Supporting Information

Photocatalytic Radical Aroylation of Unactivated Alkenes: Pathway to β-Functionalized 1,4-, 1,6-, and 1,7-Diketones

Satavisha Sarkar,[‡], Arghya Banerjee,[‡] Wang Yao, Eric V. Patterson, Ming-Yu Ngai*

ming-yu.ngai@stonybrook.edu

Department of Chemistry and Institute of Chemical Biology and Drug Discovery,
The State University of New York, Stony Brook, New York 11794-3400

Table of Contents

General Information

All air- and moisture-insensitive reactions were carried out under an ambient atmosphere, magnetically stirred, and monitored by thin layer chromatography (TLC) using Agela Technologies TLC plates pre-coated with 250 μm thickness silica gel 60 F254 plates and visualized by fluorescence quenching under UV light. Flash chromatography was performed on SiliaFlash® Silica Gel 40-63μm 60Å particle size using a forced flow of eluent at 0.3–0.5 bar pressure.[1] Preparative TLC was performed on Uniplate® UV254 (20 x 20 cm) with 1000 μm thickness and visualized fluorescence quenching under UV light.

All air and moisture-sensitive manipulations were performed using oven-dried glassware, including standard Schlenk and glovebox techniques under an atmosphere of nitrogen. All reaction vials were capped using green caps with F-217 PTFE liners. Diethyl ether and THF were distilled from deep purple sodium benzophenone ketyl. Acetonitrile were dried over CaH_2 and distilled. Acetonitrile was degassed *via* three freeze-pump-thaw cycles. Dry DMA was degassed *via* three freeze-pump-thaw cycles. All other chemicals were used as received.

All deuterated solvents were purchased from Cambridge Isotope Laboratories. NMR spectra were recorded on either a Bruker Ascend 700 spectrometer operating at 700 MHz for ^{1}H acquisitions and 175 MHz for ^{13}C acquisitions, a Bruker 500 Advance spectrometer operating at 500 MHz, 125 MHz, and 470 MHz for ^{1}H, ^{13}C, and ^{19}F acquisitions, respectively, a Bruker 400 Nanobay spectrometer operating at 400 MHz, 100 MHz, and 376 MHz for ^{1}H, ^{13}C, and ^{19}F acquisitions, respectively. Chemical shifts were referenced to the residual proton solvent peaks (^{1}H: $CDCl_3$, δ 7.26) solvent ^{13}C signals ($CDCl_3$, δ 77.23),[2] dissolved or external neat $PhCF_3$ (^{19}F, δ –63.3 relative to $CFCl_3$)[3] or *m*-fluoronitrobenzene (19F, –112.01)[4]. Signals are listed in ppm, and multiplicity identified as s = singlet, br = broad, d = doublet, t = triplet, q = quartet, m = multiplet; coupling constants in Hz; integration.

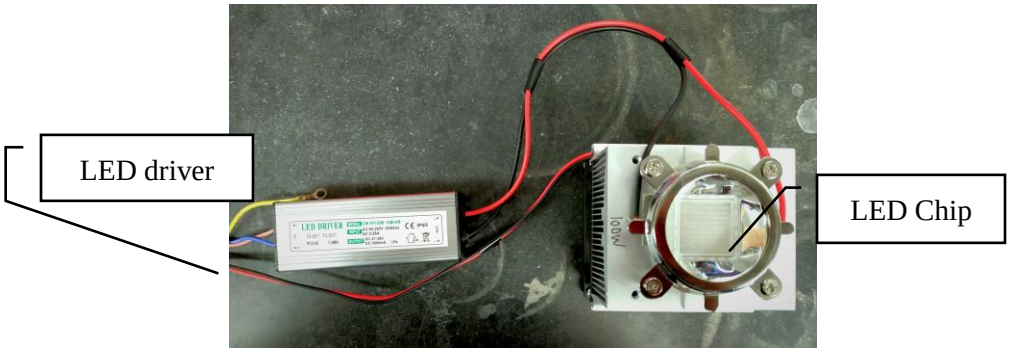
High-resolution mass spectra were performed at Mass Spectrometry Services at Stony Brook University and were obtained using Agilent LC-UV-TOF mass spectrometer. Concentration under reduced pressure was performed by rotary evaporation at 25–30 °C at the appropriate pressure. Purified compounds were further dried under high vacuum (0.01–0.05 Torr). Yields refer to purified and spectroscopically pure compounds.

Enantiomeric excesses were determined by chiral High-Performance Liquid Chromatography (HPLC) analysis with chiral Lux Cellouse-4 column with hexane and isopropanol as solvents. The UV detection was monitored at 254 nm. HPLC samples were dissolved in ethanol.

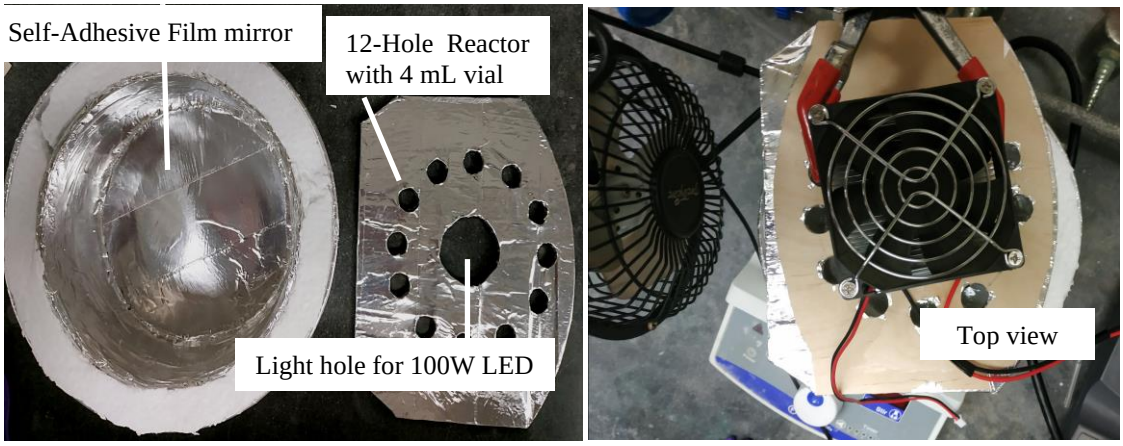
Photoredox Reaction Setup

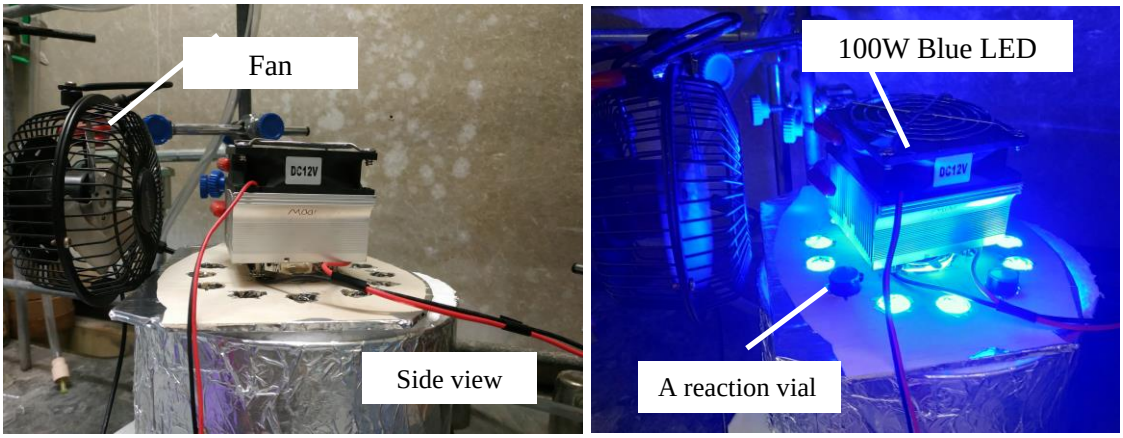
Heat sink and AC LED driver: purchased from ebay (seller babaoshop) http://stores.ebay.com/babaoshop/

LED Light: purchased from ebay (seller due20150801) http://stores.ebay.com/due20150801/



A picture of 100W blue LED light





Reaction setup

Detailed Reaction Optimizations

General reaction procedures: All optimization reactions were set up in a glove box under an N_2 atmosphere.

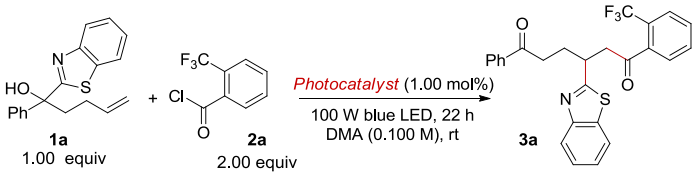
An oven dried 4 mL clear borosilicate glass vial (Fisher scientific FS60910D-1) was used for all the optimization reactions, and the vial was sealed with a green PTFE thermoset cap (Qopak 00546). The reaction scale was 0.0200 mmol with respect to the amount of 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol. Photoredox catalyst was added into the reaction vial. After mixing all the reaction components, the reaction vial was capped and then taken out of the glovebox. Unless it is indicated, optimization reactions were run using 100 W blue LED for 22 hours. Yields were determined by ^{19}F NMR using benzotrifluoride ($PhCF_3$) as the internal standard (IS).

