Supporting Information

Gold(I)-Catalyzed Route to α-Sulfenylated Carbonyl Compounds from Propargylic Alcohols and Aryl Thiols.

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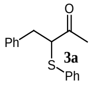
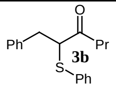
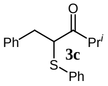
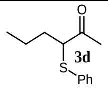
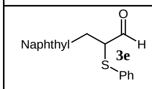
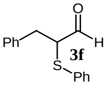
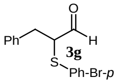
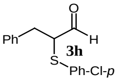
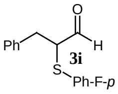
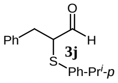
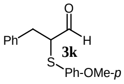
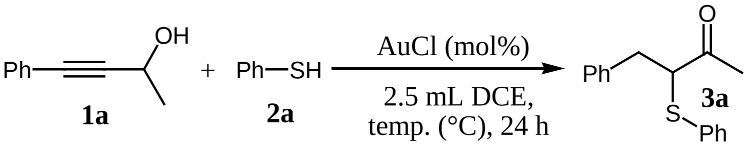
A. Checklist of Characterization data of all compounds:

Compounds	*Known / Unknown*	*IR*	*^{1}H NMR*	*^{13}C NMR*	*HRMS*	*CHN Analysis*
 **3a**	Known	–	√	√	–	–
 **3b**	Unknown	√	√	√	√	√
 **3c**	Unknown	√	√	√	√	√
 **3d**	Known	–	√	√	–	–
 **3e**	Unknown	√	√	√	√	√
 **3f**	Known	–	√	√	–	–
 **3g**	Unknown	√	√	√	√	√
 **3h**	Unknown	√	√	√	√	√
 **3i**	Unknown	√	√	√	√	√
 **3j**	Unknown	√	√	√	√	√
 **3k**	Unknown	√	√	√	√	√
	Unknown	√	√	√	√	√
	Known	–	√	√	–	–
	Known	–	√	√	–	–

B. General considerations: ^{1}H and ^{2}H NMR spectra were recorded with a Varian 300 (300 MHz), Varian 400 (400 MHz) and Varian 500 (500 MHz) spectrometer as solutions in $CDCl_3$. Chemical shifts are expressed in parts per million (ppm, δ) and are referenced to $CHCl_3$ (δ = 7.26 ppm) as an internal standard. All coupling constants are absolute values and are expressed in Hz. The description of the signals include: s = singlet, d = doublet, t = triplet, m = multiplet and dd = doublet of doublets, at = apparent triplet. ^{13}C NMR spectra were recorded with a Varian 300 (75 MHz) and Varian 400 (100 MHz) spectrometer as solutions in $CDCl_3$ with complete proton decoupling. Chemical shifts are expressed in parts per million (ppm, δ) and are referenced to $CDCl_3$ (δ = 77.0 ppm) as an internal standard. IR spectra were recorded by a Perkin Elmer FT-IR Spectrometer. High-Resolution Mass Spectra (HRMS) were performed with a micrOTOF (Bruker) spectrometer by Na-formate. The molecular fragments are quoted as the relation between mass and charge (*m*/*z*). CHN analysis were performed at eurofins MikroKemi, in Uppsala, Sweden. The routine monitoring of reactions was performed with silica gel pre-coated Al plate, which was analyzed with iodine and/or uv light respectively. Solvents, reagents and chemicals were purchased from Aldrich. Au^I-SPh was prepared according to a literature procedure.[1] All reactions were executed with oven-dried glassware under argon atmosphere. Solvent 1,2-Dichloroethane and chloroform was dried by distilling over anhydrous phosphorus pentoxide prior to use. $NaBD_4$ 98 atom % D 90% (CP) purchased from Aldrich was used for reduction of aldehyde to prepare alcohol having one deuterium at the hydridic position. D_2O (99 atom % D) was purchased from Aldrich and was used to incorporate deuterium at the protic position of alcohol and thiophenol.

C. Table of optimization of catalyst loading and reaction temperature:[a]

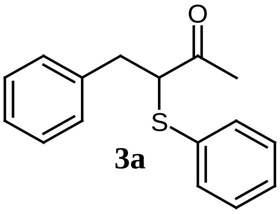


Entry	Catalyst (mol%)	Temp (°C)	Yield (%)[b]
1	AuCl (10 mol%)	65	92
2	AuCl (5 mol%)	65	91
3	**AuCl (2 mol%)**	**65**	**92**
4	AuCl (1 mol%)	65	71
5	AuCl (2 mol%)	65	39[c]
6	AuCl (2 mol%)	reflux	92
7	AuCl (2 mol%)	50	40

[a] Reaction condition: **1a** (1 mmol), **2a** (1.5 mmol) and AuCl (x mol%) was run in 2.5 mL 1,2-DCE solvent for 24 h under argon atmosphere. [b] Yields refer to isolated yields. [c] The reaction was performed open to air.

D. Experimental procedures for the synthesis of all compounds including their spectroscopic data are provided below:

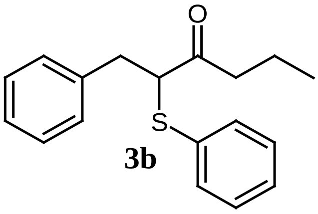
1. 4-Phenyl-3-(phenylthio)butan-2-one (3a):[2]



3a

At first, the catalyst AuCl (5 mg, 2 mol%) was weighed and transferred to a 5 mL microwave vial containing a small magnet in a glove box under argon atmosphere. After that, the cap of the vial was closed tightly and the vial was taken out from the glove-box. 2.5 mL of dry 1,2-dichloroethane solvent followed by alcohol **1a** (145 µL, 1 mmol) and benzenethiol **2a** (154 µL, 1.5 mmol) were added to the vial by syringe and was stirred using a magnetic stirrer at 65 °C for 24 h. After completion of the reaction (by TLC or crude NMR), 1,2 dichloroethane was evaporated under reduced pressure and the residue was purified by silica-gel (100–200 mess) column chromatography using 3% (*v*/*v*) ethyl acetate / pentane solution to afford the desired product **3a** as a pale yellow oil (236 mg, 0.92 mmol, 92%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.20 (s, 3 H, H-1), 3.00 (dd, J = 6.9 Hz, 14.4 Hz, 1 H, H-4), 2.68 (dd, J = 8.4 Hz, 14.1 Hz, 1 H, H-4), 3.90 (dd, J = 6.9 Hz, 8.4 Hz, 1 H, H-3), 7.18–7.37 (m, 10 H, H-arom) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 28.1, 36.9, 59.0, 127.1, 128.5, 128.8, 129.4, 133.0, 133.3, 138.3, 204.5 ppm.

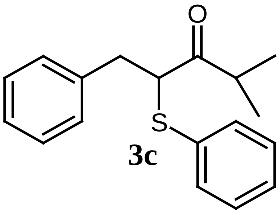
2. 1-Phenyl-2-(phenylthio)hexan-3-one (3b):



3b

Alcohol **1b** (184 µL, 1 mmol), benzenethiol **2a** (154 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3b** as a yellowish oil (255 mg, 0.89 mmol, 89%). IR (Neat): $\tilde{\upsilon}$ = 2962, 1706, 1439, 690 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 0.80 (t, J = 7.2 Hz, 3 H, H-6), 1.43–1.54 (m, 2 H, H-5), 2.29–2.40 (m, 1 H, H-4), 2.47–2.58 (m, 1 H, H-4), 2.98 (dd, J = 6.3, 14.1 Hz, 1 H, H-1), 3.19 (dd, J = 8.7, 14.1 Hz, 1 H, H-1), 3.88 (dd, J = 6.6, 8.7 Hz, 1 H, H-2), 7.16–7.37 (m, 10 H, H-arom) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.5, 17.2, 37.0, 42.8, 58.0, 126.6, 128.0, 128.4, 129.0, 129.1, 133.0, 133.1, 138.3, 206.0 ppm. HRMS: calcd. for $C_{18}H_{20}OSNa$ 307.1133; found 307.1115. Anal. calcd. for $C_{18}H_{20}OS$ (284.4): C 76.0, H 7.1; found C 76.0, H 7.0.

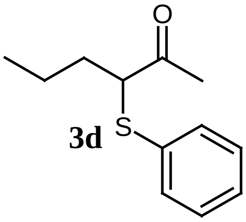
3. 4-Methyl-1-phenyl-2-(phenylthio)pentan-3-one (3c):



3c

Alcohol **1c** (128 µL, 1 mmol), benzenethiol **2a** (154 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3c** as a yellowish oil (248 mg, 0.88 mmol, 88%). IR (Neat): $\tilde{\nu}$ = 2969, 1707, 1439, 699 cm^{-1}. ^{1}H NMR (300 MHz, CDCl$_3$): δ = 0.76 (d, J = 6.9 Hz, 3 H, H-5), 1.04 (d, J = 6.7 Hz, 3 H, CH$_3$), 2.70–2.79 (m, 1 H, H-4), 3.00 (dd, J = 5.7 Hz, 13.8 Hz, 1 H, H-1), 3.22 (dd, J = 9.6 Hz, 13.8 Hz, 1 H, H-1), 3.97 22 (dd, J = 5.7 Hz, 9.6 Hz, 1 H, H-2), 7.42–7.38 (m, 2 H, H-arom), 7.14–7.35 (m, 8 H, H-arom) ppm. ^{13}C NMR (100 MHz, CDCl$_3$): δ = 17.8, 18.3, 37.3, 39.3, 56.5, 126.5, 128.3, 129.0, 129.2, 132.8, 133.6, 138.5, 208.7 ppm. HRMS: calcd. for $C_{18}H_{20}OSNa$ 307.1133; found 307.1115. Anal. calcd. for $C_{18}H_{20}OS$ (284.4): C 76.0, H 7.1; found C 76.0, H 7.4.

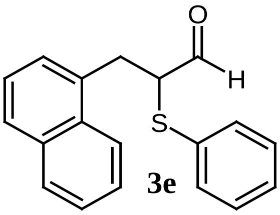
4. 3-(Phenylthio)hexan-2-one (3d):[3]



3d

Alcohol **1d** (324 µL, 3 mmol), benzenethiol **2a** (103 µL, 1 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3d** as a yellowish oil (105 mg, 0.50 mmol, 50%). ^{1}H NMR (300 MHz, CDCl$_3$): δ = 0.96 (t, J = 7.2 Hz, 3 H, H-6), 1.38–1.60 (m, 2 H, H-5), 1.64–1.86 (m, 2 H, H-4), 2.26 (s, 3 H, H-1), 3.65 (t, J = 7.5 Hz, 1 H, H-3), 7.24–7.44 (m, 5 H, H-arom) ppm. ^{13}C NMR (75 MHz, CDCl$_3$): δ = 14.0, 20.8, 26.6, 32.7, 57.8, 128.1, 129.3, 132.4, 133.4, 205.8 ppm.

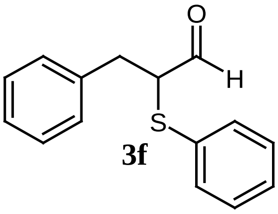
5. 3-(Naphthalen-4-yl)-2-(phenylthio)propanal (3e):



3e

Alcohol **1e** (182 mg, 1 mmol), benzenethiol **2a** (154 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3e** as a reddish brown oil (260 mg, 0.90 mmol, 90%). IR (Neat): ῦ = 3056, 1716, 1439, 776 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.47 (dd, *J* = 6.0 Hz, 14.7 Hz, 1 H, H-3), 3.66 (dd, *J* = 8.1 Hz, 14.7 Hz, 1 H, H-3), 3.98–4.04 (m, 1 H, H-2), 7.29–7.33 (m, 3 H, H-arom), 7.38–7.46 (m, 4 H, H-arom), 7.50–7.60 (m, 2 H, H-arom), 7.80 (dd, *J* = 2.4 Hz, 7.2 Hz, 1 H, H-arom), 7.89–7.92 (m, 1 H, H-arom), 7.99 (dd, *J* = 1.2 Hz, 7.8 Hz, 1 H, H-arom), 9.54 (d, *J* = 3.6 Hz, 1 H, H-1) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 31.7, 57.3, 123.3, 125.6, 125.7, 126.1, 126.7, 127.9, 128.2, 128.7, 129.4, 131.7, 131.9, 133.4, 133.7, 134.3, 194.3 ppm. HRMS: calcd. for $C_{19}H_{16}OSNa$ 315.0820; found 315.0813. Anal. calcd. for $C_{19}H_{16}OS$ (292.4): C 78.1, H 5.5; found C 77.7, H 5.5.

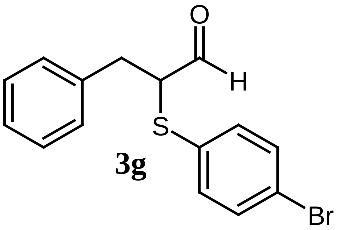
6. 3-Phenyl-2-(phenylthio)propanal (3f):[4]



3f

Alcohol **1f** (125 µL, 1 mmol), benzenethiol **2a** (154 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3f** as a reddish brown oil (225 mg, 0.93 mmol, 93%). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 3.00 (dd, *J* = 6.9 Hz, 14.4 Hz, 1 H, H-3), 3.22 (dd, *J* = 8.1 Hz, 14.4 Hz, 1 H, H-3), 3.81–3.87 (m, 1 H, H-2), 7.23–7.41 (m, 10 H, H-arom), 9.50 (d, *J* = 3.6 Hz, 1 H, H-1) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 34.4, 58.1, 127.1, 128.6, 128.8, 129.3, 129.3, 131.6, 133.4, 137.3, 194.2 ppm.

