Supporting Information

for

Gold-catalyzed intermolecular coupling of sulfonylacetylene with allyl ethers: [3,3]- and [1,3]-rearrangements

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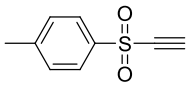
Characterization of starting materials, general procedure for the carboalkoxylation, characterization of products, and ^{1}H and ^{13}C NMR spectra of all new compounds

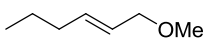
1. Characterization of starting materials
2. General procedure for the carboalkoxylation
3. Characterization of products
4. Scanned copies of the spectra for substrates
5. Scanned copies of the spectra for products

1. Characterization of starting materials



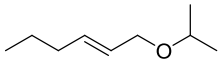
1

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.90 (d, *J* = 8.6 Hz, 2H), 7.40 (d, *J* = 8.2 Hz, 2H), 3.47 (s, H), 2.48 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 146.1, 138.0, 130.2, 127.8, 81.2, 80.5, 21.9.



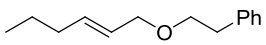
2a

^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.70 (dt, *J* = 15.6, 7.7 Hz, H), 5.55 (dt, *J* = 15.2, 6.2 Hz, H), 3.86 (d, *J* = 6.2 Hz, 2H), 3.32 (s, 3H), 2.03 (q, *J* = 7.0 Hz, 2H), 1.41 (sextet, *J* = 7.4 Hz, 2H), 0.90 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 134.8, 126.3, 73.4, 57.7, 34.5, 22.3, 13.8.



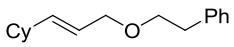
2b

^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.68 (dt, *J* = 15.2, 6.7 Hz, H), 5.56 (dt, *J* = 15.7, 5.8 Hz, H), 3.91 (d, *J* = 5.9, 2H), 3.61 (septet, *J* = 6.2 Hz, H), 2.02 (q, *J* = 7.0 Hz, 2H), 1.40 (sextet, *J* = 7.4 Hz, 2H), 1.16 (d, *J* = 5.8, 6H), 0.90 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 134.0, 127.2, 70.7, 69.1, 34.5, 22.4, 22.3, 13.9.



2c

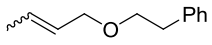
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32-7.19 (m, 5H), 5.69 (dt, *J* = 15.3, 6.6 Hz, H), 5.55 (dt, *J* = 15.2, 6.3 Hz, H), 3.95 (d, *J* = 6.2 Hz, 2H), 3.64 (t, *J* = 7.4 Hz, 2H), 2.91 (t, *J* = 7.4 Hz, 2H), 2.03 (q, *J* = 7.0 Hz, 2H), 1.41 (sextet, *J* = 7.5 Hz, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.1, 134.6, 129.0, 128.5, 126.6, 126.3, 71.8, 71.1, 36.5, 34.5, 22.4, 13.8.



2d

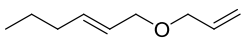
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.40-7.16 (m, 5H), 5.63 (dd, *J* = 15.7, 6.3 Hz, H), 5.49 (dt, *J* = 15.6, 6.2 Hz, H), 3.93 (d, *J* = 5.8, 2H), 3.62 (t, *J* =7.4 Hz, 2H), 2.90 (t, *J* = 7.4 Hz, 2H), 2.08-1.88 (m, H), 1.82-1.59 (m, 5H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.4, 139.1, 129.0, 128.5, 126.3, 123.8, 72.0, 71.1, 40.5, 36.5, 32.9, 26.3, 26.2.

(E/Z = 16:1)



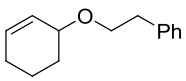
2f

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.40-7.32 (m, E&Z isomer 5H), 5.70 (dq, *J* = 15.2, 6.6 Hz, E isomer H), 5.57 (dtd, *J* = 15.3, 6.3, 1.2 Hz, E isomer H), 4.05 (d, *J* = 6.7 Hz, Z isomer 2H), 3.91 (d, *J* = 6.2 Hz, E isomer 2H), 3.62 (t, *J* = 7.4 Hz, E isomer 2H), 2.90 (t, *J* = 7.5 Hz, E isomer 2H), 1.71 (d, *J* = 6.2 Hz, E isomer 3H), 1.62 (d, *J* = 6.7 Hz, Z isomer 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.0, 129.4, 128.9, 128.3, 127.6, 126.2, 71.6, 71.0, 36.4, 17.8.



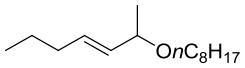
2h

^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.92 (ddt, *J* = 16.0, 10.6, 5.9 Hz, H), 5.70 (dt, *J* = 15.2, 6.3 Hz, H), 5.56 (dt, *J* = 15.2, 6.3 Hz, H), 5.27 (dd, *J* = 17.2, 1.6 Hz, H), 5.18 (dd, *J* = 10.6, 1.2 Hz, H), 3.97 (d, *J* = 5.8 Hz, 2H), 3.93 (d, *J* = 6.3 Hz, 2H), 2.03 (q, *J* = 7.0 Hz, 2H), 1.41 (sextet, *J* = 7.4 Hz, 2H), 0.90 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 135.0, 134.9, 126.4, 117.1, 71.1, 71.0, 34.5, 22.4, 13.9.



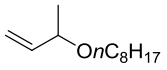
2j

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.32-7.17 (m, 5H), 5.88-5.81 (m, H), 5.76 (dd, *J* = 2.3, 10.1 Hz, H), 3.85 (s br, H), 3.76-3.60 (m, 2H), 2.90 (t, *J* = 7.4 Hz, 2H),2.10-1.88 (m, 2H), 1.88-1.48 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.2, 130.9, 129.0, 128.4, 127.9, 126.2, 73.1, 69.4, 36.9, 28.4, 25.3, 19.3.



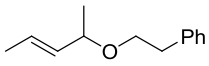
2k

^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.56 (td, *J* = 6.6, 15.6 Hz, H), 5.32 (dd, *J* = 7.8, 15.6 Hz, H), 3.80-3.70 (m, H), 3.48-3.36 (m, H), 3.36-3.18 (m, H), 2.00 (app q, *J* = 7.0 Hz, 2H), 1.60-1.49 (m, 2H), 1.41 (sextet, *J* = 7.4 Hz, 2H), 1.39-1.18 (m, 10H), 1.21 (d, *J* = 6.3 Hz, 3H), 0.90 (t, *J* = 7.4 Hz, 3H), 0.88 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 132.6, 132.4, 76.6, 68.2, 34.4, 32.0, 30.1, 29.6, 29.4, 26.4, 22.8, 22.5, 21.9, 14.2, 13.8.



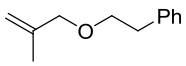
2l

^{1}H NMR ($CDCl_3$, 400 MHz): δ 5.74 (ddd, *J* = 7.0. 10.2, 17.2 Hz, H), 5.16 (d, *J* = 17.2 Hz, H), 5.11 (d, *J* = 10.6 Hz, H), 3.84-3.73 (m, H), 3.49-3.85 (m, H), 3.84-3.72 (m, H), 1.60-1.50 (m, 2H), 1.38-1.20 (m, 10H), 1.23 (d, *J* = 6.7 Hz, 3H), 0.88 (t, *J* = 6.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.9, 115.5, 76.9, 68.6, 32.0, 30.1, 29.6, 29.4, 26.4, 22.8, 21.5, 14.2.



2m

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35-7.13 (m, 5H), 5.64-5.52 (m, H), 5.40-5.28 (m, H), 3.83-3.73 (m, H), 3.69-3.57 (m, H), 3.51-3.42 (m, H), 2.94-2.80 (m, 2H), 1.68 (d, *J* = 6.3 Hz, 3H), 1.22 (d, *J* = 6.3 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.2, 133.5, 129.1, 128.4, 127.5, 126.2, 76.7, 69.1, 36.7, 21.6, 17.8.



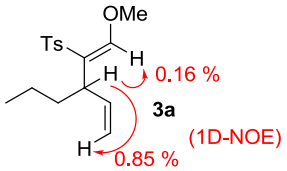
2n

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.35-7.14 (m, 5H), 4.93 (s, 1H), 4.87 (s, 1H), 3.89 (s, 2H), 3.62 (t, *J* = 7.1 Hz, 2H), 1.70 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.5, 139.2, 129.1, 128.4, 126.3, 112.1, 75.0, 71.1, 36.5, 19.6.

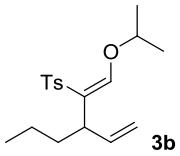
2. General procedure for the carboalkoxylation

A flame-dried test tube was charged with $Au(PPh_3)Cl$ (2.5 mg, 0.005 mmol) and $AgSbF_6$ (1.7 mg, 0.005 mmol). The content was dissolved in anhydrous $CHCl_3$ (1 mL), and allyl ether **2c** (61.3 mg, 0.30 mmol) was added to the mixture. After cooling the mixture to −15 ^{o}C, *p*-toluenesulfonylacetylene **1** (18.0 mg, 0.10 mmol) was added in one-lot. The reaction mixture was allowed to warm slowly to ca. 15 ^{o}C over 2 h. After the reaction was complete by TLC analysis, the solvent was evaporated and the residue was purified by chromatography (EtOAc:Hex = 1:10) to give 27.7 mg (72%, as a mixture of [3,3]- and [1,3]-product (8:1)) of **3c** as a colorless liquid.

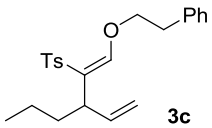
3. Characterization of products



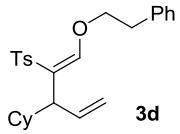
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 2H), 6.23 (s, H), 5.74 (ddd, *J* = 17.2, 9.8, 7.4 Hz), 5.10 (d, *J* = 18.4 Hz, H), 5.06 (d, *J* = 10.9 Hz, H), 3.68 (s, 3H), 3.37 (q, *J* = 7.0 Hz, H), 2.42 (s, 3H), 1.66-1.49 (m, 2H), 1.42-1.30 (m, 2H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 154.5, 143.4, 140.4, 140.1, 129.1, 127.9, 122.9, 115.5, 62.0, 42.3, 37.0, 21.7, 20.6, 14.0; HRMS (FAB) Calcd for $C_{16}H_{22}O_3S$ (M + H), 295.1368; found 295.1368.



^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81 (d, *J* = 8.5 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 6.31 (s, H), 5.79 (ddd, *J* = 17.1, 10.1, 7.4 Hz, H), 5.12 (d, *J* = 17.2 Hz, H), 5.07 (d, *J* = 10.5 Hz, H), 3.96 (septet, *J* = 6.2 Hz, H), 3.43 (q, *J* = 7.4 Hz, H), 2.42 (s, 3H), 1.69-1.52 (m, 2H), 1.42-1.33 (m, 2H), 1.11 (d, *J* = 6.2 Hz, 3H), 1.05 (d, *J* = 6.2 Hz, 3H), 0.93 (t, *J* =7.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.9, 143.2, 140.8, 140.4, 128.8, 128.4, 122.7, 115.3, 78.3, 42.2, 37.1, 22.3, 22.2, 21.7, 20.7, 14.0; HRMS (FAB) Calcd for $C_{18}H_{26}O_3S$ (M + H), 323.1681; found 323.1682.

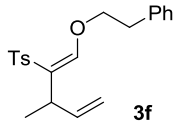


^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.28-7.20 (m, 5H), 6.90 (d, *J* = 7.4 Hz, 2H), 6.08 (s, H), 5.61 (ddd, *J* = 17.6, 10.1, 7.8 Hz, H), 5.04 (d, *J* = 16.8 Hz, H), 5.01 (d, *J* = 9.8 Hz, H), 4.09 (dt, *J* = 10.6, 6.6 Hz, H), 4.04 (dt, *J* = 10.2, 7.0 Hz, H), 3.32 (q, *J* = 7.4 Hz, H), 2.79 (t, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 1.53-1.38 (m, 2H), 1.38-1.22 (m, 2H), 0.88 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.6, 143.3, 140.5, 137.0, 129.1, 128.9, 128.7, 128.4, 128.3, 128.2, 126.8, 115.4, 76.2, 42.2, 36.9, 36.4, 21.7, 20.6, 14.0; HRMS (FAB) Calcd for $C_{23}H_{28}O_3S$ (M + H), 385.1837; found 385.1835.



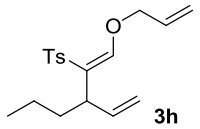
3d

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.24-7.19 (m, 5H), 6.98 (d, *J* = 7.9 Hz, 2H), 6.08 (s, H), 5.68 (ddd, *J* = 17.1, 9.4, 8.5 Hz, H), 5.00 (d, *J* = 15.2 Hz, H), 5.00 (d, *J* = 11.3 Hz, H), 4.08 (dt, *J* = 10.1, 6.6 Hz, H), 4.02 (dt, *J* = 10.1, 7.0 Hz, H), 2.98 (t, *J* = 9.0 Hz, H), 2.77 (td, *J* = 6.6, 1.6 Hz, 2H), 2.41 (s, 3H), 1.77-1.62 (m, 4H), 1.52-1.44 (m, 4H), 1.25-1.05 (m, 4H), 0.89-0.75 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.5, 143.3, 140.2, 139.7, 137.0, 129.1, 128.9, 128.8, 128.2, 126.9, 121.4, 116.2, 76.3, 50.1, 40.9, 36.4, 31.5, 31.2, 26.5, 26.4, 26.3, 21.7; HRMS (FAB) Calcd for $C_{26}H_{32}O_3S$ (M + H), 425.2150; found 425.2151.



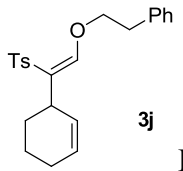
3f

^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.79 (d, *J* = 8.2 Hz, 2H), 7.26-7.21 (m, 5H), 7.00 (d, *J* = 7.8 Hz, 2H), 6.08 (s, H), 5.68 (ddd, *J* = 16.4, 10.2, 5.9 Hz, H), 5.04 (d, *J* = 17.6 Hz, H), 5.00 (d, *J* = 10.5 Hz, H), 4.09 (dt, *J* = 10.1, 7.1 Hz, H), 4.06 (dt, *J* = 10.5, 6.7 Hz, H), 3.53 (quintet, *J* = 6.3 Hz, H), 2.80 (t, *J* = 6.6 Hz, 2H), 2.42 (s, 3H), 1.18 (d, *J* = 7.0 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.7, 143.5, 141.0, 140.0, 137.0, 129.1, 129.0, 128.7, 128.1, 126.8, 122.6, 114.5, 76.3, 36.4, 36.0, 21.7, 20.2; HRMS (FAB) Calcd for $C_{21}H_{24}O_3S$ (M + H), 357.1524; found 357.1526.



3h

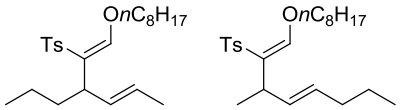
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.6 Hz, 2H), 6.27 (s, H), 5.75 (ddd, *J* = 17.6, 10.2, 7.4 Hz, H), 5.67 (ddt, *J* = 17.2, 11.7, 5.1 Hz, H), 5.17 (dd, *J* = 15.6, 1.1 Hz, H), 5.14 (dd, *J* = 16.0, 1.2 Hz, H), 5.09 (d, *J* = 11.0 Hz, H), 5.06 (d, *J* = 11.1 Hz, H), 4.34-4.33 (m, 2H), 3.40 (q, *J* = 7.5 Hz, H), 2.43 (s, 3H), 1.66-1.50 (m, 2H), 1.41-1.26 (m, 2H), 0.91 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 152.8, 143.4, 140.5, 140.0, 132.2, 129.0, 128.2, 123.1, 118.9, 115.5, 75.2, 42.3, 37.0, 21.7, 20.6, 14.0; HRMS (FAB) Calcd for $C_{18}H_{24}O_3S$ (M + H), 321.1524; found 321.1525.



3j

Inseparable mixture with **4**, **5** (R = $(CH_2)_2Ph$) and $Ph(CH_2)_2OH$

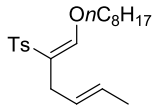
^1H NMR ($CDCl_3$, 400 MHz): δ 7.78 (d, *J* = 8.2 Hz, 2H), 7.35-7.18 (m, 5H), 7.00 (d, *J* = 7.9 Hz, 2H), 6.10 (s, H), 5.77-5.72 (m, H), 5.27-5.21 (m, H), 4.02 (t, *J* = 7.2 Hz, 2H), 3.55-3.46 (m, H), 2.79 (t, *J* = 7.0 Hz, 2H), 2.43 (s, 3H), 2.01-1.87 (m, 4H), 1.58-1.38 (m, 2H). LRMS (EI^+, GC-MS) Calcd for $C_{23}H_{27}O_3S$ (M + H), 383; found 383.



3k **3k'**

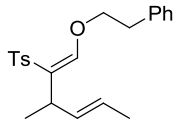
3k and **3k'** (1:1.4), inseparable mixture with **4** (R = C_8H_{17})

^1H NMR ($CDCl_3$, 400 MHz): δ 6.28 (s, H, **3k'**), 6.26 (s, H, **3k**), 5.58-5.29 (m, 2H, **3k** and **3k'**), 3.64 (t, *J* = 6.6 Hz, 2H, **3k** and **3k'**), 3.53-3.40 (m, H, **3k**), 3.33 (app q, *J* = 7.1 Hz, H, **3k'**). LRMS (EI^+, GC-MS) Calcd for $C_{24}H_{39}O_3S$ (M + H), 407; found 407.



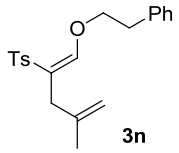
3l

^1H NMR ($CDCl_3$, 400 MHz): δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.26 (d, *J* = 8.2 Hz, 2H), 6.29 (s, H), 5.60-5.48 (m, H), 5.45-5.35 (m, H), 3.84 (t, *J* = 6.7 Hz, 2H), 3.04 (d, *J* = 5.8 Hz, 2H), 2.42 (s, 3H), 1.67 (d, *J* = 5.5 Hz, 3H), 1.56-1.48 (m, 2H), 1.36-1.12 (m, 10H), 0.89 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.0, 143.1, 139.7, 128.7, 127.8, 127.7, 127.4, 117.6, 75.3, 31.6, 31.2, 29.4, 29.0, 28.9, 25.3, 22.4, 21.4, 17.6, 13.9; HRMS (FAB) Calcd for $C_{21}H_{33}O_3S$ (M + H), 365.2150; found 365.2151.



3m

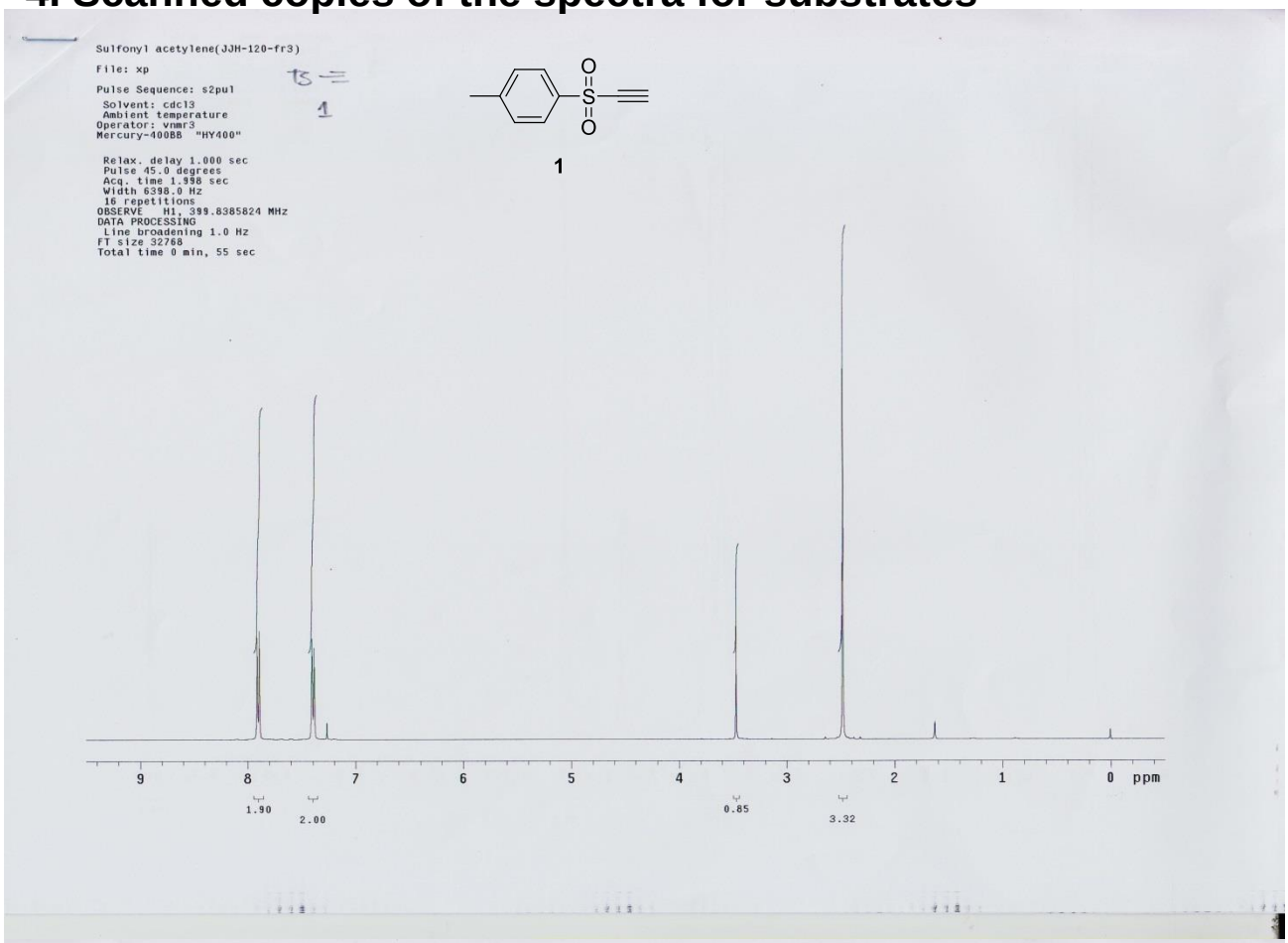
^1H NMR ($CDCl_3$, 400 MHz): δ 7.77 (d, *J* = 7.8 Hz, 2H), 6.99 (d, *J* = 7.1 Hz, 2H), 6.05 (s, H), 5.50-5.39 (m, H), 5.28-5.19 (m, H), 4.02 (t, *J* = 7.0 Hz, 2H), 3.52-3.45 (m, H), 3.00 (t, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 1.62 (d, *J* = 6.2 Hz, 3H), 1.15 (d, *J* = 7.0 Hz, 3H). LRMS (EI^+, GC-MS) Calcd for $C_{22}H_{27}O_3S$ (M + H), 371; found 371.