Optimization for 1,4-Migration:

Table S1. Control Reactions

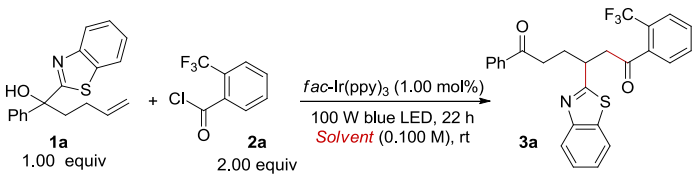
Entry	Photocatalyst	Photocatalyst Amount	Solvent	Deviation	Yield [%]
1	$Ir(ppy)_3$	1.00 mol%	DMA	No Deviation	91
2	-	-	DMA	No Photocatalyst	11
3	$Ir(ppy)_3$	1.00 mol%	DMA	No light	NR
4	-	-	DMA	No light & Photocatalyst	NR

Table S2. Screening of Different Photocatalysts



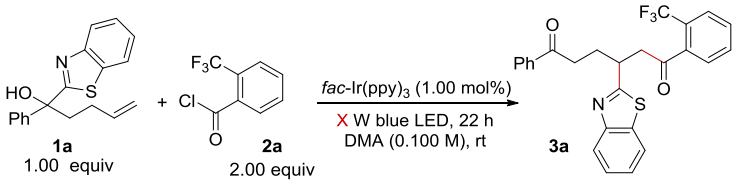
Entry	Photocatalyst	Photocatalyst Amount	Yield [%]
1	$Ir(ppy)_3$	1.00 mol%	91
2	$Ir(dF(CF_3)ppy)_2(dtbbpy)PF_6$	1.00 mol%	90
3	$Ir(Fppy)_3$	1.00 mol%	92
4	$Ir(dmppy)_2(dtbbpy)PF_6$	1.00 mol%	57
5	$Ir(dtbppy)_2(dtbbpy)PF_6$	1.00 mol%	91
6	$Ru(bpy)_3(PF_6)_2$	1.00 mol%	32
7	$Ru(bpz)_3(PF_6)_2$	1.00 mol%	0
8	$Ru(dtbpy)_3(PF_6)_2$	1.00 mol%	62
9	$Ru(phen)_3(PF_6)_2$	1.00 mol%	12

Table S3. Screening of Different Solvents



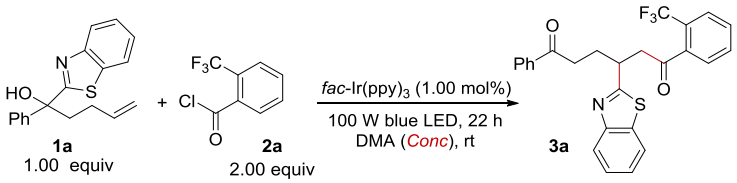
Entry	Solvent	Solvent Concentration	Yield [%]
1	MeCN	0.100 M	46
2	$CHCl_3$	0.100 M	37
3	DCM	0.100 M	48
4	DCE	0.100 M	53
5	DMA	0.100 M	90
6	Toluene	0.100 M	23
7	THF	0.100 M	49
8	Acetone	0.100 M	21
9	Chlorobenzene	0.100 M	33
10	DMF	0.100 M	78

Table S4. Strength of the Light



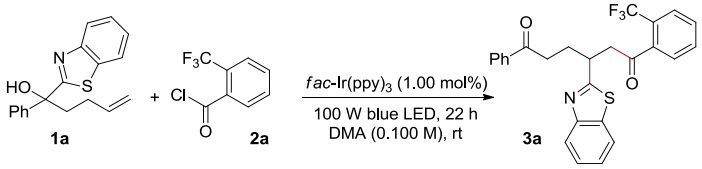
Entry	Power	Yield [%]
1	30 W	77
2	50 W	79
3	100 W	90

Table S5. Screening of Concentration of DMA



Entry	Solvent	Solvent Concentration	Yield [%]
1	DMA	0.100 M	91
2	DMA	0.200 M	82
3	DMA	0.400 M	44
4	DMA	0.0500 M	51

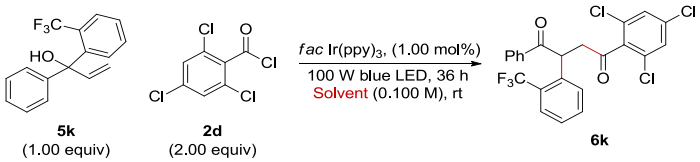
Table S6. Screening of Different Stoichiometry of Reactants



Entry	Amount of 1a	Amount of 2a	Yield [%]
1	1.00 equiv	1.00 equiv	78
2	1.00 equiv	1.50 equiv	89
3	1.00 equiv	2.00 equiv	91
4	1.00 equiv	2.50 equiv	86
5	1.00 equiv	3.00 equiv	82
6	2.00 equiv	1.00 equiv	86

Optimization for 1,2-Migration:

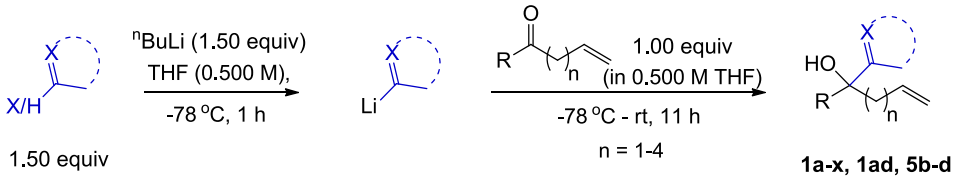
Table S7. Screening of Solvent for 1,2 Migration



Entry	Solvent	Solvent Concentration	Yield [%]
1	DMA	0.100 M	57
2	DMA : PhCl (1:1)	0.100 M	68

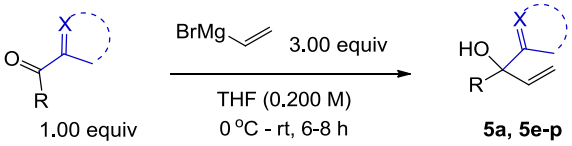
Experimental Data

General Procedure A for Starting Material Synthesis:



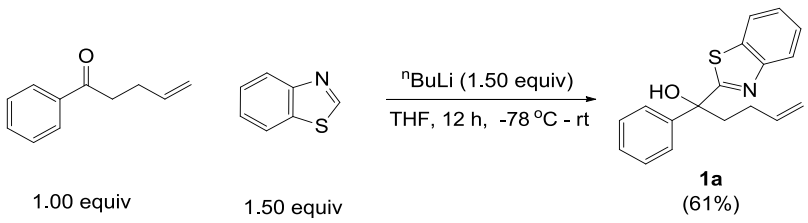
To an oven-dried 100 mL double neck round bottom flask was added heterocycle (1.50 equiv) in dry THF (0.500 M) under N_2 atmosphere and cooled to -78 °C. ^{n}BuLi (1.50 equiv, 2.50 M in hexane) dropwise added to this solution at -78 °C. After the addition was complete, the solution was kept stirring at the same temperature until complete lithiation. To this stirred solution was added a solution of ketone (1.00 equiv) in dry THF (0.500 M) at -78 °C and stirred continued at this temperature for 1-3 h. Next, the reaction temperature was gradually increased to room temperature and stirred for another 8-10 h. After the reaction completion, the reaction was quenched with saturated NH_4Cl solution, extracted with EtOAc and dried before purified on a silica column using an eluent of EtOAc:Hexanes (v/v) to afford the desired product.

General Procedure B for Starting Material Synthesis:



To an oven-dried 100 mL double neck round bottom flask, vinyl magnesium bromide (3.00 equiv) was added dropwise to a solution of ketone (1.00 equiv) in dry THF (0.200 M) under N_2 atmosphere at 0 °C. The resulting mixture was warmed gradually to room temperature and stirred for 6-8 h. After completion of the reaction, the reaction mixture was quenched with a saturated NH_4Cl solution, extracted with EtOAc and dried before purified on a silica column using an eluent of EtOAc:Hexanes (v/v) to afford the desired product.