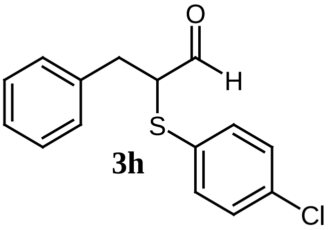
7. 2-(4-Bromophenylthio)-3-phenylpropanal (3g):



3g

Alcohol **1f** (125 µL, 1 mmol), 4-bromobenzenethiol **2b** (284 mg, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3g** as a yellowish oil (282 mg, 0.88 mmol, 88%). IR (Neat): ῦ = 3421, 1716, 1471, 1007, 697 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.99 (dd, *J* = 6.9 Hz, 14.4 Hz, 1 H, H-3), 3.21 (dd, *J* = 8.1 Hz, 14.4 Hz, 1 H, H-3), 3.79–3.85 (m, 1 H, H-2), 7.21–7.38 (m, 7 H, H-arom), 7.42–7.45 (m, 2 H, H-arom), 9.48 (d, *J* = 3.6 Hz, 1 H, H-1) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 34.3, 57.9, 122.8, 127.0, 128.6, 129.0, 132.3, 134.5, 136.9, 137.7, 193.6 ppm. HRMS: calcd. for $C_{15}H_{13}BrOSNa$ 342.9768; found 342.9746. Anal. calcd. for $C_{15}H_{13}BrOS$ (321.2): C 56.1, H 4.1; found C 55.9, H 3.8.

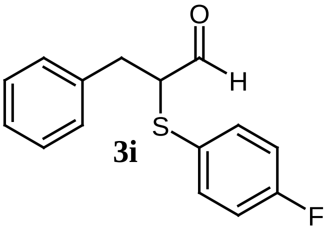
8. 2-(4-Chlorophenylthio)-3-phenylpropanal (3h):



3h

Alcohol **1f** (125 µL, 1 mmol), 4-chlorobenzenethiol **2c** (218 mg, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3h** as a yellowish oil (255 mg, 0.92 mmol, 92%). IR (Neat): ῦ = 3415, 2923, 1717, 1474, 1092, 715 cm^{-1}. ^{1}H NMR (400 MHz, CDCl$_3$): δ = 2.98 (dd, J = 6.8 Hz, 14.4 Hz, 1 H, H-3), 3.21 (dd, J = 8.0 Hz, 14.4 Hz, 1 H, H-3), 3.77–3.82 (m, 1 H, H-2), 7.22–7.35 (m, 9 H, H-arom), 9.49 (d, J = 3.2 Hz, 1 H, H-1) ppm. ^{13}C NMR (100 MHz, CDCl$_3$): δ = 34.3, 58.1, 127.0, 128.6, 129.0, 129.3, 130.1, 134.5, 134.7, 136.9, 193.6 ppm. HRMS: calcd. for $C_{15}H_{13}ClOSNa$ 299.0273; found 299.0272. Anal. calcd. for $C_{15}H_{13}ClOS$ (276.8): C 65.1, H 4.7; found C 65.3, H 4.7.

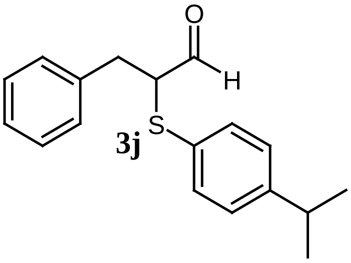
9. 2-(4-Fluorophenylthio)-3-phenylpropanal (3i):



3i

Alcohol **1f** (125 µL, 1 mmol), 4-fluorobenzenethiol **2d** (160 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** for 48 h to obtain **3i** as a yellowish oil (125 mg, 0.48 mmol, 48%). IR (Neat): ῦ = 3065, 1704, 1588, 1487, 1223, 826, 697 cm^{-1}.^{1}H NMR (400 MHz, CDCl$_3$): δ = 2.98 (dd, J = 6.8 Hz, 14.4 Hz, 1 H, H-3), 3.20 (dd, J = 8.0 Hz, 14.8 Hz, 1 H, H-3), 3.74–3.78 (m, 1 H, H-2), 6.99–7.04 (m, 2 H, H-arom), 7.22–7.40 (m, 7 H, H-arom), 9.51 (d, J = 3.6 Hz, 1 H, H-1) ppm. ^{13}C NMR (100 MHz, CDCl$_3$): δ = 34.5, 58.8, 116.5, 116.7, 127.2, 128.9, 129.3, 136.4, 136.5, 137.4, 164.6, 193.9 ppm. HRMS: calcd. for $C_{15}H_{13}FOSNa$ 283.0569; found 283.0582. Anal. calcd. for $C_{15}H_{13}FOS$ (260.3): C 69.2, H 5.0; found C 68.9, H 5.2.

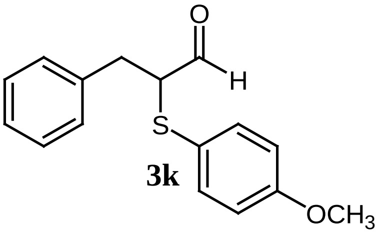
10. 2-(4-Isopropylphenylthio)-3-phenylpropanal (3j):



3j

Alcohol **1f** (125 µL, 1 mmol), 4-isopropylbenzenethiol **2e** (233 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3j** reddish yellow oil (216 mg, 0.76 mmol, 76%). IR (Neat): ṽ = 2960, 1719, 825 cm^{-1}. ^{1}H NMR (400 MHz, CDCl$_3$): δ = 1.27 (d, J = 6.8 Hz, 6 H, H-methyl), 2.88–2.95 (m, 1 H, C<u>*H*</u>(CH$_3$)$_2$), 3.01 (dd, J = 6.8 Hz, 14.8 Hz, 1 H, H-3), 3.23 (dd, J = 7.6 Hz, 14.4 Hz, 1 H, H-3), 3.78–3.82 (m, 1 H, H-2), 7.19 (d, J = 8.0 Hz, 2 H, H-arom), 7.25–7.29 (at, 3 H, H-arom), 7.32–7.35 (at, 4 H, H-arom), 9.53 (d, J = 3.6 Hz, 1 H, H-1) ppm. ^{13}C NMR (100 MHz, CDCl$_3$): δ = 24.0, 34.0, 34.6, 58.6, 127.1, 127.6, 128.4, 128.8, 129.4, 134.0, 137.7, 149.8, 194.3 ppm. HRMS: calcd. for $C_{18}H_{20}OSNa$ 307.1133; found 307.1164. Anal. calcd. for $C_{18}H_{20}OS$ (284.4): C 76.0, H 7.1; found C 76.2, H 7.0.

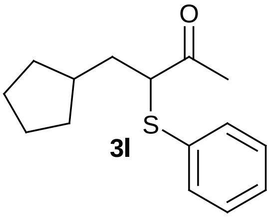
11. 2-(4-Methoxyphenylthio)-3-phenylpropanal (3k):



3k

Alcohol **1f** (125 µL, 1 mmol), 4-methoxybenzenethiol **2f** (184 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** to obtain **3k** as reddish yellow oil (117 mg, 0.43 mmol, 43%). IR (Neat): ṽ = 2836, 1717, 1590, 1490, 1248, 824, 698 cm^{-1}. ^{1}H NMR (400 MHz, CDCl$_3$): δ = 2.96 (dd, J = 6.8 Hz, 14.4 Hz, 1 H, H-3), 3.16 (dd, J = 8 Hz, 14.4 Hz, 1 H, H-3), 3.68–3.79 (m, 1 H, H-2), 3.82 (s, 3 H, H-methoxy), 6.85–6.88 (m, 2 H, H-arom), 7.25–7.28 (m, 2 H, H-arom), 7.32–7.35 (m, 3 H, H-arom), 7.36–7.44 (m, 2 H, H-arom), 9.51 (d, J = 3.2 Hz, 2 H, H-1) ppm. ^{13}C NMR (100 MHz, CDCl$_3$): δ = 33.9, 55.3, 58.7, 114.6, 114.7, 126.8, 128.6, 129.0, 132.6, 136.7, 193.7 ppm. HRMS: calcd. for $C_{16}H_{16}O_2SNa$ 295.0769; found 295.0770. Anal. calcd. for $C_{16}H_{16}O_2S$ (272.4): C 70.6, H 5.9; found C 70.5, H 5.8.

12. 4-Cyclopentyl-3-(phenylthio)butan-2-one (3l):



3l

Alcohol **1g** (138 mg, 1 mmol), benzenethiol **2a** (154 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated as described for **3a** for 48 h to obtain **3l** as a yellowish oil (119 mg, 0.48 mmol, 48%). IR (Neat): ῡ = 2947, 1705, 1353, 1209, 1025, 739, 690 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.08–1.18 (m, 2 H, H-aliphatic), 1.50–1.68 (m, 4 H, H-aliphatic), 1.71–1.90 (m, 4 H, H-aliphatic), 1.93–2.26 (m, 1 H, H-aliphatic), 2.26 (s, 3 H, H-1), 3.69 (t, *J* = 7.6 Hz, 1 H, H-3), 7.23–7.35 (m, 3 H, H-arom), 7.36–7.39 (m, 2 H, H-arom) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ = 24.9, 25.0, 26.2, 36.5, 37.7, 57.0, 127.7, 129.0, 132.1, 133.2, 205.6 ppm. HRMS: calcd. for $C_{15}H_{20}NaOS$ 271.1133; found 271.1131. Anal. calcd. for $C_{15}H_{20}OS$ (248.4): C 72.5, H 8.1; found C 72.3, H 8.0.

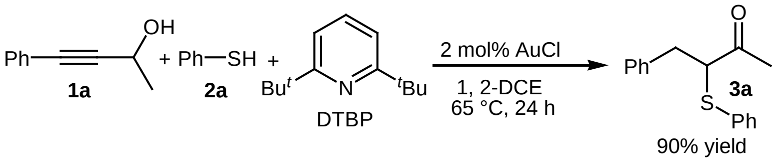
12. (*Z*)-3-Phenyl-2-(phenylthio)prop-2-en-1-ol (5-*Z*):[5]

Alcohol **1f** (125 µL, 1 mmol), benzenethiol **2a** (154 µL, 1.5 mmol) and the catalyst AuCl (5 mg, 2 mol%) were treated in 2.5 mL DCE solvent as described for **3f** at 65 °C for 2 h. Column chromatographic purification afforded the *E*- and *Z*- isomers of **5** (73 mg., 0.30 mmol, 30%) as a colorless oil (*Z* : *E* = 7 : 1). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.33 (bs, 1 H, H-alcohol), 4.23 (s, 2 H, H-1), 7.20 (s, 1 H, H-3), 7.26–7.43 (m, 8 H, H-aromatic), 7.68–7.70 (m, 2 H, H-arom) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 66.3, 126.9, 127.8, 128.1, 129.1, 129.2, 129.3, 130.3, 133.2, 133.3, 133.4, ppm.

13. (*E*)-3-Phenyl-2-(phenylthio)prop-2-en-1-ol (5-*E*):[5]

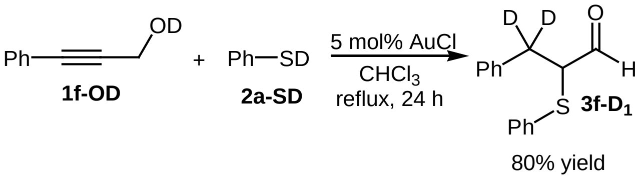
^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.09 (brs, 1 H, H-alcohol), 4.37 (s, 2 H, H-1), 6.96 (s, 1 H, H-3), 7.28–7.39 (m, 8 H, H-arom), 7.49–7.51 (m, 2 H, H-arom) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 60.3, 127.6, 127.7, 128.1, 128.5, 128.7, 128.8, 129.1, 129.3 129.4, 131.5, 135.5, 135.9, 136.7 ppm.

E. Experimental procedures for the AuCl catalyzed reaction between 1a and 2a in presence of 2, 6-di-*tert*-butylpyridine (DTBP):



At first, the catalyst AuCl (5 mg, 2 mol%) was weighed and transferred to a 5 mL microwave vial containing a small magnet in a glove box under argon atmosphere. After that, the cap of the vial was closed tightly and the vial was taken out from the glove-box. 2.5 mL of dry 1,2-dichloroethane solvent followed by DTBP (65 µL, 30 mol%) was added and stirred at r. t. for 15 mint. After that, alcohol **1a** (145 µL, 1 mmol) and benzenethiol **2a** (154 µL, 1.5 mmol) were added to the vial by syringe and was stirred using a magnetic stirrer at 65 °C for 24 h. After completion of the reaction (by TLC), 1,2 dichloroethane was evaporated under reduced pressure and the residue was purified by silica-gel (100–200 mess) column chromatography using 3% (*v*/*v*) ethyl acetate / pentane solution to afford the desired product **3a** as a pale yellow oil (231 mg, 0.90 mmol, 90%).

F. Experimental procedures for the AuCl catalyzed reaction between 1f-OD and 2a-SD:



Preparation of 1f-OD from 1f:

1f (125 µL, 1 mmol) dissolving in 1.5 mL $CDCl_3$ was taken in a oven-dried (pre-rinsed by D_2O) slink tube attached with argon line and high vacuum pump. D_2O (180 µL, 10 mmol) was added and the reaction mixture was stirred vigorously for 30 mint maintaining complete argon atmosphere inside the reaction vessel. Excess D_2O and $CDCl_3$ were completely removed carefully under vacuum and kept under high vacuum for 2 h. ^{1}H NMR of a small amount of this reveals the formation of **1f-OD** (80% deuterium incorporation). The residue was dissolved in 1.5 mL freshly distilled $CHCl_3$.

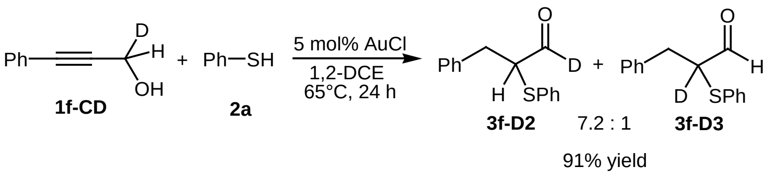
Preparation of 2a-SD from 2a:

2a (154 µL, 1.5 mmol) and D_2O (270 µL, 15 mmol) was treated in $CDCl_3$ (1.5 mL) following the same method described above for the synthesis of **1f-OD** to obtain **2a-SD** (80% deuterium incorporation).

Reaction between 1f-OD and 2a-SD:

2a-SD dissolved in 1 mL freshly distilled $CHCl_3$ was added to the 1.5 mL $CHCl_3$ solution of **1f-OD**. AuCl (13 mg, 5 mol%) was added and the reaction mixture was refluxed under argon for 24 h. Usual purification yielded **3f-D1** (195 mg, 0.80 mmol, 80%). ^{1}H NMR and ^{2}H NMR spectroscopic studies of the purified product revealed that the total deuterium content was 75%, of which deuterium incorporation at the benzylic position (**3f-D1**) was 90%.