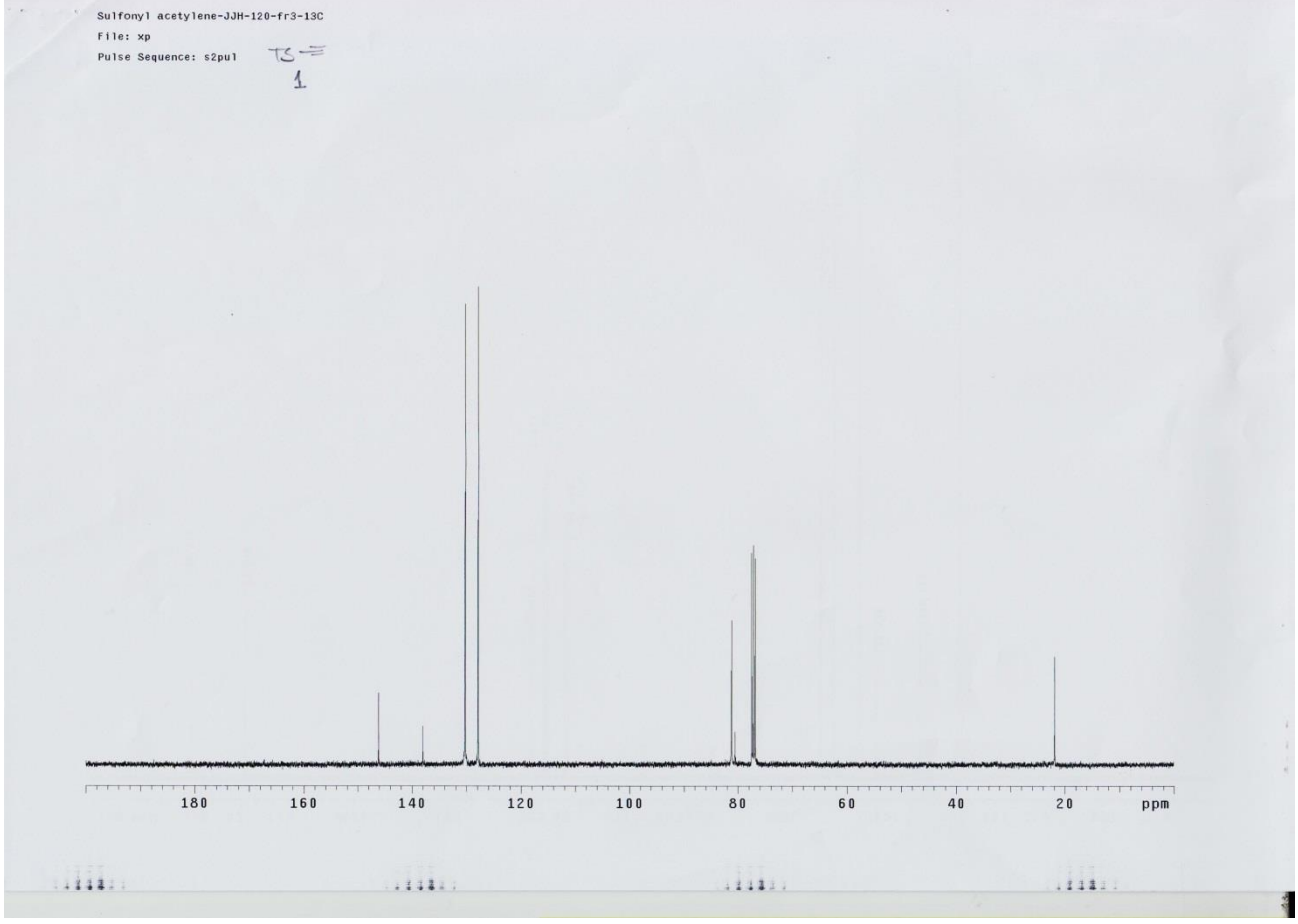


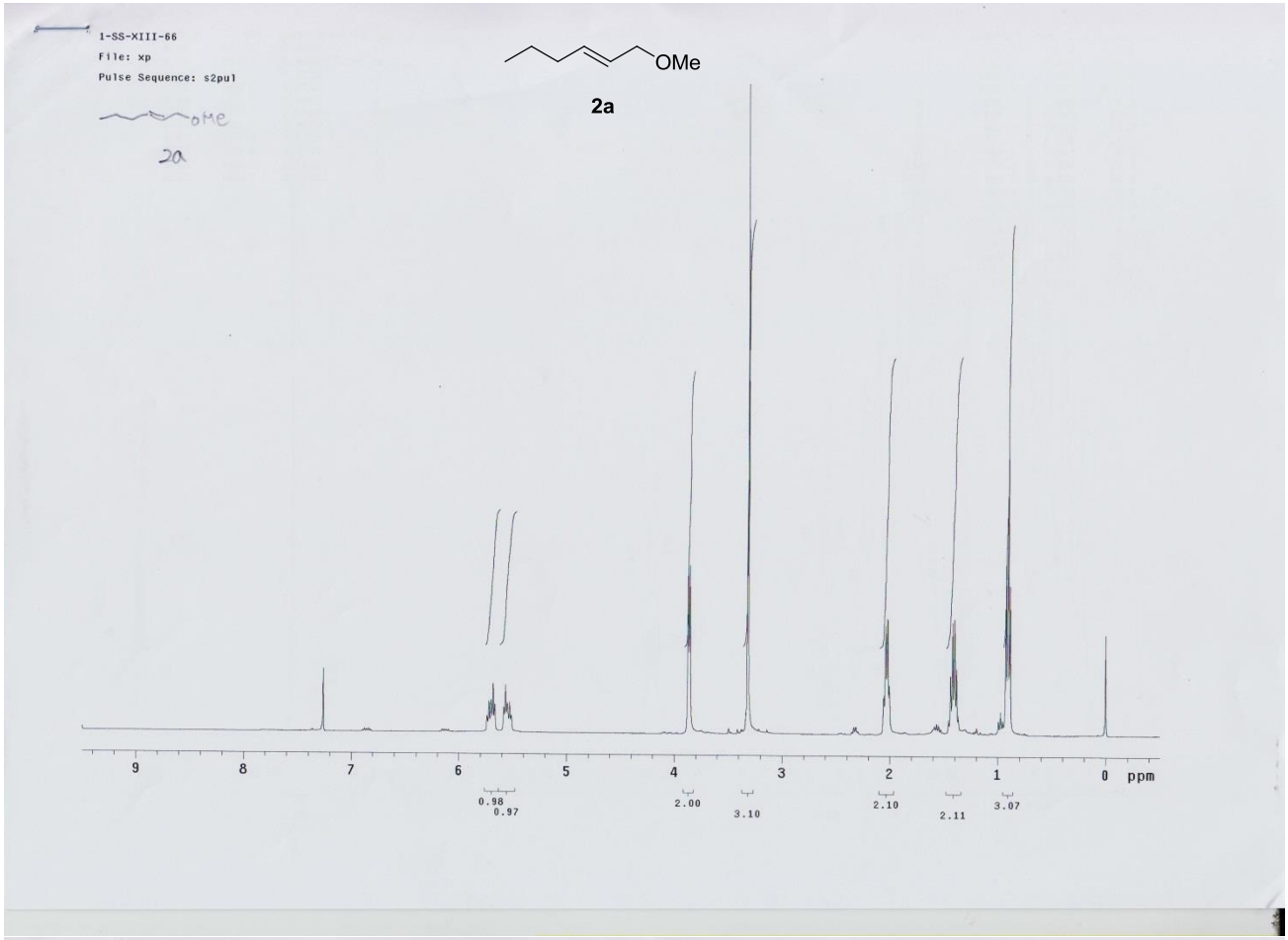
3n

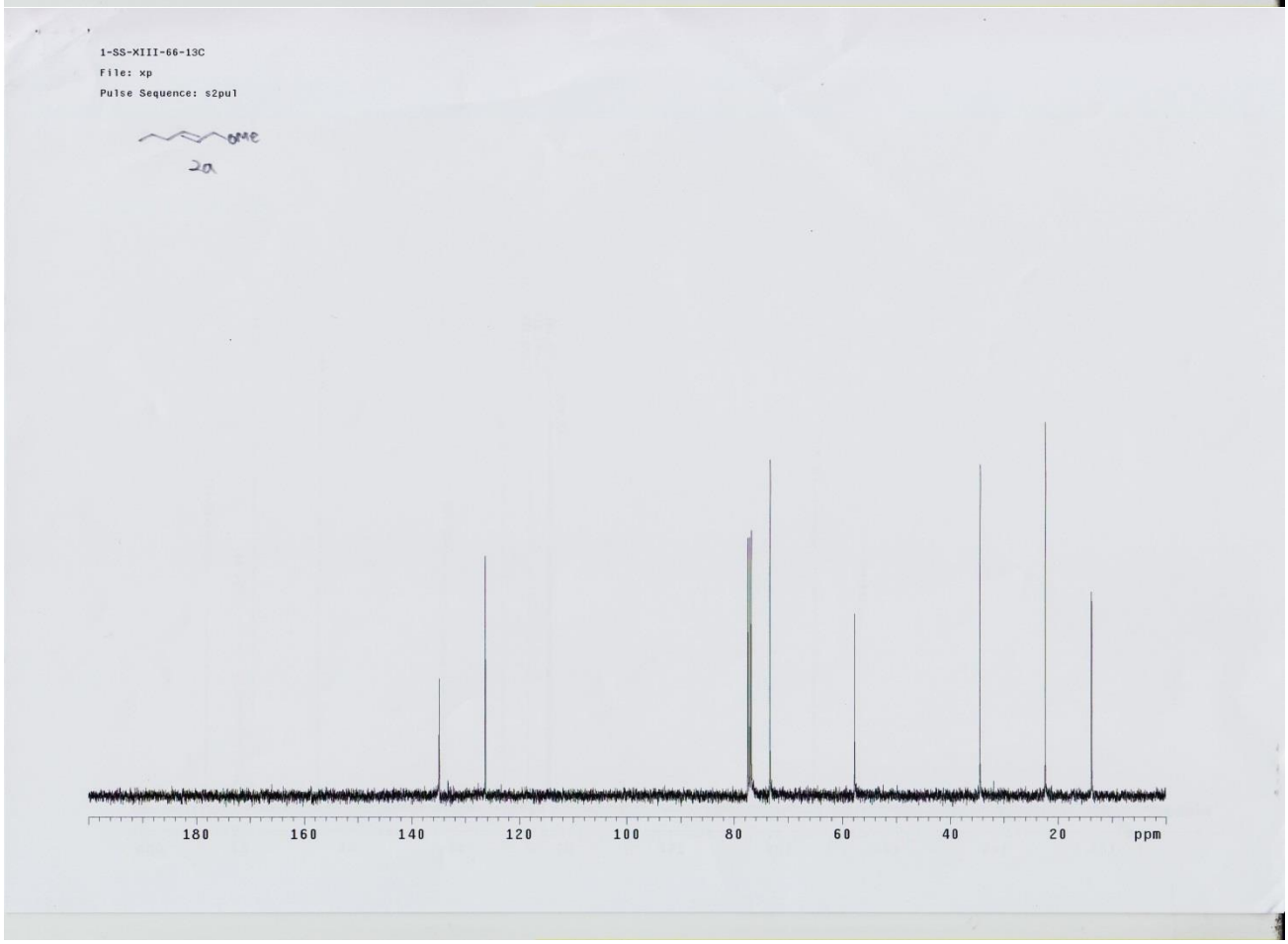
^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.77 (d, *J* = 8.2 Hz, 2H), 7.26-7.22 (m, 5H), 7.06 (d, *J* = 6.3 Hz, 2H), 6.21 (s, 1H), 4.82 (s, 1H), 4.76 (s, 1H), 4.10 (t, *J* = 6.6 Hz, 2H), 2.98 (s, 2H), 2.85 (t, *J* = 7.0 Hz, 2H), 2.42 (s, 3H), 1.60 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.7, 143.4, 142.3, 139.6, 136.9, 129.0, 128.6, 128.0, 126.8, 116.6, 113.4, 76.1, 36.2, 21.7, 21.6; HRMS (FAB) Calcd for $C_{21}H_{24}O_3S$ (M + H), 357.1524; found 357.1537.

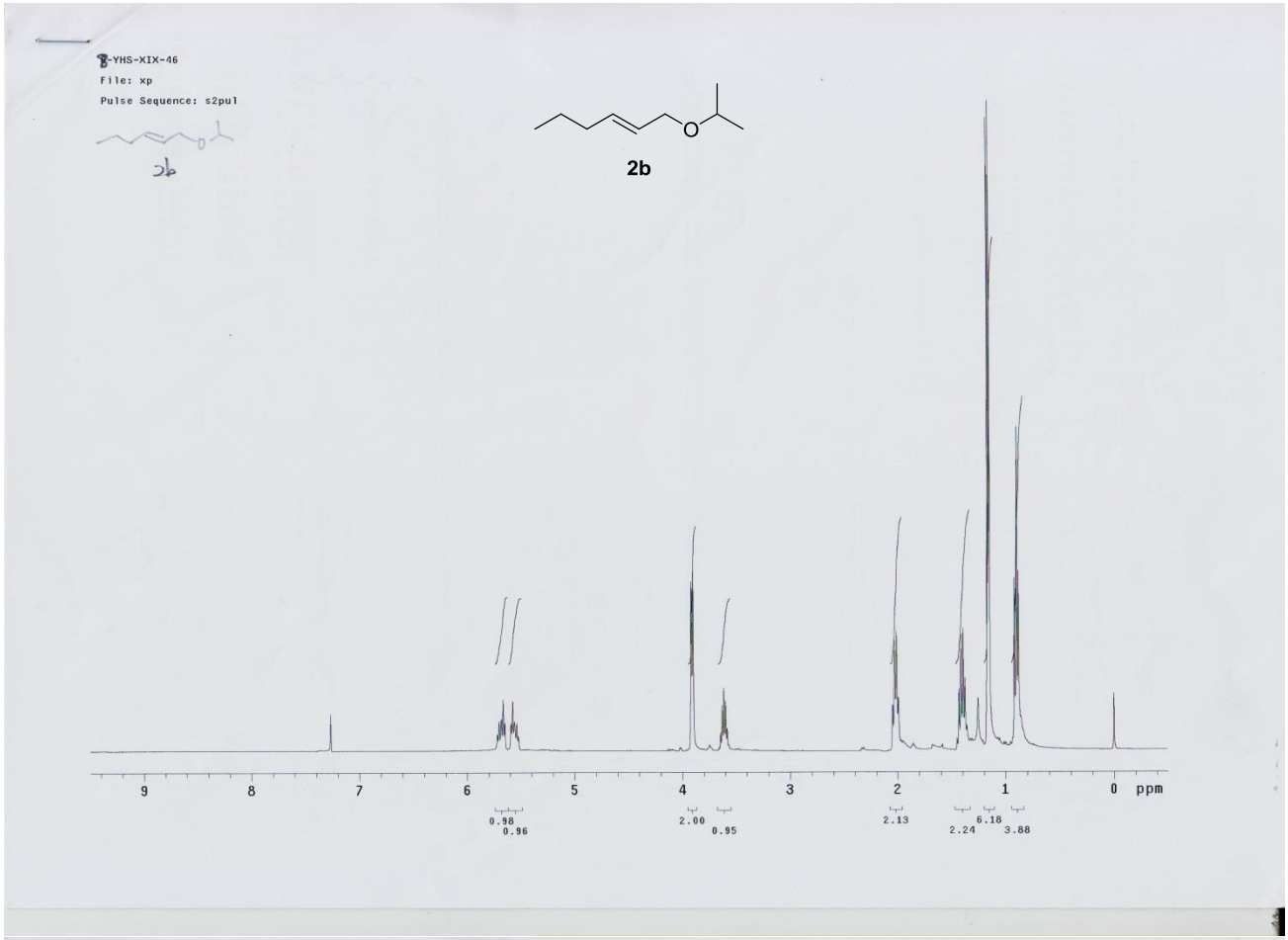
4. Scanned copies of the spectra for substrates