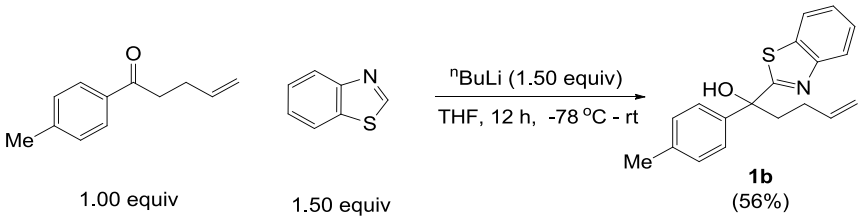
1-(Benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (1a)



The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (1.60 g, 10.0

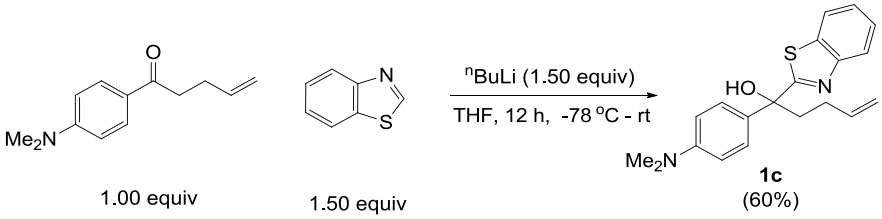
mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a white solid (1.80 g, 6.10 mmol, 61% yield). $\mathbf{R}_f$ = 0.51 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.03 (d, *J* = 7.70 Hz, 1H), 7.84 (d, *J* = 7.70 Hz, 1H), 7.73 (d, *J* = 7.00 Hz, 2H), 7.47 (t, *J* = 7.00 Hz, 1H), 7.40-7.35 (m, 3H), 7.30 (t, *J* = 7.00 Hz, 1H), 5.92-5.88 (m, 1H), 5.08-5.00 (m, 2H), 4.17 (s, 1H), 2.64-2.60 (m, 2H), 2.23-2.20 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 178.37, 152.80, 143.90, 138.28, 135.81, 128.58, 127.81, 126.15, 125.70, 125.16, 123.25, 121.85, 115.35, 79.15, 41.70, 28.28. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-1-(*p*-tolyl)pent-4-en-1-ol (1b)



The reaction was performed according to the general procedure A using 1-(*p*-tolyl)pent-4-en-1-one (348 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (346 mg, 1.12 mmol, 56% yield). $\mathbf{R}_f$ = 0.51 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.00 (d, *J* = 8.50 Hz, 1H), 7.82 (d, *J* = 8.00 Hz, 1H), 7.56 (d, *J* = 8.50 Hz, 2H), 7.46 (t, *J* = 7.50 Hz, 1H), 7.35 (t, *J* = 7.50 Hz, 1H), 7.17 (d, *J* = 8.50 Hz, 2H), 5.91-5.83 (m, 1H), 5.05-4.96 (m, 2H), 3.92 (bs, 1H), 2.59-2.51 (m, 2H), 2.33 (s, 3H), 2.25-2.11 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 178.50, 152.79, 141.08, 138.40, 137.64, 135.94, 129.37, 126.20, 125.65, 125.21, 123.31, 121.90, 115.38, 79.13, 41.71, 28.35, 21.23. These spectroscopic data correspond to previously reported data.[5]

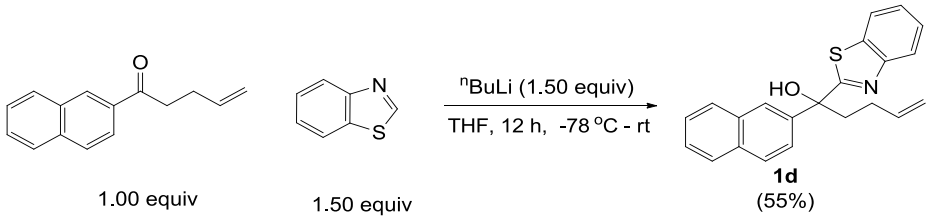
1-(Benzo[*d*]thiazol-2-yl)-1-(4-(dimethylamino)phenyl)pent-4-en-1-ol (1c)



The reaction was performed according to the general procedure A using 1-(4-(dimethylamino)phenyl)pent-4-en-1-one (407 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (406 mg, 1.20 mmol, 60% yield). $\mathbf{R}_f$ = 0.43 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.29 (d, *J* = 8.19 Hz, 1H), 7.84 (d, *J* = 7.98 Hz, 1H), 7.55 (d, *J* = 9.10 Hz, 2H), 7.46 (t, *J* = 7.35 Hz, 1H), 7.35 (t, *J* = 7.00 Hz, 1H), 6.73 (d, *J* = 8.96 Hz, 2H), 5.94-5.89 (m, 1H), 5.09-5.08 (m, 1H), 5.01-4.99 (m, 1H), 4.08 (s,

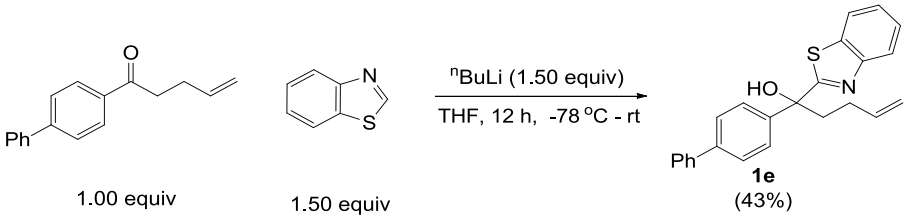
1H), 2.94 (s, 6H), 2.64-2.56 (m, 2H), 2.31-2.27 (m, 1H), 2.22-2.17 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 179.37, 152.94, 149.99, 138.53, 135.81, 131.71, 126.56, 125.95, 124.90, 123.12, 121.76, 115.02, 112.34, 78.79, 41.39, 40.57, 28.30. **HRMS** (ESI-TOF) *m/z* calcd for $C_{20}H_{23}N_2OS$ [$(M + H)^+$], 339.15256, found, 339.15306.

1-(Benzo[*d*]thiazol-2-yl)-1-(naphthalen-2-yl)pent-4-en-1-ol (1d)



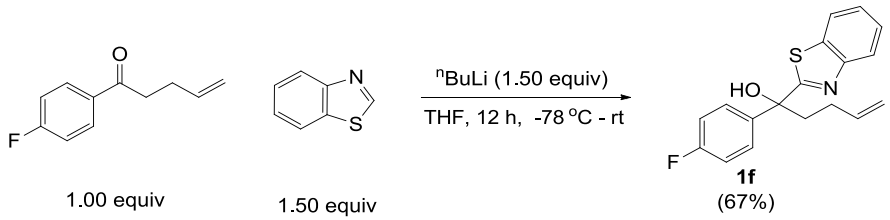
The reaction was performed according to the general procedure A using 1-(naphthalen-2-yl)pent-4-en-1-one (420 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with DCM:Hexanes [1:1 (v/v)] to afford the title compound as a gummy solid (380 mg, 1.10 mmol, 55% yield). $\mathbf{R_f}$ = 0.38 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.16 (s, 1H), 8.02 (d, *J* = 8.20 Hz, 1H), 7.87-7.76 (m, 5H), 7.49-7.45 (m, 3H), 7.35 (t, *J* = 7.60 Hz, 1H), 5.93-5.85 (m, 1H), 5.06-5.02 (m, 1H), 4.99-4.97 (m, 1H), 4.02 (s, 1H), 2.69-2.66 (m, 2H), 2.23-2.17 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 178.10, 152.81, 141.25, 138.35, 135.97, 133.31, 132.93, 128.63, 128.48, 127.72, 126.46, 126.44, 126.27, 125.30, 124.51, 124.00, 123.38, 121.94, 115.54, 79.37, 41.67, 28.38. These spectroscopic data correspond to previously reported data.[5]

1-([1,1'-Biphenyl]-4-yl)-1-(benzo[*d*]thiazol-2-yl)pent-4-en-1-ol (1e)



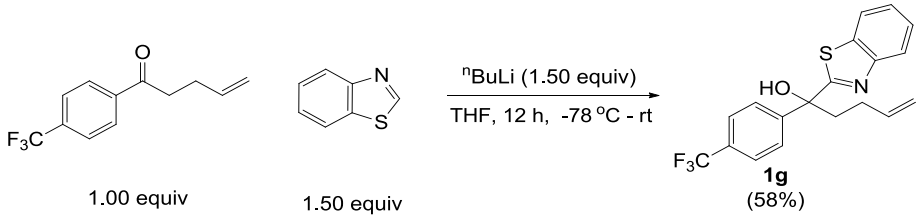
The reaction was performed according to the general procedure A using 1-([1,1'-biphenyl]-4-yl)pent-4-en-1-one (472 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (319 mg, 0.860 mmol, 43% yield). $\mathbf{R_f}$ = 0.36 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.06 (d, *J* = 8.26 Hz, 1H), 7.86 (d, *J* = 7.98 Hz, 1H), 7.81-7.80 (m, 2H), 7.63-7.60 (m, 4H), 7.49 (t, *J* = 7.70 Hz, 1H), 7.45 (t, *J* = 7.52 Hz, 2H), 7.39-7.36 (m, 2H), 5.95-5.91 (m, 1H), 5.10-5.08 (m, 1H), 5.04-5.02 (m, 1H), 4.20 (bs, 1H), 2.69-2.62 (m, 2H), 2.31-2.22 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 178.30, 152.87, 142.96, 140.68, 140.63, 138.28, 135.82, 128.91, 127.52, 127.30, 127.23, 126.19, 125.20, 123.29, 121.89, 115.43, 79.12, 41.73, 28.32. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-1-(4-fluorophenyl)pent-4-en-1-ol (1f)