G. Experimental procedures for the AuCl catalyzed reaction between 1f-CD and 2a:



Preparation of 1f-CD:

1f-CD (90% deuterium purity) was prepared by usual reduction of the corresponding aldehyde by $NaBD_4$ (98 atom % D 90% CP) in methanol solvent.

Reaction between 1f-CD and 2a:

Alcohol **1f-CD** (125 µL, 1 mmol), benzenethiol **2a** (154 µL, 1.5 mmol) and the catalyst AuCl (13 mg, 5 mol%) in 1,2-dichloroethane solvent (2.5 mL) were treated at 65 °C as described for **3a**. Usual purification was carried out to obtain a mixture of **3f-D2** and **3f-D1** as yellowish oil (221 mg, 0.91 mmol, 91%). ^{1}H NMR and ^{2}H NMR spectroscopic studies of the purified product show that the total deuterium content of the product was 90%, of which deuterium incorporation at the aldehyde position (**3f-D2**) was 79% and the remaining 11% deuterium was incorporated at the α-position of the product (**3f-D3**).

H. Deuterium Kinetic Isotope Effect.

For kinetic experiments, a total of 6 sets of reactions were investigated simultaneously for better reproducibility; 3 of them were reaction between the deuterated alcohol **1f-CD** and **2a** and other 3 were reaction between non-deuterated **1f** and **2a**.

For each reaction, **1f-CD** (133 mg, 1 mmol) or **1f** (132 mg, 1 mmol), **2a** (154 µL, 1.5 mmol) and AuCl (13 mg, 5 mol%) were used in 2.5 mL DCE solvent in a similar way as described for the synthesis of **3a**. During the course of the reaction, 100 µL of the reaction mixture was taken our by syringe in different time intervals and passed through a short silica packed pipette eluting with 50% ethyl acetate / pentane. The solvent was evaporated out and crude NMR was checked in $CDCl_3$. The disappearance of **1f-CD** or **1f** as well as formation of the product was calculated by comparing the integration of proton signals at 4.52 (singlet; starting alcohol), 4.24 (singlet; major intermediate), 4.37 (singlet; minor intermediate) and 3.83 (multiplate; product) ppm.

When substrate **1f-CD** was used in the kinetic experiments, two different products were generated (**3f-D2** and **3f-D3**). The rate constants $k_{\mathbf{H}}^{\mathbf{D}}$ and $k_{\mathbf{D}}^{\mathbf{H}}$ for the generation of **3f-D2** and **3f-D3** together with $k_{\mathbf{H}}^{\mathbf{H}}$ were investigated by different experiments. The consumption of **1f** and also generation of **3f** followed first-order kinetics over three half-lives and the rate constant was determined ($k_{\mathbf{H}}^{\mathbf{H}} = 1.39 \times 10^{-2} \pm 0.007$).

To determine the ratio between rate constants $k_{\mathbf{H}}^{\mathbf{D}}$ and $k_{\mathbf{D}}^{\mathbf{H}}$ the reaction of substrate **1f-CD** was performed and the ratio between the products **3f-D2** and **3f-D3** were determined by ^{1}H NMR and ^{2}H NMR (7.2:1). We make the assumption that the product ratio is due to difference in rate constants.

The ratio between $k_{\mathrm{H}}^{\mathrm{H}}$ to ($k_{\mathrm{H}}^{\mathrm{D}}$ + $k_{\mathrm{D}}^{\mathrm{H}}$) was studied by running kinetic experiments and plotting them to determine the difference in the corresponding rate constants. The observed ratio in rate $k_{\mathrm{H}}^{\mathrm{H}} \div k_{\mathrm{H}}^{\mathrm{D}}$ + $k_{\mathrm{D}}^{\mathrm{H}}$) was determined to 1.3.

Solving $k_{\mathrm{D}}^{\mathrm{H}}$: The ratio $k_{\mathrm{H}}^{\mathrm{H}} \div$ ($k_{\mathrm{H}}^{\mathrm{D}}$ + $k_{\mathrm{D}}^{\mathrm{H}}$) was determined to 1.3. Making the assumption that the observed ratio between the product distribution of **3f-D2** and **3f-D3** is reflected by the relative rate constants $k_{\mathrm{H}}^{\mathrm{D}} \div k_{\mathrm{D}}^{\mathrm{H}}$ the following equation was obtained:

$$1.3 = \frac{k_{\mathrm{H}}^{\mathrm{H}}}{\frac{1}{8}.2k_{\mathrm{D}}^{\mathrm{H}}} + \frac{k_{\mathrm{H}}^{\mathrm{H}}}{7.\frac{2}{8}.2k_{\mathrm{H}}^{\mathrm{D}}}$$

$k_{\mathrm{D}}^{\mathrm{H}} = 1.65 \times 10^{-3} \pm 0.0045$

Giving a primary kinetic isotope effect of ($k_{\mathrm{H}}^{\mathrm{H}} \div k_{\mathrm{D}}^{\mathrm{H}}$):

$$\frac{k_{\mathrm{H}}^{\mathrm{H}}}{k_{\mathrm{D}}^{\mathrm{H}}} = \frac{1.39 \times 10^{-2}}{1.65 \times 10^{-3}}$$

$$\frac{k_{\mathrm{H}}^{\mathrm{H}}}{k_{\mathrm{D}}^{\mathrm{H}}} = 8.4 \pm 0.2$$

Solving $k_{\mathbf{H}}^{\mathbf{D}}$: We use the value obtained for $k_{\mathbf{D}}^{\mathbf{H}}$ and the ratio $k_{\mathbf{H}}^{\mathbf{D}} \div k_{\mathbf{D}}^{\mathbf{H}}$ discussed above.

$$\frac{k_{\mathbf{H}}^{\mathbf{D}}}{k_{\mathbf{D}}^{\mathbf{H}}} = \frac{7.2}{1}$$

$$k_{\mathbf{H}}^{\mathbf{D}} = 7.2 \times 1.65 \times 10^{-3}$$

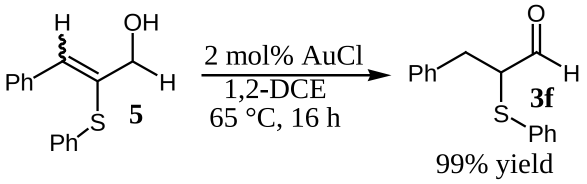
$$k_{\mathbf{H}}^{\mathbf{D}} = 1.18 \times 10^{-2} \pm 0.003$$

Giving a secondary kinetic isotope effect of ($k_{\mathbf{H}}^{\mathbf{H}} \div k_{\mathbf{H}}^{\mathbf{D}}$):

$$\frac{k_{\mathbf{H}}^{\mathbf{H}}}{k_{\mathbf{H}}^{\mathbf{D}}} = \frac{1.39 \times 10^{-2}}{1.18 \times 10^{-2}}$$

$$\frac{k_{\mathbf{H}}^{\mathbf{H}}}{k_{\mathbf{H}}^{\mathbf{D}}} = 1.17 \pm 0.1$$

I. Conversion of intermediate 5 to the product 3f:

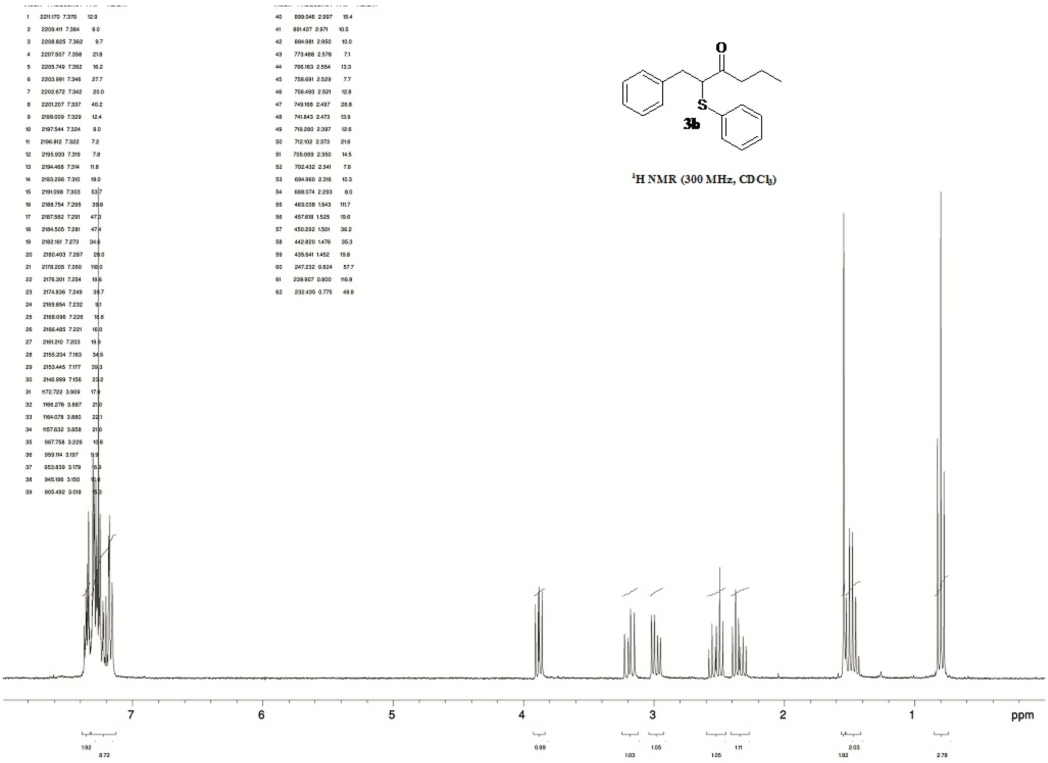


Intermediate **5** (242 mg, 1 mmol) and AuCl (5 mg, 2 mol%) was treated in DCE solvent (2.5 mL) at 65 °C follwing the standard method described for the synthesis of **3a** to afford the product **3f** as a yellow oil (240 mg, 0.99 mmol, 99%). Attempt to use gold(I) benzenethiolate (Au-SPh), acetic acid and thiophenol as catalyst towards this transformation were not successful and no product formation was observed.

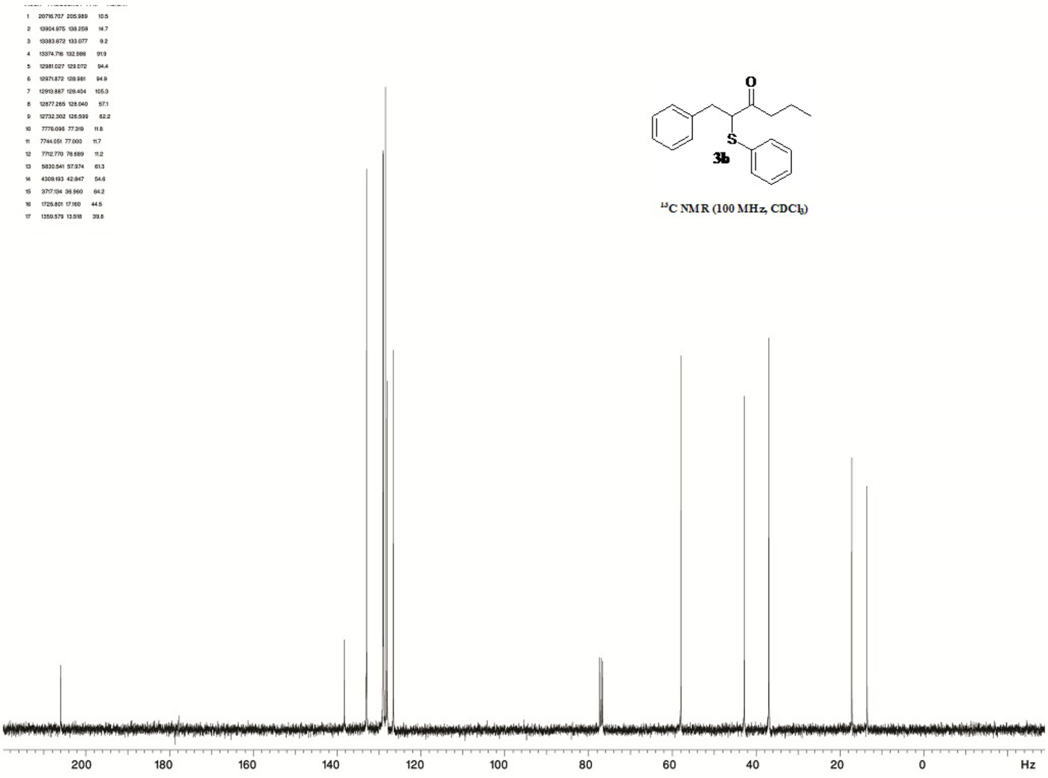
J. A cross-over experiment to investigate the intramolecularity of the hydride migration:

To investigate the intramolecularity of the reaction, a cross over experiment was carried using **1f-CD** (1 mmol), **1e** (1 mmol), **2a** (3 mmol) and AuCl (10 mol%) in 2.5 mL DCE solvent. The reaction was run for 24 h at 65 °C following the standard method. The two products resulting from the reactions between each alcohol and thiophenol have distinguishable differences in chemical shift in ^{1}H NMR spectra for aldehydic as well as the *α*- and *ß*-protons. Usual purification followed by ^{1}H and ^{2}H NMR spectroscopy clearly indicated no deuterium incorporation in any position of the product **3e**, whereas deuterium incorporation in **3f** was obtained in the aldehydic position and in the *α*- position in a similar ratios as mentioned in **Scheme 4** of the manuscript.