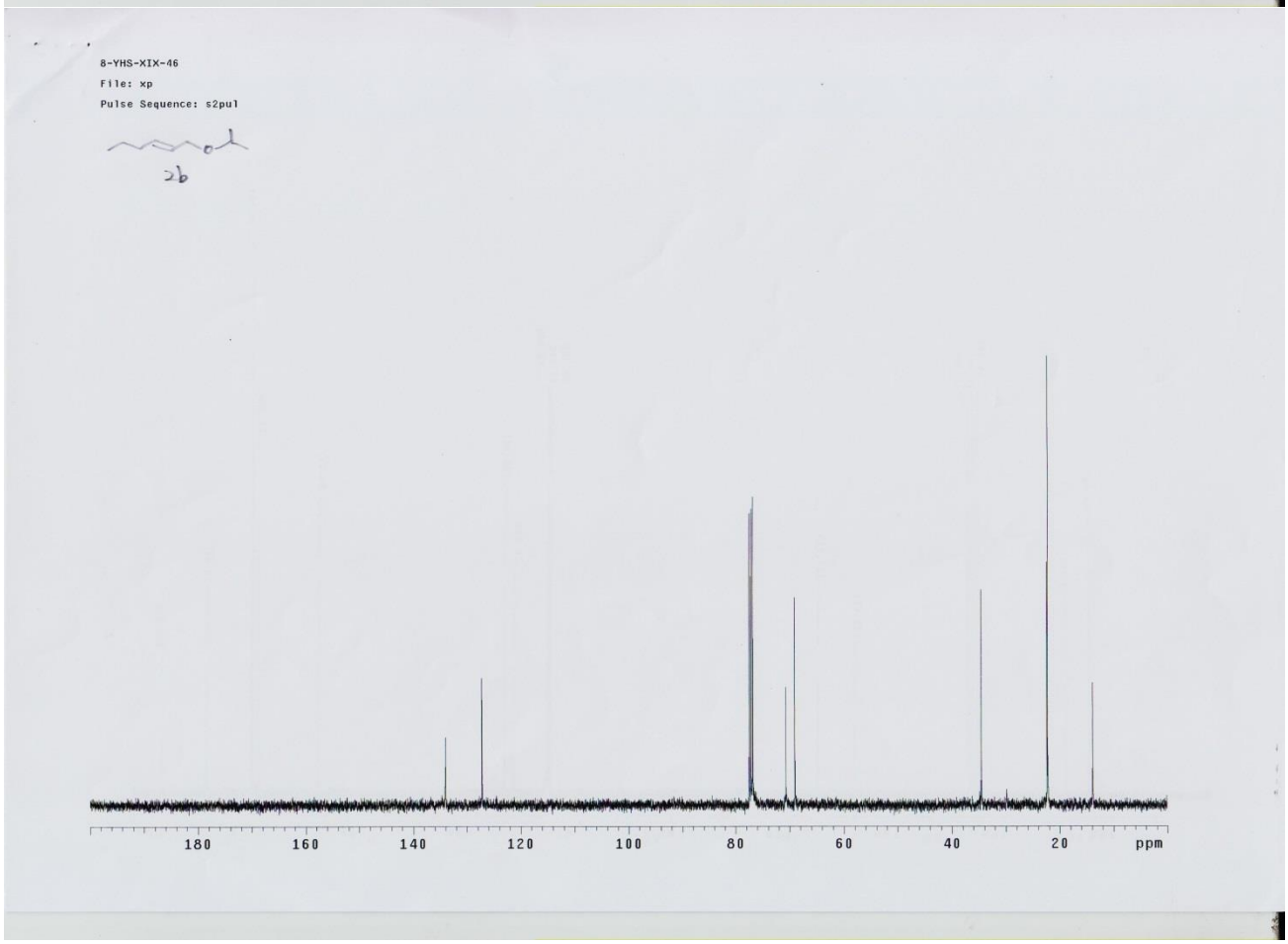


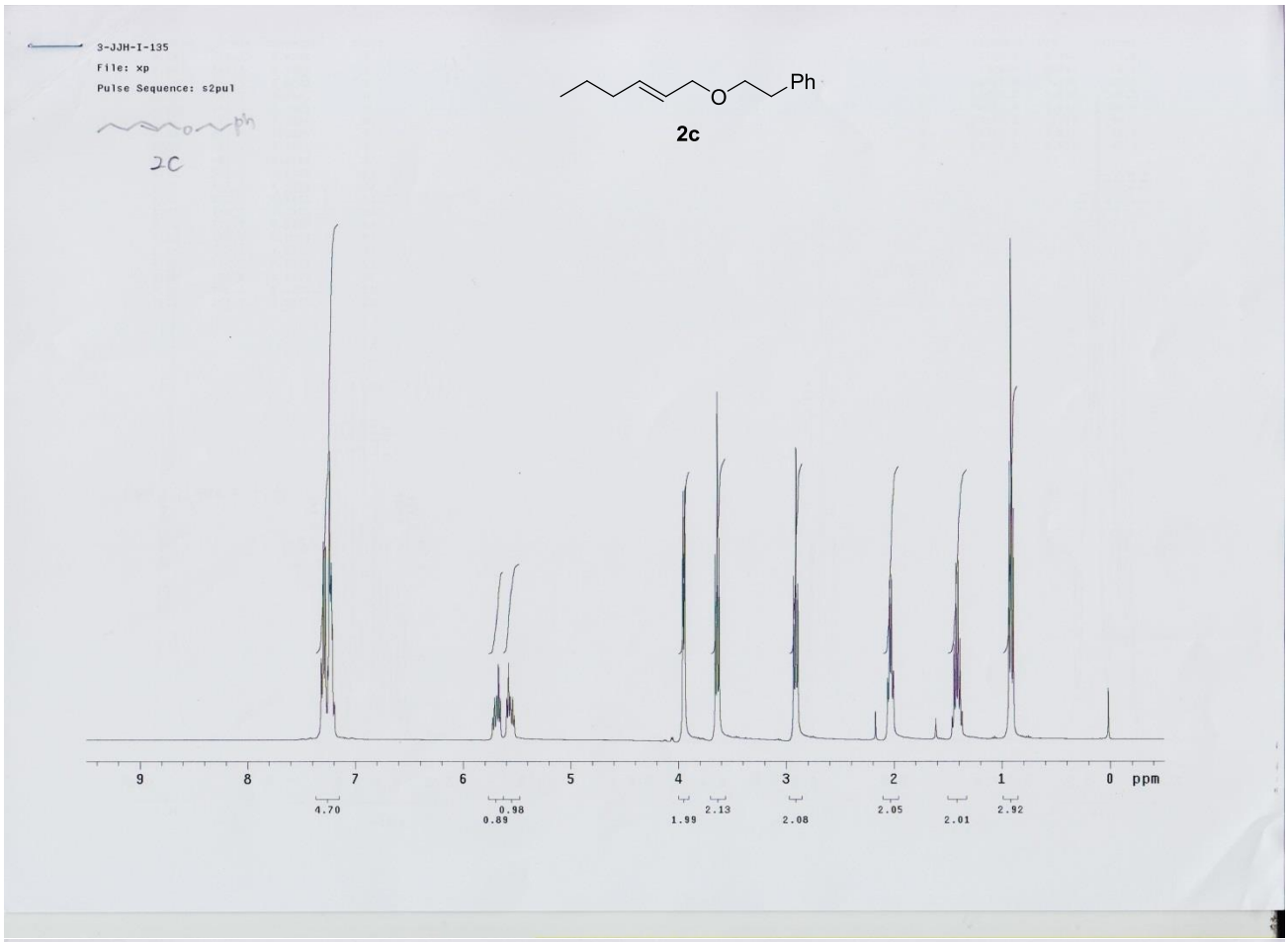


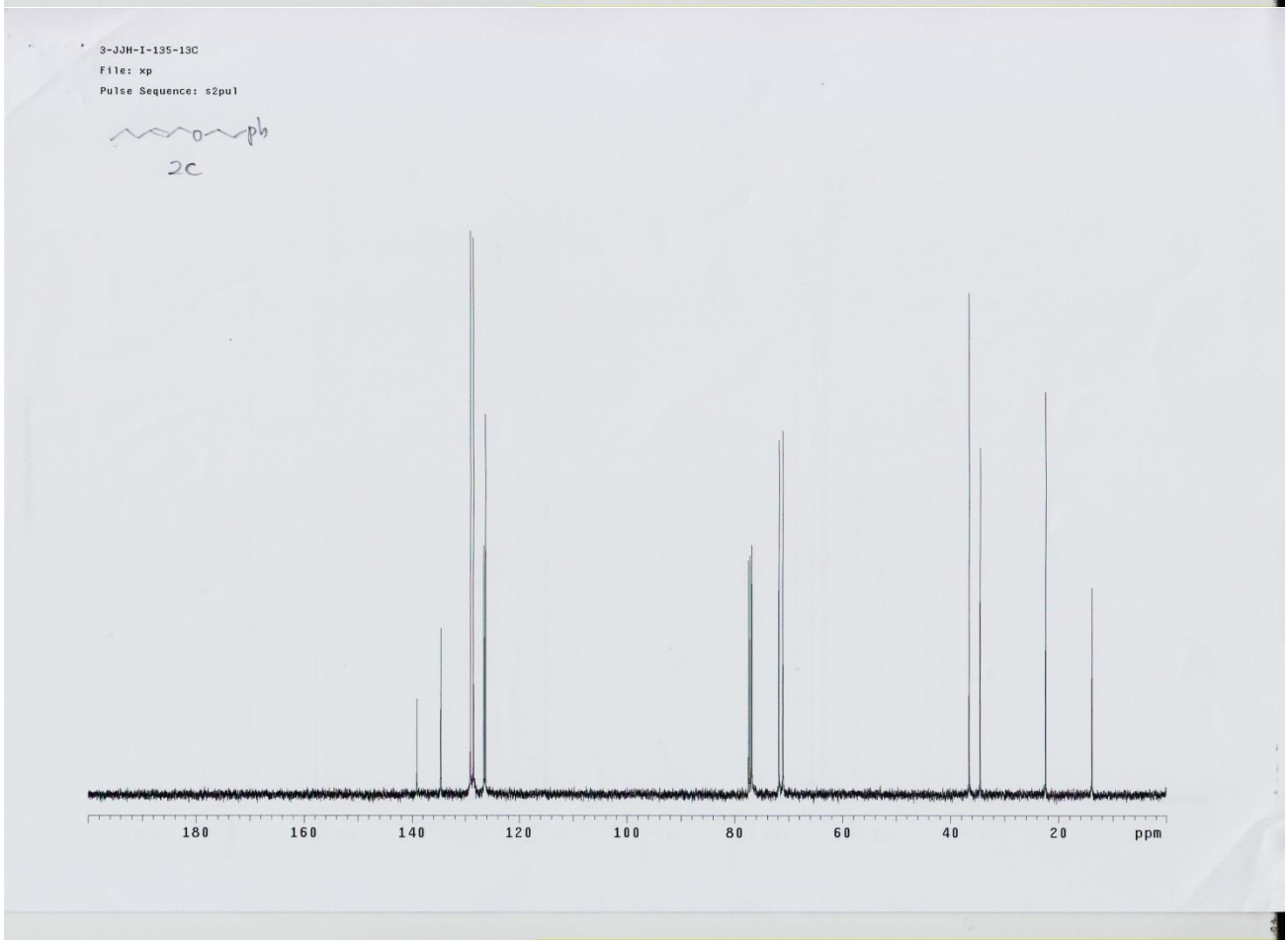

1-SS-XIII-66
File: xp
Pulse Sequence: s2pul
OMe
2a
9
8
7
6
5
4
3
2
1
0
ppm
0.98
0.97
2.00
3.10
2.10
2.11
3.07

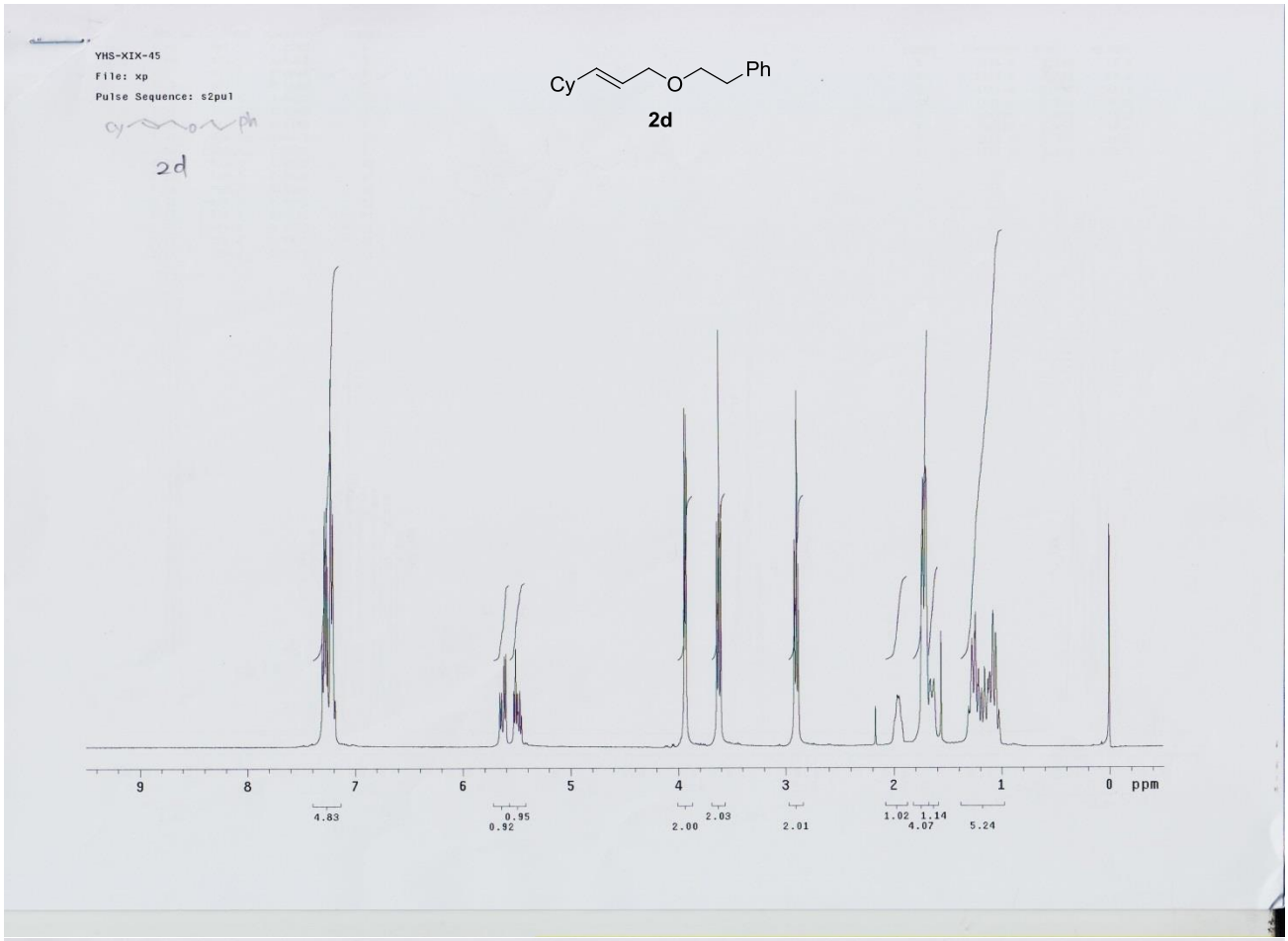

1-SS-XIII-66-13C
File: xp
Pulse Sequence: s2pul
OMe
2a
180
160
140
120
100
80
60
40
20
ppm

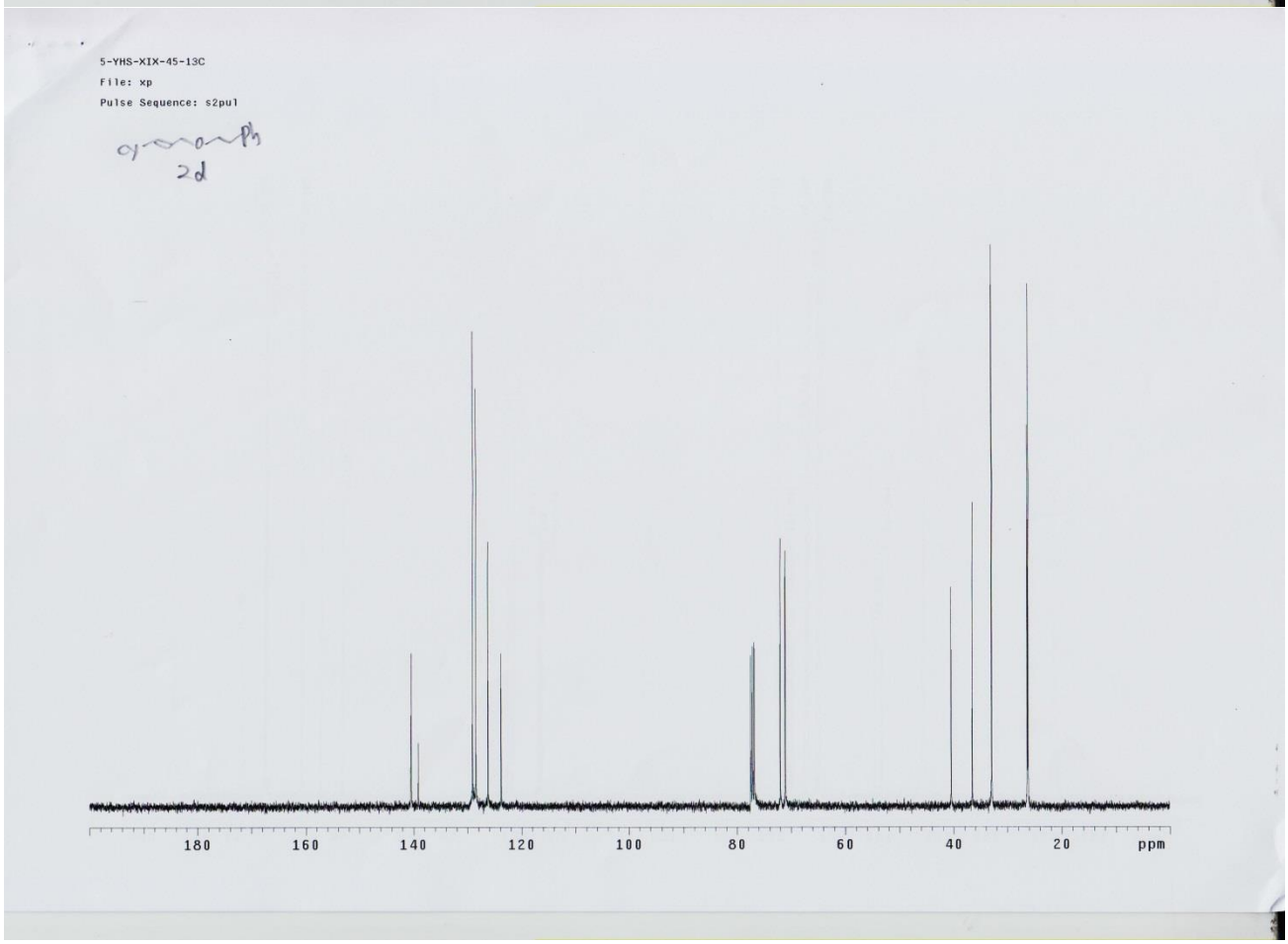

8-YHS-XIX-46
File: xp
Pulse Sequence: s2pul
2b
9
8
7
6
5
4
3
2
1
0 ppm
0.98
0.96
2.00
0.95
2.13
6.18
2.24
3.88

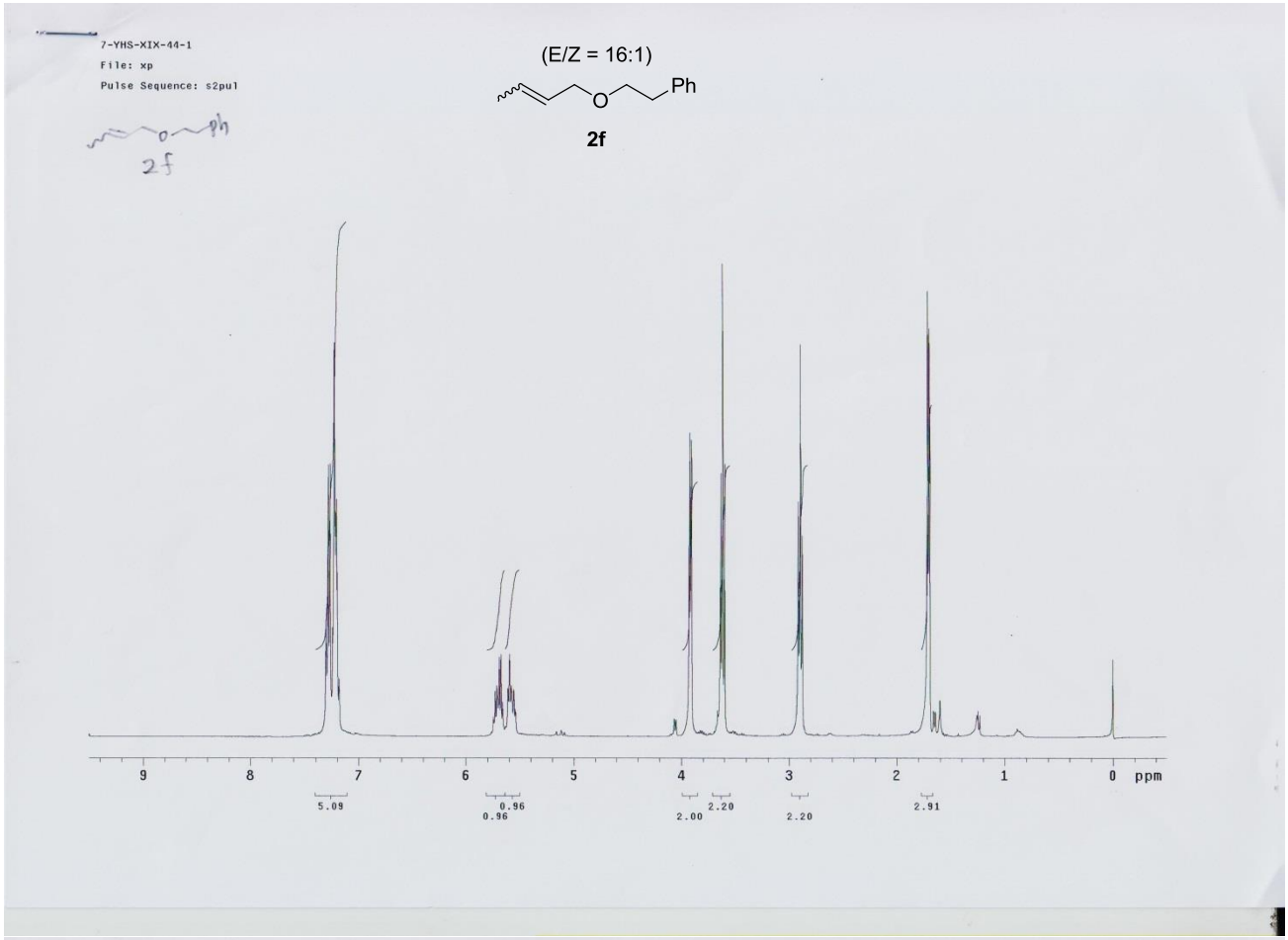

8-YHS-XIX-46
File: xp
Pulse Sequence: s2pul
2b
180
160
140
120
100
80
60
40
20
ppm

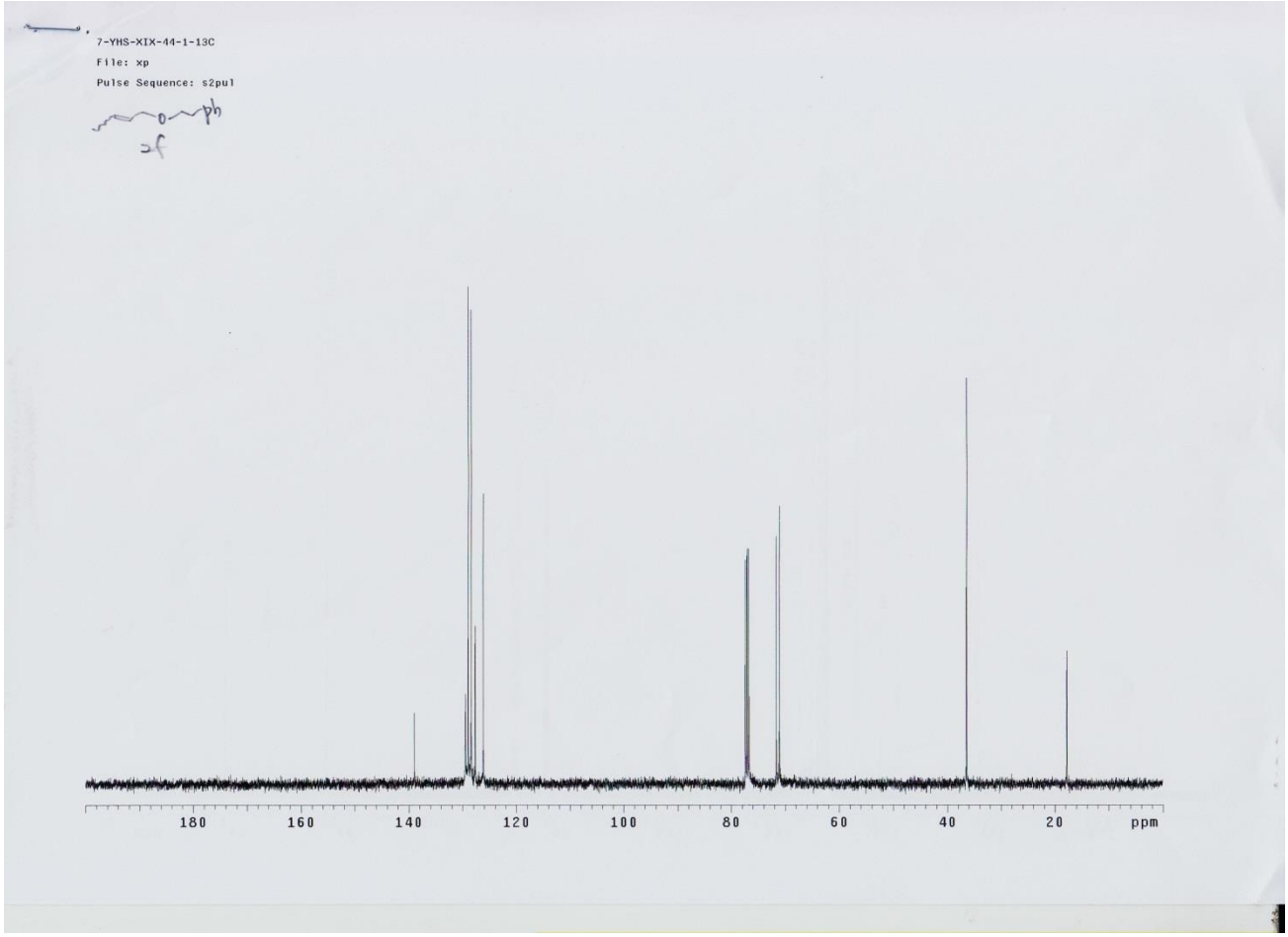

3-JJH-I-135
File: xp
Pulse Sequence: s2pul
2C
Ph
O
2c
9
8
7
6
5
4
3
2
1
0
ppm
4.70
0.98
0.89
1.99
2.13
2.08
2.05
2.01
2.92

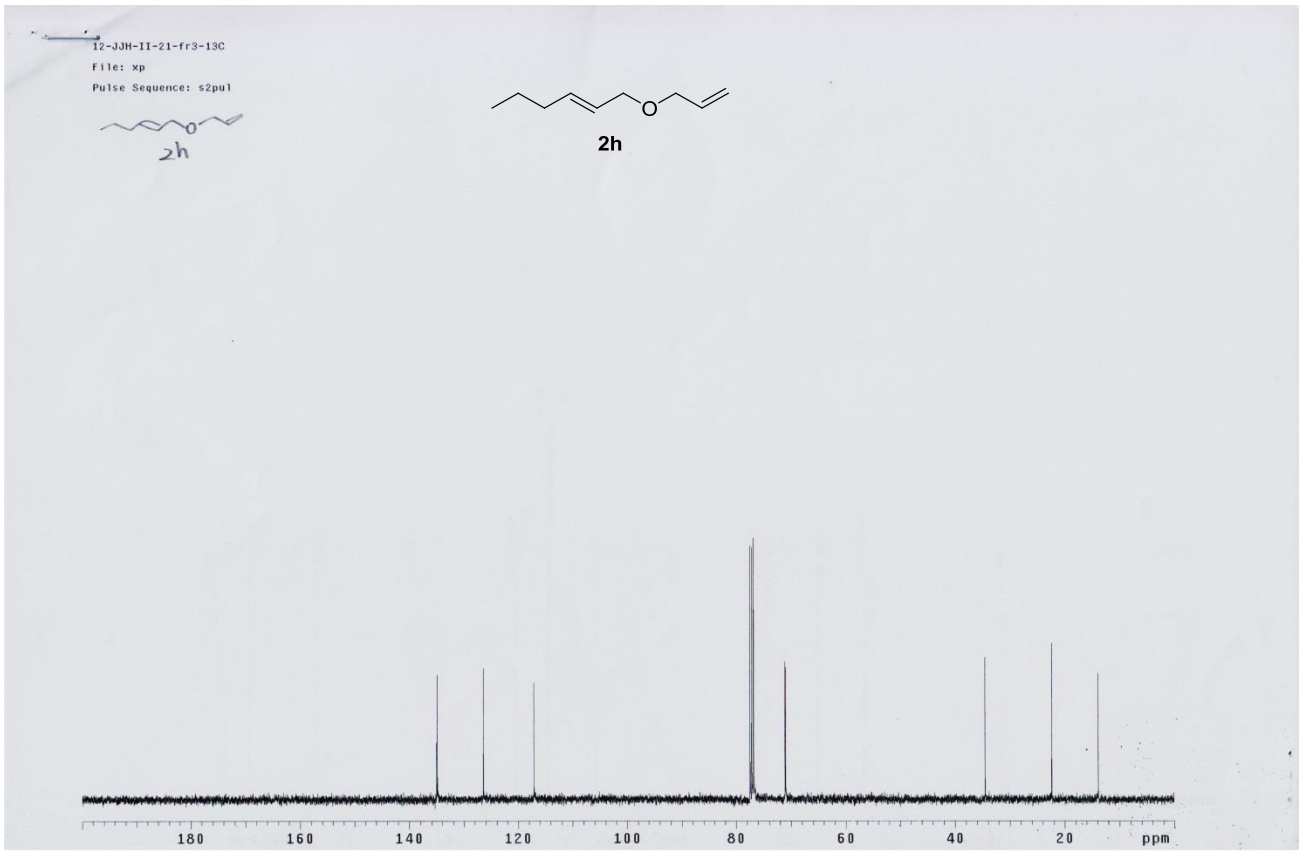

3-JJH-I-135-13C
File: xp
Pulse Sequence: s2pul
2C
180
160
140
120
100
80
60
40
20
ppm