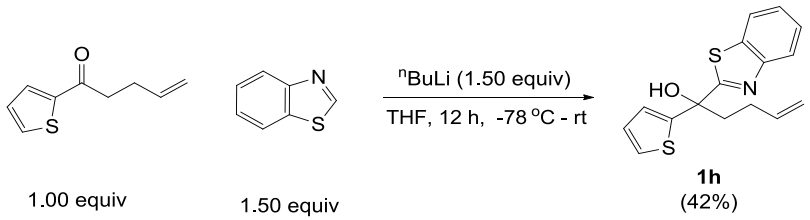
The reaction was performed according to the general procedure A using 1-(4-fluorophenyl)pent-4-en-1-one (356 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (419 mg, 1.34 mmol, 67% yield). $\mathbf{R_f}$ = 0.41 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.00 (d, *J* = 8.00 Hz, 1H), 7.84 (d, *J* = 8.00 Hz, 1H), 7.67-7.64 (m, 2H), 7.47 (t, *J* = 7.50 Hz, 1H), 7.36 (t, *J* = 7.50 Hz, 1H), 7.03 (t, *J* = 8.50 Hz, 2H), 5.88-5.82 (m, 1H), 5.04-4.97 (m, 2H), 3.95 (s, 1H), 2.58-2.49 (m, 2H), 2.19-2.13 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 178.06, 162.38 (d, $J^1_{C\text{-}F}$ = 245.41 Hz), 152.83, 139.76 (d, $J^4_{C\text{-}F}$ = 2.80 Hz), 138.18, 135.83, 127.62 (d, $J^3_{C\text{-}F}$ = 8.07 Hz), 126.32, 125.34, 123.35, 121.95, 115.56 (d, $J^2_{C\text{-}F}$ = 16.42 Hz), 115.33, 78.93, 41.92, 28.31. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –115.01 (s). These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-1-(4-(trifluoromethyl)phenyl)pent-4-en-1-ol (1g)



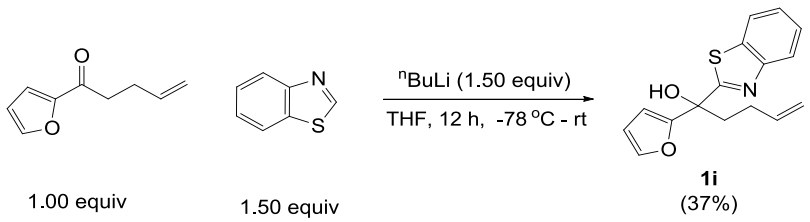
The reaction was performed according to the general procedure A using 1-(4-(trifluoromethyl)phenyl)pent-4-en-1-one (456 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a white solid (421 mg, 1.16 mmol, 58% yield). $\mathbf{R_f}$ = 0.38 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.01 (d, *J* = 8.19 Hz, 1H), 7.85-7.83 (m, 3H), 7.61 (d, *J* = 8.40 Hz, 2H), 7.48 (t, *J* = 7.00 Hz, 1H), 7.39 (t, *J* = 7.00 Hz, 1H), 5.89-5.85 (m, 1H), 5.05-4.99 (m, 2H), 3.98 (bs, 1H), 2.60-2.55 (m, 2H), 2.18-2.17 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 177.24, 152.79, 147.78, 138.01, 135.79, 130.05 (q, $J^2_{C\text{-}F}$ = 32.41 Hz), 126.46, 126.23, 125.60 (q, $J^3_{C\text{-}F}$ = 3.54 Hz), 125.52, 124.25 (q, $J^1_{C\text{-}F}$ = 270.50 Hz), 123.43, 122.01, 115.94, 79.19, 41.89, 28.31. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –62.60 (s). These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-1-(thiophen-2-yl)pent-4-en-1-ol (1h)



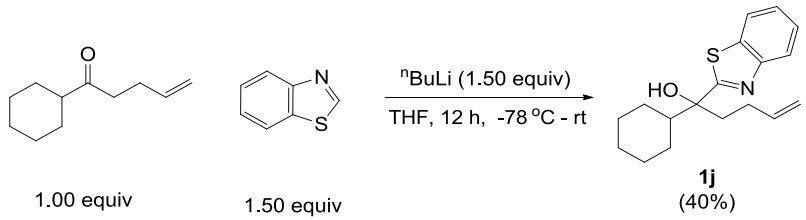
The reaction was performed according to the general procedure A using 1-(thiophen-2-yl)pent-4-en-1-one (332.4 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (253 mg, 0.840 mmol, 42% yield). $\mathbf{R_f}$ = 0.40 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.01 (d, *J* = 8.20 Hz, 1H), 7.85 (d, *J* = 8.00 Hz, 1H), 7.48 (t, *J* = 8.50 Hz, 1H), 7.38 (t, *J* = 8.00 Hz, 1H), 7.26-7.25 (m, 1H), 7.17-7.16 (m, 1H), 6.99-6.98 (m, 1H), 5.89-5.83 (m, 1H), 5.06-4.97 (m, 2H), 4.44-4.41 (m, 1H), 2.60-2.53 (m, 2H), 2.34-2.31 (m, 1H), 2.17-2.15 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 177.14, 152.56, 149.53, 138.00, 136.03, 127.24, 126.36, 125.54, 125.42, 124.33, 123.41, 121.99, 115.51, 78.01, 43.04, 28.33. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-1-(furan-2-yl)pent-4-en-1-ol (1i)



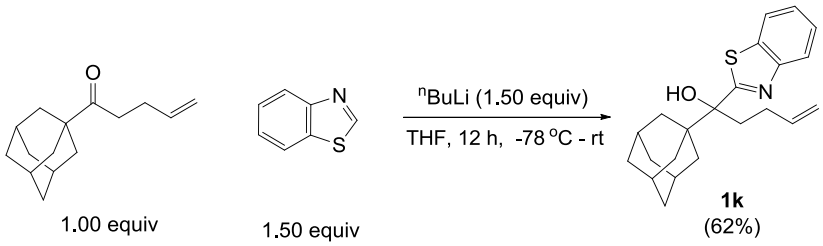
The reaction was performed according to the general procedure A using 1-(furan-2-yl)pent-4-en-1-one (300.2 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (210.9 mg, 0.740 mmol, 37% yield). $\mathbf{R_f}$ = 0.37 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.02 (d, *J* = 8.15 Hz, 1H), 7.87 (d, *J* = 7.90 Hz, 1H), 7.48 (t, *J* = 7.70 Hz, 1H), 7.40-7.36 (m, 2H), 6.43-6.42 (m, 1H), 6.35-6.35 (m, 1H), 5.86-5.79 (m, 1H), 5.04-4.94 (m, 2H), 4.22 (s, 1H), 2.57-2.51 (m, 1H), 2.47-2.42 (m, 1H), 2.31-2.23 (m, 1H), 2.11-2.04 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 175.13, 155.73, 152.44, 142.77, 137.96, 136.07, 126.31, 125.42, 123.44, 121.96, 115.30, 110.71, 107.14, 77.47, 40.12, 27.86. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-1-cyclohexylpent-4-en-1-ol (1j)



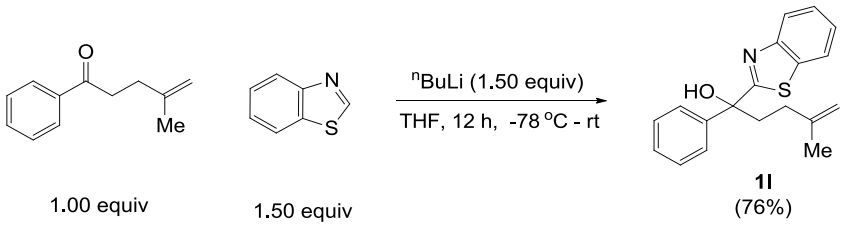
The reaction was performed according to the general procedure A using 1-cyclohexylpent-4-en-1-one (332 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (240.8 mg, 0.800 mmol, 40% yield). $\mathbf{R_f}$ = 0.54 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ºC, δ): 7.99 (d, *J* = 7.92 Hz, 1H), 7.88 (d, *J* = 7.96 Hz, 1H), 7.48 (t, *J* = 7.28 Hz, 1H), 7.37 (t, *J* = 8.08 Hz, 1H), 5.83-5.73 (m, 1H), 4.98-4.93 (m, 1H), 4.92-4.89 (m, 1H), 3.41 (s, 1H), 2.24-2.11 (m, 2H), 2.05-1.98 (m, 2H), 1.87-1.73 (m, 3H), 1.70-1.62 (m, 2H), 1.40-1.10 (m, 6H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 178.54, 152.69, 138.58, 135.72, 126.14, 125.03, 123.08, 121.92, 115.08, 80.60, 48.79, 38.99, 28.12, 27.31, 26.69, 26.65, 26.61, 26.48. These spectroscopic data correspond to previously reported data.[5]

1-(Adamantan-1-yl)-1-(benzo[*d*]thiazol-2-yl)pent-4-en-1-ol (1k)



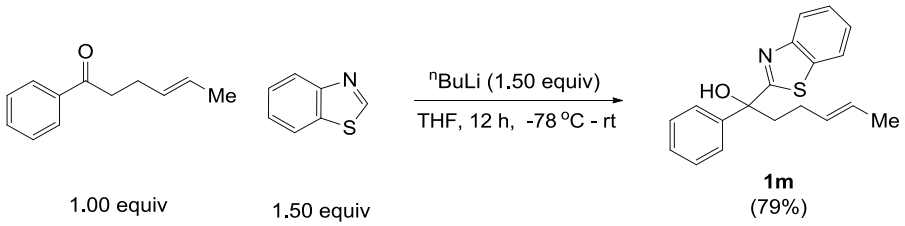
The reaction was performed according to the general procedure A using 1-(adamantan-1-yl)pent-4-en-1-one (218.3 mg, 1.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (220 mg, 0.620 mmol, 62% yield). $\mathbf{R_f}$ = 0.60 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.01 (d, *J* = 8.15 Hz, 1H), 7.88 (d, *J* = 7.95 Hz, 1H), 7.47 (t, *J* = 7.67 Hz, 1H), 7.38 (t, *J* = 7.15 Hz, 1H), 5.83-5.75 (m, 1H), 4.96-4.89 (m, 2H), 3.64 (s, 1H), 2.18-2.04 (m, 3H), 1.99-1.94 (m, 6H), 1.67-1.57 (m, 10H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 177.04, 152.38, 138.89, 135.84, 126.00, 124.97, 123.11, 121.68, 115.07, 82.81, 40.71, 37.12, 36.75, 34.19, 28.79, 28.24. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{28}NOS$ [$(M + H)^+$], 354.18861, found, 354.18833.