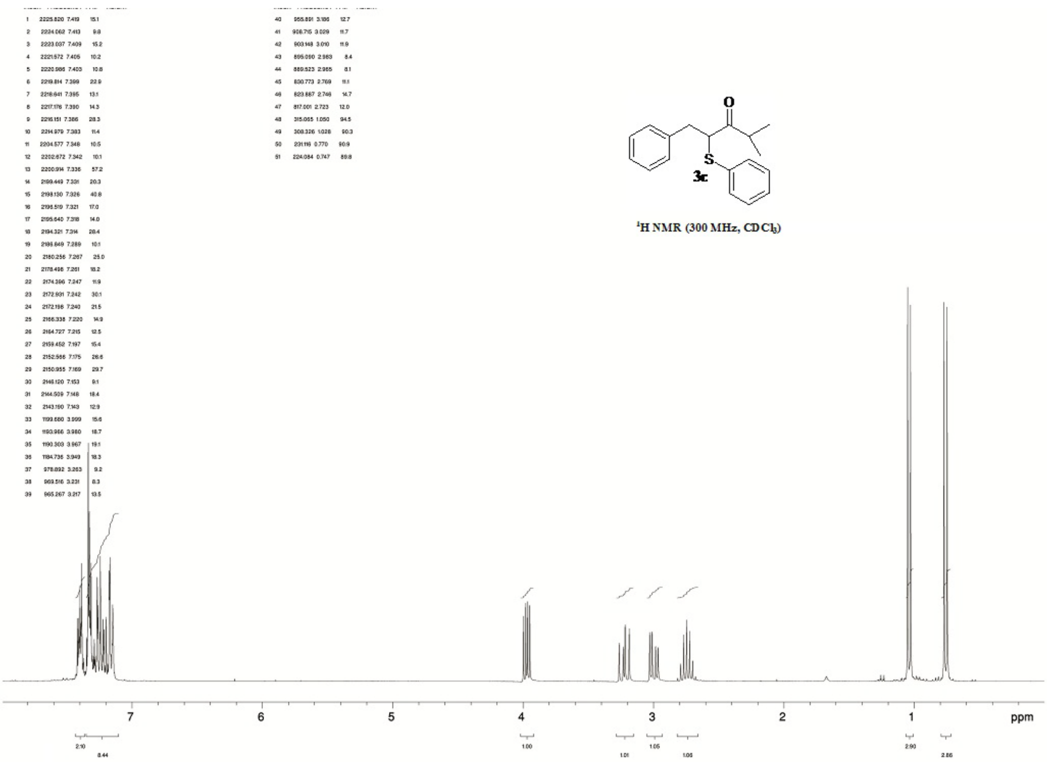
K. Copies of ^{1}H and ^{13}C NMR Spectra of all Unknown Products-



1	2211.170	7.370	12.9
2	2209.411	7.364	9.0
3	2208.825	7.362	9.7
4	2207.507	7.358	21.8
5	2205.749	7.352	16.2
6	2203.991	7.346	27.7
7	2202.672	7.342	20.0
8	2201.207	7.337	40.2
9	2199.009	7.329	12.4
10	2197.544	7.324	9.0
11	2196.812	7.322	7.2
12	2195.933	7.319	7.8
13	2194.468	7.314	11.8
14	2193.296	7.310	19.0
15	2191.098	7.303	53.7
16	2188.754	7.295	39.6
17	2187.582	7.291	47.3
18	2184.505	7.281	47.4
19	2182.161	7.273	34.6
20	2180.403	7.267	26.0
21	2178.205	7.260	118.0
22	2176.301	7.254	19.6
23	2174.836	7.249	39.7
24	2169.854	7.232	9.1
25	2168.096	7.226	18.8
26	2166.485	7.221	16.0
27	2161.210	7.203	19.9
28	2155.204	7.183	34.5
29	2153.445	7.177	39.3
30	2146.999	7.156	23.2
31	1172.722	3.909	17.9
32	1166.276	3.887	21.0
33	1164.078	3.880	22.1
34	1157.632	3.858	21.0
35	967.758	3.226	10.8
36	959.114	3.197	9.9
37	953.839	3.179	16.9
38	945.196	3.150	15.4
39	905.492	3.018	15.3
40	899.046	2.997	15.4
41	891.427	2.971	10.5
42	884.981	2.950	10.0
43	773.468	2.578	7.1
44	766.163	2.554	13.3
45	758.691	2.529	7.7
46	756.493	2.521	12.8
47	749.168	2.497	26.8
48	741.843	2.473	13.9
49	719.280	2.397	12.6
50	712.102	2.373	21.6
51	705.069	2.350	14.5
52	702.432	2.341	7.8
53	694.960	2.316	10.3
54	688.074	2.293	8.0
55	463.038	1.543	111.7
56	457.618	1.525	19.6
57	450.292	1.501	36.2
58	442.820	1.476	35.3
59	435.641	1.452	19.8
60	247.232	0.824	57.7
61	239.907	0.800	116.9
62	232.435	0.775	49.8



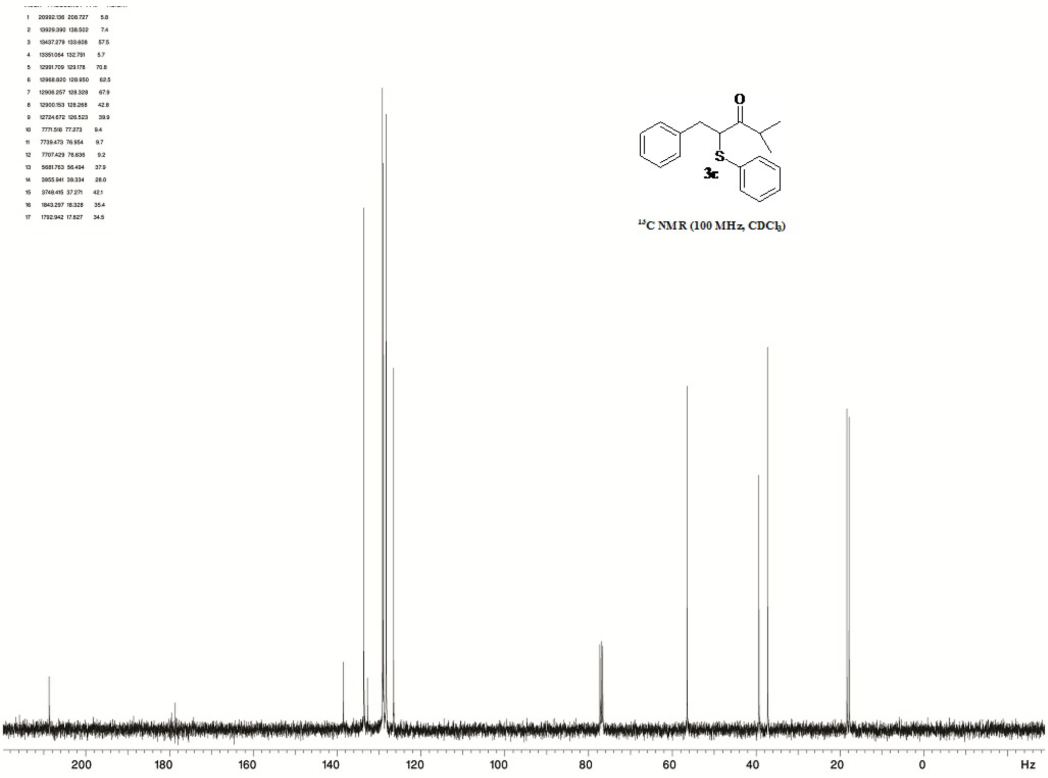
1	20716.707	205.989	10.5
2	13904.975	138.259	14.7
3	13383.872	133.077	9.2
4	13374.716	132.986	91.9
5	12981.027	129.072	94.4
6	12971.872	128.981	94.9
7	12913.887	128.404	105.3
8	12877.265	128.040	57.1
9	12732.302	126.599	62.2
10	7776.096	77.319	11.8
11	7744.051	77.000	11.7
12	7712.770	76.689	11.2
13	5830.541	57.974	61.3
14	4309.193	42.847	54.6
15	3717.134	36.960	64.2
16	1725.801	17.160	44.5
17	1359.579	13.518	39.8



3c

^{1}H NMR (300 MHz, CDCl$_3$)

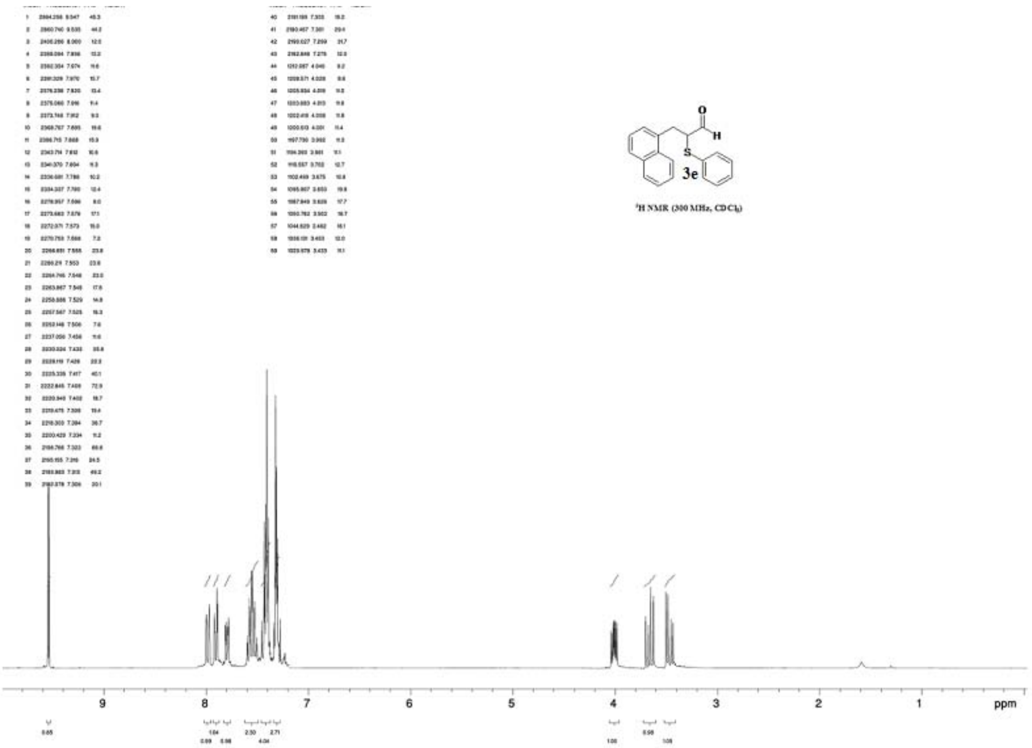
1	2225.820	7.419	15.1
2	2224.062	7.413	9.8
3	2223.037	7.409	15.2
4	2221.572	7.405	10.2
5	2220.986	7.403	10.8
6	2219.814	7.399	22.9
7	2218.641	7.395	13.1
8	2217.176	7.390	14.3
9	2216.151	7.386	28.3
10	2214.979	7.383	11.4
11	2204.577	7.348	10.5
12	2202.672	7.342	10.1
13	2200.914	7.336	57.2
14	2199.449	7.331	20.3
15	2198.130	7.326	40.8
16	2196.519	7.321	17.0
17	2195.640	7.318	14.0
18	2194.321	7.314	28.4
19	2186.849	7.289	10.1
20	2180.256	7.267	25.0
21	2178.498	7.261	18.2
22	2174.396	7.247	11.9
23	2172.931	7.242	30.1
24	2172.198	7.240	21.5
25	2166.338	7.220	14.9
26	2164.727	7.215	12.5
27	2159.452	7.197	15.4
28	2152.566	7.175	26.6
29	2150.955	7.169	29.7
30	2146.120	7.153	9.1
31	2144.509	7.148	18.4
32	2143.190	7.143	12.9
33	1199.880	3.999	15.6
34	1193.966	3.980	18.7
35	1190.303	3.967	19.1
36	1184.736	3.949	18.3
37	978.892	3.263	9.2
38	969.516	3.231	8.3
39	965.267	3.217	13.5
40	955.891	3.186	12.7
41	908.715	3.029	11.7
42	903.148	3.010	11.9
43	895.090	2.983	8.4
44	889.523	2.965	8.1
45	830.773	2.769	11.1
46	823.887	2.746	14.7
47	817.001	2.723	12.0
48	315.065	1.050	94.5
49	308.326	1.028	90.3
50	231.116	0.770	90.9
51	224.084	0.747	89.8