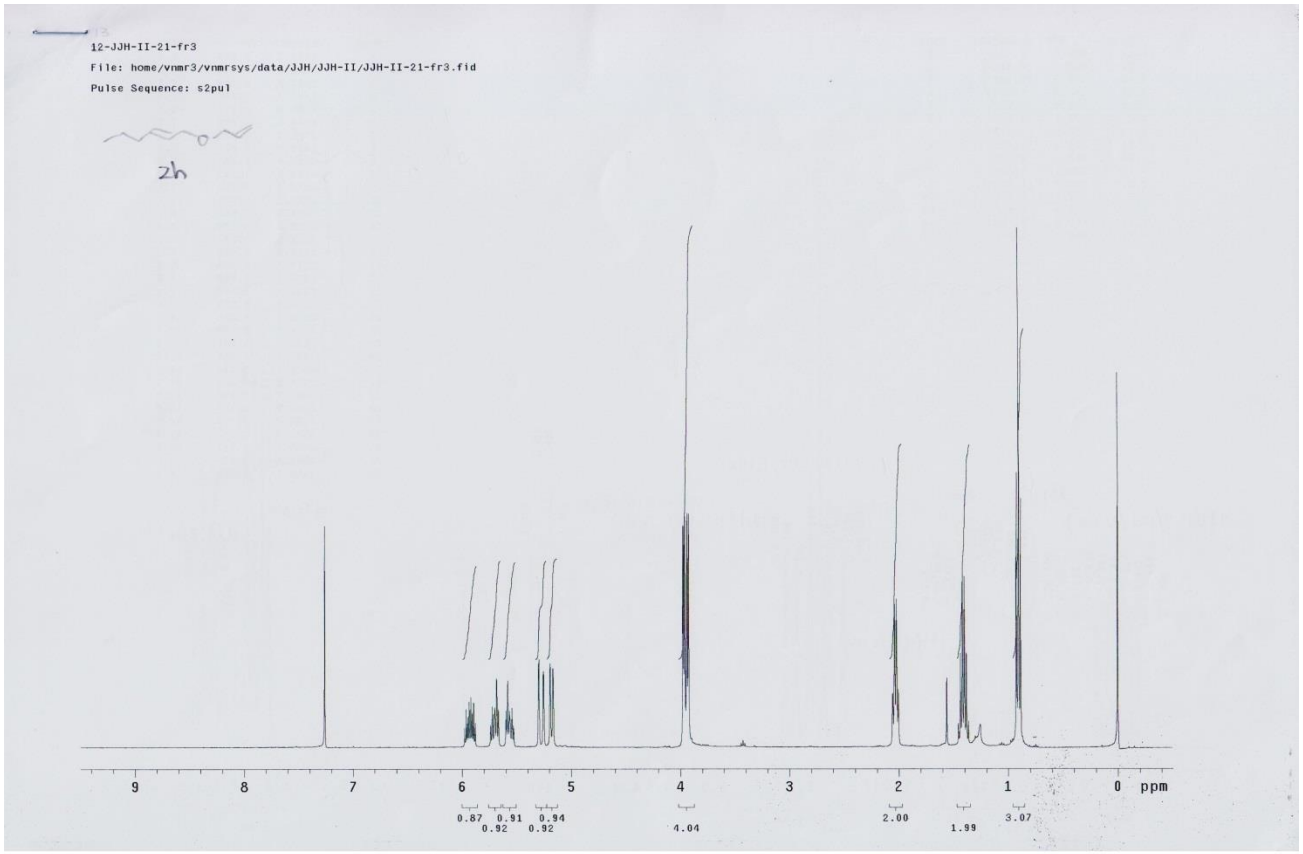

YHS-XIX-45
File: xp
Pulse Sequence: s2pul
2d
Cy
O
Ph
2d
9
8
7
6
5
4
3
2
1
0 ppm
4.83
0.92
0.95
2.00
2.03
2.01
1.02
4.07
1.14
5.24

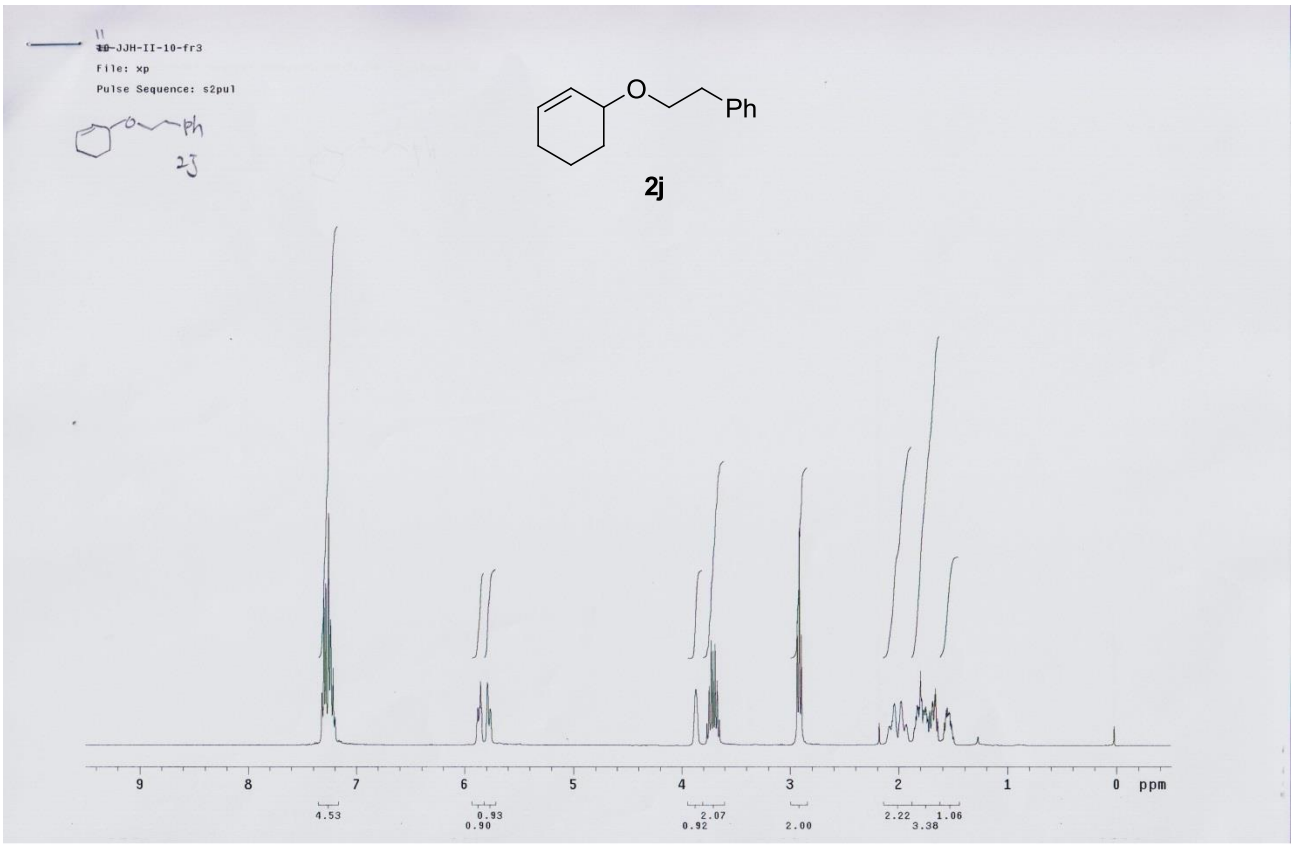

5-YHS-XIX-45-13C
File: xp
Pulse Sequence: s2pul
2d
180
160
140
120
100
80
60
40
20
ppm

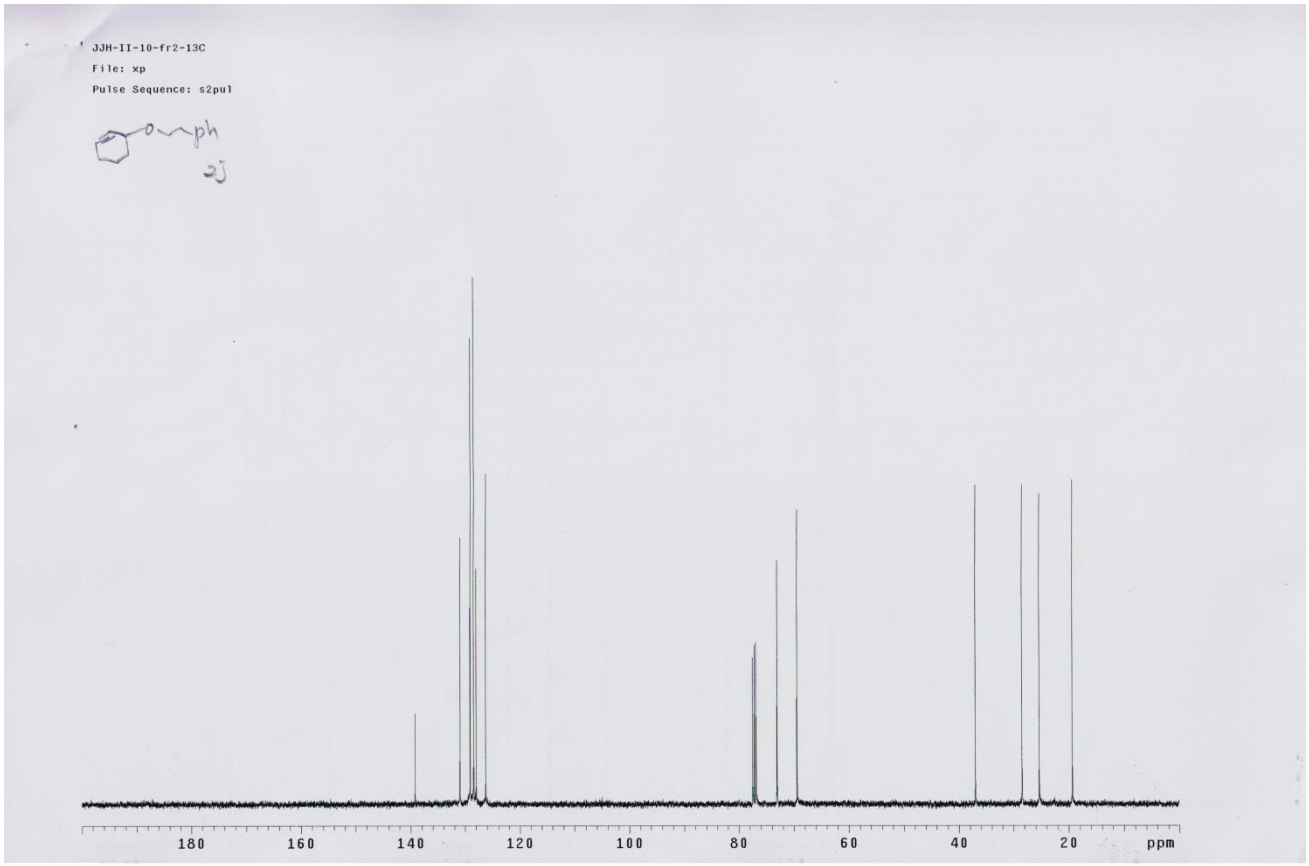

7-YHS-XIX-44-1
File: xp
Pulse Sequence: s2pul
(E/Z = 16:1)
Ph
2f
9
8
7
6
5
4
3
2
1
0
ppm
5.09
0.96
0.96
2.00
2.20
2.20
2.91

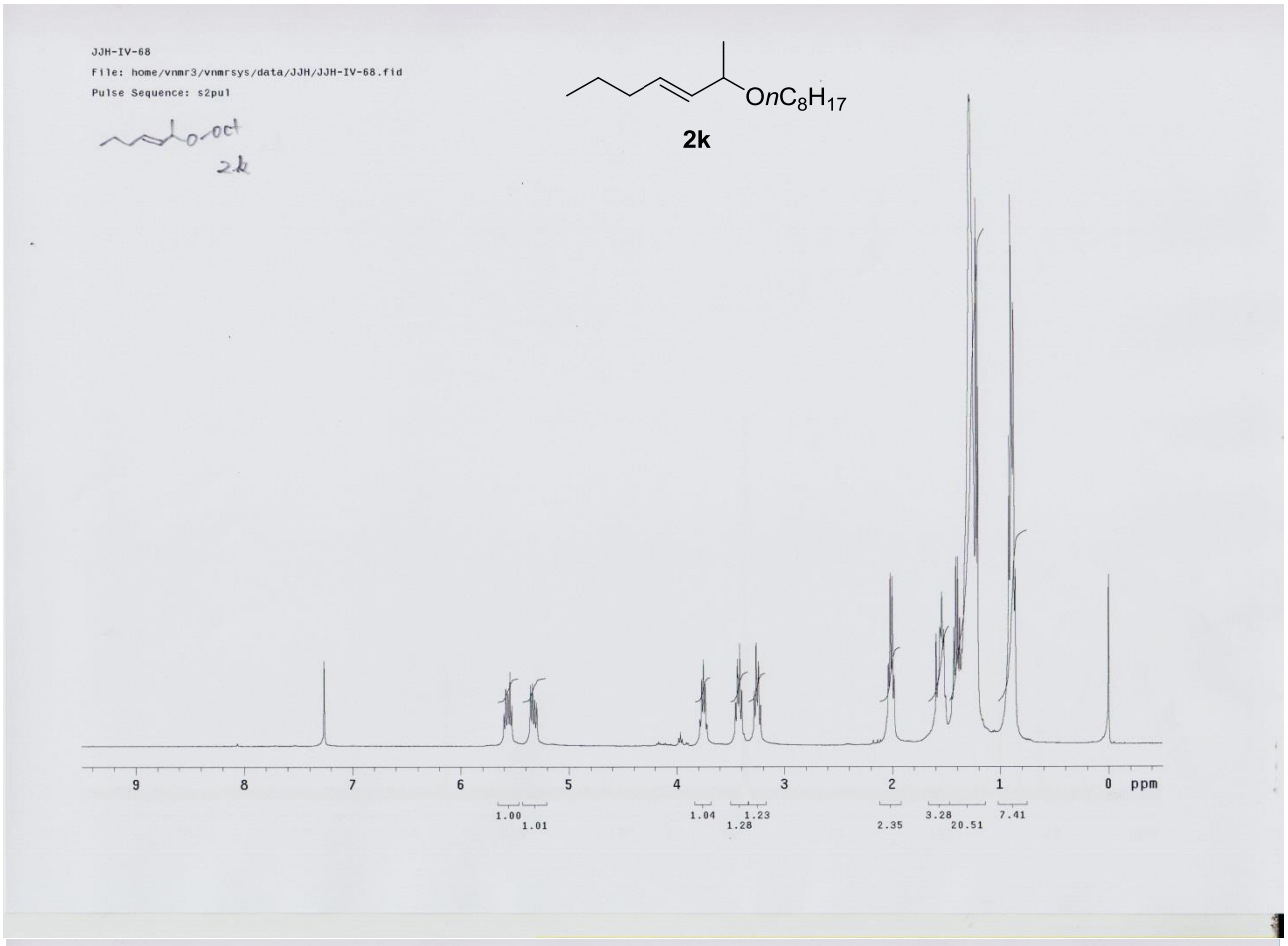

7-YHS-XIX-44-1-13C
File: xp
Pulse Sequence: s2pul
2f
180
160
140
120
100
80
60
40
20
ppm

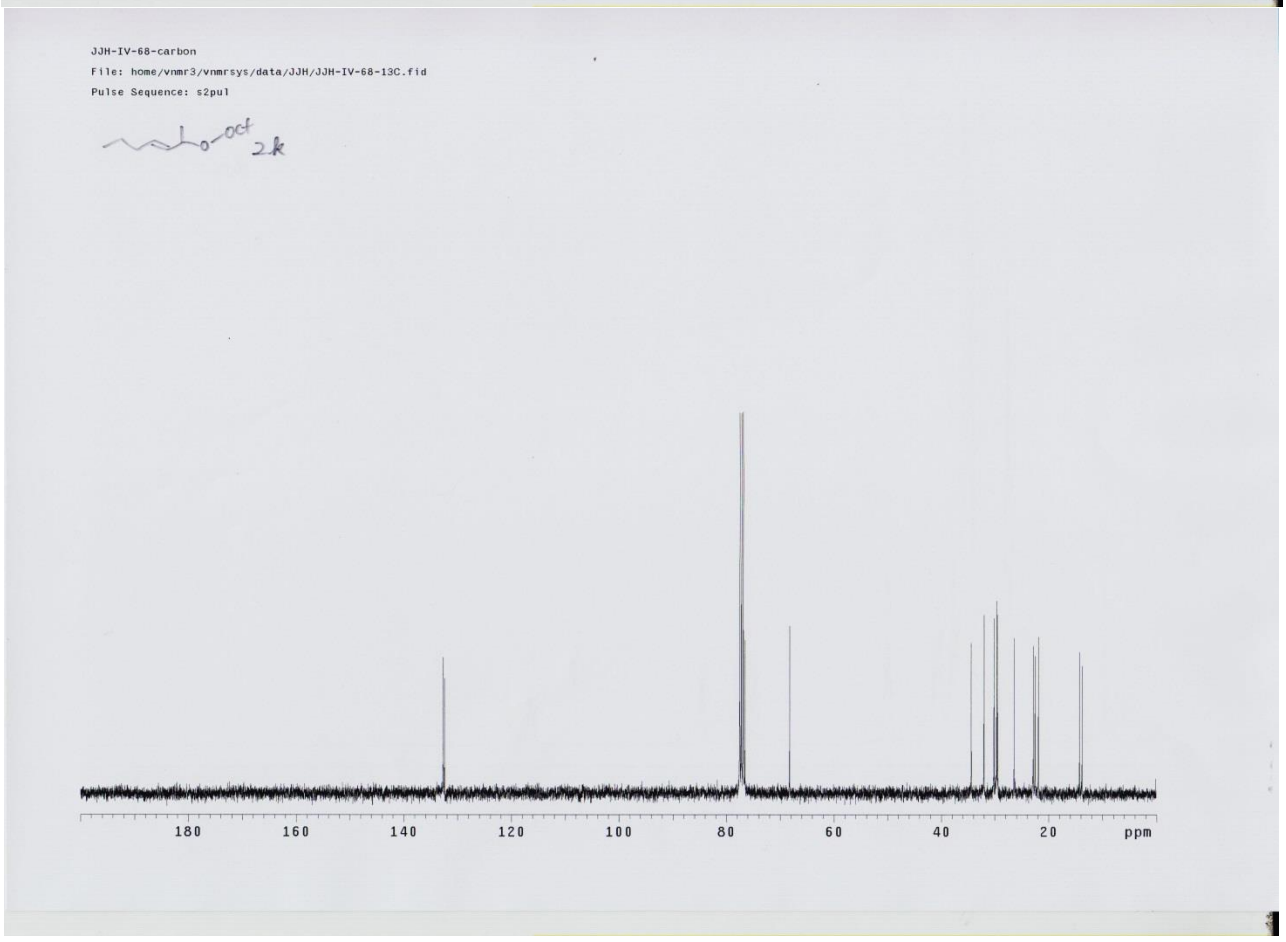

12-JJH-II-21-fr3-13C
File: xp
Pulse Sequence: s2pul
2h
2h
180
160
140
120
100
80
60
40
20
ppm

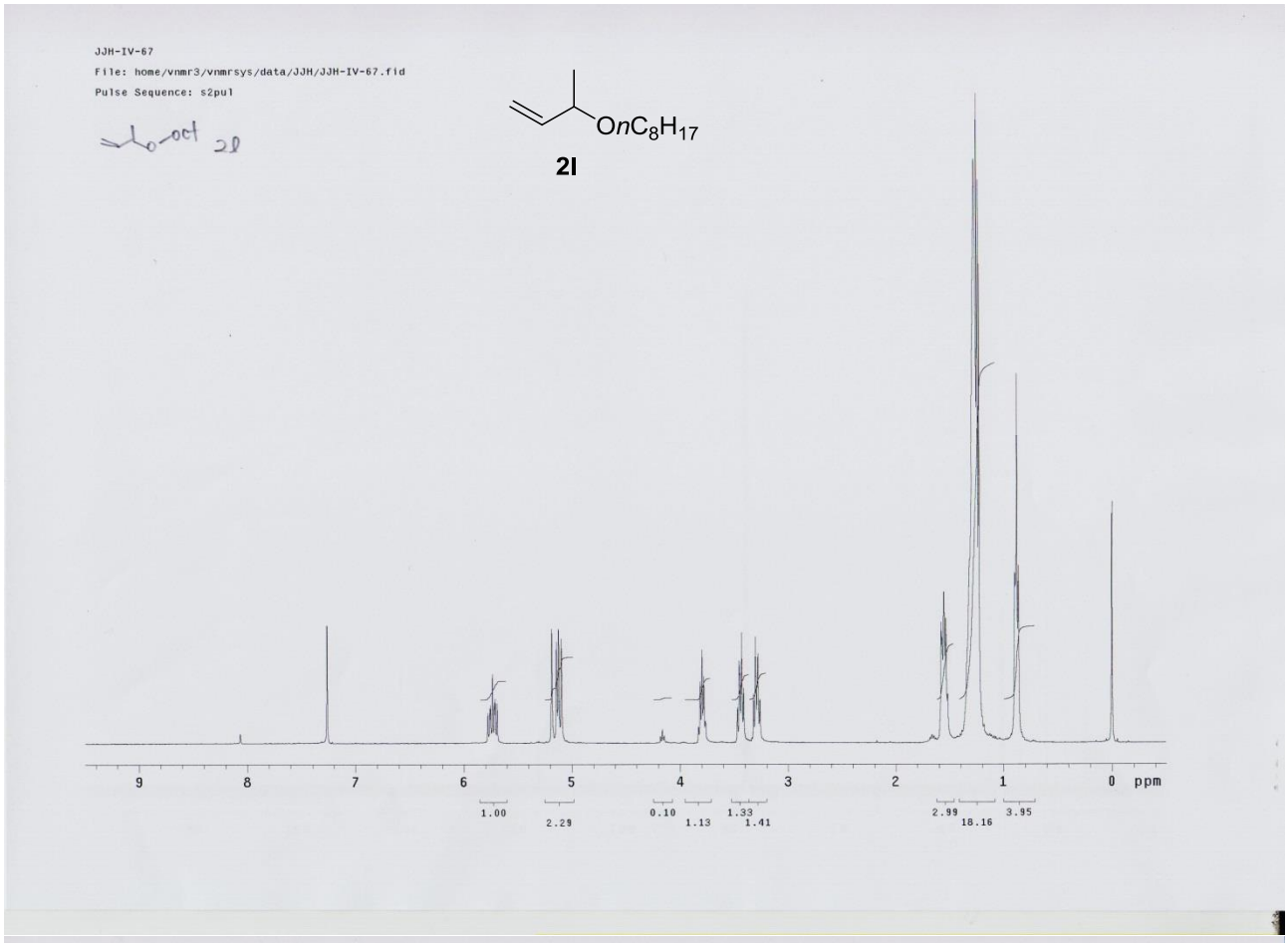

12-JJH-II-21-fr3
File: home/vnmr3/vnmrsys/data/JJH/JJH-II/JJH-II-21-fr3.fid
Pulse Sequence: s2pul
2h
9
8
7
6
5
4
3
2
1
0
ppm
0.87
0.91
0.94
0.92
0.92
4.04
2.00
1.99
3.07