1-(Benzo[*d*]thiazol-2-yl)-4-methyl-1-phenylpent-4-en-1-ol (1l)



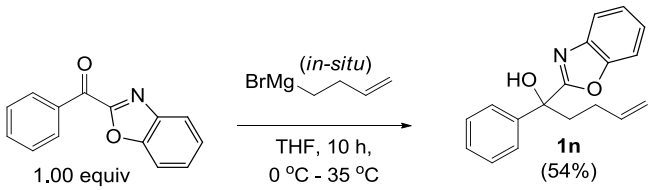
The reaction was performed according to the general procedure A using 4-methyl-1-phenylpent-4-en-1-one (348.4 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (469 mg, 1.52 mmol, 76% yield). $\mathbf{R}_f$ = 0.42 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.02 (d, *J* = 8.20 Hz, 1H), 7.84 (d, *J* = 8.05 Hz, 1H), 7.73-7.71 (m, 2H), 7.47 (t, *J* = 7.50 Hz, 1H), 7.39-7.34 (m, 3H), 7.29 (t, *J* = 7.50 Hz, 1H), 4.75 (d, *J* = 10.75 Hz, 2H), 4.09-4.08 (m, 1H), 2.67-2.62 (m, 2H), 2.18-2.12 (m, 2H), 1.76 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 178.35, 152.85, 145.91, 144.01, 135.92, 128.64, 127.84, 126.19, 125.72, 125.20, 123.32, 121.90, 110.67, 79.32, 40.62, 30.07, 22.86. These spectroscopic data correspond to previously reported data.[5]

(*E*)-1-(Benzo[*d*]thiazol-2-yl)-1-phenylhex-4-en-1-ol (1m)



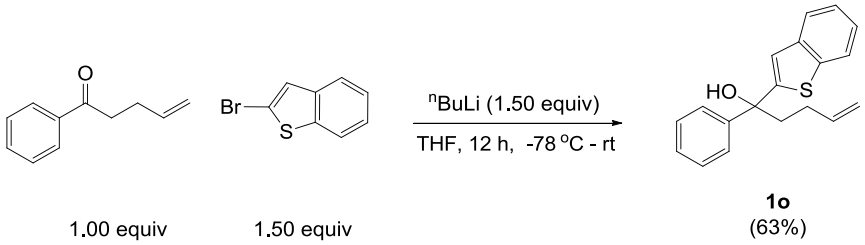
The reaction was performed according to the general procedure A using (*E*)-1-phenylhex-4-en-1-one (348.4 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (489 mg, 1.58 mmol, 79% yield). $\mathbf{R}_f$ = 0.44 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (400 MHz, $CDCl_3$, 25 ºC, δ): 8.05 (d, *J* = 7.92 Hz, 1H), 7.84 (d, *J* = 7.96 Hz, 1H), 7.70 (d, *J* = 8.64 Hz, 2H), 7.47 (t, *J* = 7.16 Hz, 1H), 7.39-7.34 (m, 3H), 7.29-7.27 (m, 1H), 5.54-5.40 (m, 2H), 3.99 (s, 1H), 2.62-2.49 (m, 2H), 2.18-2.09 (m, 2H), 1.63 (d, *J* = 4.80 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 ºC, δ): 178.48, 152.93, 144.10, 135.91, 130.82, 128.59, 127.78, 126.28, 126.16, 125.71, 125.15, 123.31, 121.88, 79.42, 42.32, 27.22, 18.10. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]oxazol-2-yl)-1-phenylpent-4-en-1-ol (1n)



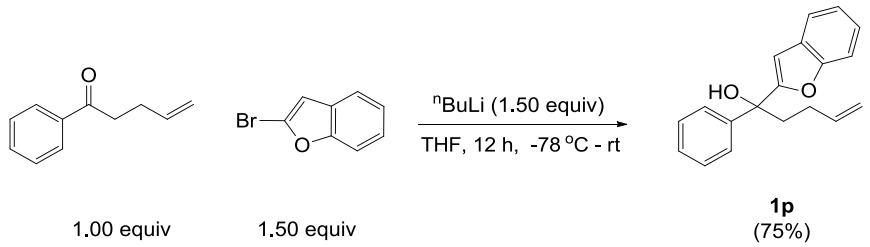
To an oven-dried 100 mL double neck round bottom flask was added magnesium (216.0 mg, 9.00 mmol, 3.60 equiv) in dry THF (0.700 M) under N_2 atmosphere and cooled to 0 ℃.[6] Then 4-bromo-1-butene (301 mg, 2.25 mmol, 0.900 equiv) was added. The rest of 4-bromo-1-butene (703 mg, 5.25 mmol, 2.10 equiv) was added dropwise to the mixture after the exothermal reaction began in the flask. The mixture was stirred for additional 1 hour at room temperature. After that, the prepared Grignard solution was added to THF (0.200 M) solution of benzo[*d*]oxazol-2-yl(phenyl)methanone (557 mg, 2.50 mmol, 1.00 equiv) at 0 ℃. The reaction mixture stirred at 35 °C for 10 hours and quenched with sat. NH_4Cl, extract with EtOAc, dried with Na_2SO_4, concentrated under vacuum. The reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a white solid (377 mg, 1.35 mmol, 54% yield). $\mathbf{R_f}$ = 0.38 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 °C, δ): 7.74-7.70 (m, 1H), 7.64 (d, *J* = 9.00 Hz, 2H), 7.53-7.50 (m, 1H), 7.38-7.32 (m, 4H), 7.29 (t, *J* = 7.50 Hz, 1H), 5.87-5.79 (m, 1H), 5.03-4.92 (m, 2H), 4.01 (s, 1H), 2.58-2.42 (m, 2H), 2.25-2.09 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 °C, δ): 169.00, 151.44, 142.79, 140.49, 137.98, 128.66, 128.05, 125.49, 125.39, 124.81, 120.36, 115.14, 111.12, 77.48, 40.38, 28.14. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*b*]thiophen-2-yl)-1-phenylpent-4-en-1-ol (1o)



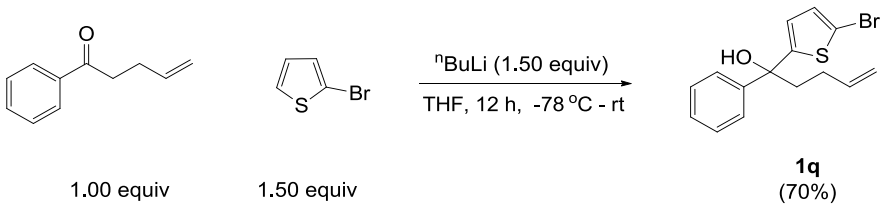
The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (160.2 mg, 1.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (185 mg, 0.630 mmol, 63% yield). $\mathbf{R_f}$ = 0.47 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 °C, δ): 7.79 (d, *J* = 7.90 Hz, 1H), 7.72 (d, *J* = 8.00 Hz, 1H), 7.58 (d, *J* = 7.50 Hz, 2H), 7.40-7.30 (m, 5H), 7.20 (s, 1H), 5.95-5.87 (m, 1H), 5.09-5.02 (m, 2H), 2.66 (s, 1H), 2.53-2.50 (m, 2H), 2.32-2.24 (m, 1H), 2.14-2.07 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 °C, δ): 153.53, 145.23, 139.79, 139.69, 138.45, 128.42, 127.54, 125.78, 124.42, 124.36, 123.76, 122.47, 120.52, 115.26, 77.65, 42.29, 28.49. **HRMS** (ESI-TOF) *m/z* calcd for $C_{19}H_{18}NaOS$ [$(M + H)^+$], 317.09706, found, 317.09826.