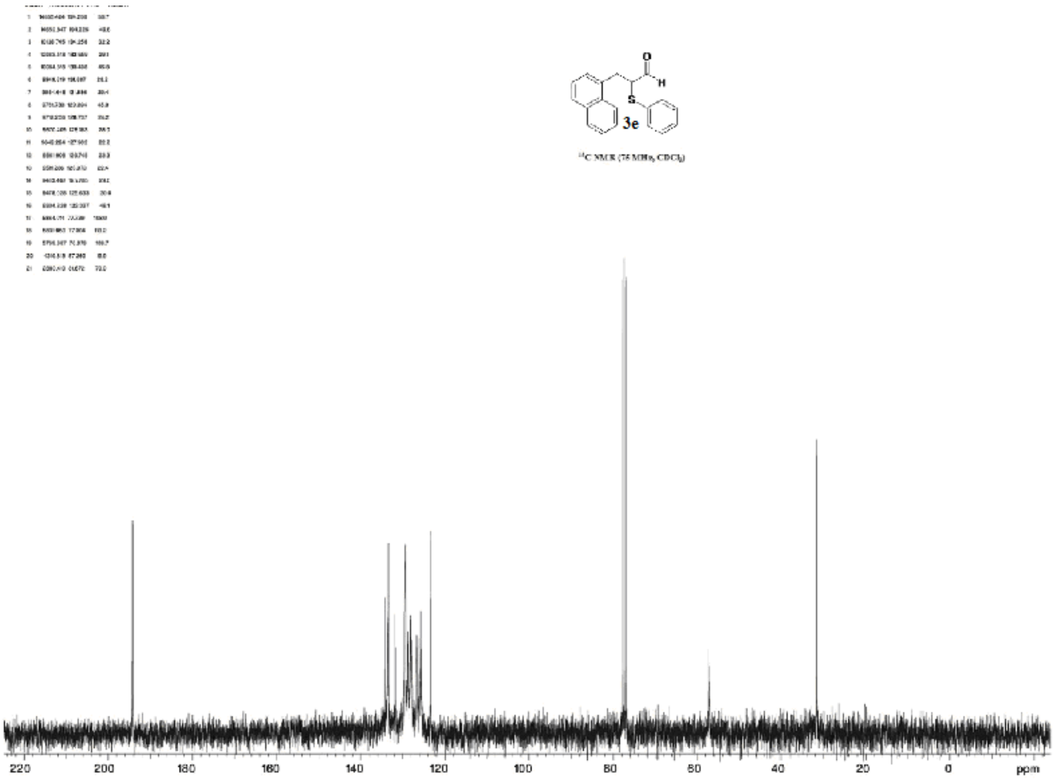


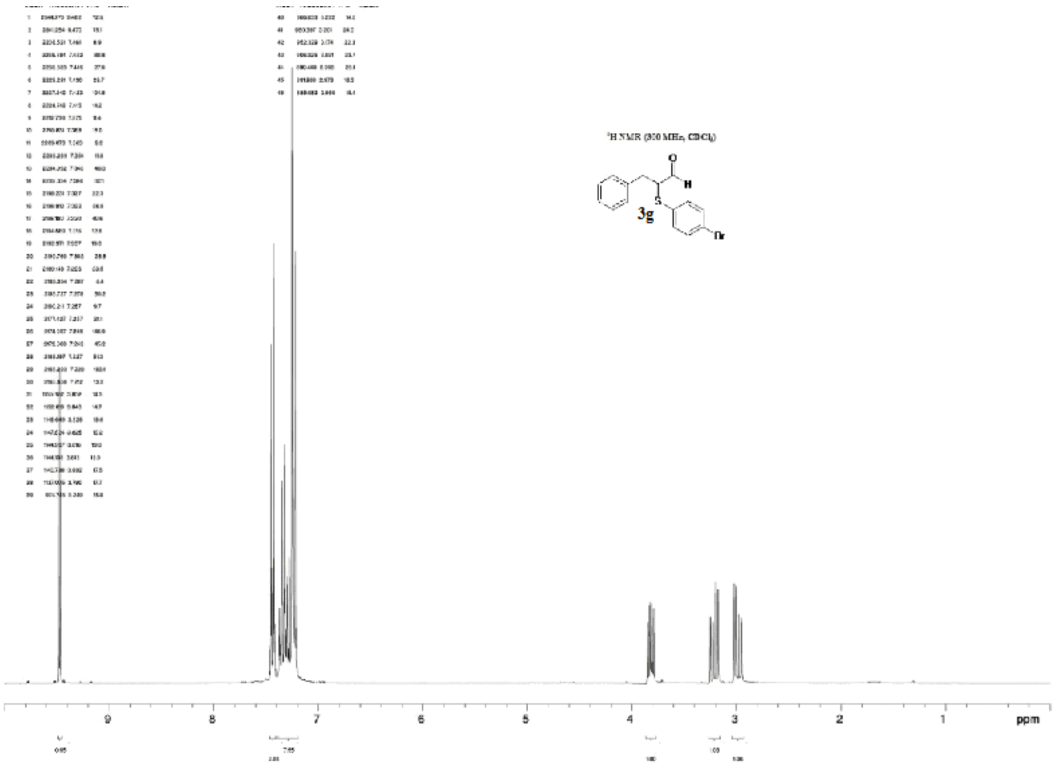
3c

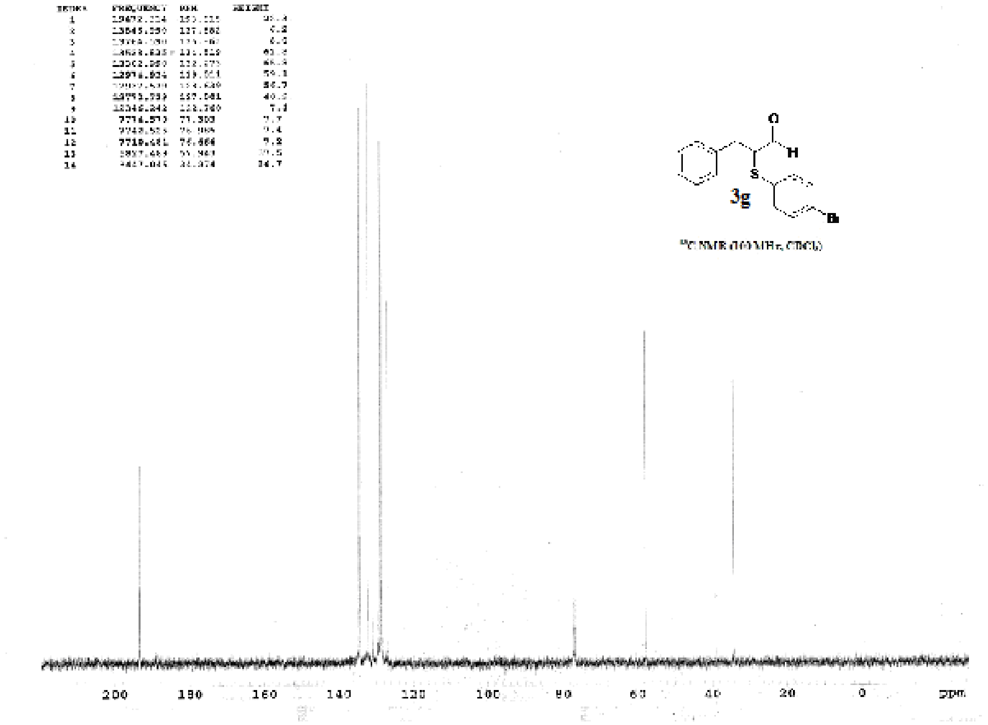
^{13}C NMR (100 MHz, CDCl$_3$)

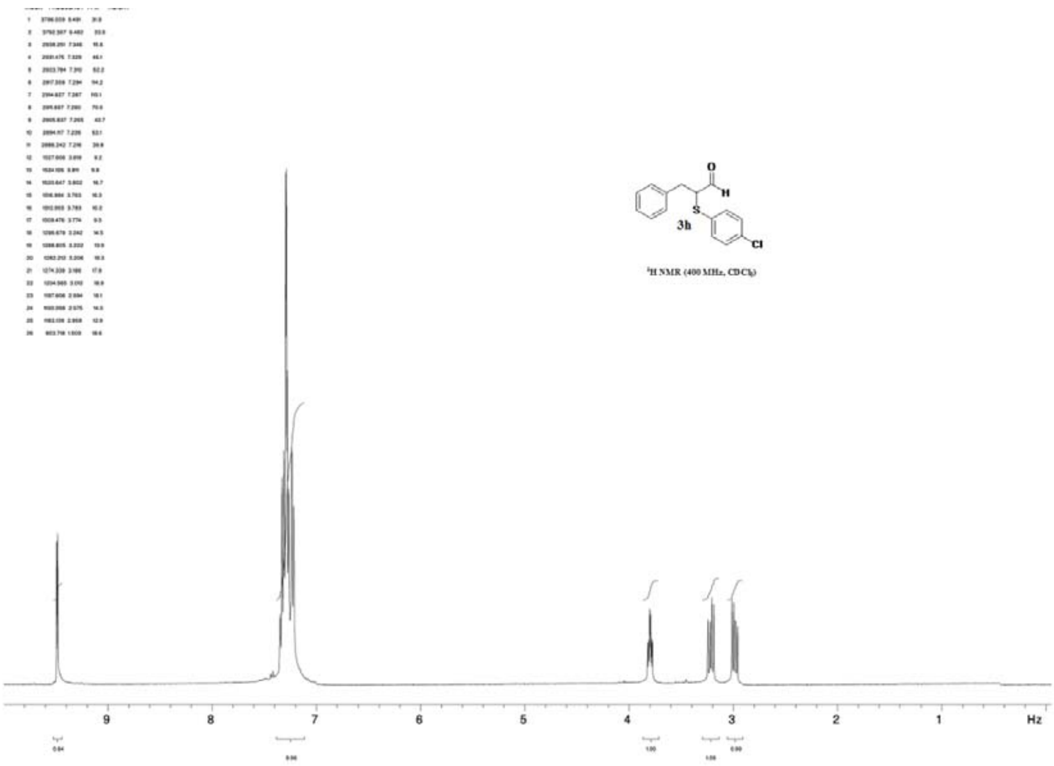
1	20992.136	208.727	5.8
2	13929.390	138.502	7.4
3	13437.279	133.608	57.5
4	13351.064	132.751	5.7
5	12991.709	129.178	70.8
6	12968.820	128.950	62.5
7	12906.257	128.328	67.9
8	12900.153	128.268	42.8
9	12724.672	126.523	39.9
10	7771.518	77.273	9.4
11	7739.473	76.954	9.7
12	7707.429	76.636	9.2
13	5681.763	56.494	37.9
14	3955.941	39.334	28.0
15	3748.415	37.271	42.1
16	1843.297	18.328	35.4
17	1792.942	17.827	34.5


3e
¹H NMR (300 MHz, CDCl₃)
9
8
7
6
5
4
3
2
1
ppm
0.65
1.04
0.99
0.98
2.30
2.71
4.04
1.00
0.98
1.00

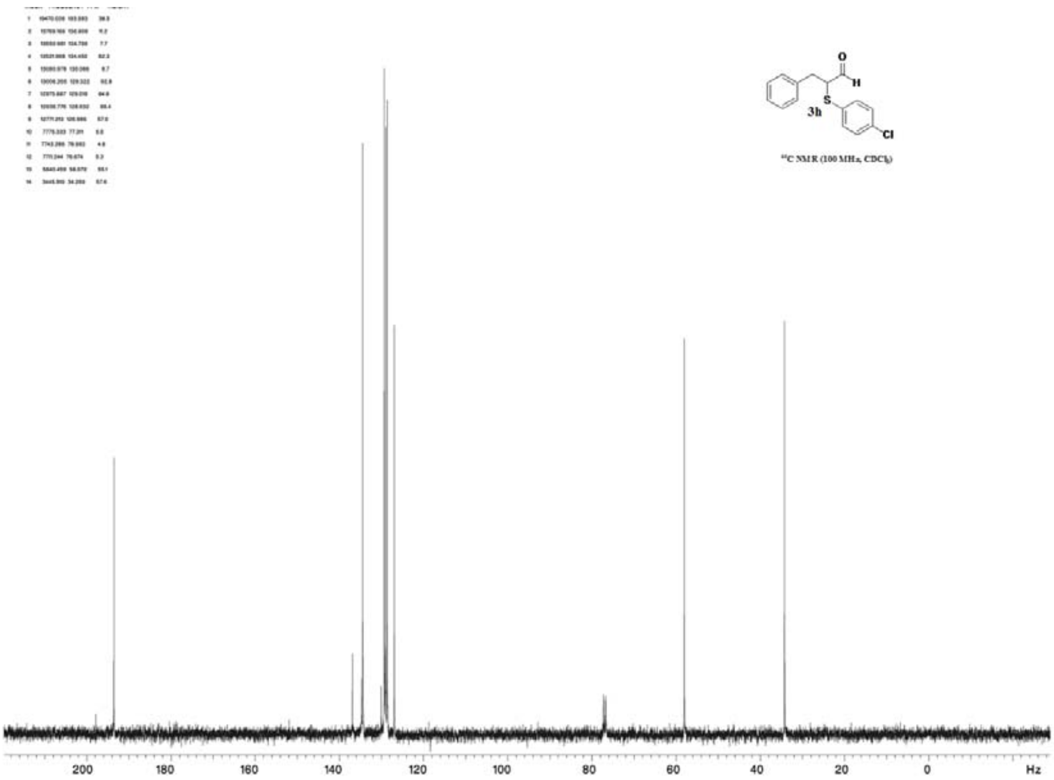

3e
¹³C NMR (75 MHz, CDCl₃)
220
200
180
160
140
120
100
80
60
40
20
0
ppm


^{1}H NMR (300 MHz, CDCl$_3$)
O
H
S
3g
Br
9
8
7
6
5
4
3
2
1
ppm

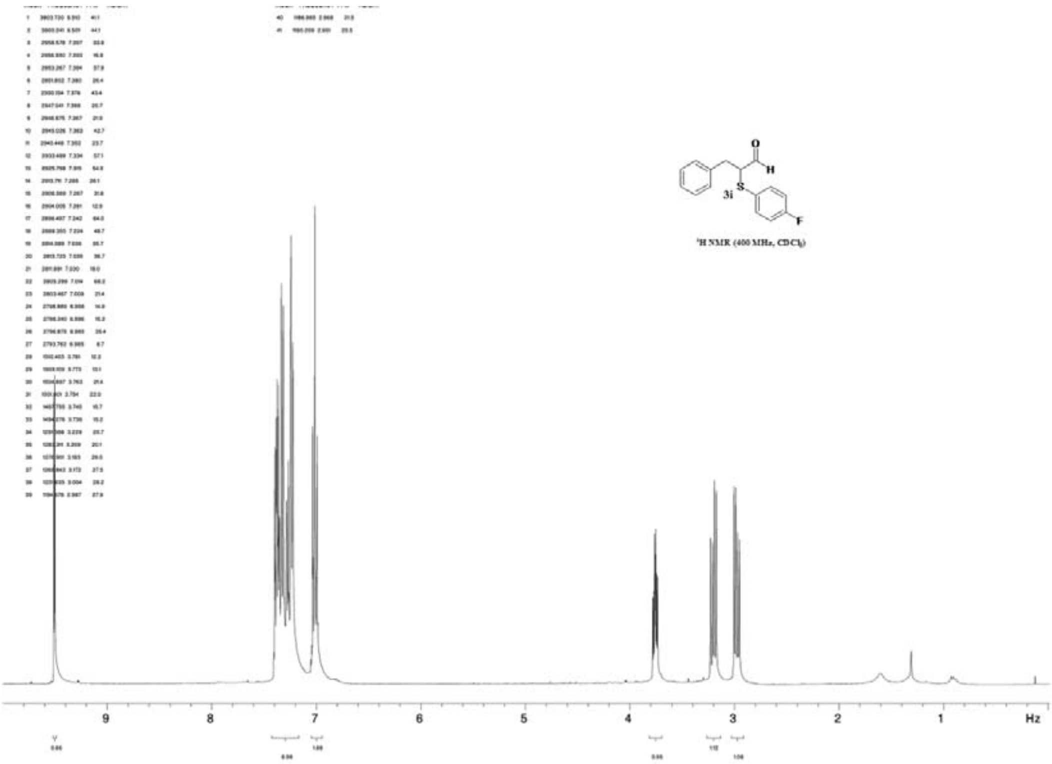

O
H
S
3g
Br
^{13}C NMR (100 MHz, CDCl$_3$)
200
180
160
140
120
100
80
60
40
20
0
ppm

