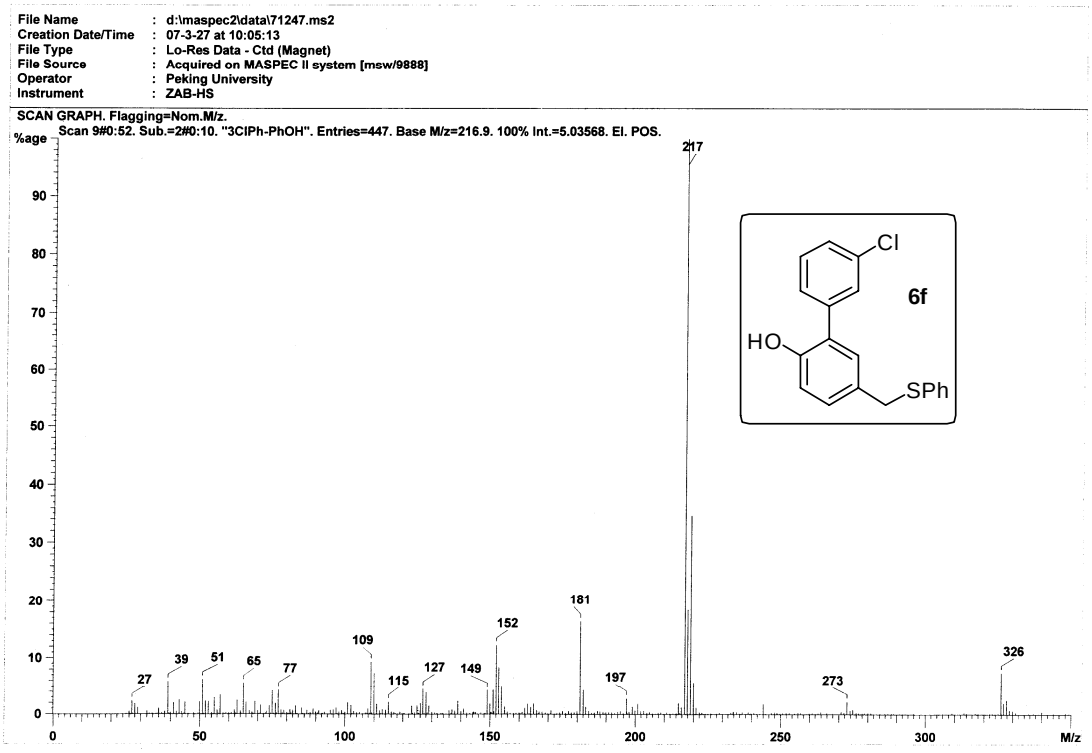


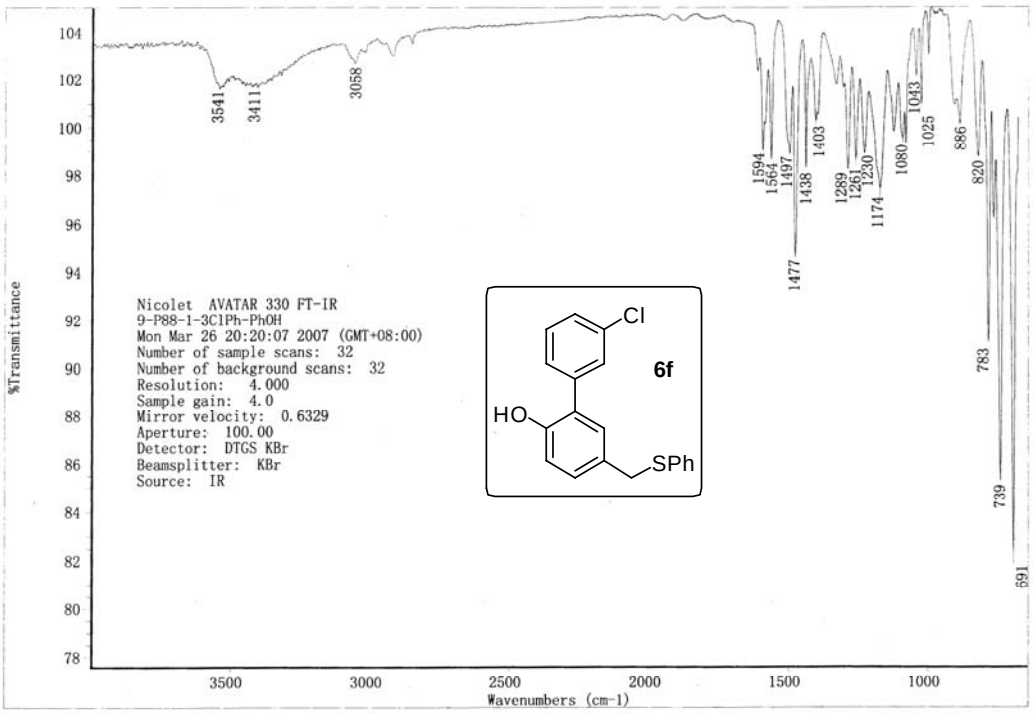


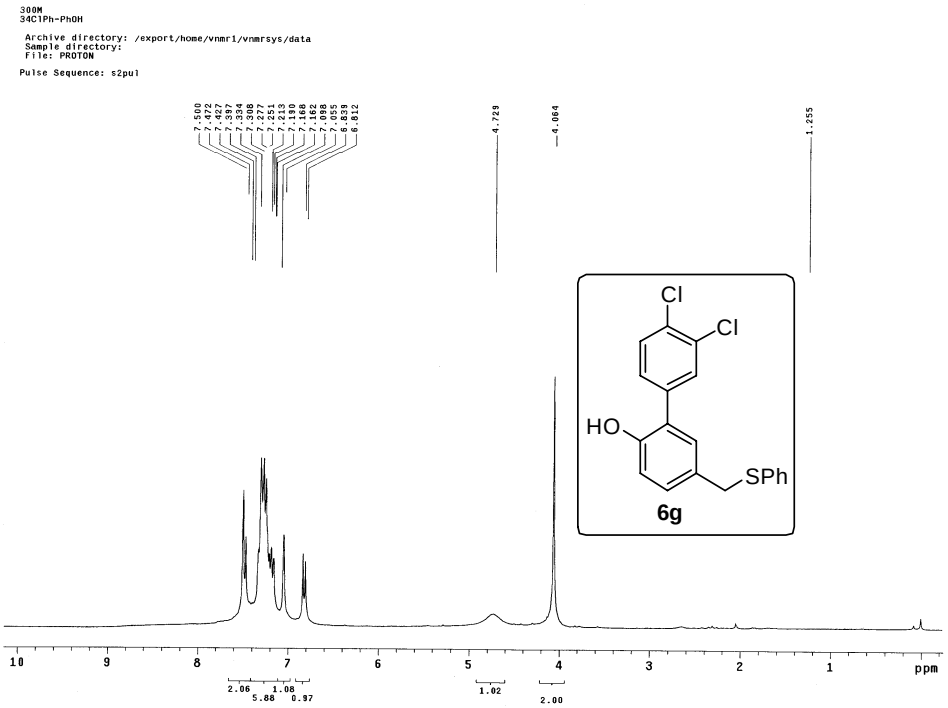


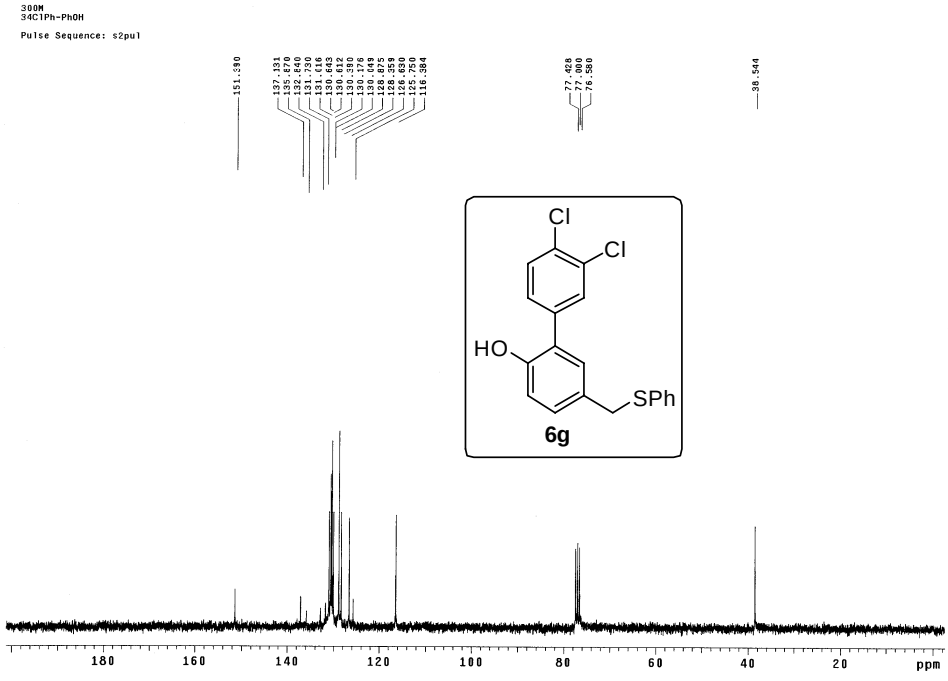