1-(Benzofuran-2-yl)-1-phenylpent-4-en-1-ol (1p)



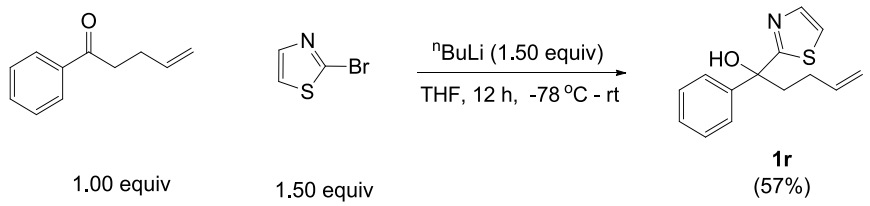
The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (160.2 mg, 1.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (210 mg, 0.750 mmol, 75% yield). $\mathbf{R}_f$ = 0.45 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.56 (d, *J* = 7.70 Hz, 1H), 7.51 (d, *J* = 7.0 Hz, 2H), 7.44 (d, *J* = 7.70 Hz, 1H), 7.37 (t, *J* = 7.70 Hz, 2H), 7.31-7.26 (m, 2H), 7.24-7.22 (m, 1H), 6.68 (s, 1H), 5.90-5.84 (m, 1H), 5.05-4.97 (m, 2H), 2.79 (bs, 1H), 2.53-2.47 (m, 1H), 2.36-2.32 (m, 1H), 2.23-2.20 (m, 1H), 2.08-2.06 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 161.30, 154.97, 143.81, 138.49, 128.44, 128.26, 127.67, 125.82, 124.37, 123.04, 121.30, 115.09, 111.53, 103.35, 76.05, 40.11, 28.17. **HRMS** (ESI-TOF) *m/z* calcd for $C_{19}H_{18}NaO_2$ [$(M + Na)^+$], 301.11990, found, 301.12093.

1-(5-Bromothiophen-2-yl)-1-phenylpent-4-en-1-ol (1q)



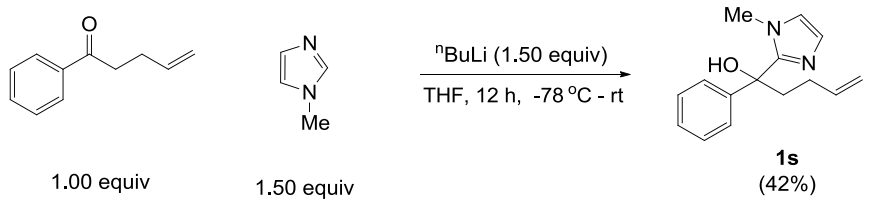
The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (160.2 mg, 1.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (225 mg, 0.700 mmol, 70% yield). $\mathbf{R}_f$ = 0.64 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.46 (d, *J* = 7.70 Hz, 2H), 7.35 (t, *J* = 7.70 Hz, 2H), 7.29-7.26 (m, 1H), 6.88 (d, *J* = 3.50 Hz, 1H), 6.65 (d, *J* = 3.50 Hz, 1H), 5.87-5.81 (m, 1H), 5.02-4.97 (m, 2H), 2.50-2.49 (m, 1H), 2.40-2.31 (m, 2H), 2.20-2.15 (m, 1H), 2.04-2.01 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 154.68, 145.05, 138.36, 129.59, 128.51, 127.64, 125.72, 124.26, 115.41, 111.99, 77.50, 42.39, 28.49. **HRMS** (ESI-TOF) *m/z* calcd for $C_{15}H_{15}BrNaOS$ [$(M + Na)^+$], 344.99192, found, 344.99282.

1-Phenyl-1-(thiazol-2-yl)pent-4-en-1-ol (1r)



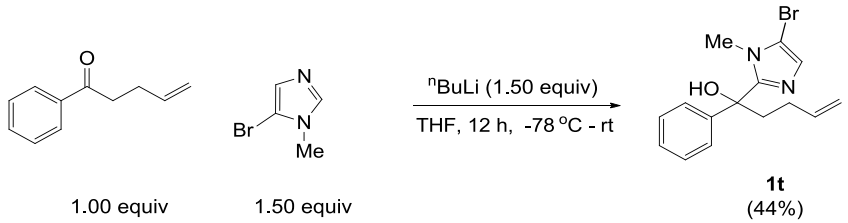
The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (240.3 mg, 1.50 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (209.7 mg, 0.855 mmol, 57% yield). $\mathbf{R_f}$ = 0.45 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.71 (d, *J* = 3.20 Hz, 1H), 7.61 (d, *J* = 7.75 Hz, 2H), 7.35 (t, *J* = 7.50 Hz, 2H), 7.27-7.24 (m, 2H), 5.88-5.80 (m, 1H), 5.02-4.94 (m, 2H), 3.68 (s, 1H), 2.53-2.43 (m, 2H), 2.13-2.08 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 177.73, 144.48, 142.26, 138.39, 128.59, 127.70, 125.59, 119.77, 115.34, 78.96, 42.24, 28.35. These spectroscopic data correspond to previously reported data.[5]

1-(1-Methyl-1*H*-imidazol-2-yl)-1-phenylpent-4-en-1-ol (1s)



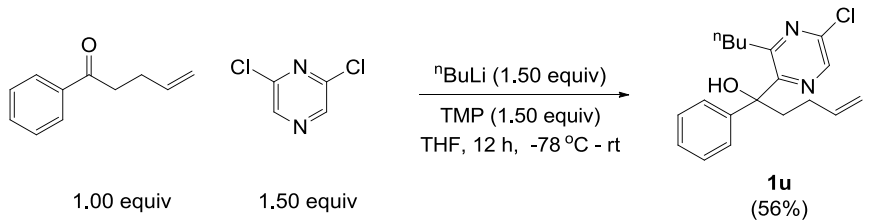
The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (240.3 mg, 1.50 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:1 (v/v)] to afford the title compound as a gummy solid (152.6 mg, 0.630 mmol, 42% yield). $\mathbf{R_f}$ = 0.20 EtOAc:Hexanes [1:1 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.31-7.27 (m, 4H), 7.23 (t, *J* = 6.65 Hz, 1H), 6.89 (s, 1H), 6.75 (s, 1H), 5.84-5.78 (m, 1H), 5.01-4.91 (m, 2H), 3.56 (s, 1H), 3.26 (s, 3H), 2.51-2.46 (m, 2H), 2.18-2.12 (m, 1H), 1.98-1.94 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 150.84, 143.57, 138.81, 128.35, 127.27, 125.98, 125.71, 123.06, 114.91, 75.68, 41.03, 34.27, 27.87. These spectroscopic data correspond to previously reported data.[5]

1-(5-Bromo-1-methyl-1*H*-imidazol-2-yl)-1-phenylpent-4-en-1-ol (1t)



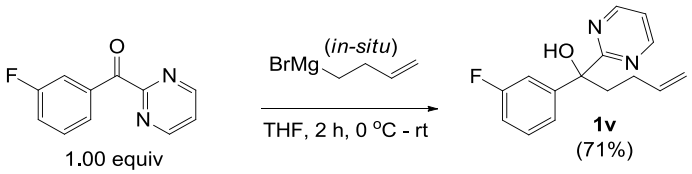
The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (160.2 mg, 1.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (141 mg, 0.440 mmol, 44% yield). $\mathbf{R_f}$ = 0.36 EtOAc:Hexanes [1:4 (v/v)] **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.32 (t, *J* = 7.70 Hz, 2H), 7.28-7.25 (m, 3H), 6.98 (s, 1H), 5.85-5.80 (m, 1H), 5.03-4.94 (m, 2H), 3.23 (s, 3H), 2.89 (s, 1H), 2.50-2.46 (m, 2H), 2.18-2.13 (m, 1H), 2.02-1.96 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 151.56, 142.98, 138.60, 128.55, 127.56, 126.75, 125.63, 115.31, 105.98, 76.26, 40.96, 32.78, 27.88. **HRMS** (ESI-TOF) *m/z* calcd for $C_{15}H_{18}BrN_2O$ [$(M + H)^+$], 321.05970, found, 321.05921.

1-(3-Butyl-5-chloropyrazin-2-yl)-1-phenylpent-4-en-1-ol (1u)



The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (160.2 mg, 1.00 mmol, 1.00 equiv) as the substrate and 2,2,6,6-tetramethylpiperidine (TMP) (211.5 mg, 1.50 mmol, 1.50 equiv) as additive. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (185.2 mg, 0.560 mmol, 56% yield). $\mathbf{R_f}$ = 0.57 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.56 (s, 1H), 7.54 (t, *J* = 7.0 Hz, 2H), 7.36 (t, *J* = 7.70 Hz, 2H), 7.28-7.26 (m, 1H), 5.87-5.81 (m, 1H), 5.02-4.95 (m, 2H), 4.18 (s, 1H), 2.93 (t, *J* = 8.05 Hz, 2H), 2.48-2.37 (m, 2H), 2.16-2.06 (m, 2H), 1.74-1.70 (m, 2H), 1.46-1.40 (m, 2H), 0.97 (t, *J* = 7.00 Hz, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 156.98, 154.54, 146.86, 144.57, 139.71, 138.37, 128.71, 127.59, 125.91, 115.14, 77.00, 40.53, 34.48, 29.99, 28.18, 22.71, 14.06. **HRMS** (ESI-TOF) *m/z* calcd for $C_{19}H_{24}ClN_2O$ [$(M + H)^+$], 331.15717, found, 331.15743.