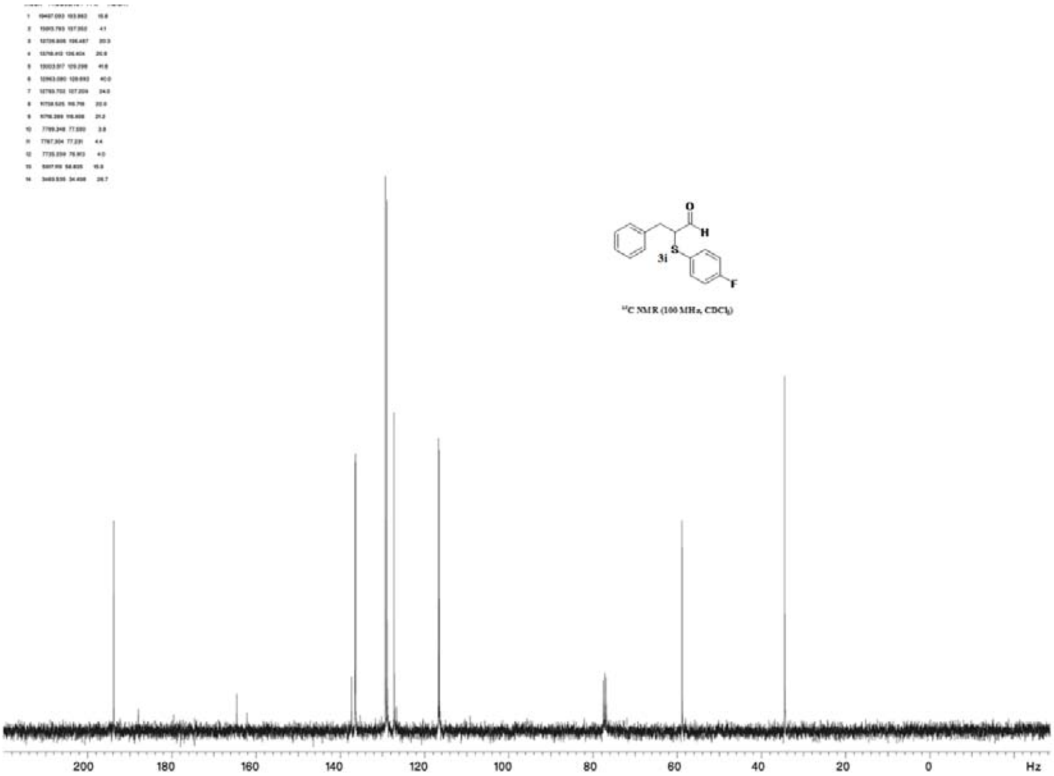


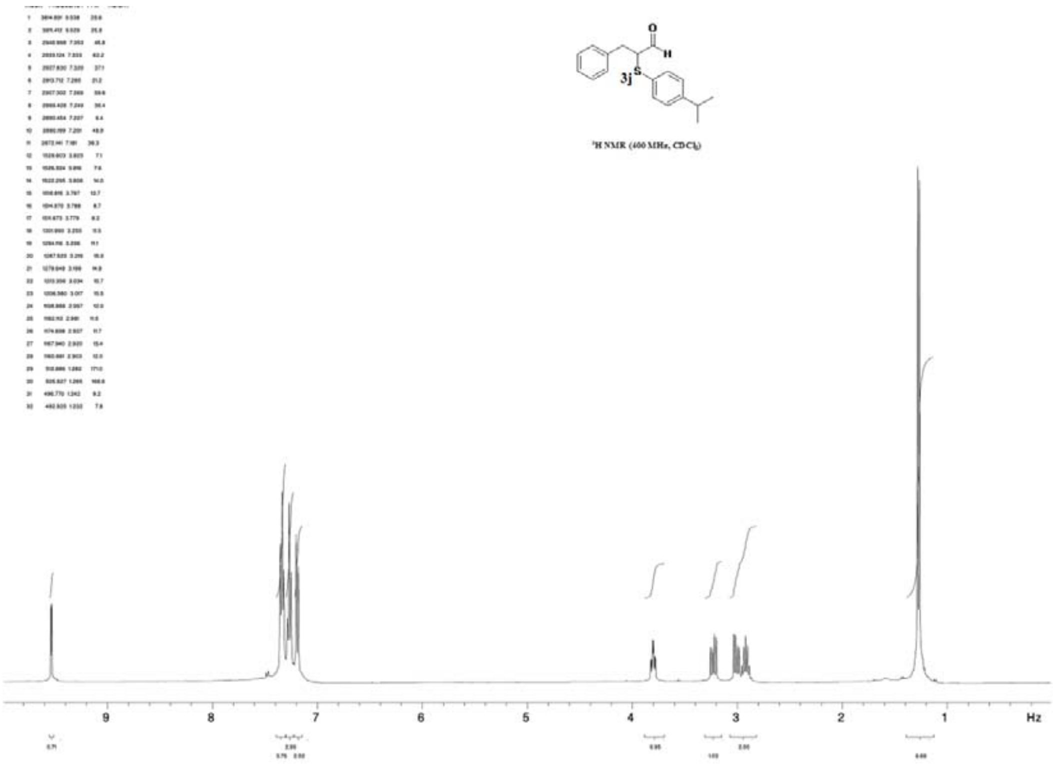
^{1}H NMR (400 MHz, CDCl$_3$)

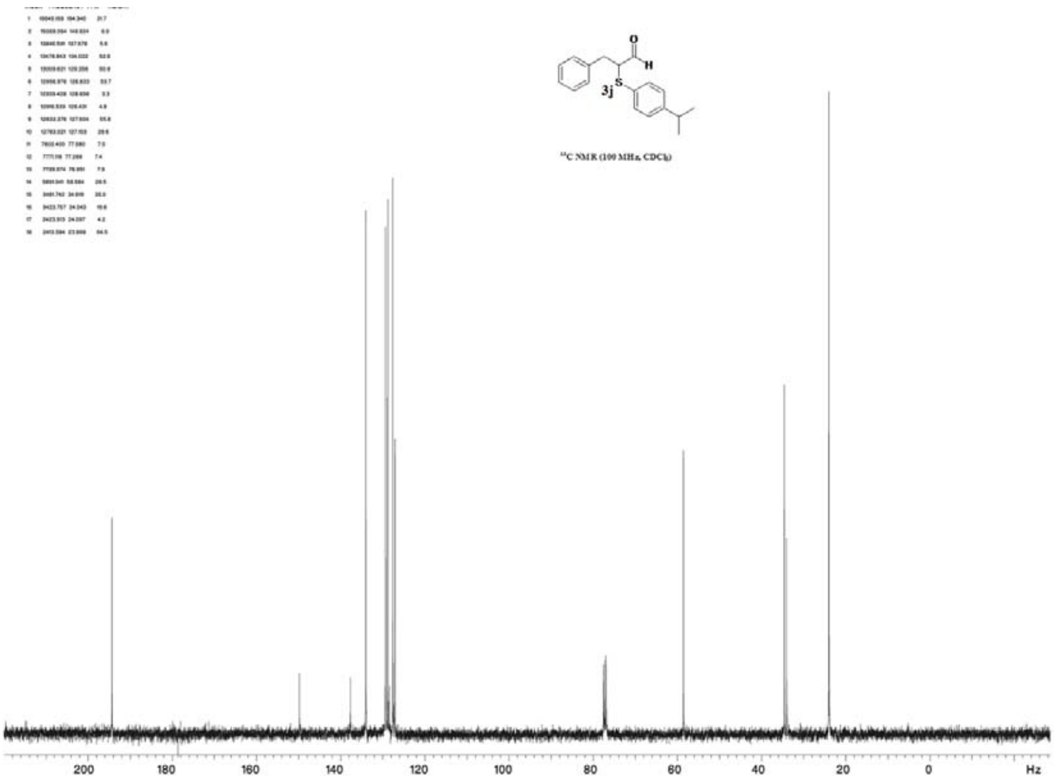


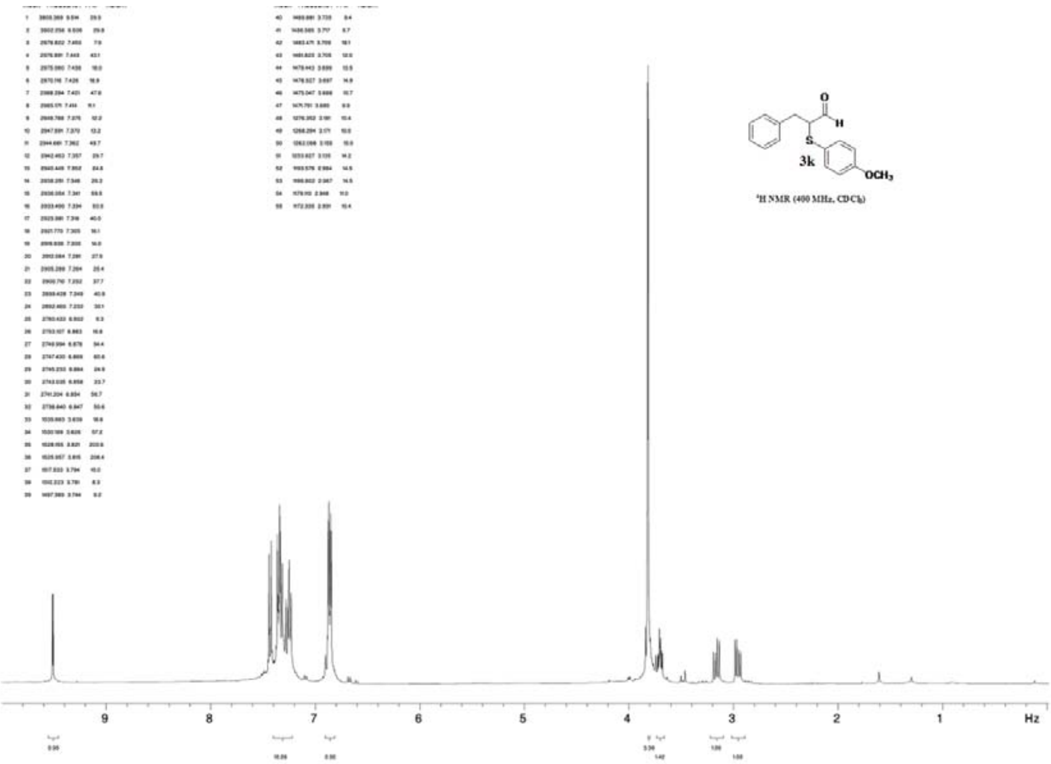
^{13}C NMR (100 MHz, CDCl$_3$)