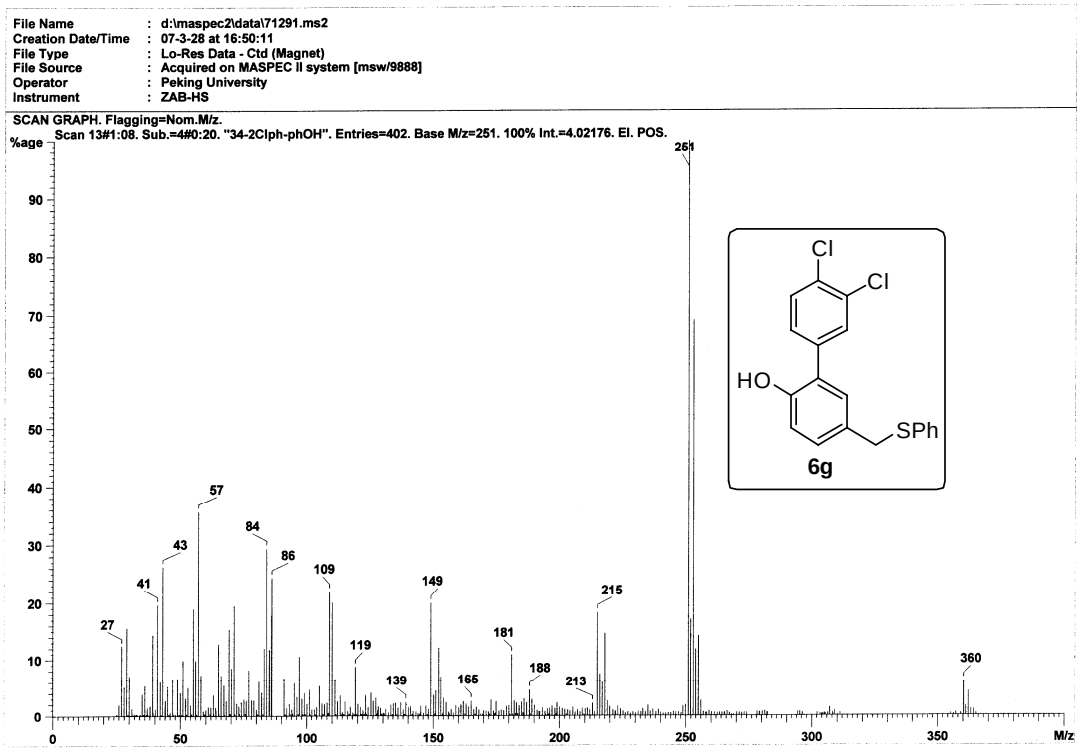


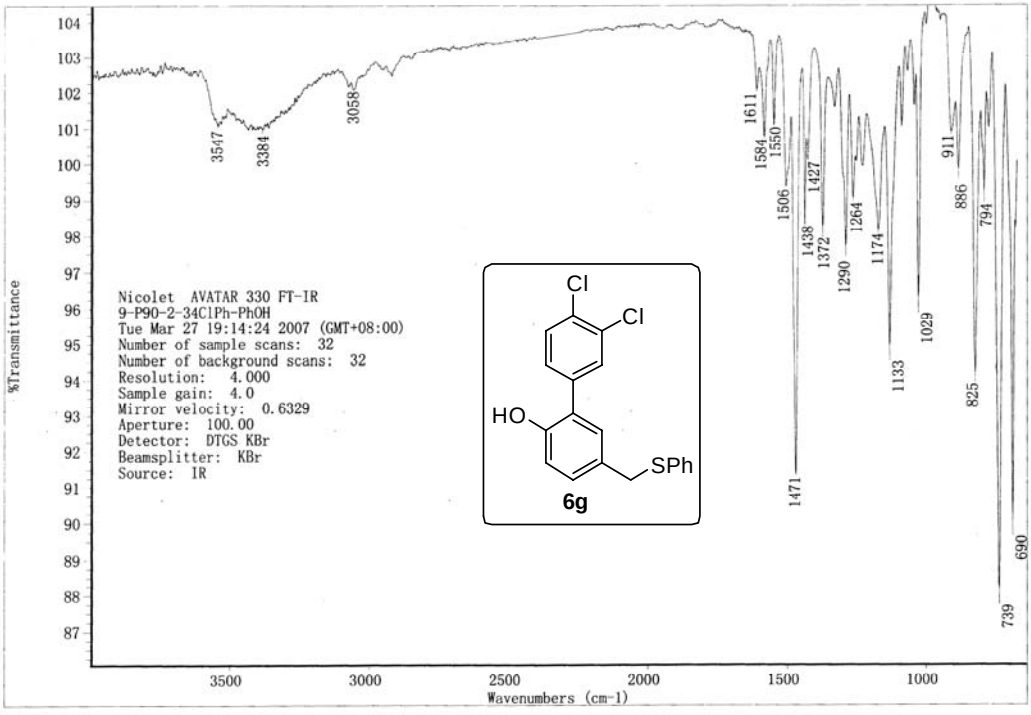


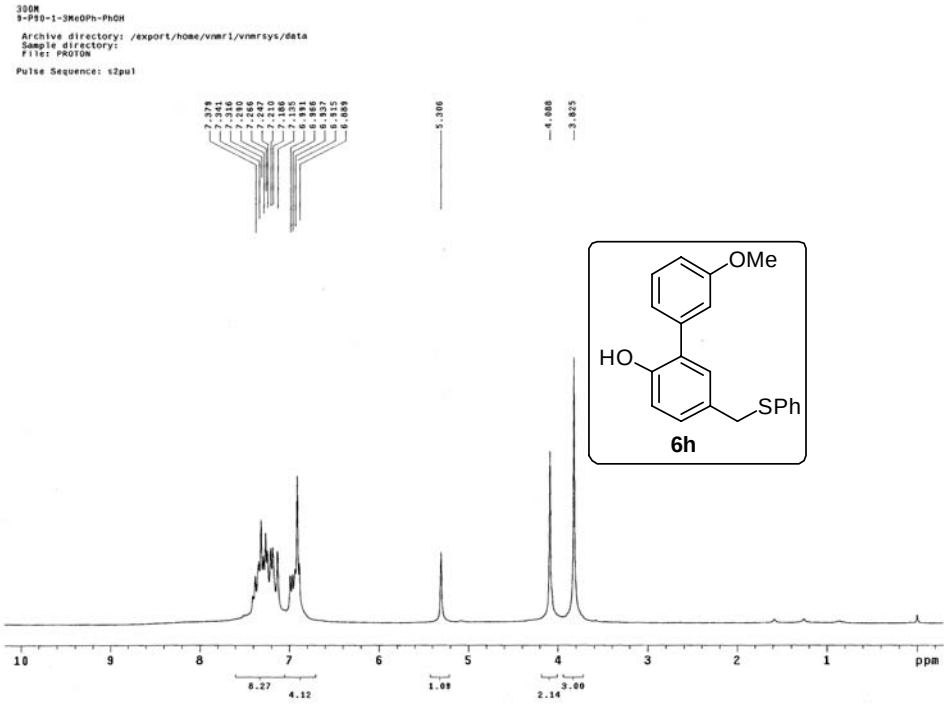


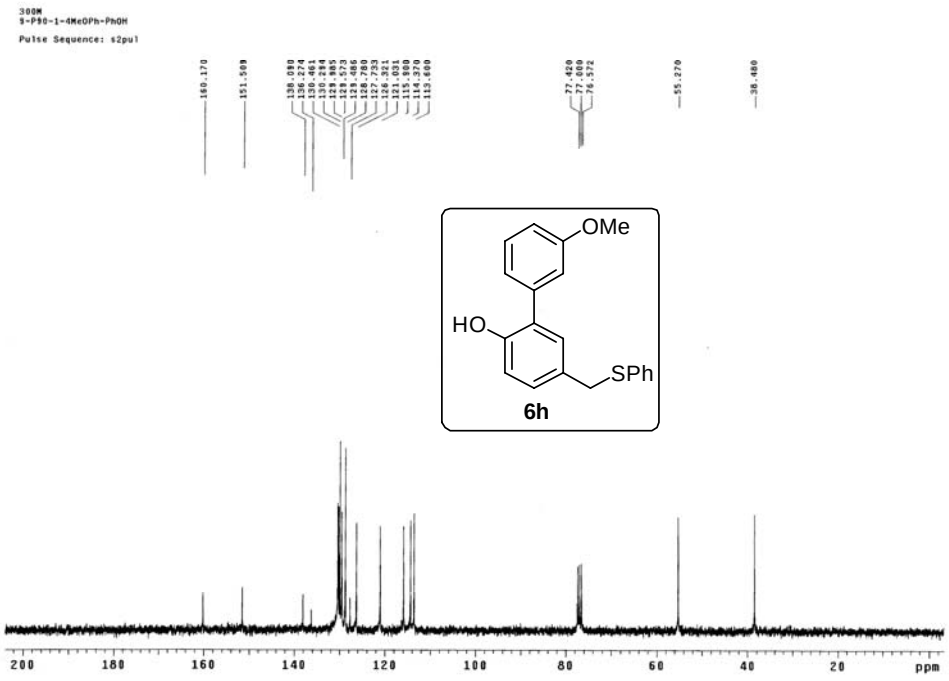