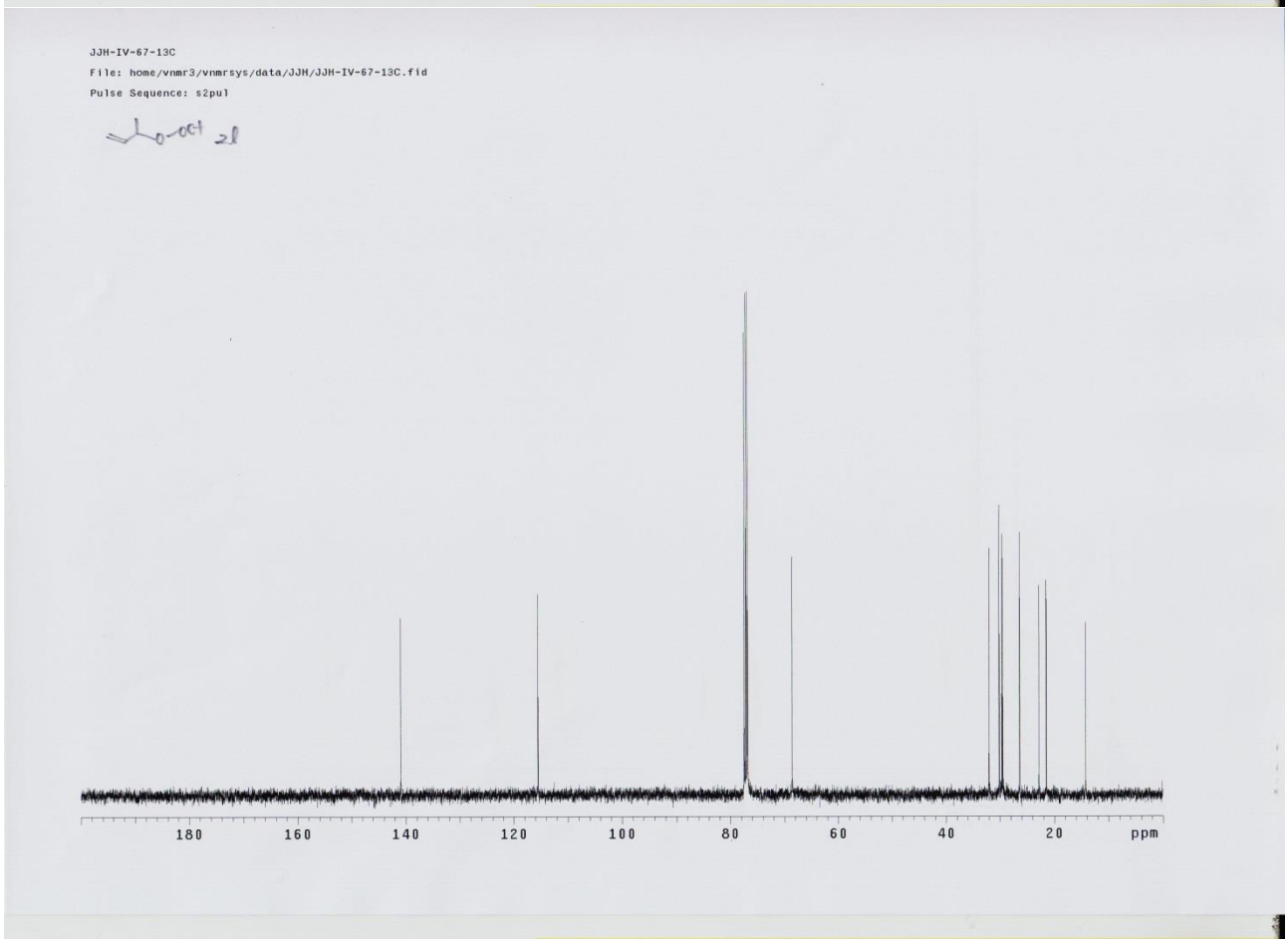

JJH-II-10-fr3
File: xp
Pulse Sequence: s2pul
Ph
2j
9
8
7
6
5
4
3
2
1
0
ppm
4.53
0.93
0.90
2.07
0.92
2.00
2.22
1.06
3.38

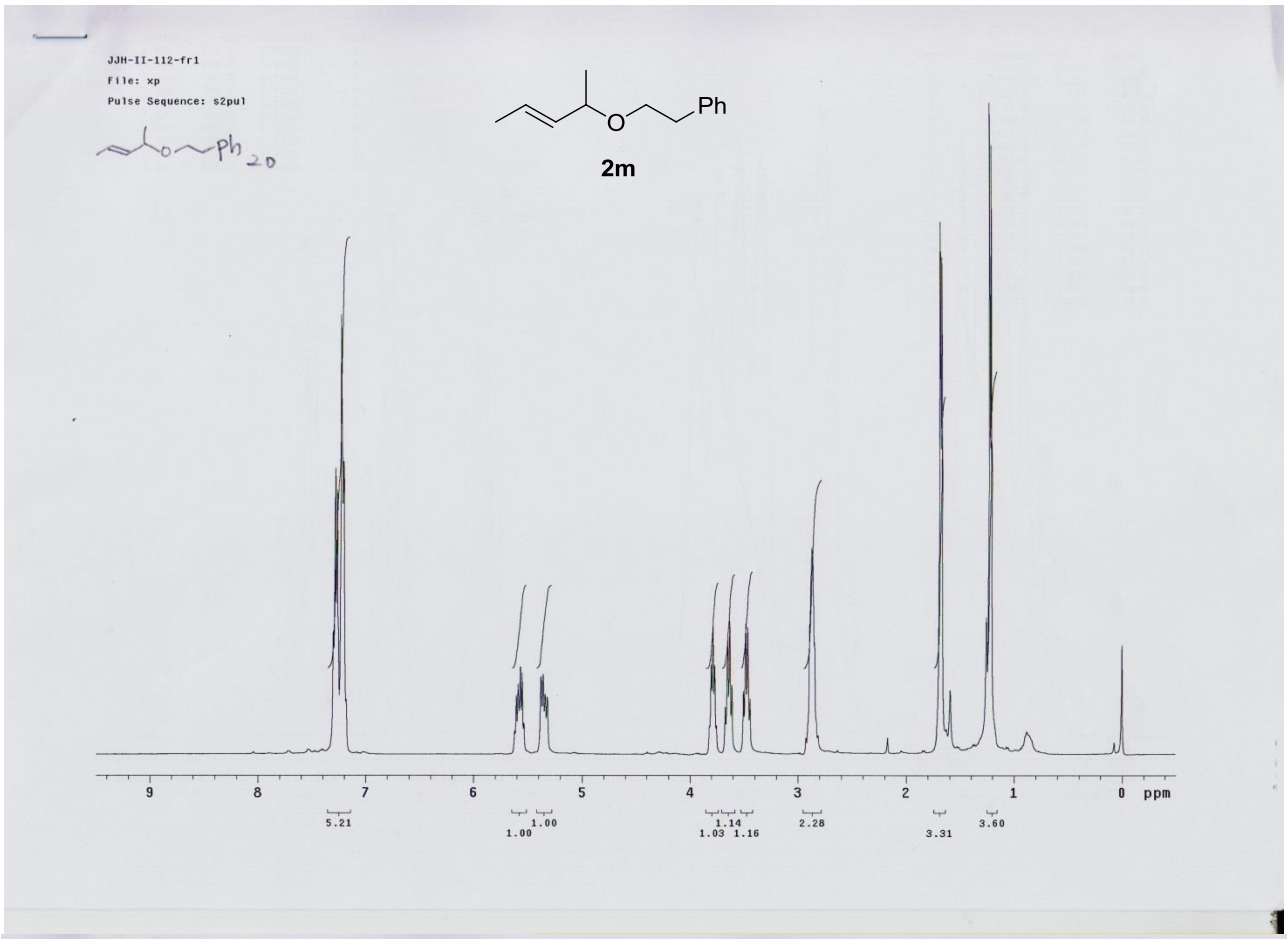

JJH-II-10-fr2-13C
File: xp
Pulse Sequence: s2pul
180
160
140
120
100
80
60
40
20
ppm

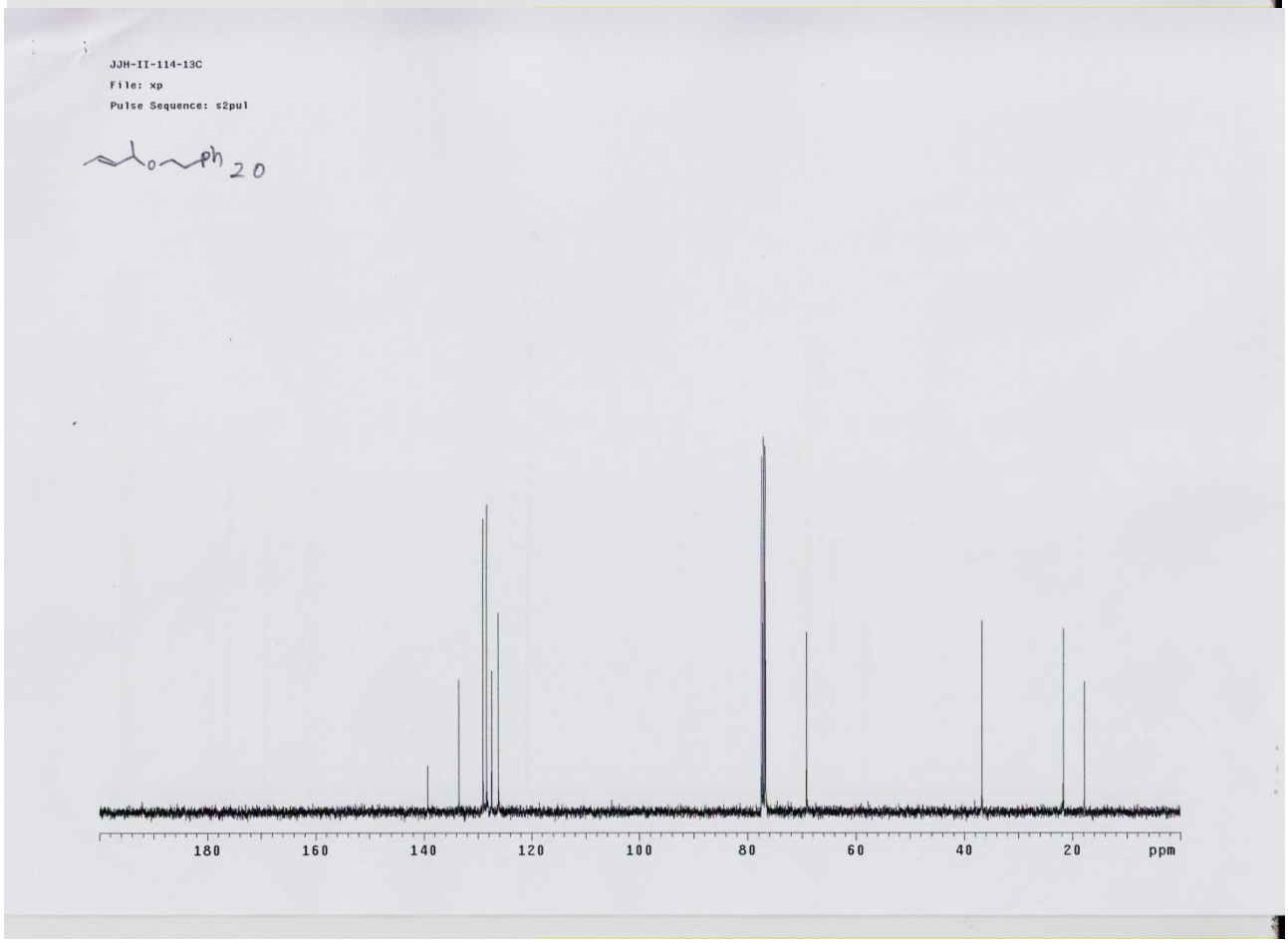

JJH-IV-68
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-68.fid
Pulse Sequence: s2pul
2k
OnC8H17
2k
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.04
1.23
1.28
2.35
3.28
20.51
7.41

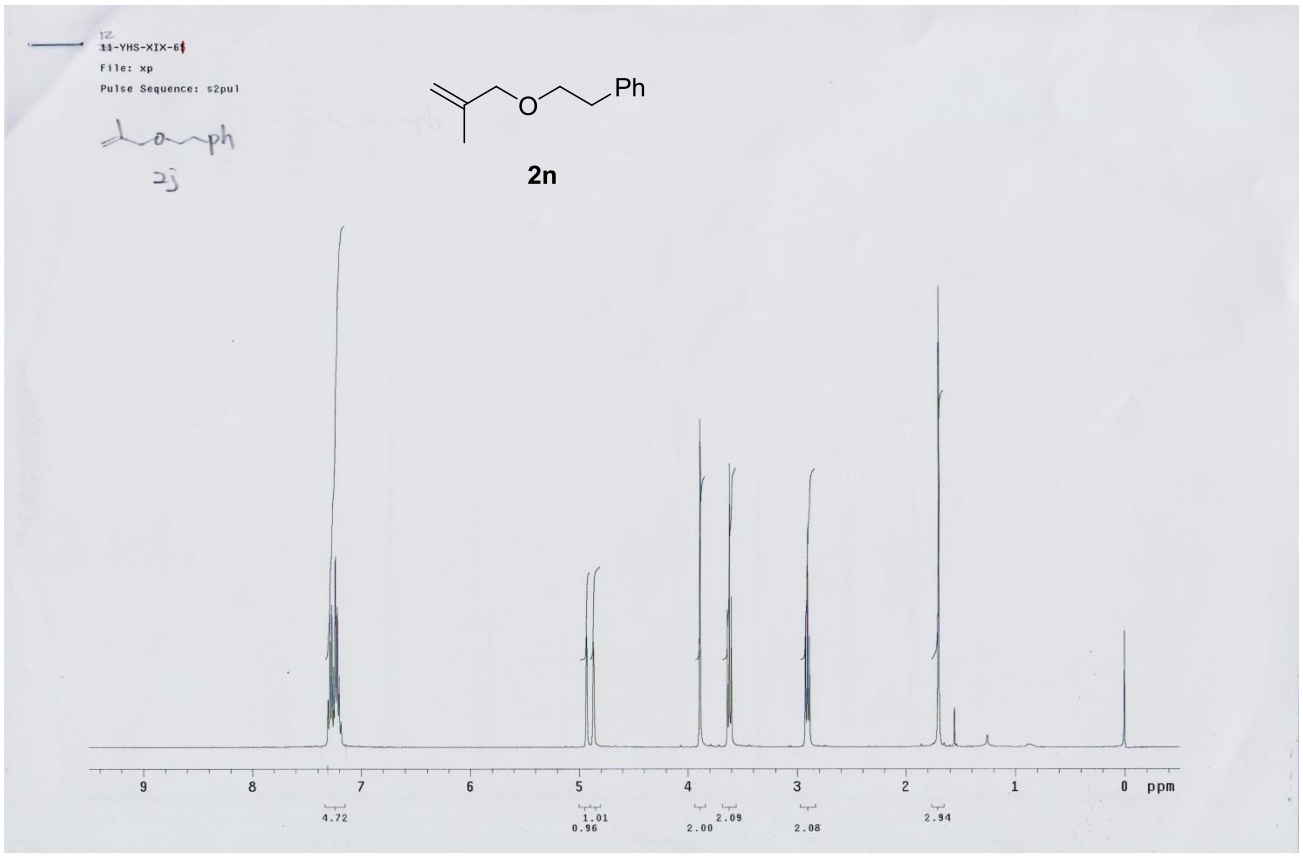

JJH-IV-68-carbon
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-68-13C.fid
Pulse Sequence: s2pul
2k
180
160
140
120
100
80
60
40
20
ppm

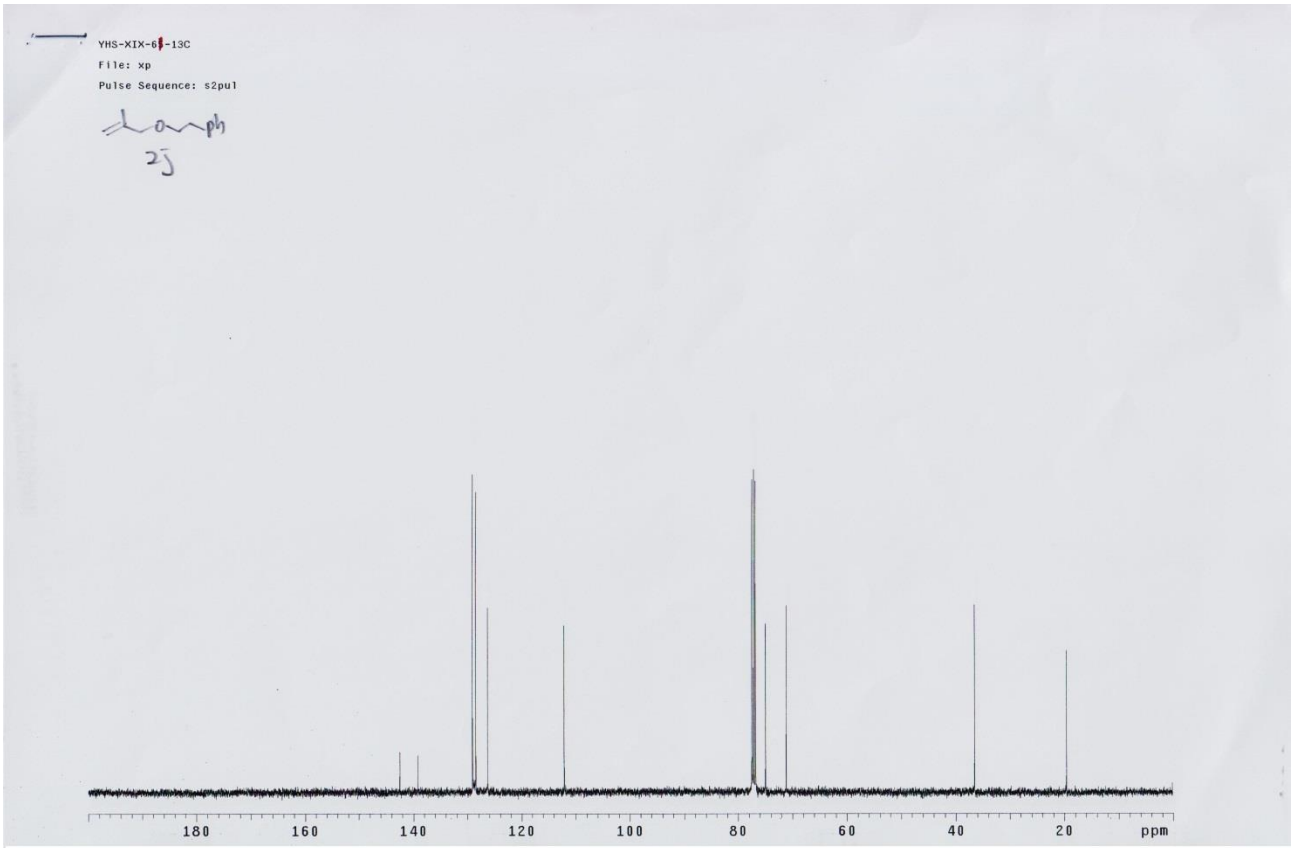

JJH-IV-67
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-67.fid
Pulse Sequence: s2pul
2l
OnC8H17
2l
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.29
0.10
1.13
1.33
1.41
2.99
18.16
3.95


JJH-IV-67-13C
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-67-13C.fid
Pulse Sequence: s2pul
2l
180
160
140
120
100
80
60
40
20
ppm

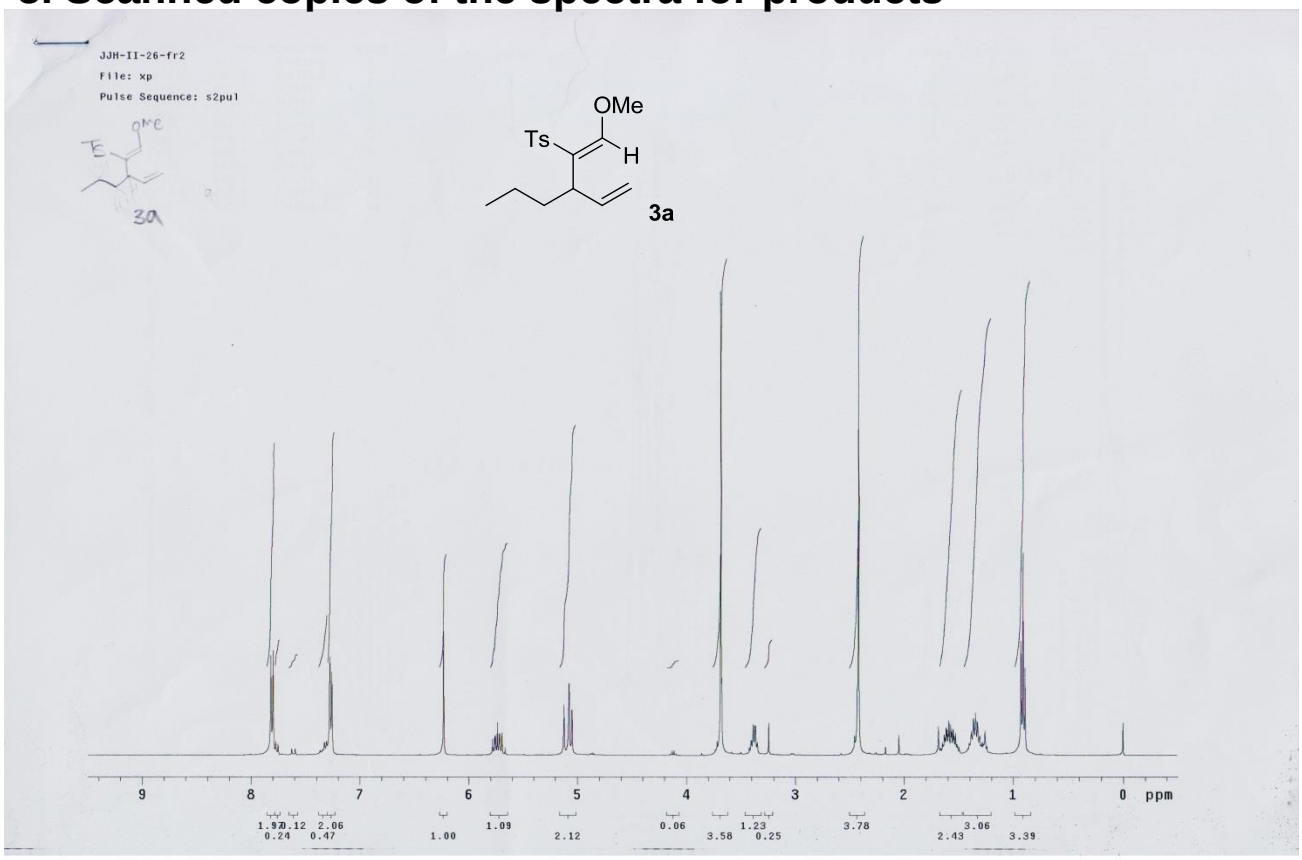

JJH-II-112-fr1
File: xp
Pulse Sequence: s2pul
Ph
O
2m
9
8
7
6
5
4
3
2
1
0
ppm
5.21
1.00
1.00
1.03
1.14
1.16
2.28
3.31
3.60