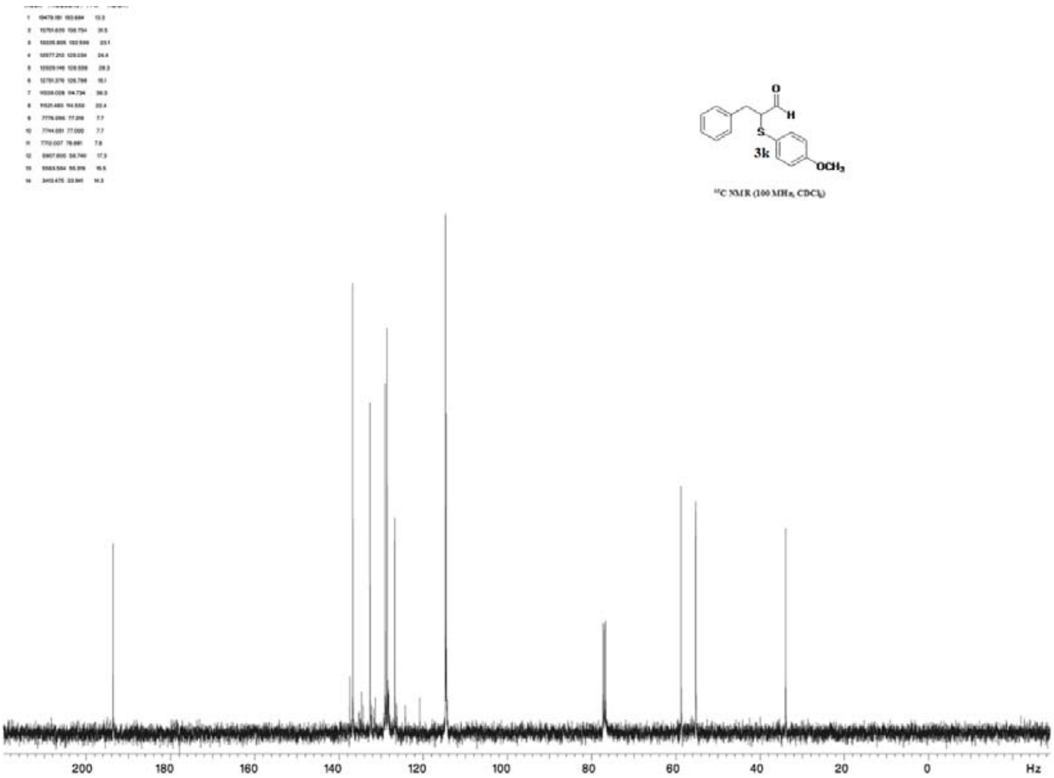

O
H
S
3i
F
¹H NMR (400 MHz, CDCl₃)
9
8
7
6
5
4
3
2
1
Hz

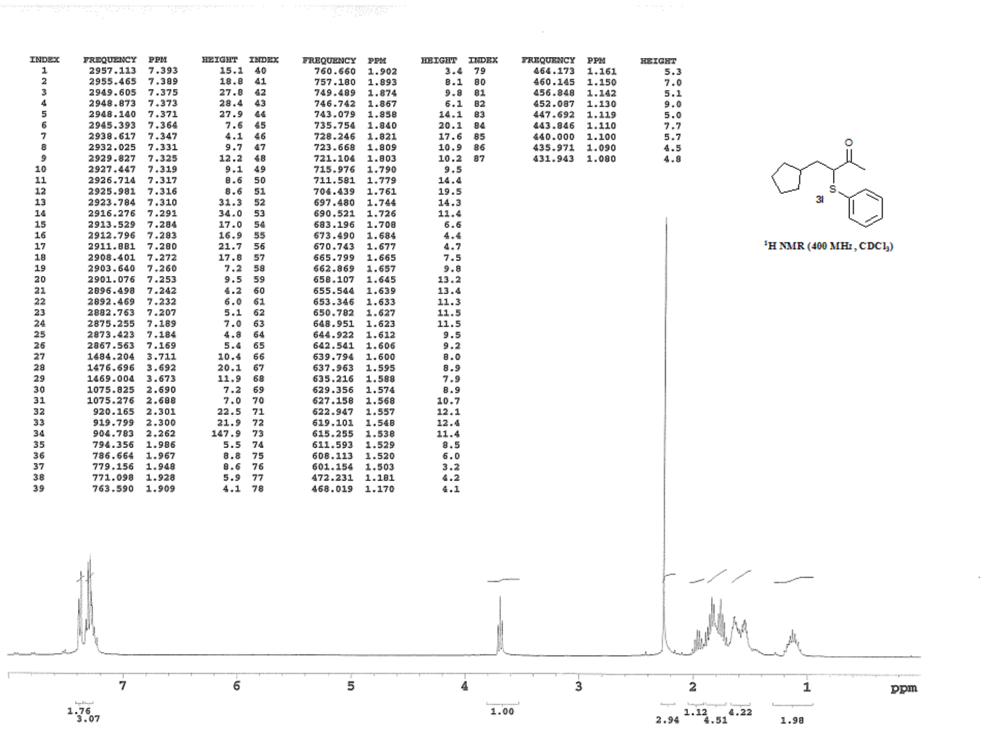

O
H
S
3i
F
¹³C NMR (100 MHz, CDCl₃)
200
180
160
140
120
100
80
60
40
20
0
Hz


O
H
S
3j
1H NMR (400 MHz, CDCl3)
9
8
7
6
5
4
3
2
1
Hz


O
H
S
3j
13C NMR (100 MHz, CDCl3)
200
180
160
140
120
100
80
60
40
20
0
Hz

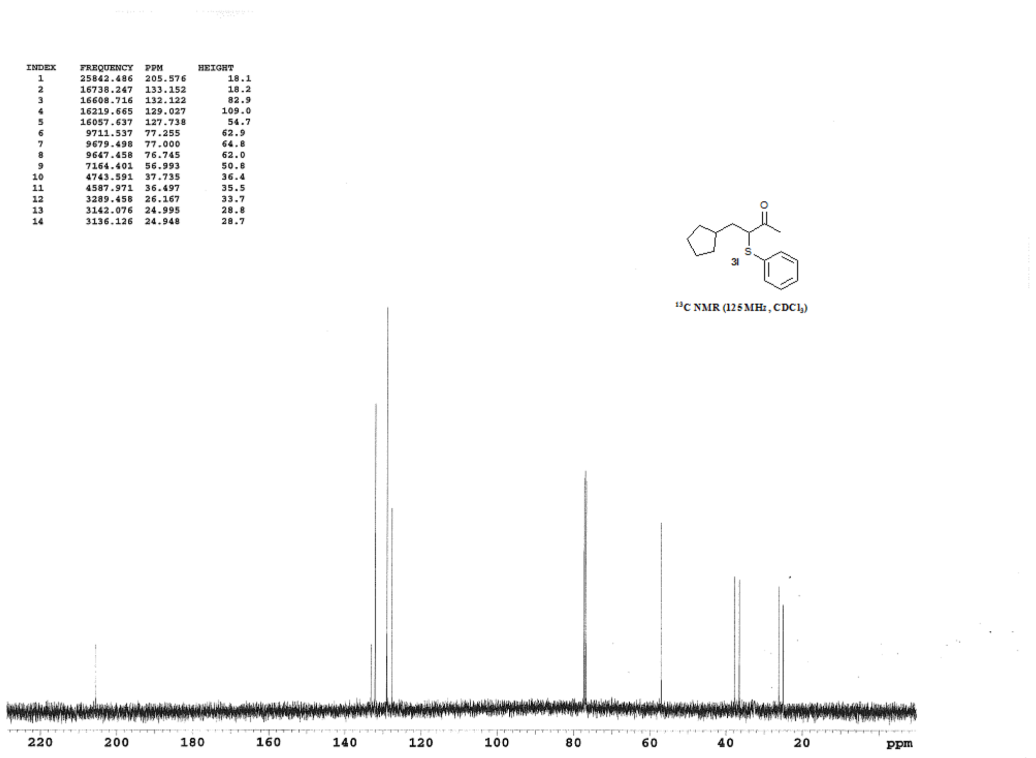

O
H
S
3k
OCH$_3$
^{1}H NMR (400 MHz, CDCl$_3$)
9
8
7
6
5
4
3
2
1
Hz


O
H
S
3k
OCH$_3$
^{13}C NMR (100 MHz, CDCl$_3$)
200
180
160
140
120
100
80
60
40
20
0
Hz



¹H NMR (400 MHz, CDCl$_3$)

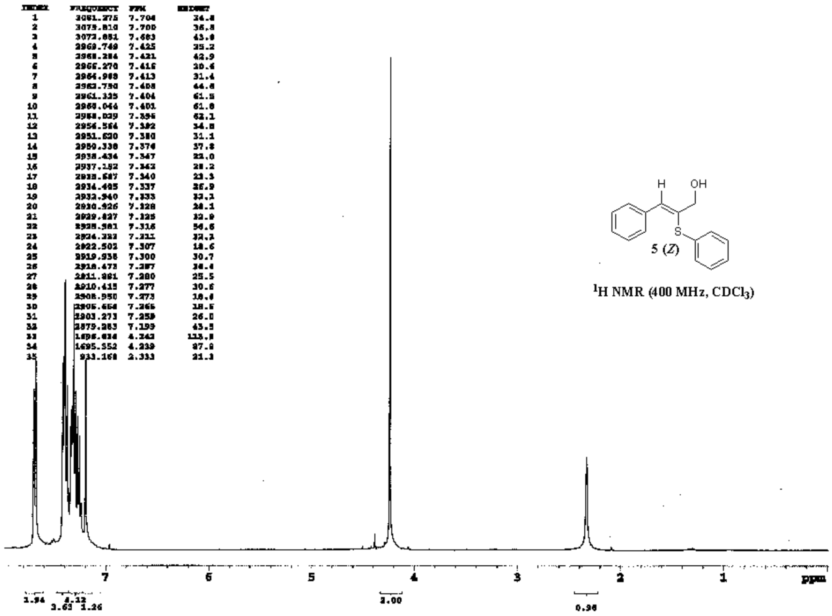
INDEX	FREQUENCY	PPM	HEIGHT
1	2957.113	7.393	15.1
2	2955.465	7.389	18.8
3	2949.605	7.375	27.8
4	2948.873	7.373	28.4
5	2948.140	7.371	27.9
6	2945.393	7.364	7.6
7	2938.617	7.347	4.1
8	2932.025	7.331	9.7
9	2929.827	7.325	12.2
10	2927.447	7.319	9.1
11	2926.714	7.317	8.6
12	2925.981	7.316	8.6
13	2923.784	7.310	31.3
14	2916.276	7.291	34.0
15	2913.529	7.284	17.0
16	2912.796	7.283	16.9
17	2911.881	7.280	21.7
18	2908.401	7.272	17.8
19	2903.640	7.260	7.2
20	2901.076	7.253	9.5
21	2896.498	7.242	4.2
22	2892.469	7.232	6.0
23	2882.763	7.207	5.1
24	2875.255	7.189	7.0
25	2873.423	7.184	4.8
26	2867.563	7.169	5.4
27	1484.204	3.711	10.4
28	1476.696	3.692	20.1
29	1469.004	3.673	11.9
30	1075.825	2.690	7.2
31	1075.276	2.688	7.0
32	920.165	2.301	22.5
33	919.799	2.300	21.9
34	904.783	2.262	147.9
35	794.356	1.986	5.5
36	786.664	1.967	8.8
37	779.156	1.948	8.6
38	771.098	1.928	5.9
39	763.590	1.909	4.1
40	760.660	1.902	3.4
41	757.180	1.893	8.1
42	749.489	1.874	9.8
43	746.742	1.867	6.1
44	743.079	1.858	14.1
45	735.754	1.840	20.1
46	728.246	1.821	17.6
47	723.668	1.809	10.9
48	721.104	1.803	10.2
49	715.976	1.790	9.5
50	711.581	1.779	14.4
51	704.439	1.761	19.5
52	697.480	1.744	14.3
53	690.521	1.726	11.4
54	683.196	1.708	6.6
55	673.490	1.684	4.4
56	670.743	1.677	4.7
57	665.799	1.665	7.5
58	662.869	1.657	9.8
59	658.107	1.645	13.2
60	655.544	1.639	13.4
61	653.346	1.633	11.3
62	650.782	1.627	11.5
63	648.951	1.623	11.5
64	644.922	1.612	9.5
65	642.541	1.606	9.2
66	639.794	1.600	8.0
67	637.963	1.595	8.9
68	635.216	1.588	7.9
69	629.356	1.574	8.9
70	627.158	1.568	10.7
71	622.947	1.557	12.1
72	619.101	1.548	12.4
73	615.255	1.538	11.4
74	611.593	1.529	8.5
75	608.113	1.520	6.0
76	601.154	1.503	3.2
77	472.231	1.181	4.2
78	468.019	1.170	4.1
79	464.173	1.161	5.3
80	460.145	1.150	7.0
81	456.848	1.142	5.1
82	452.087	1.130	9.0
83	447.692	1.119	5.0
84	443.846	1.110	7.7
85	440.000	1.100	5.7
86	435.971	1.090	4.5
87	431.943	1.080	4.8



¹³C NMR (125 MHz, CDCl$_3$)

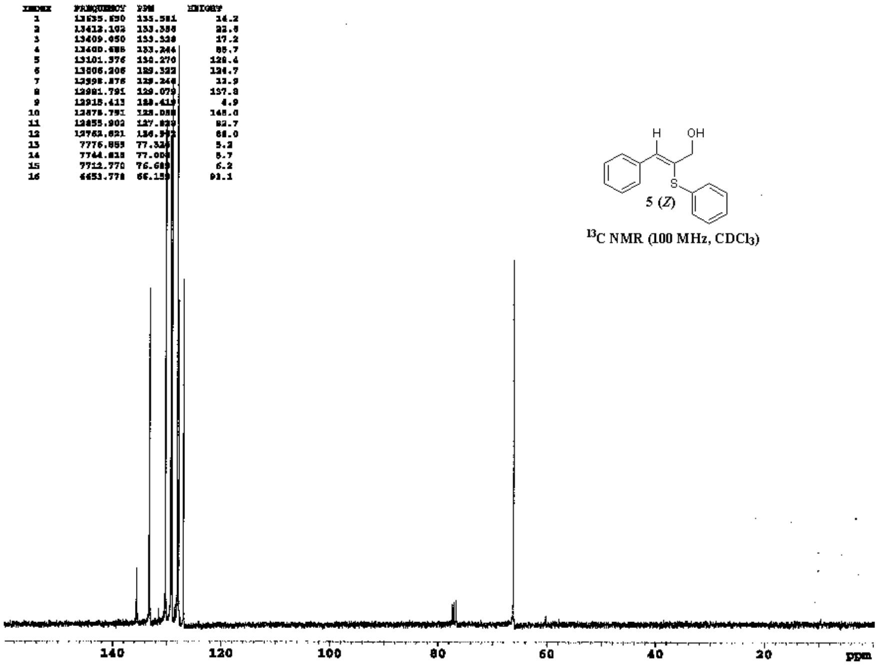
INDEX	FREQUENCY	PPM	HEIGHT
1	25842.486	205.576	18.1
2	16738.247	133.152	18.2
3	16608.716	132.122	82.9
4	16219.665	129.027	109.0
5	16057.637	127.738	54.7
6	9711.537	77.255	62.9
7	9679.498	77.000	64.8
8	9647.458	76.745	62.0
9	7164.401	56.993	50.8
10	4743.591	37.735	36.4
11	4587.971	36.497	35.5
12	3289.458	26.167	33.7
13	3142.076	24.995	28.8
14	3136.126	24.948	28.7

L. Copies of NMR spectra of isolated intermediate 5-



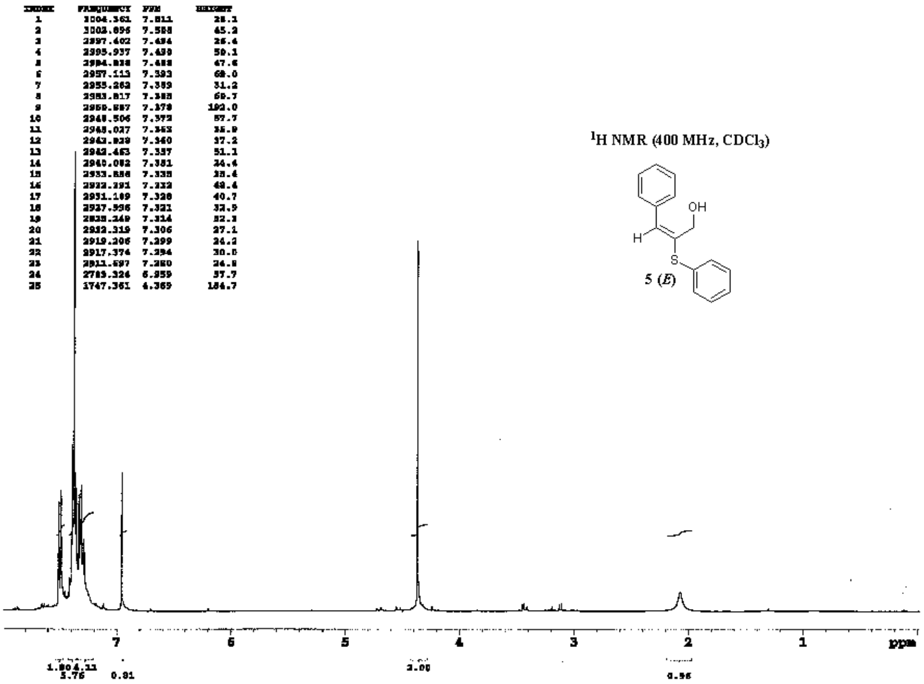
^{1}H NMR (400 MHz, CDCl$_3$)