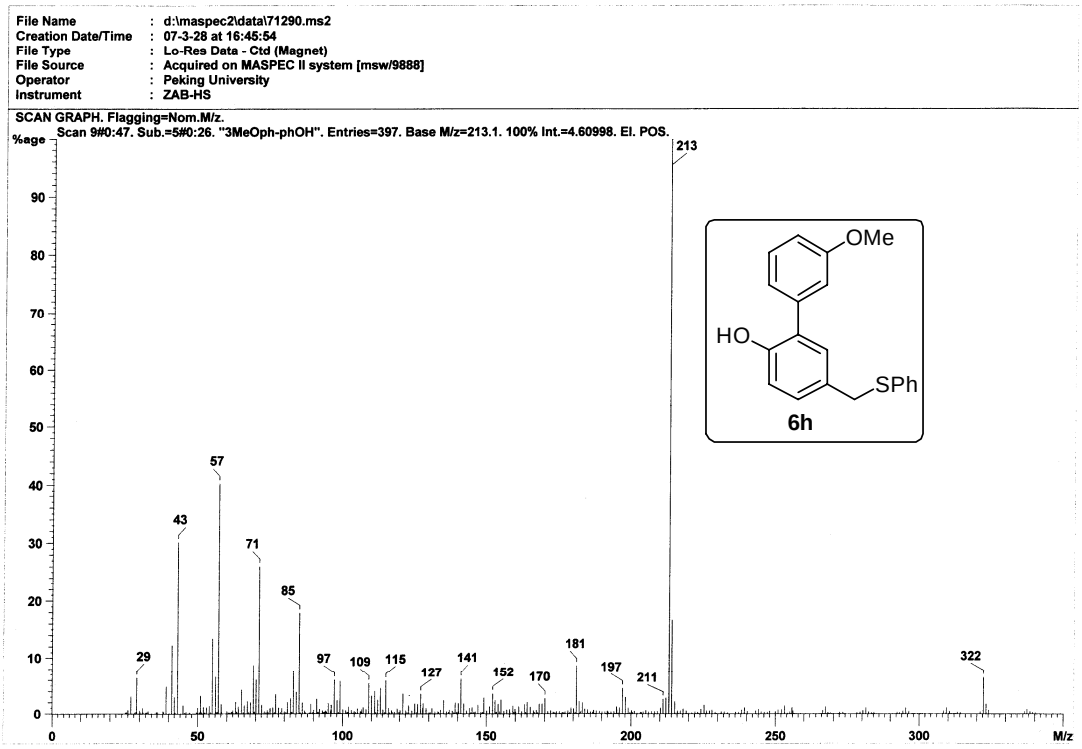


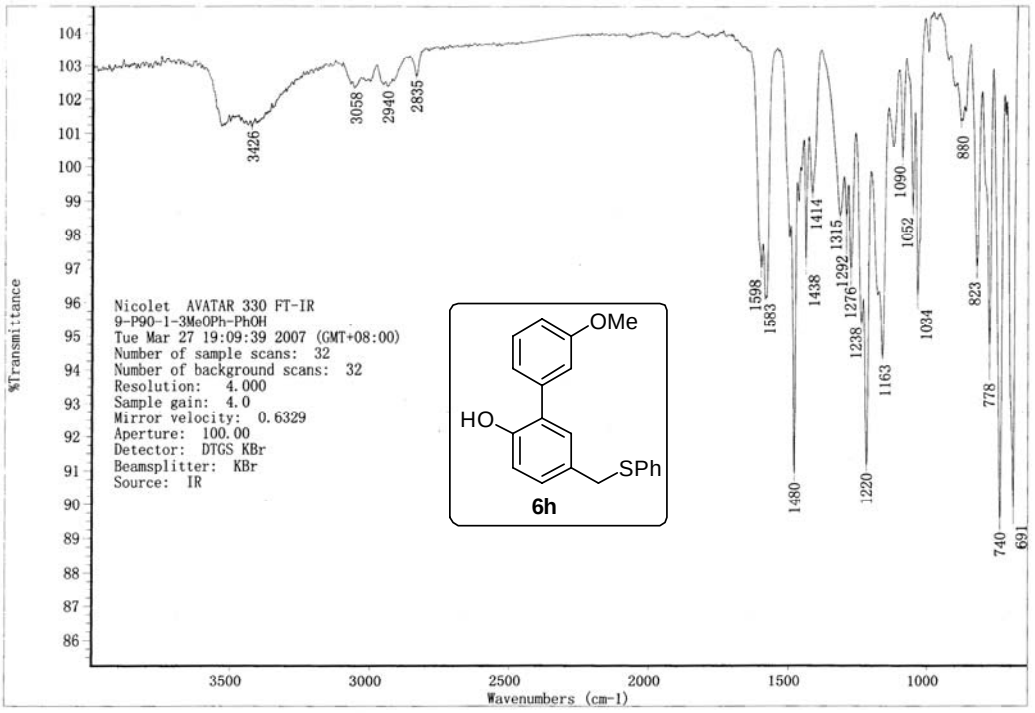


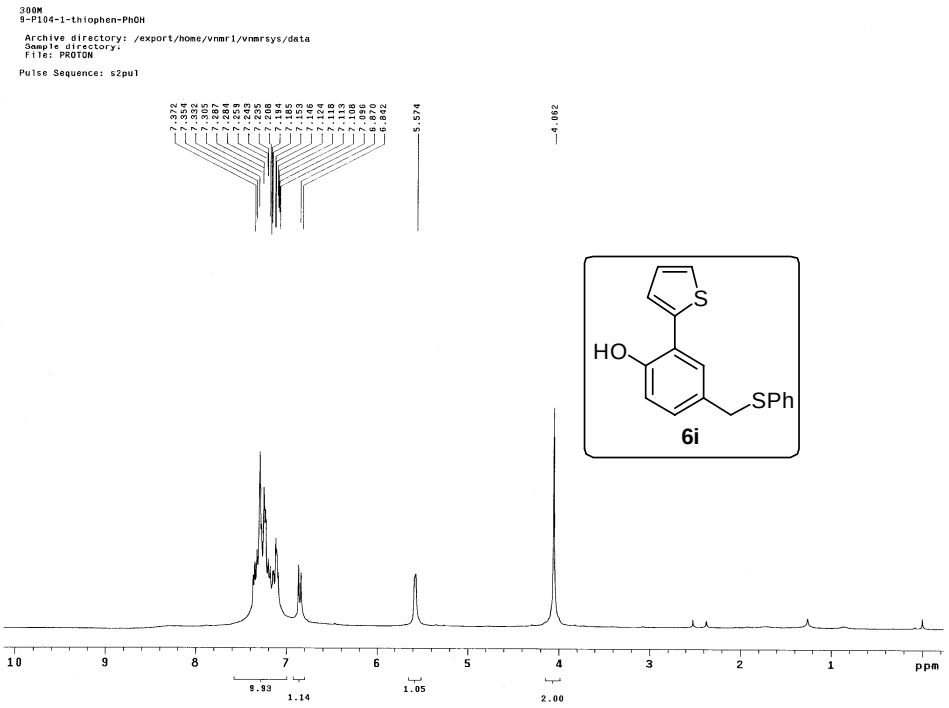


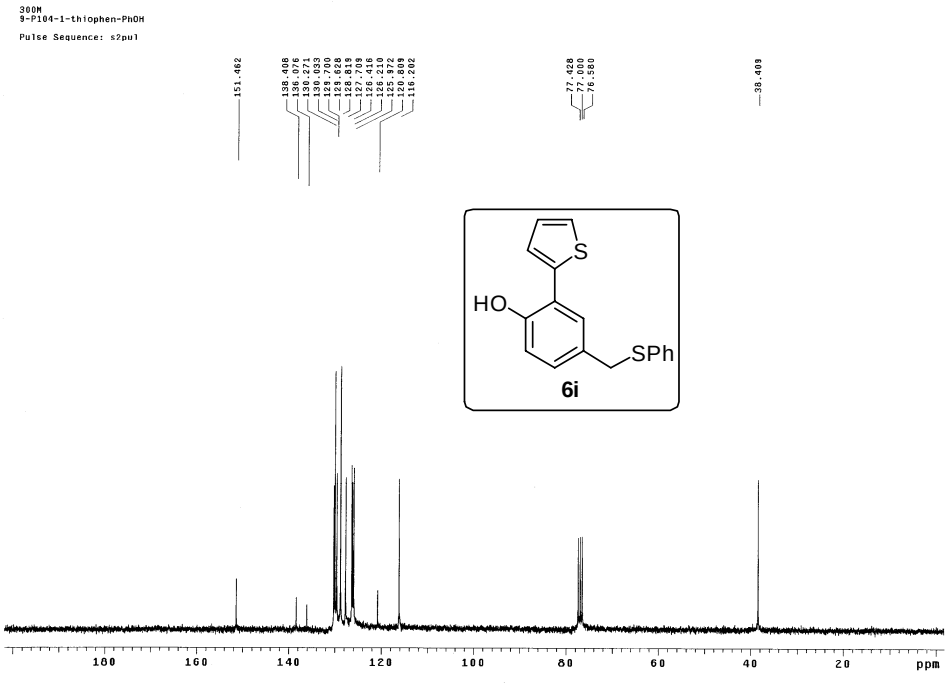

OMe
HO
SPh
6h