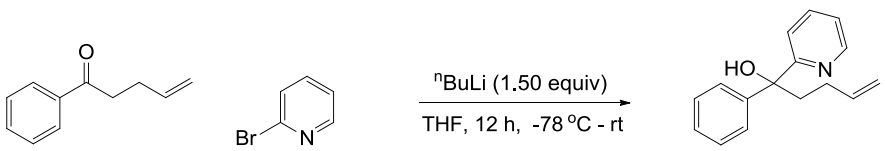
1-(3-Fluorophenyl)-1-(pyrimidin-2-yl)pent-4-en-1-ol (1v)



A dry two-neck flask equipped with a stirring bar was charged magnesium (216.0 mg, 9.00 mmol, 3.60 equiv) and then the flask was refilled with nitrogen at 0 °C.[6] The minimum amount of THF (1.00 M) was added and then 4-bromo-1-butene (301 mg, 2.25 mmol, 0.900 equiv) was added. After the exothermal reaction began in the flask, the rest of the solution of 4-bromo-1-butene (703 mg, 5.25 mmol, 2.10 equiv) in THF (2.60 M) was added dropwise to the mixture. The resulting mixture was stirred for additional 1 hour at room temperature. Then, this Grignard

solution was added to a THF solution (0.830 M) of (3-fluorophenyl)(pyrimidin-2-yl)methanone (500 mg, 2.50 mmol, 1.00 equiv) at 0 °C. After the reaction mixture was stirred at room temperature for 2 hours, it was quenched with sat. NH_4Cl, extracted with EtOAc, dried with Na_2SO_4, filtered off the Na_2SO_4, and concentrated under vacuum. The reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:15 (v/v)] to afford the title compound as a yellow solid (456 mg, 1.77 mmol, 71% yield). $\mathbf{R_f}$ = 0.30 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.74 (d, *J* = 4.90 Hz, 2H), 7.54 (d, *J* = 7.90 Hz, 1H), 7.50 (dt, *J* = 2.15 &10.70 Hz, 1H), 7.28-7.24 (m, 1H), 7.20 (d, *J* = 4.90 Hz, 1H), 6.90 (dd, *J* = 2.50 & 9.70 Hz, 1H), 5.83-5.74 (m, 1H), 5.53 (s, 1H), 4.96 (dq, *J* = 17.20 & 1.50 Hz, 1H), 4.88 (dq, *J* = 1.50 & 10.0 Hz, 1H), 2.53-2.47 (m, 1H), 2.44-2.38 (m, 1H), 2.15-2.08 (m, 1H), 1.94-1.87 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 171.74, 162.93 (d, $J^1_{C\text{-}F}$ = 245.50 Hz), 157.02, 148.35 (d, $J^{3'}_{C\text{-}F}$ = 7.50 Hz), 138.63, 129.57 (d, $J^3_{C\text{-}F}$ = 7.50 Hz), 121.74 (d, $J^4_{C\text{-}F}$ = 2.50 Hz), 119.50, 114.52, 113.97 (d, $J^{2'}_{C\text{-}F}$ = 20.0 Hz), 113.41 (d, $J^2_{C\text{-}F}$ = 23.8 Hz), 78.09 (d, $J^{4'}_{C\text{-}F}$ = 1.50 Hz), 41.05, 28.33. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –116.24 (m). **HRMS** (ESI-TOF) *m/z* calcd for $C_{15}H_{16}FN_2O$ [$(M + H)^+$], 259.12412, found, 259.12404.

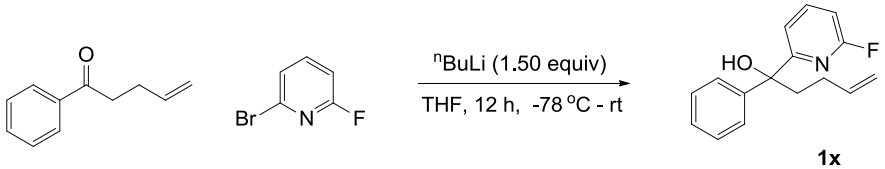
1-Phenyl-1-(pyridin-2-yl)pent-4-en-1-ol (1w)



1.00 equiv 1.50 equiv **1w** (62%)

The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (240 mg, 1.50 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (222.5 mg, 0.930 mmol, 62% yield). $\mathbf{R_f}$ = 0.56 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.51 (d, *J* = 4.98 Hz, 1H), 7.65 (t, *J* = 7.91 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 8.05 Hz, 1H), 7.32 (t, *J* = 7.56 Hz, 2H), 7.22 (t, *J* = 7.35 Hz, 1H), 7.17-7.16 (m, 1H), 6.03 (s, 1H), 5.86-5.82 (m, 1H), 5.00-4.97 (m, 1H), 4.93-4.91 (m, 1H), 2.46-2.41 (m, 1H), 2.34-2.29 (m, 1H), 2.23-2.20 (m, 1H), 1.96-1.93 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 163.57, 147.39, 146.41, 138.89, 137.23, 128.43, 127.07, 126.11, 122.22, 120.63, 114.49, 77.09, 40.58, 28.25. These spectroscopic data correspond to previously reported data.[5]

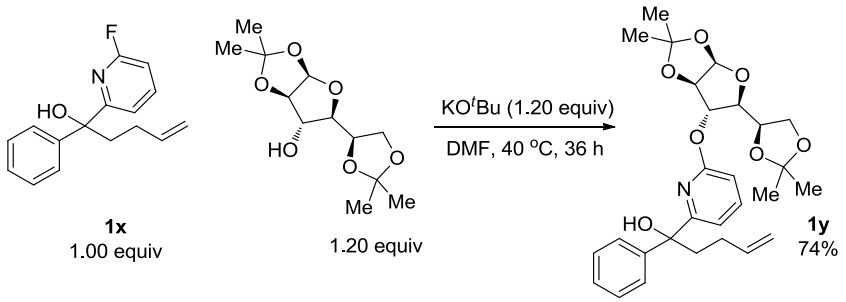
1-(6-Fluoropyridin-2-yl)-1-phenylpent-4-en-1-ol (1x)



1.00 equiv 1.50 equiv **1x** (81%)

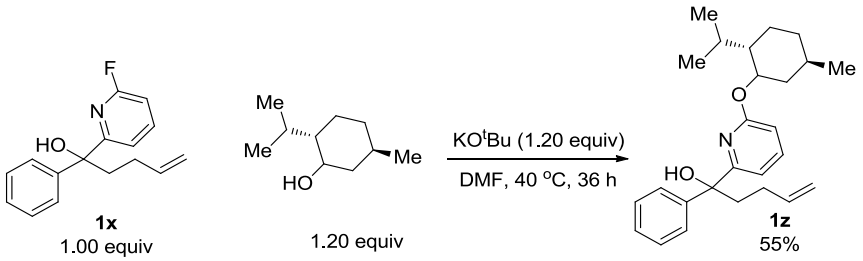
The reaction was performed according to the general procedure A using 1-phenylpent-4-en-1-one (320.4 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (411 mg, 1.62 mmol, 81% yield). $\mathbf{R}_f$ = 0.53 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.78-7.73 (m, 1H), 7.93 (d, *J* = 8.00 Hz, 2H), 7.87 (t, *J* = 7.50 Hz, 2H), 7.27-7.22 (m, 2H), 6.79 (dd, *J* = 8.0 & 2.5 Hz, 1H), 5.87-5.79 (m, 1H), 5.01-4.92 (m, 2H), 4.60 (s, 1H), 2.44-2.32 (m, 2H), 2.18-2.13 (m, 1H), 2.05-1.99 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 163.84 (d, $J^3_{C\text{-}F}$ = 9.97 Hz), 162.53 (d, $J^1_{C\text{-}F}$ = 241.1 Hz), 145.49, 142.17 (d, $J^3_{C\text{-}F}$ =7.27 Hz), 138.68, 128.52, 127.34, 126.05, 117.72 (d, $J^4_{C\text{-}F}$ =4.25 Hz), 114.80, 107.73 (d, $J^2_{C\text{-}F}$ =35.9 Hz), 77.57, 40.58, 28.25. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –68.60 (d). **HRMS** (ESI-TOF) *m/z* calcd for $C_{16}H_{17}FNO$ [$(M + H)^+$], 258.12887, found, 258.12920.