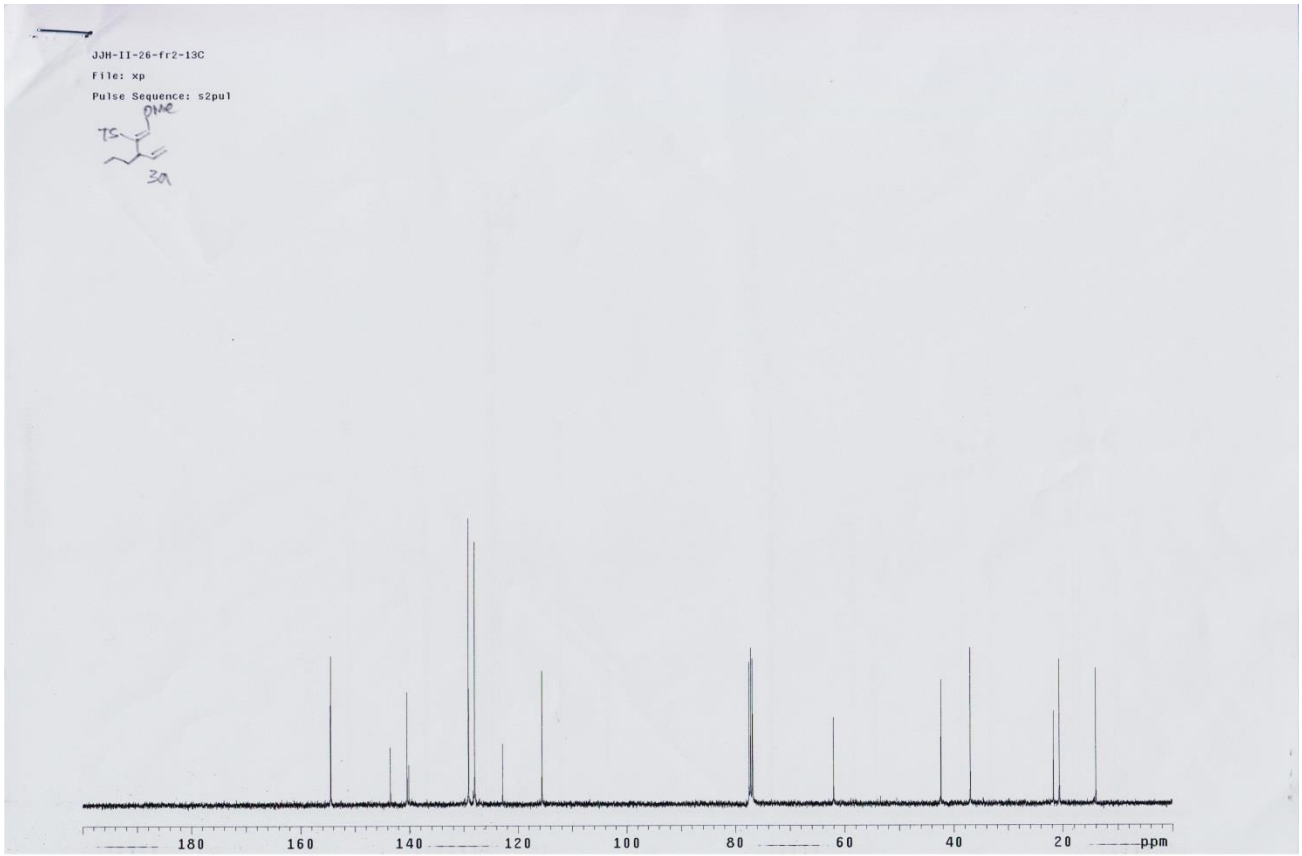

JJH-II-114-13C
File: xp
Pulse Sequence: s2pul
180
160
140
120
100
80
60
40
20
ppm

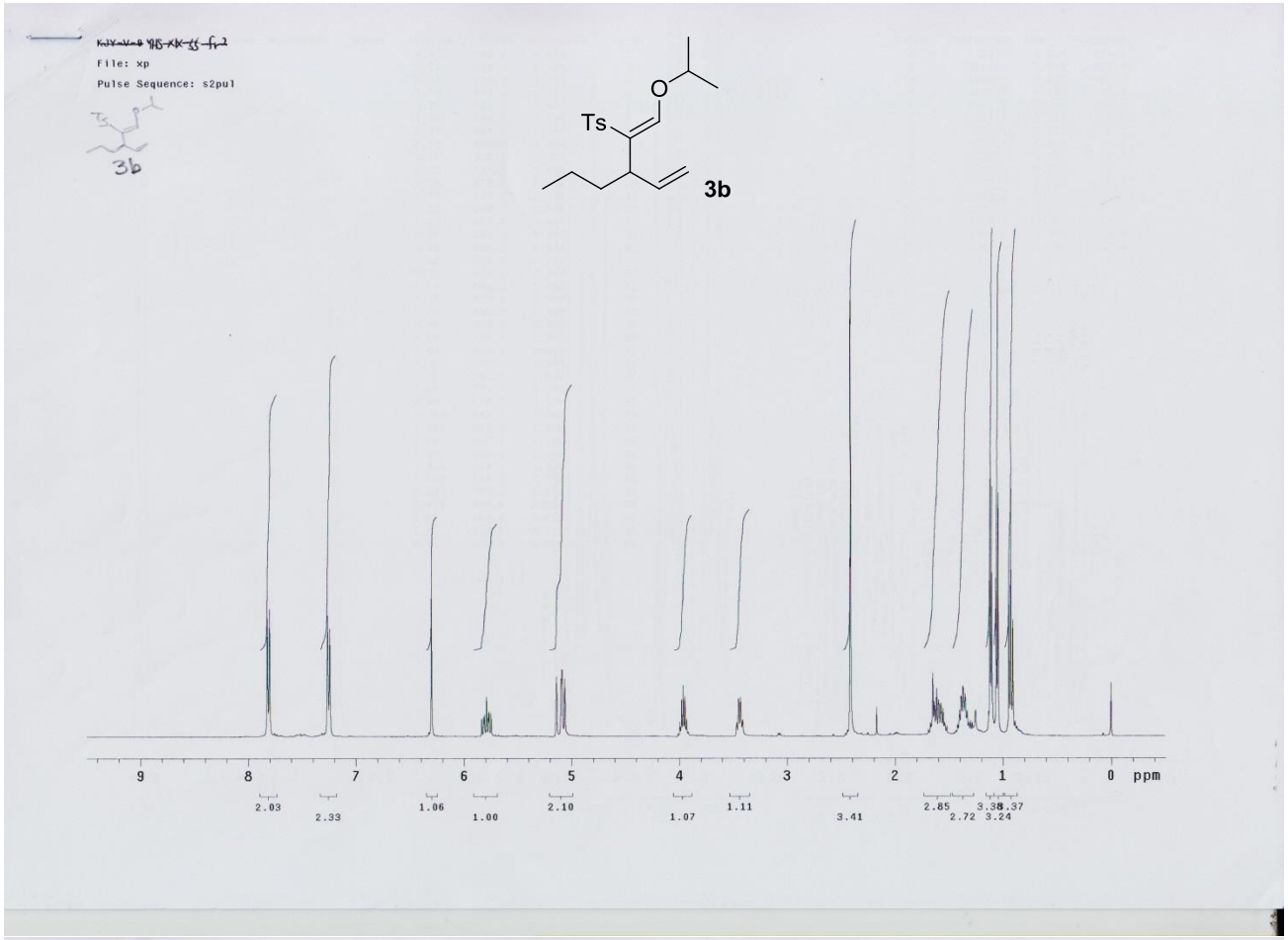

11-YHS-XIX-6
File: xp
Pulse Sequence: s2pul
Ph
2n
9
8
7
6
5
4
3
2
1
0
ppm
4.72
1.01
0.96
2.00
2.09
2.08
2.94

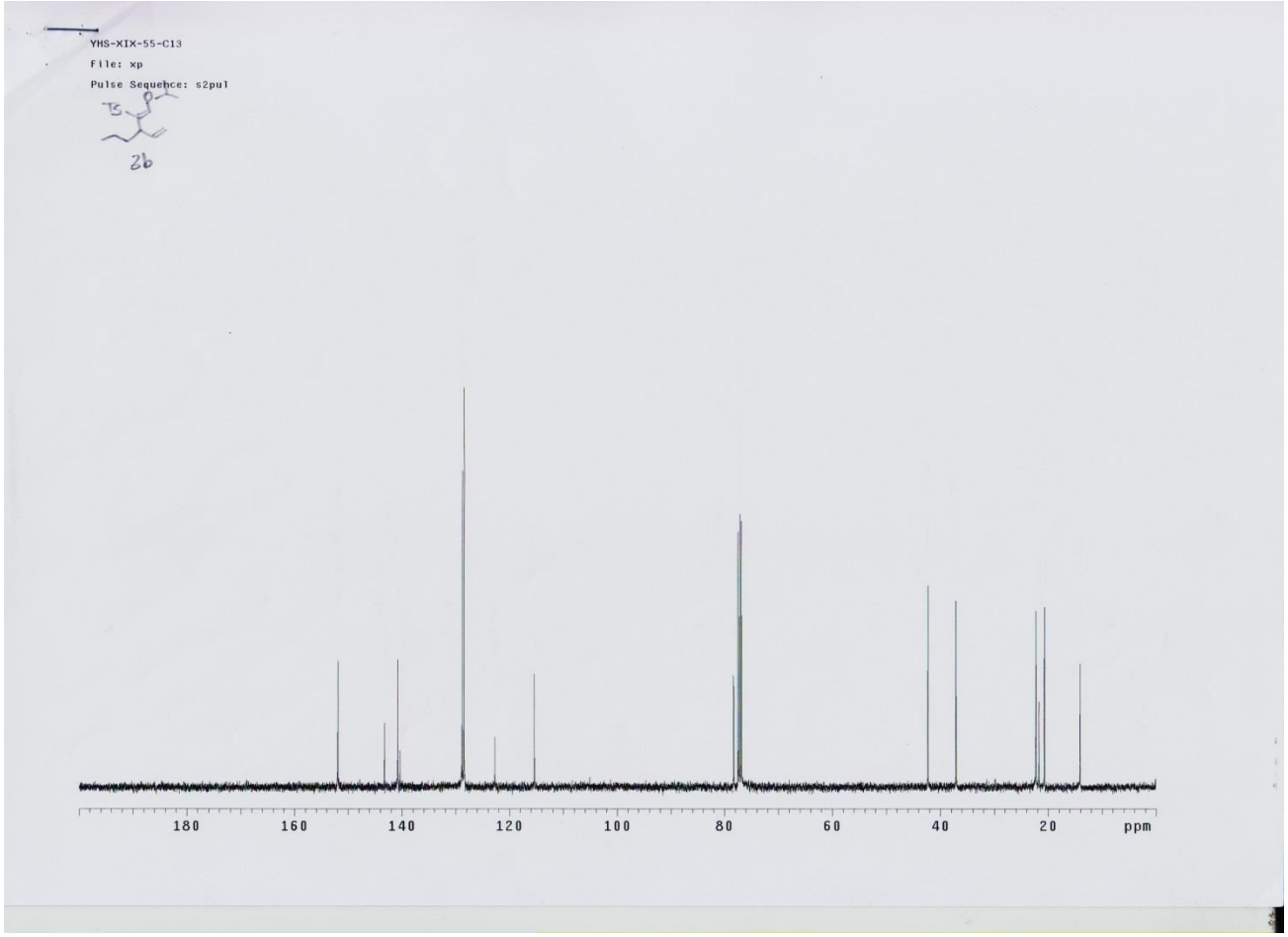

YHS-XIX-6-13C
File: xp
Pulse Sequence: s2pul
180
160
140
120
100
80
60
40
20
ppm

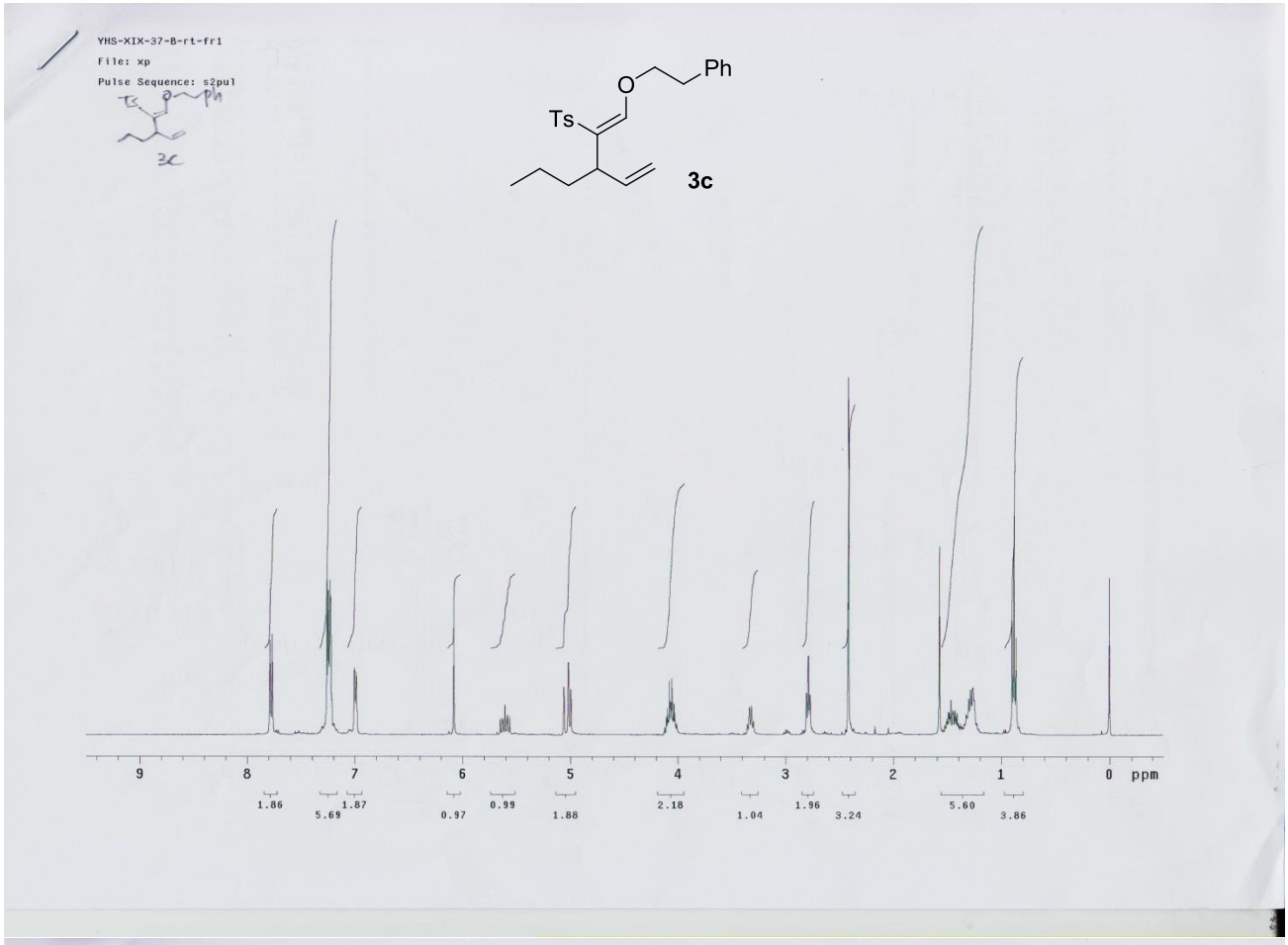
5. Scanned copies of the spectra for products



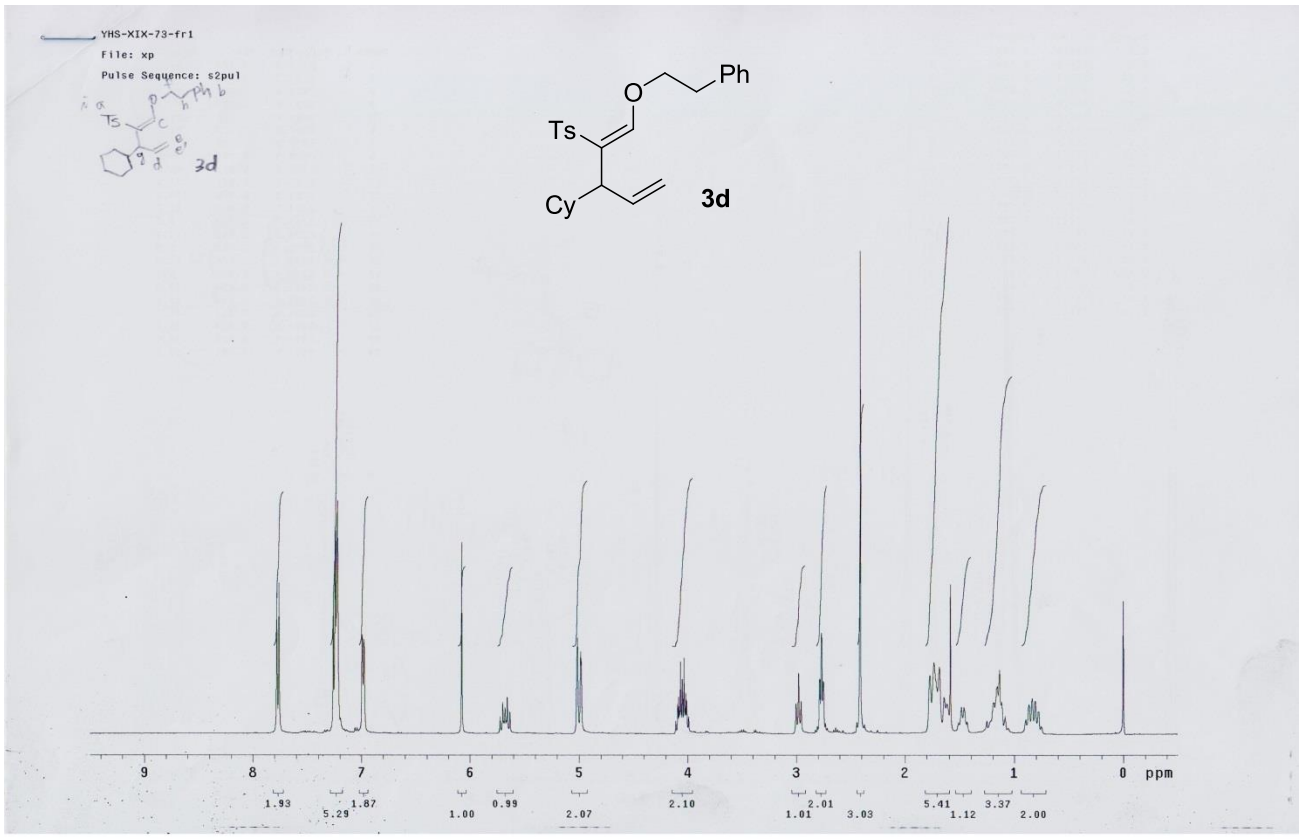


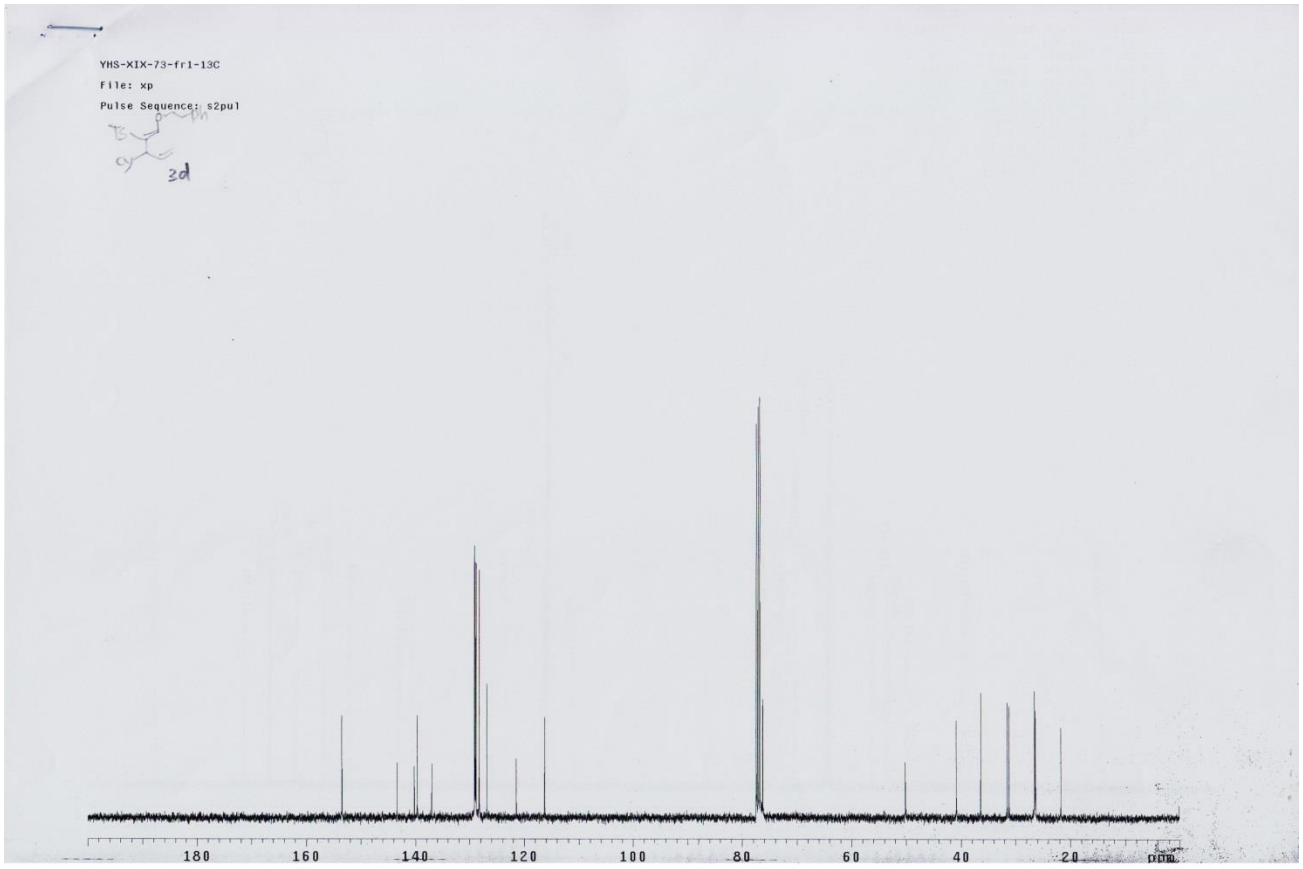

File: xp
Pulse Sequence: s2pul
3b
Ts
O
3b
9
8
7
6
5
4
3
2
1
0
ppm
2.03
2.33
1.06
1.00
2.10
1.07
1.11
3.41
2.85
2.72
3.38
3.24
3.37