INDEX	FREQUENCY	PPM	HEIGHT
1	3081.275	7.704	34.8
2	3079.810	7.700	36.8
3	3072.851	7.683	43.8
4	2969.749	7.425	35.2
5	2968.284	7.421	42.9
6	2966.270	7.416	30.6
7	2964.988	7.413	31.4
8	2962.750	7.408	44.8
9	2961.325	7.404	61.5
10	2960.044	7.401	61.8
11	2958.029	7.396	62.1
12	2956.564	7.392	34.8
13	2951.620	7.380	31.1
14	2950.338	7.376	37.8
15	2938.434	7.347	22.0
16	2937.152	7.343	28.2
17	2935.687	7.340	23.3
18	2934.405	7.337	26.9
19	2932.940	7.333	32.1
20	2930.926	7.328	28.1
21	2929.827	7.325	32.9
22	2925.981	7.316	56.6
23	2924.333	7.311	32.2
24	2922.502	7.307	18.6
25	2919.938	7.300	30.7
26	2918.473	7.297	38.4
27	2911.881	7.280	25.5
28	2910.415	7.277	30.6
29	2908.950	7.273	18.4
30	2905.654	7.265	18.5
31	2903.273	7.259	26.0
32	2879.283	7.199	43.5
33	1696.634	4.242	113.8
34	1695.352	4.239	87.0
35	933.168	2.333	21.3



^{13}C NMR (100 MHz, CDCl$_3$)

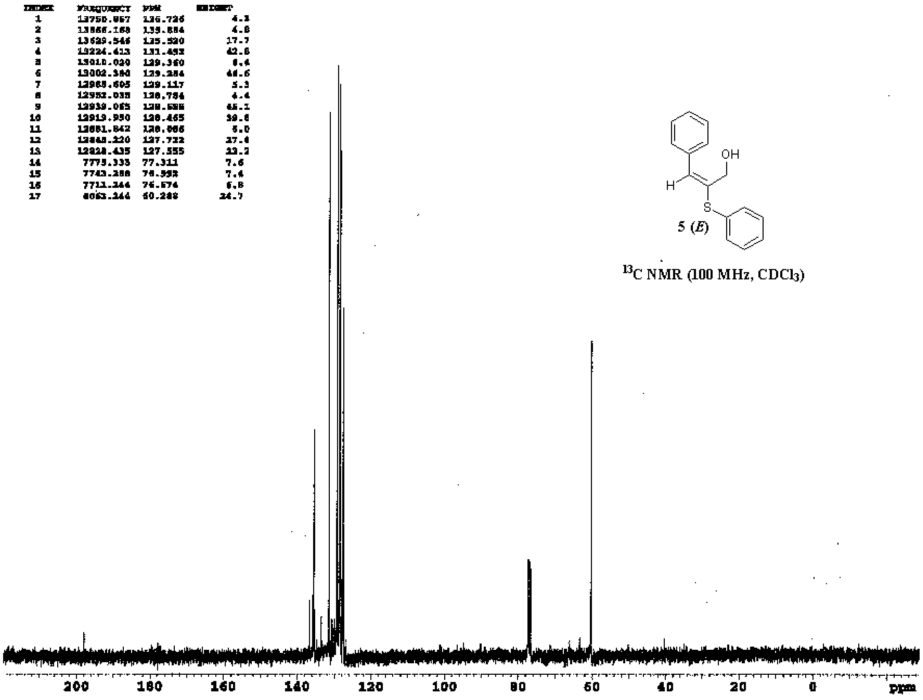
INDEX	FREQUENCY	PPM	HEIGHT
1	13635.690	135.581	14.2
2	13412.102	133.356	22.8
3	13409.050	133.326	17.2
4	13400.688	133.244	88.7
5	13101.376	130.270	128.4
6	13006.206	129.322	134.7
7	12998.876	129.248	12.9
8	12981.791	129.079	157.8
9	12918.413	128.449	4.9
10	12878.791	128.055	148.0
11	12855.902	127.828	82.7
12	12762.821	126.902	68.0
13	7776.855	77.326	5.2
14	7744.818	77.008	5.7
15	7712.770	76.689	6.2
16	6653.778	66.159	91.1



INDEX	FREQUENCY	PPM	HEIGHT
1	3004.361	7.511	28.1
2	3003.096	7.508	45.2
3	2997.402	7.494	26.4
4	2995.937	7.490	50.1
5	2994.838	7.488	47.6
6	2957.113	7.393	68.0
7	2955.262	7.389	31.2
8	2953.817	7.385	60.7
9	2950.887	7.378	192.0
10	2948.506	7.372	57.7
11	2945.027	7.363	35.9
12	2943.939	7.360	37.2
13	2942.463	7.357	51.1
14	2940.082	7.351	24.4
15	2933.886	7.335	35.4
16	2932.391	7.332	48.4
17	2931.189	7.328	40.7
18	2927.996	7.321	32.9
19	2925.249	7.314	52.3
20	2922.319	7.306	27.1
21	2919.206	7.299	24.2
22	2917.374	7.294	30.0
23	2911.697	7.280	24.8
24	2783.324	6.959	37.7
25	1747.361	4.369	184.7

^{1}H NMR (400 MHz, $CDCl_3$)

5 (*E*)

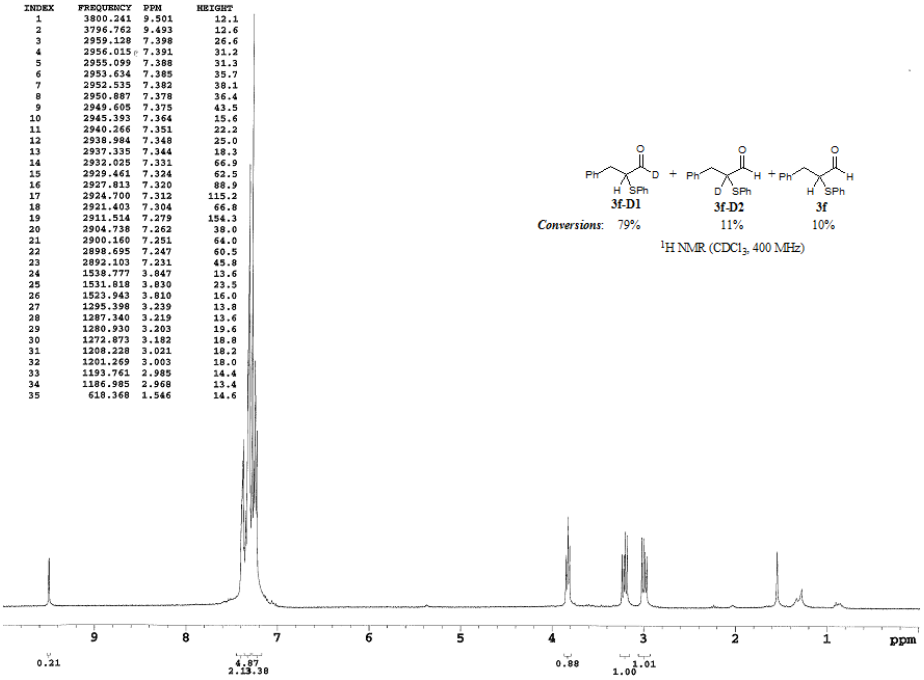


INDEX	FREQUENCY	PPM	HEIGHT
1	13750.957	136.726	4.3
2	13666.168	135.884	4.8
3	13629.546	135.520	17.7
4	13224.413	131.493	42.8
5	13010.020	129.360	8.4
6	13002.380	129.284	46.6
7	12985.605	129.117	5.3
8	12952.035	128.784	4.4
9	12939.065	128.654	45.1
10	12919.950	128.465	39.8
11	12881.842	128.086	5.0
12	12845.220	127.722	27.4
13	12828.435	127.555	33.2
14	7775.333	77.311	7.6
15	7743.288	76.993	7.4
16	7711.244	76.674	6.8
17	6063.244	60.288	24.7

5 (*E*)

^{13}C NMR (100 MHz, $CDCl_3$)

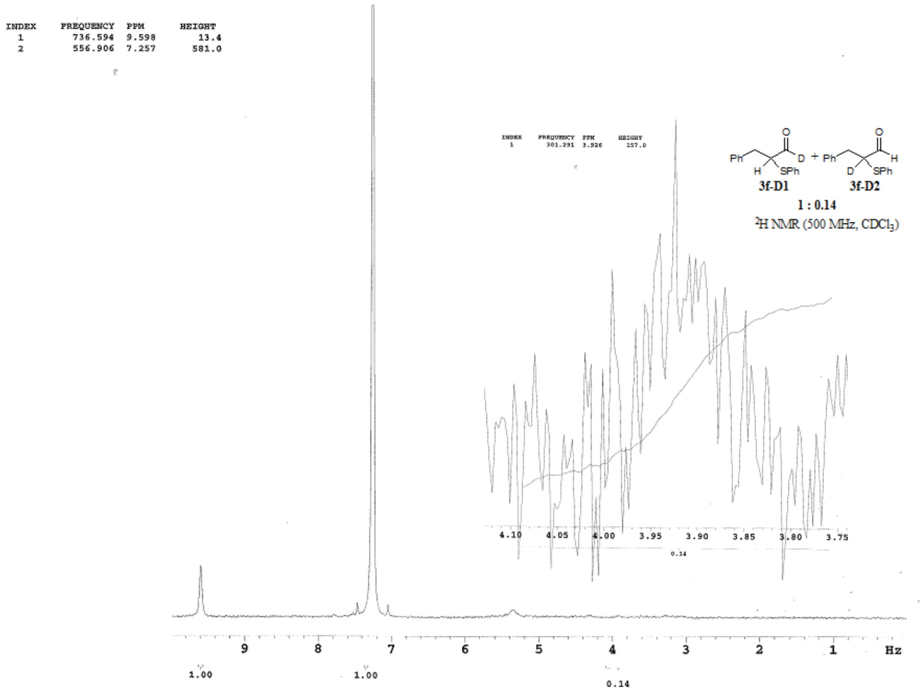
M. Copies of NMR spectra of deuterated products-



INDEX	FREQUENCY	PPM	HEIGHT
1	3800.241	9.501	12.1
2	3796.762	9.493	12.6
3	2959.128	7.398	26.6
4	2956.015	7.391	31.2
5	2955.099	7.388	31.3
6	2953.634	7.385	35.7
7	2952.535	7.382	38.1
8	2950.887	7.378	36.4
9	2949.605	7.375	43.5
10	2945.393	7.364	15.6
11	2940.266	7.351	22.2
12	2938.984	7.348	25.0
13	2937.335	7.344	18.3
14	2932.025	7.331	66.9
15	2929.461	7.324	62.5
16	2927.813	7.320	88.9
17	2924.700	7.312	115.2
18	2921.403	7.304	66.8
19	2911.514	7.279	154.3
20	2904.738	7.262	38.0
21	2900.160	7.251	64.0
22	2898.695	7.247	60.5
23	2892.103	7.231	45.8
24	1538.777	3.847	13.6
25	1531.818	3.830	23.5
26	1523.943	3.810	16.0
27	1295.398	3.239	13.8
28	1287.340	3.219	13.6
29	1280.930	3.203	19.6
30	1272.873	3.182	18.8
31	1208.228	3.021	18.2
32	1201.269	3.003	18.0
33	1193.761	2.985	14.4
34	1186.985	2.968	13.4
35	618.368	1.546	14.6

Conversions: 79% 11% 10%

^{1}H NMR ($CDCl_3$, 400 MHz)

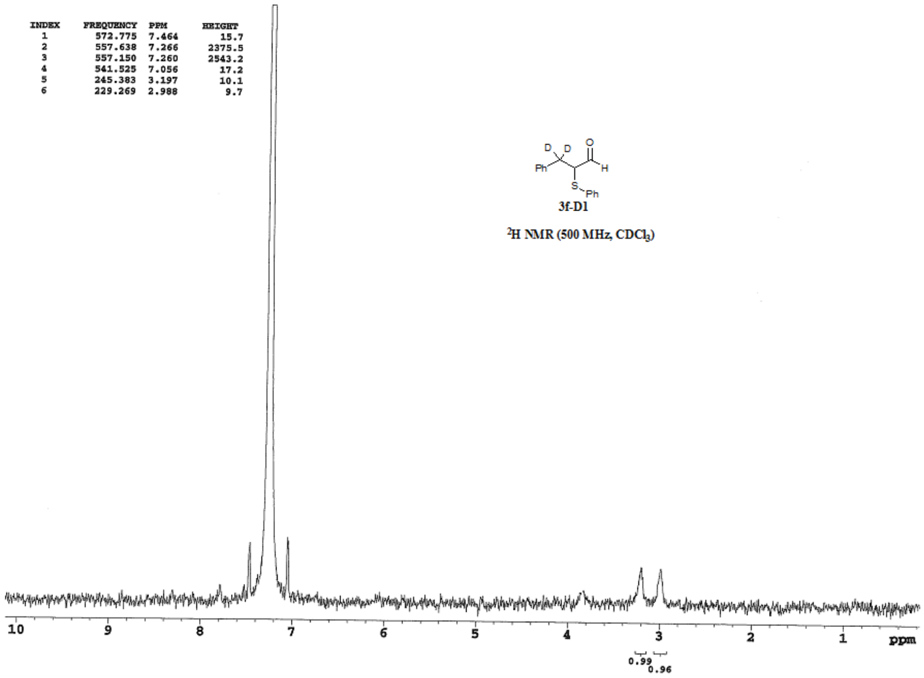


INDEX	FREQUENCY	PPM	HEIGHT
1	736.594	9.598	13.4
2	556.906	7.257	581.0

INDEX	FREQUENCY	PPM	HEIGHT
1	301.291	3.926	157.0

1 : 0.14

^{2}H NMR (500 MHz, $CDCl_3$)



INDEX	FREQUENCY	PPM	HEIGHT
1	572.775	7.464	15.7
2	557.638	7.266	2375.5
3	557.150	7.260	2543.2
4	541.525	7.056	17.2
5	245.383	3.197	10.1
6	229.269	2.988	9.7

3f-D1

^{2}H NMR (500 MHz, $CDCl_3$)

N. References-

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