ppm

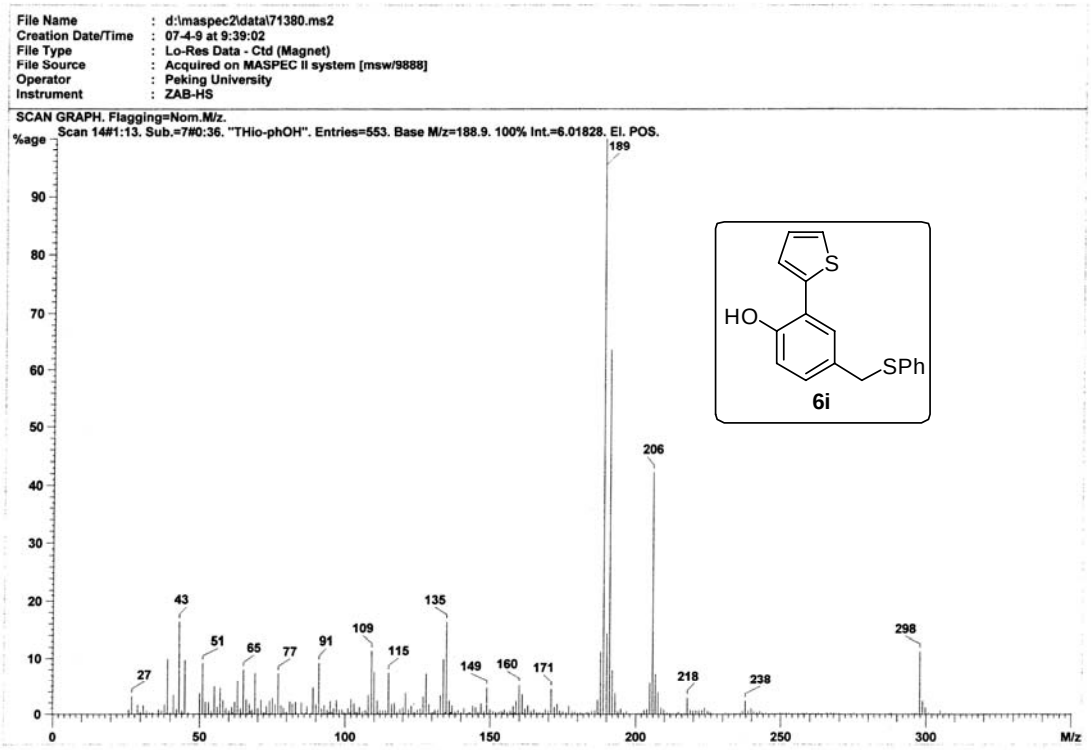

OMe
HO
SPh
6h
ppm

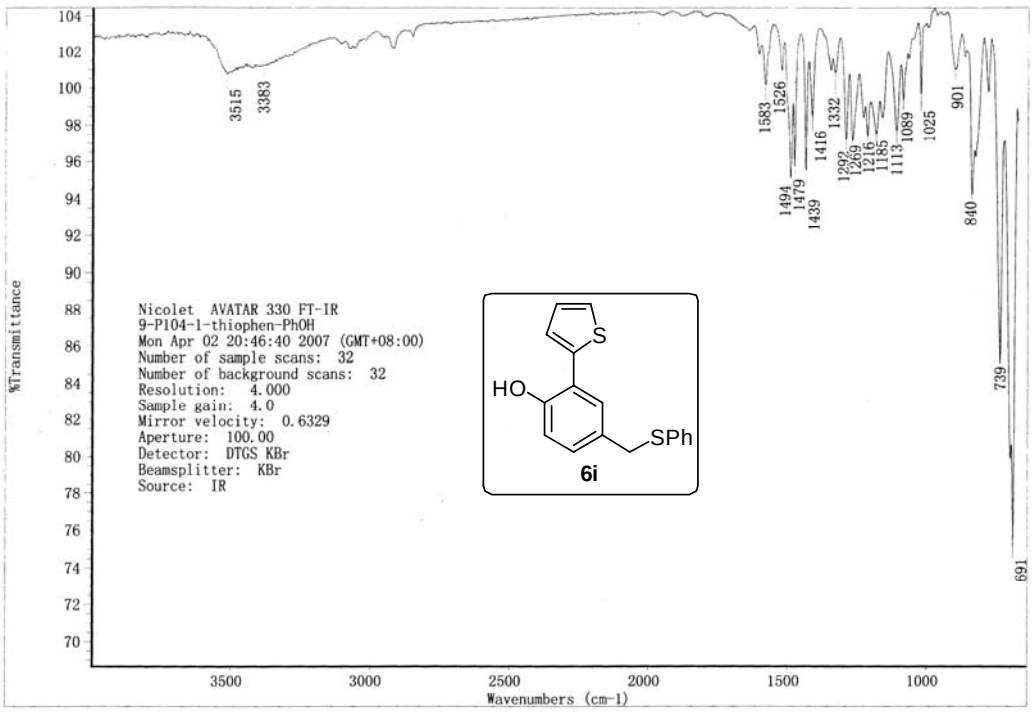


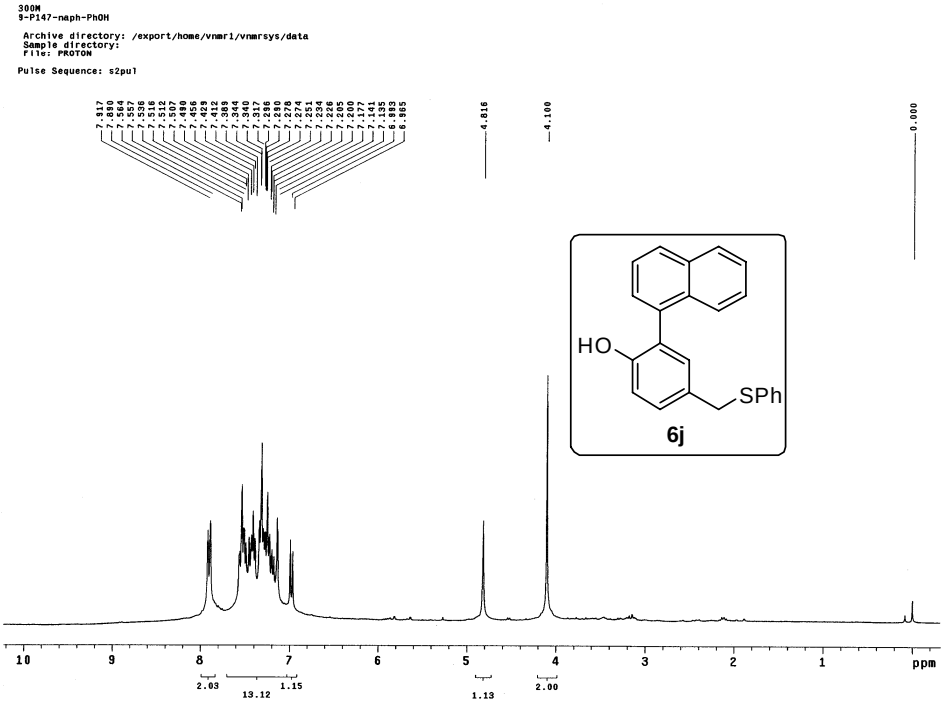


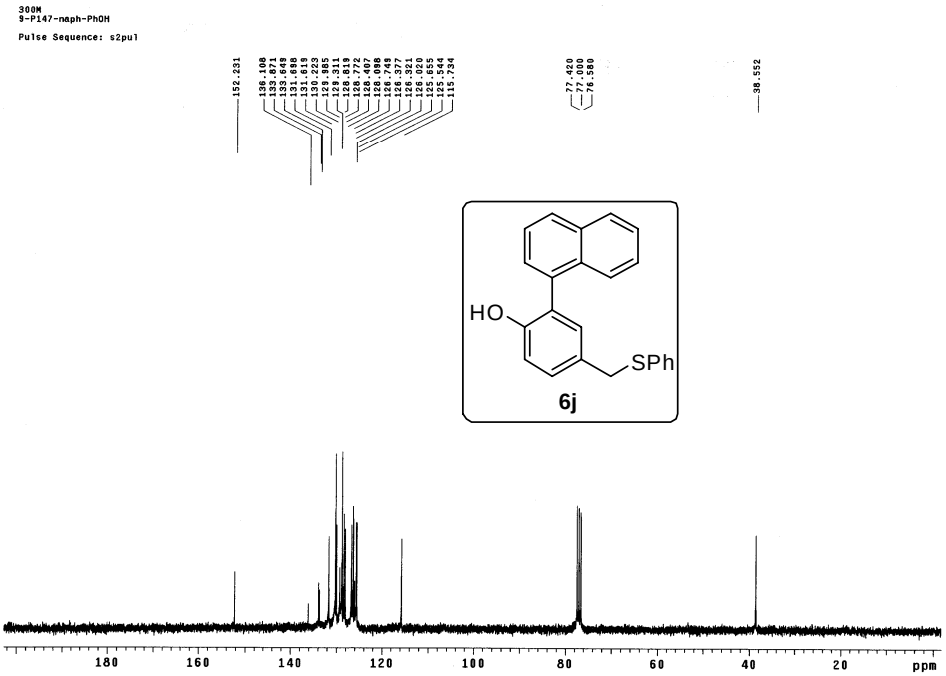