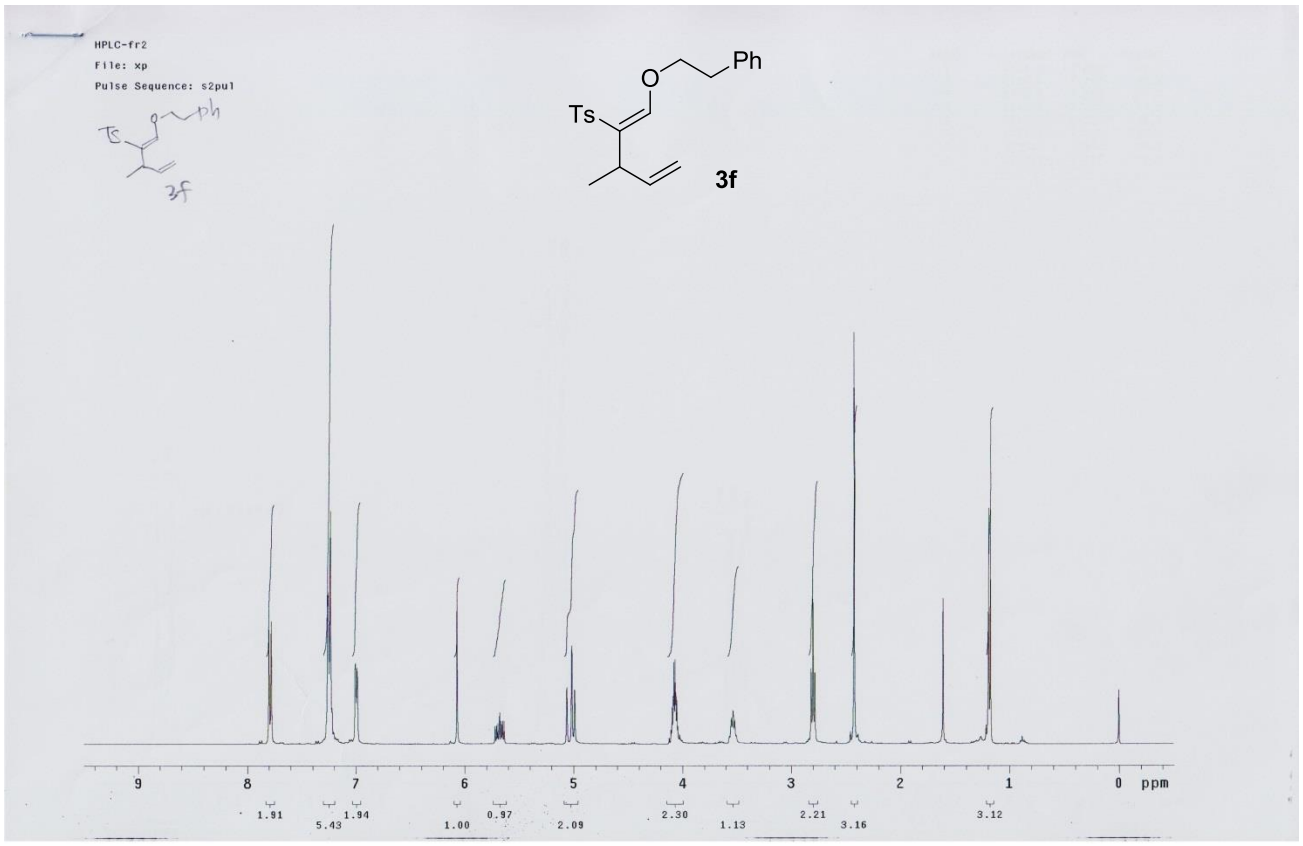

YHS-XIX-55-C13
File: xp
Pulse Sequence: s2pul
3b
180
160
140
120
100
80
60
40
20
ppm

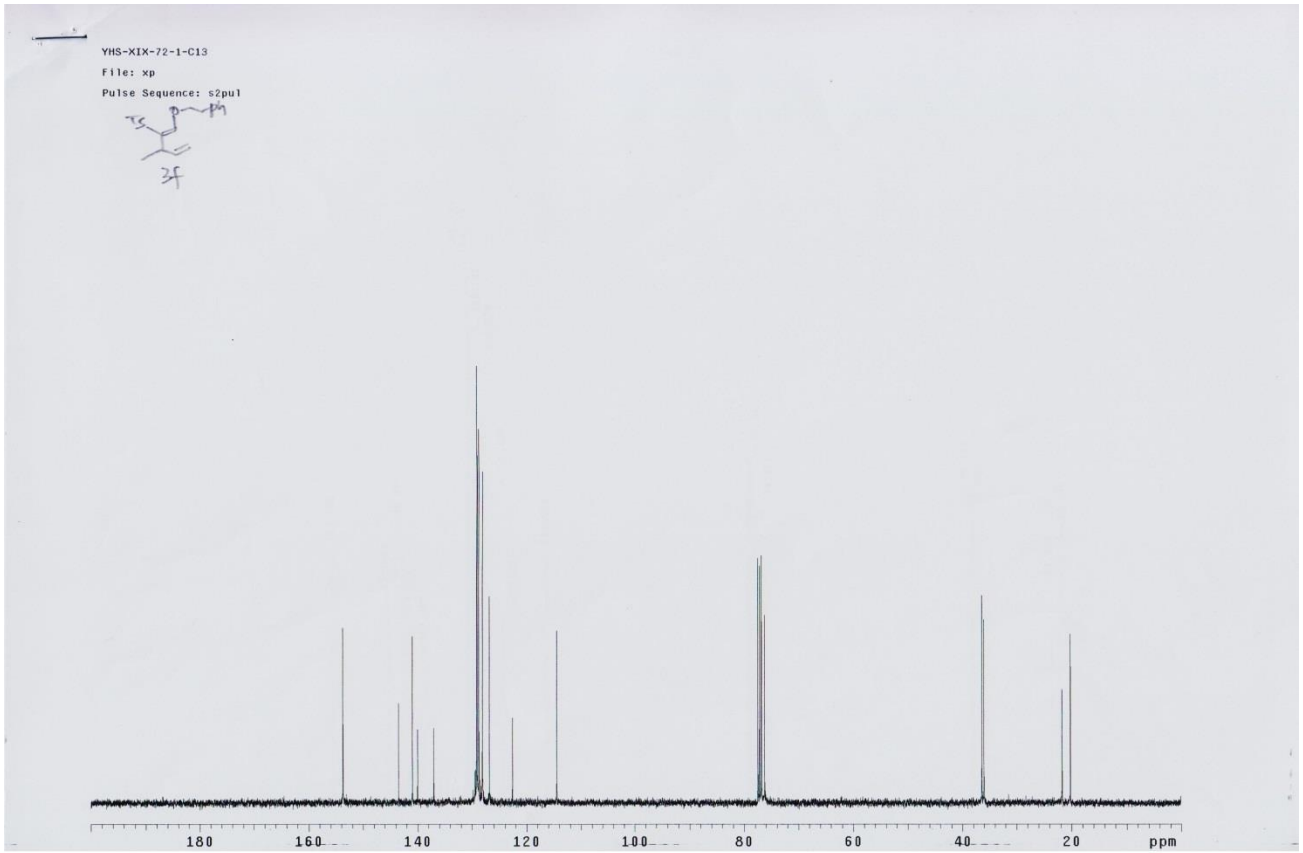

YHS-XIX-37-B-rt-fr1
File: xp
Pulse Sequence: s2pul
Ts
O
Ph
3c
9
8
7
6
5
4
3
2
1
0
ppm
1.86
5.69
1.87
0.97
0.99
1.88
2.18
1.04
1.96
3.24
5.60
3.86

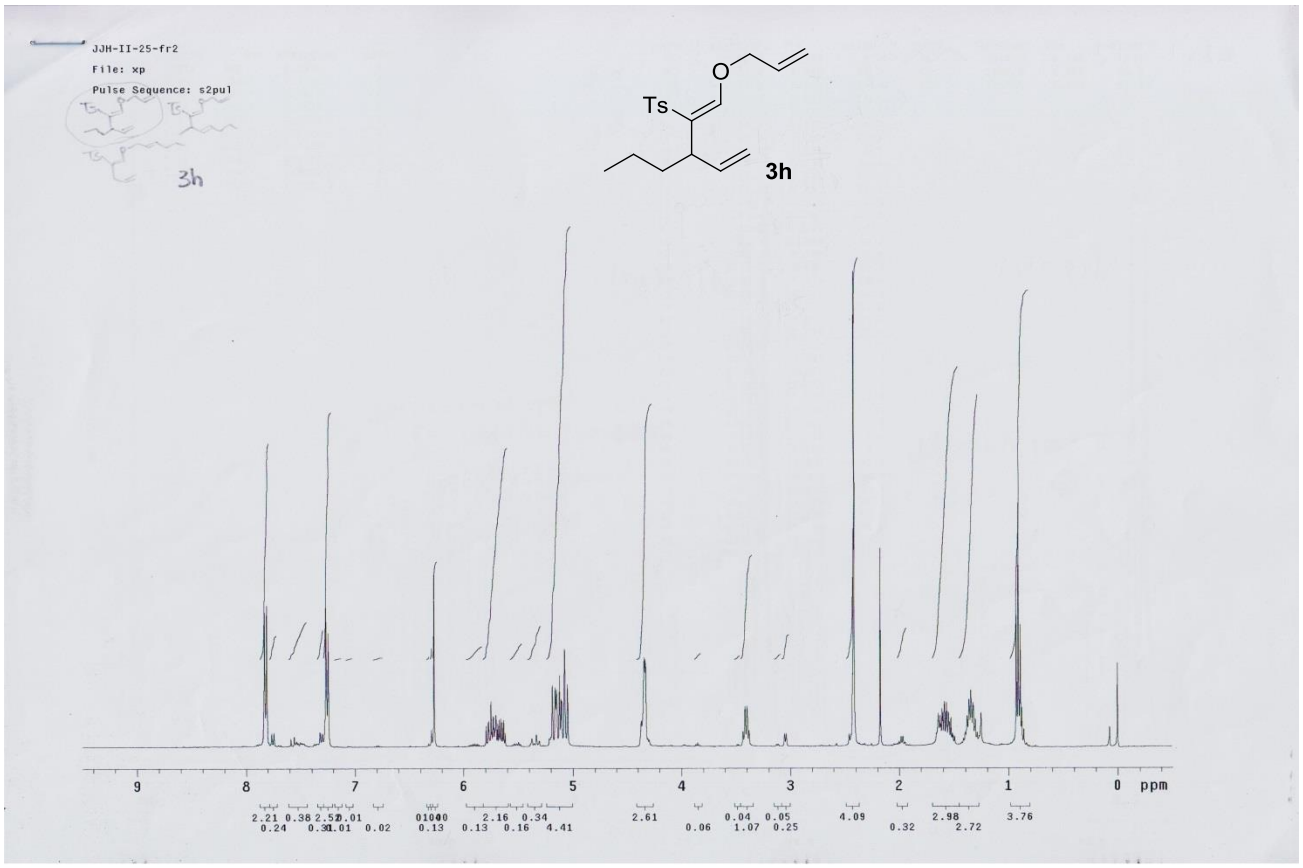

YHS-XIX-47-column-1
File: xp
Pulse Sequence: s2pul
3c
180
160
140
120
100
80
60
40
20
ppm

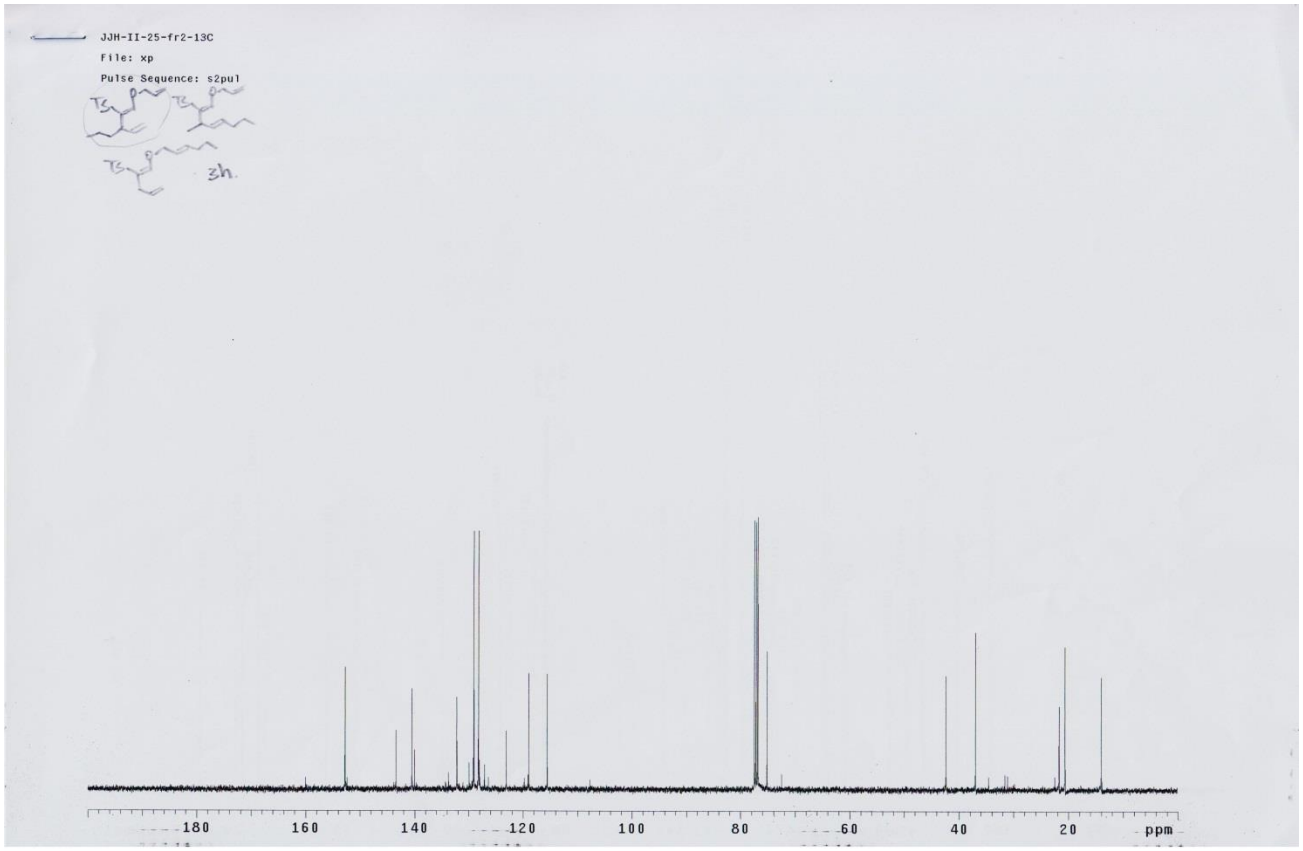

YHS-XIX-73-fr1
File: xp
Pulse Sequence: s2pul
Ts
O
Ph
Cy
3d
9
8
7
6
5
4
3
2
1
0
ppm
1.93
5.29
1.87
1.00
0.99
2.07
2.10
1.01
2.01
3.03
5.41
1.12
3.37
2.00


YHS-XIX-73-fr1-13C
File: xp
Pulse Sequence: s2pul
3d
180
160
140
120
100
80
60
40
20
ppm

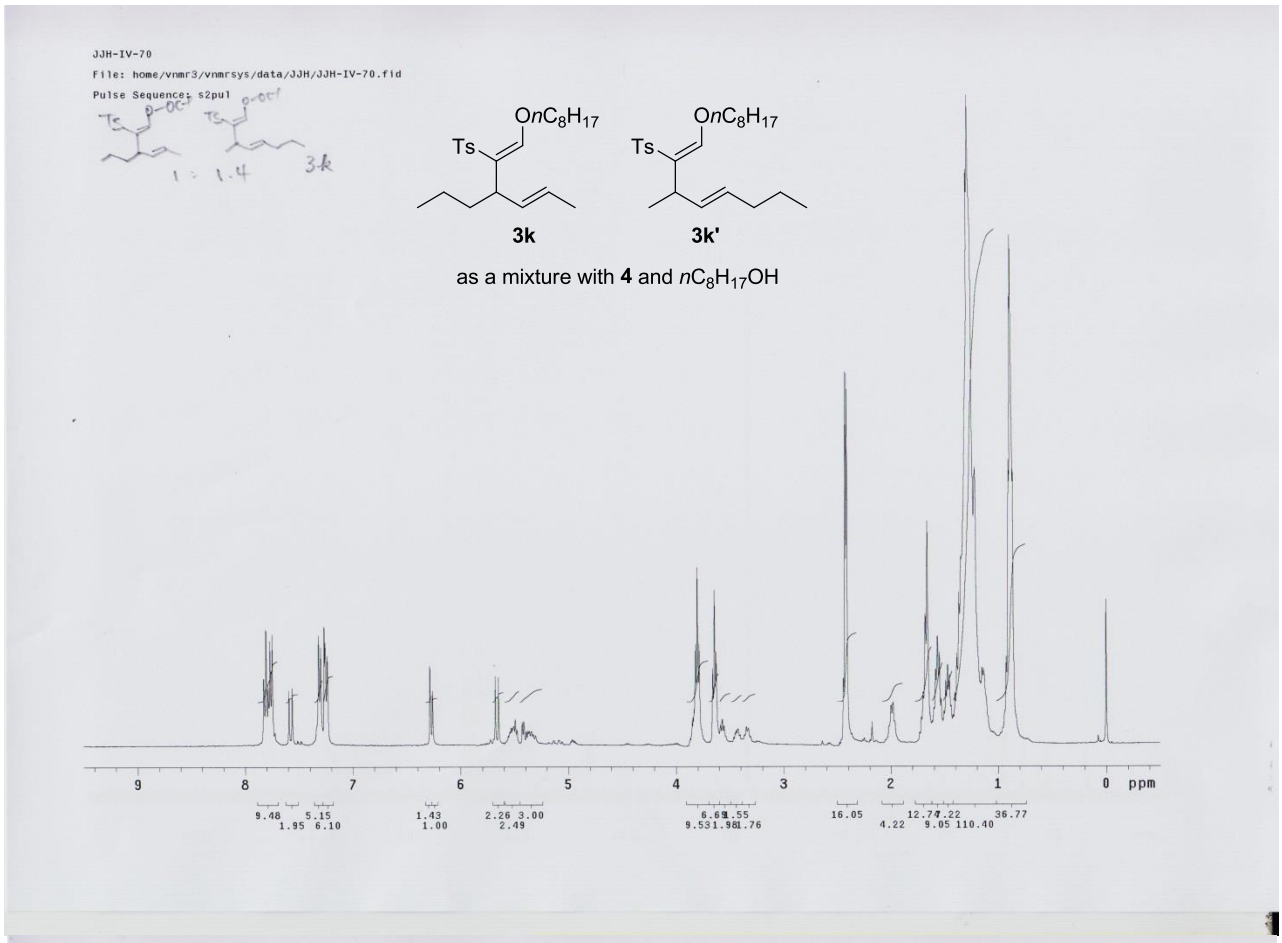

HPLC-fr2
File: xp
Pulse Sequence: s2pul
Ts
O
Ph
3f
9
8
7
6
5
4
3
2
1
0
ppm
1.91
5.43
1.94
1.00
0.97
2.09
2.30
1.13
2.21
3.16
3.12

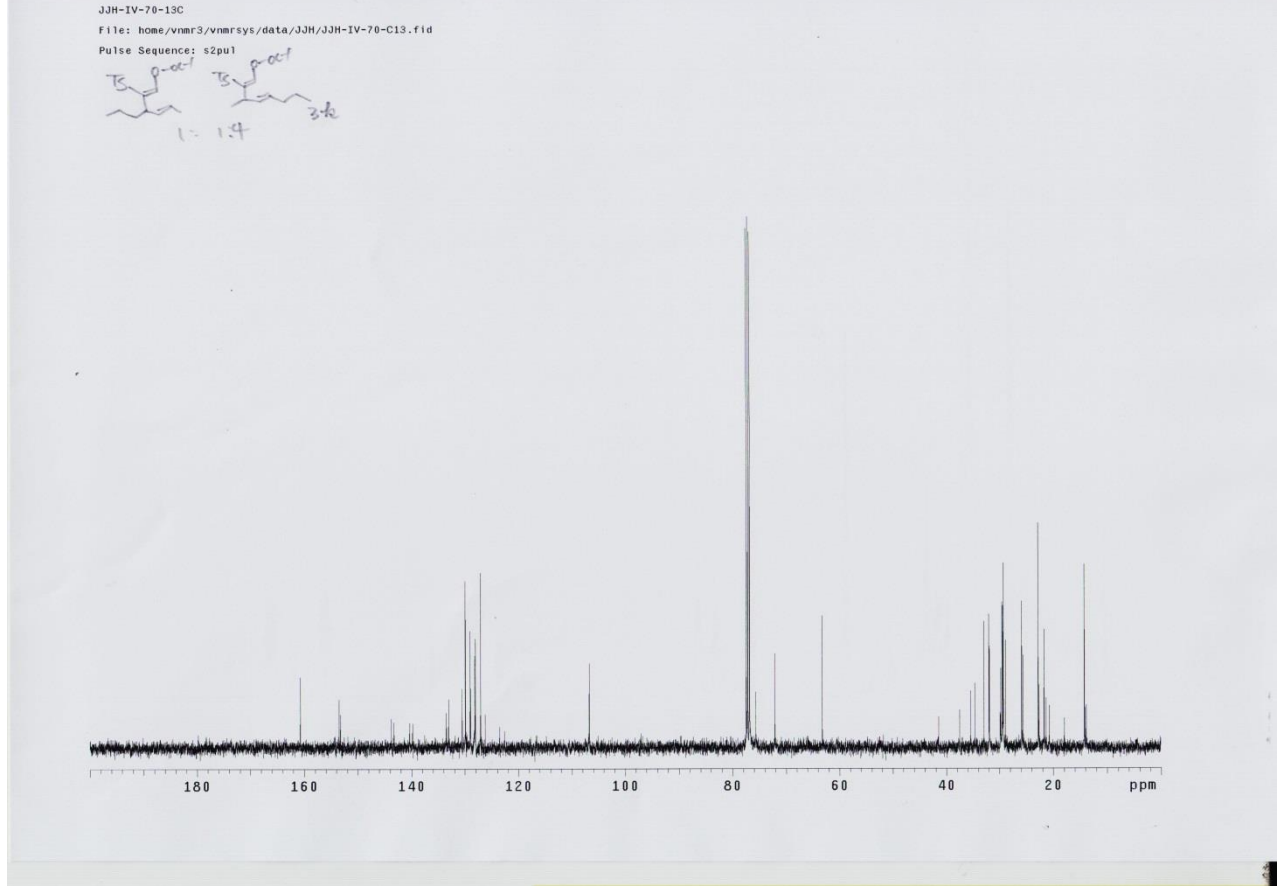

YHS-XIX-72-1-C13
File: xp
Pulse Sequence: s2pul
3f
180
160
140
120
100
80
60
40
20
ppm