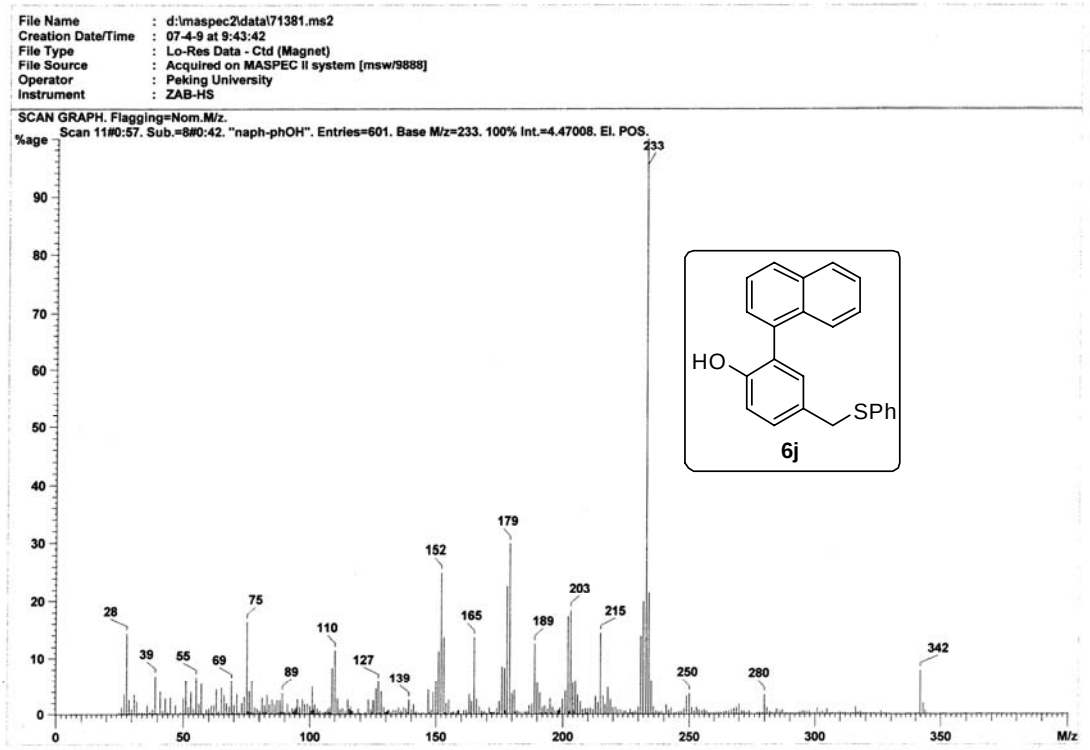


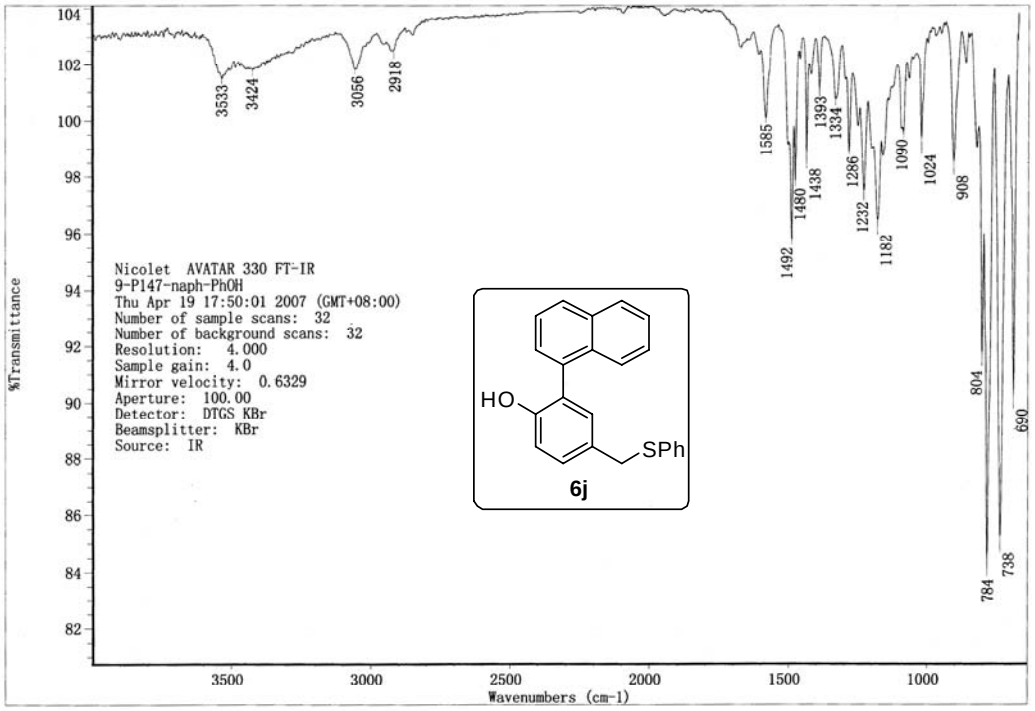

File Name : d:\maspec2\data\71380.ms2
Creation Date/Time : 07-4-9 at 9:39:02
File Type : Lo-Res Data - Ctd (Magnet)
File Source : Acquired on MASPEC II system [msw/9888]
Operator : Peking University
Instrument : ZAB-HS
SCAN GRAPH. Flagging=Nom.M/z.
Scan 14#1:13. Sub.=7#0:36. "THio-phOH". Entries=553. Base M/z=188.9. 100% Int.=6.01828. El. POS.
%age
M/z
189
206
43
135
109
51
65
77
91
115
149
160
171
27
218
238
298
S
HO
SPh
6i

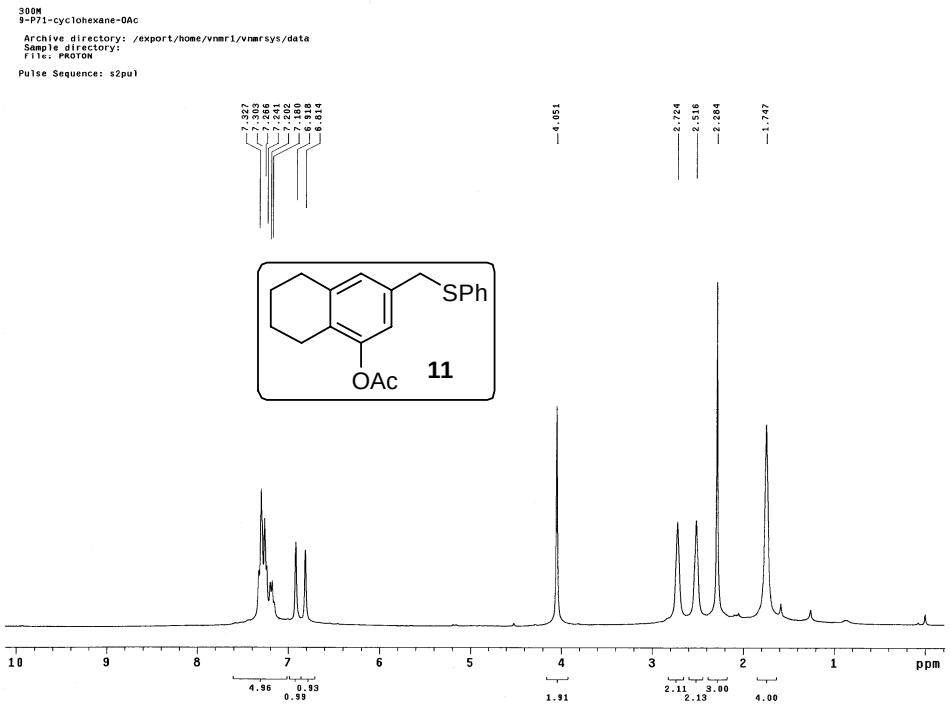

%Transmittance
Wavenumbers (cm-1)
3515
3383
1583
1526
1494
1479
1439
1416
1332
1292
1269
1216
1185
1113
1089
1025
901
840
739
691
Nicolet AVATAR 330 FT-IR
9-P104-1-thiophen-PhOH
Mon Apr 02 20:46:40 2007 (GMT+08:00)
Number of sample scans: 32
Number of background scans: 32
Resolution: 4.000
Sample gain: 4.0
Mirror velocity: 0.6329
Aperture: 100.00
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
S
HO
SPh
6i

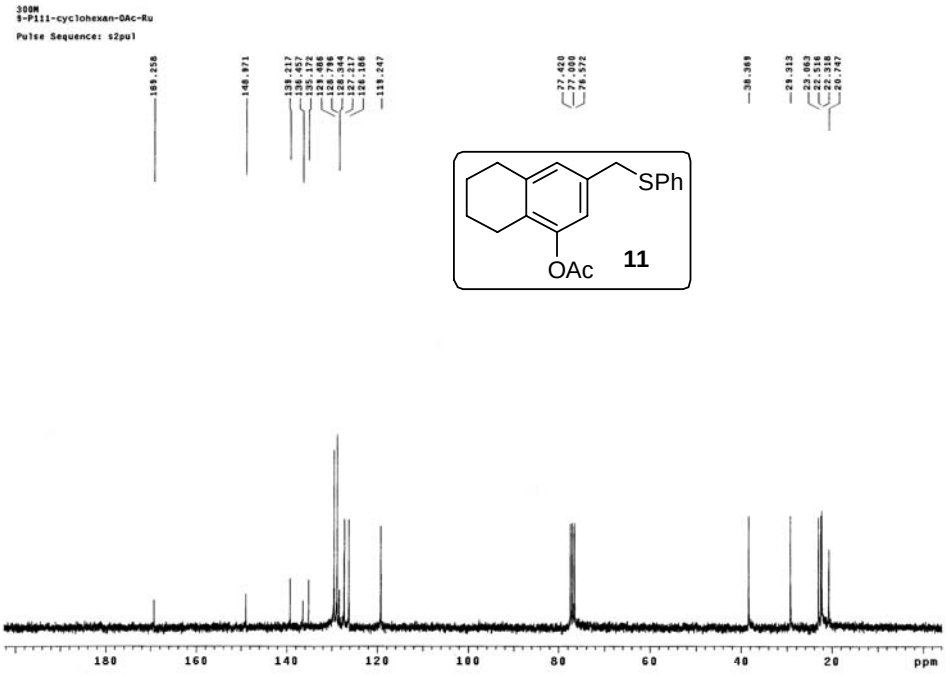

300M
9-P147-naph-PhOH
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
7.817
7.800
7.564
7.557
7.536
7.516
7.512
7.507
7.490
7.456
7.429
7.412
7.383
7.364
7.340
7.317
7.296
7.280
7.278
7.274
7.251
7.234
7.226
7.205
7.200
7.177
7.141
7.135
6.883
6.865
4.816
4.100
0.000
HO
SPh
6j
10
9
8
7
6
5
4
3
2
1
ppm
2.03
13.12
1.15
1.13
2.00


300M
9-P147-naph-PhOH
Pulse Sequence: s2pul
152.231
136.106
133.871
133.648
131.818
131.618
130.223
129.385
128.811
128.613
128.772
128.497
128.408
128.249
126.377
126.321
126.030
125.855
125.544
115.734
77.420
77.000
76.580
38.552
HO
SPh
6j
180
160
140
120
100
80
60
40
20
ppm






300M
9-P71-cyclohexane-OAc
Archive directory: /export/home/vnmr1/vnmrsys/data
Sample directory:
File: PROTON
Pulse Sequence: s2pul
7.327
7.303
7.286
7.241
7.202
7.180
6.818
6.814
4.051
2.724
2.516
2.284
1.747
SPh
OAc
11
10
9
8
7
6
5
4
3
2
1
ppm
4.96
0.83
0.99
1.91
2.11
3.00
2.13
4.00


300M
9-P111-cyclohexan-OAc-Ru
Pulse Sequence: s2pul
169.258
140.971
139.217
138.457
135.172
130.466
128.796
128.344
127.217
124.106
119.247
77.420
77.000
76.572
30.369
29.313
23.063
22.516
22.318
20.747
SPh
OAc
11
180
160
140
120
100
80
60
40
20
ppm