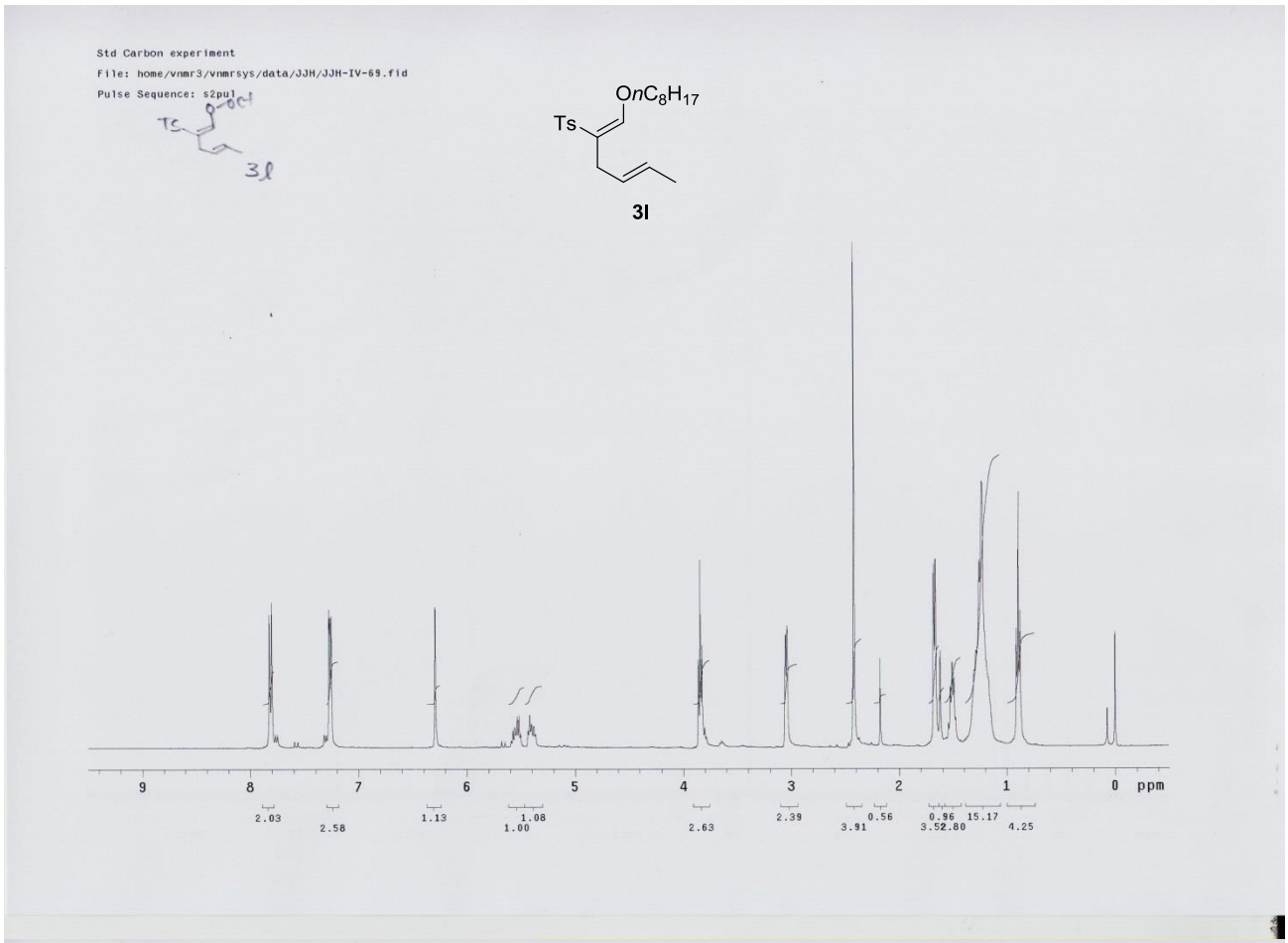

JJH-II-25-fr2
File: xp
Pulse Sequence: s2pul
3h
Ts
O
3h
9
8
7
6
5
4
3
2
1
0
ppm
2.21 0.38 2.52 2.01 0.24 0.30 1.01 0.02
0.13 2.16 0.34 0.13 0.16 4.41
2.61
0.04 0.05 0.06 1.07 0.25
4.09 0.32
2.98 2.72
3.76

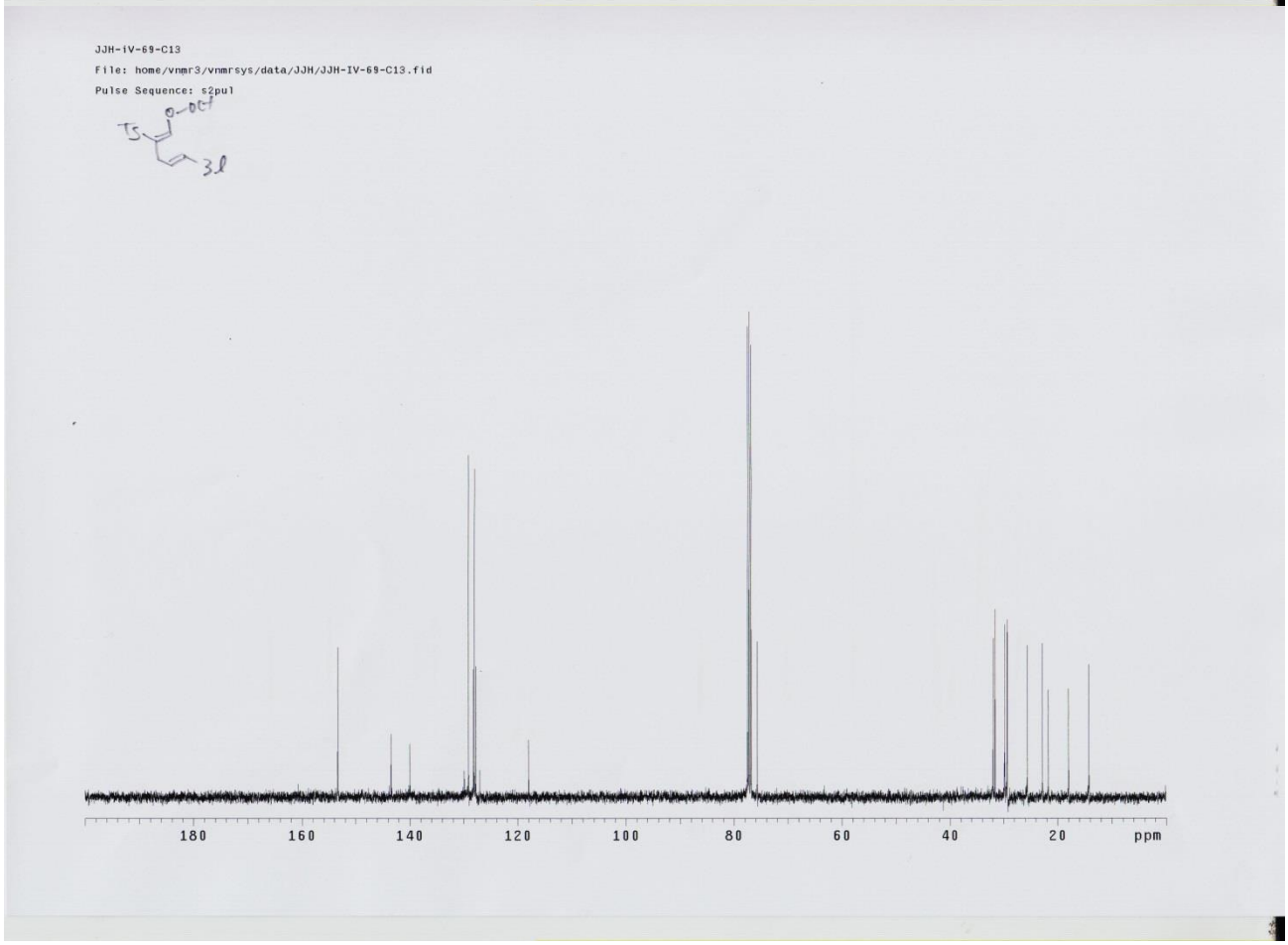

JJH-II-25-fr2-13C
File: xp
Pulse Sequence: s2pul
3h
180
160
140
120
100
80
60
40
20
ppm

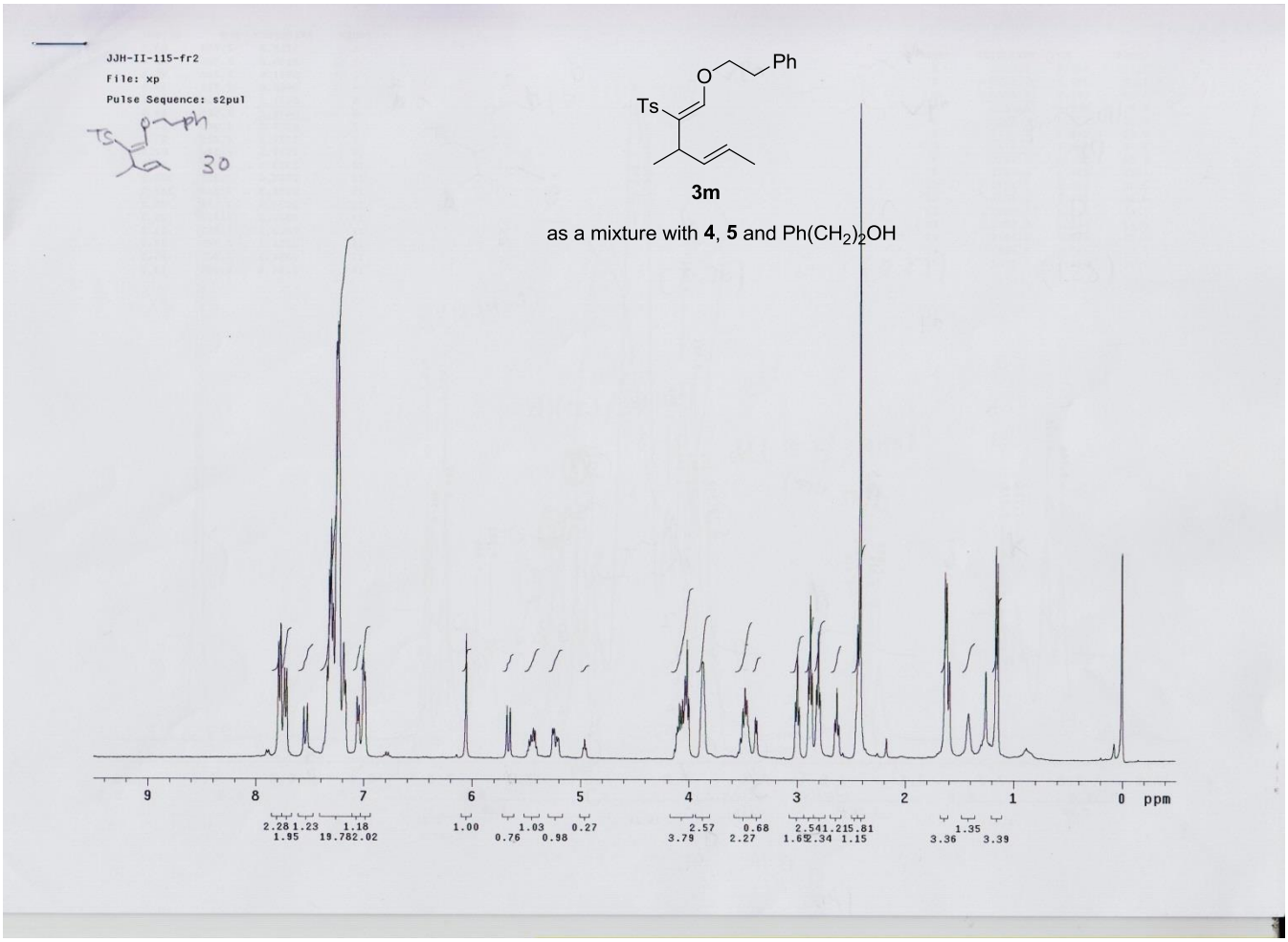

JJH-II-12-fr2
File: xp
Pulse Sequence: s2pul
Ts
Ph
O
3j
3j
as a mixture with 4, 5 and Ph(CH2)2OH
10 9 8 7 6 5 4 3 2 1 0 ppm
0.04
0.83 3.61
3.76 20.06
1.07 1.01
1.00 0.46 0.41
3.24 3.31 1.18 1.46 6.20 3.34
3.27 1.15 3.43 1.96 4.07

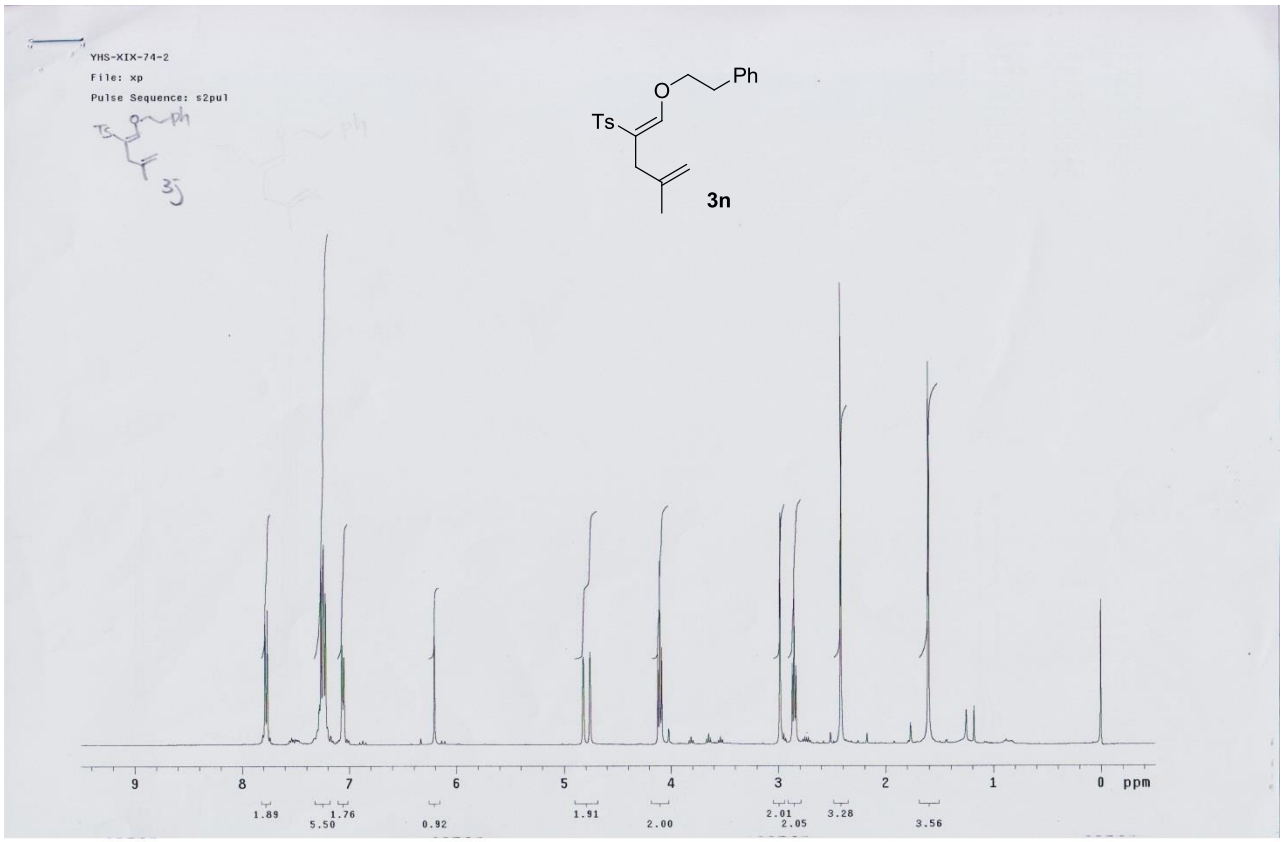

JJH-IV-70
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-70.fid
Pulse Sequence: s2pul
Ts
OnC8H17
3k
3k'
as a mixture with 4 and nC8H17OH
9 8 7 6 5 4 3 2 1 0 ppm
9.48 5.15 1.43 2.26 3.00 6.69 1.55 16.05 12.77 7.22 36.77
1.95 6.10 1.00 2.49 9.53 1.98 1.76 4.22 9.05 10.40

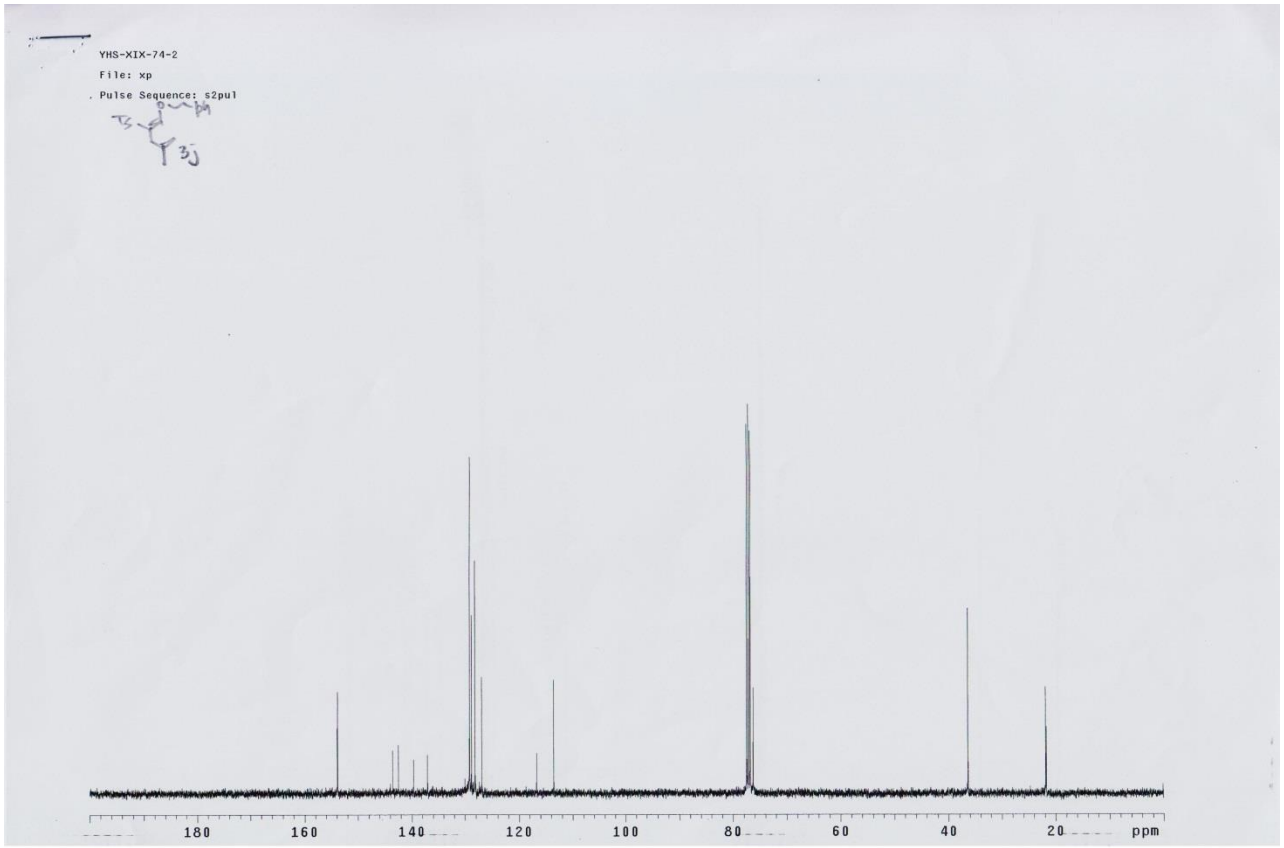

JJH-IV-70-13C
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-70-C13.fid
Pulse Sequence: s2pul
180 160 140 120 100 80 60 40 20 ppm


Std Carbon experiment
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-69.fid
Pulse Sequence: s2pul
Ts
OnC8H17
3l
9
8
7
6
5
4
3
2
1
0 ppm
2.03
2.58
1.13
1.08
1.00
2.63
2.39
3.91
0.56
0.96
3.52
15.17
2.80
4.25


JJH-iV-69-C13
File: home/vnmr3/vnmrsys/data/JJH/JJH-IV-69-C13.fid
Pulse Sequence: s2pul
Ts
3l
180
160
140
120
100
80
60
40
20
ppm


JJH-II-115-fr2
File: xp
Pulse Sequence: s2pul
Ts
O
Ph
3m
as a mixture with 4, 5 and Ph(CH2)2OH
9
8
7
6
5
4
3
2
1
0
ppm
2.28 1.23 1.18
1.95 19.78 2.02
1.00
0.76 1.03 0.98 0.27
3.79 2.57
2.27 0.68
1.65 2.54 2.34 1.21 1.15 5.81
3.36 1.35 3.39


YHS-XIX-74-2
File: xp
Pulse Sequence: s2pul
Ts
O
Ph
3n
9
8
7
6
5
4
3
2
1
0
ppm
1.89
5.50
1.76
0.92
1.91
2.00
2.01
2.05
3.28
3.56


YHS-XIX-74-2
File: xp
Pulse Sequence: s2pul
180
160
140
120
100
80
60
40
20
ppm