1-(6-(((3a*R*,5*S*,6*S*,6a*R*)-5-((*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxo-6-yl)oxy)pyridin-2-yl)-1-phenylpent-4-en-1-ol (1y)



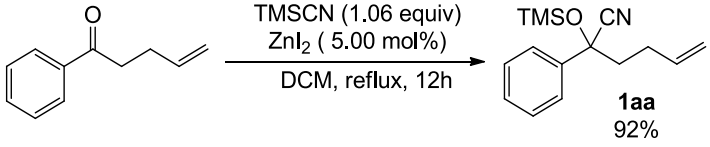
The reaction was performed according to the above procedure using 1-(6-fluoropyridin-2-yl)-1-phenylpent-4-en-1-ol (77.1 mg, 0.300 mmol, 1.00 equiv) (**1w**) and (3a*R*,5*R*,6*S*,6a*R*)-5-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-ol (93.7 mg, 0.360 mmol, 1.20 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as an gummy solid (110 mg, 0.222 mmol, 74% yield). $\mathbf{R}_f$ = 0.10 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.58-7.53 (m, 3H), 7.34-7.29 (m, 2H), 7.24-7.19 (m, 1H), 7.03-6.96 (m, 1H), 6.63-6.61 (m, 1H), 5.91-5.83 (m, 2H), 5.49-5.48 (m, 1H), 5.12 (s, 1H), 5.02-4.97 (m, 1H), 4.94-4.88 (m, 1H) , 4.65-4.64 (m, 1H), 4.59-4.58 (m, 1H), 4.36-4.34 (m, 2H), 4.13-4.08 (m, 2H), 2.40-2.31 (m, 2H), 2.19-2.03 (m, 2H), 1.58-1.57 (m, 3H), 1.46-1.42 (m, 3H), 1.34-1.27 (m, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 162.25, 162.20, 161.25, 161.16, 146.48, 145.98, 140.34, 140.25, 138.96, 128.36, 127.11, 126.96, 126.19, 125.87, 114.63, 114.55, 113.92, 113.54, 112.27, 112.22, 109.64, 109.60, 109.58, 109.50, 105.15, 105.10, 83.62, 83.53, 80.35, 80.27, 78.03, 78.01, 77.74, 77.54, 72.60, 72.52, 67.28, 67.19, 40.92, 40.18, 28.38, 28.35, 27.07, 27.01, 26.99, 26.52, 26.41, 25.44. **HRMS** (ESI-TOF) *m/z* calcd for $C_{28}H_{36}NO_7$ [$(M + H)^+$], 498.24863, found, 498.24793.

1-(6-(((2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)oxy)pyridin-2-yl)-1-phenylpent-4-en-1-ol (1z)



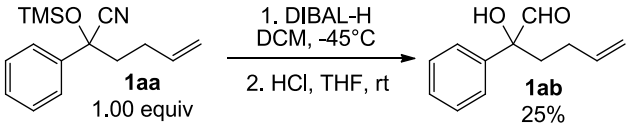
The reaction was performed according to the above procedure using 1-(6-fluoropyridin-2-yl)-1-phenylpent-4-en-1-ol (51.4 mg, 0.200 mmol, 1.00 equiv) (**1w**) and (2*S*,5*R*)-2-isopropyl-5-methylcyclohexanol (37.4 mg, 0.240 mmol, 1.20 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (43.2 mg, 0.110 mmol, 55% yield). $\mathbf{R}_f$ = 0.45 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.57-7.54 (m, 2H), 7.50-7.48 (m, 1H), 7.32-7.29 (m, 2H), 7.21 (t, *J* = 7.00 Hz, 1H), 6.89-6.84 (m, 1H), 6.53-6.51 (m, 1H), 5.57-5.55 (m, 1H), 5.38-5.33 (m, 1H), 5.03-4.97 (m, 1H), 3.08-3.05 (m, 2H), 2.15-2.03 (m, 2H), 1.74-1.70 (m, 2H), 1.63-1.62 (m, 3H), 1.55-1.50 (m, 3H), 1.17-1.11 (m, 1H), 1.03-0.99 (m, 1H), 0.93-0.88 (m, 7H), 0.75-0.70 (m, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 162.50, 162.48, 161.74, 146.33, 146.27, 139.80, 139.74, 130.08, 129.84, 128.26, 128.22, 127.63, 127.33, 127.04, 127.02, 126.23, 126.17, 125.50, 125.43, 112.60, 112.44, 109.60, 77.54, 77.51, 75.27, 75.03, 47.75, 47.72, 45.08, 44.88, 41.02, 40.96, 39.15, 38.96, 34.72, 31.75, 26.48, 26.44, 23.98, 23.94, 22.45, 22.44, 20.92, 18.37, 18.34, 16.82, 16.76, 13.42. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{36}NO_2$ [$(M + H)^+$], 394.27406, found, 394.27358.

2-Phenyl-2-((trimethylsilyl)oxy)hex-5-enenitrile (1aa)



A solution of 1-phenylpent-4-en-1-one (510 mg, 3.20 mmol, 1.00 equiv) TMSCN (0.420 mL, 3.39 mmol) and ZnI_2 (50.0 mg, 0.160 mmol) in anhydrous CH_2Cl_2 (4.00 mL) were heated to reflux for 12 h and cooled down to room temperature. The solvent was removed to afford the crude product, which was purified by flash column chromatography to afford the product as a colorless oil (770 mg, 2.94 mmol, 92%). $\mathbf{R}_f$ = 0.86 EtOAc:Hexanes [1:10 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.52 (d, *J* = 7.88 Hz, 1H), 7.40 (t, *J* = 7.40 Hz, 1H), 7.35 (d, *J* = 7.20 Hz, 2H), 7.79-7.73 (m, 1H), 5.79-5.74 (m, 1H), 5.15 (dd, *J* = 17.10, 1.14 Hz, 1H), 4.96 (d, *J* = 10.17 Hz, 1H), 2.30-2.22 (m, 1H), 2.18-2.07 (m, 2H), 2.05-1.96 (m, 1H), 0.14 (s, 9H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 141.07, 136.91, 128.91, 128.79, 125.26, 120.95, 115.54, 75.45, 45.28, 28.83, 1.13. These spectroscopic data correspond to previously reported data.[7]

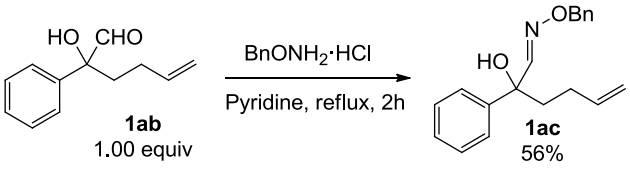
2-Hydroxy-2-phenylhex-5-enal (1ab)



2-Phenyl-2-((trimethylsilyl)oxy)hex-5-enenitrile (680 mg, 2.60 mmol, 1.00 equiv) was dissolved in anhydrous CH_2Cl_2 (4.00 mL). To this solution was added diisobutylaluminium hydride (DIBALH) (1M/hexane, 4.16 mL, 4.16 mmol) at -45 °C. The reaction mixture was stirred for 2 h and quenched with H_2O (0.200 mL) and potassium sodium tartrate (1.00 M, 4.00 mL) with vigorously stirring. Dichloromethane was used to extract the product from the aqueous layer (3 × 5.00 mL). The combined organic layer was washed with brine (3.00 mL), dried over anhydrous Na_2SO_4, filtered and concentrated to afford the crude product, which was dissolved in THF (4.00 mL). To this solution was added HCl (3.00 M, 0.70 mL) at room temperature and the reaction mixture was stirred for 1 h and quenched with H_2O (1.00 mL). EtOAc was used to extract the product from the aqueous layer (3 × 4.00 mL). The combined organic layer was washed with brine (3.00 mL), dried over anhydrous Na_2SO_4, filtered and concentrated to afford the crude product, which was purified by flash column chromatography to afford the product (110 mg, 0.650 mmol, 25% yield) as a yellow oil.

R_f = 0.40 EtOAc:Hexanes [1:10 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 9.61 (d, *J* = 0.96 Hz, 1H), 7.51-7.48 (m, 2H), 7.43-7.40 (m, 2H), 7.34-7.31 (m, 1H), 5.84-5.77 (m, 1H), 5.03 (dd, *J* = 1.38, 17.21 Hz, 1H), 4.98 (dd, *J* = 10.14 & 1.38 Hz, 1H), 3.86 (s, 1H), 2.22-2.16 (m, 1H), 2.13-2.04 (m, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 200.28, 138.38, 137.79, 129.11, 128.23, 125.96, 115.63, 81.83, 36.27, 27.25. These spectroscopic data correspond to previously reported data.[7]

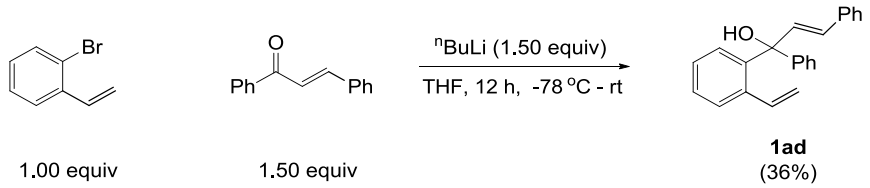
2-Hydroxy-2-phenylhex-5-enal *O*-benzyl oxime (1ac)



A solution of 2-hydroxy-2-phenylhex-5-enal (70.0 mg, 0.400 mmol, 1.00 equiv) and *O*-Benzylhydroxylamine hydrochloride (130 mg, 0.800 mmol) in pyridine (0.400 mL) was heated at 80 °C for 2 h and then cooled down to room temperature. The solvent was evaporated under reduced pressure. EtOAc (3.00 mL) was added to dissolve the crude product, which was washed with HCl (1.00 M, 1.00 mL) and brine (1.00 mL) sequentially. The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated to afford the crude product, which was purified by flash column chromatography to afford the product (70.0 mg, 0.224 mmol, 56% yield, *E*/*Z* isomers) as a colorless oil. R_f = 0.60 EtOAc:Hexanes [1:10 (v/v)]. 1H NMR (700 MHz, CDCl3, 25 ºC, δ): 7.69 (s, 2H, two isomers), 7.44-7.41 (m, 4H, two isomers), 7.38-7.27 (m, 16H, two isomers), 5.82-5.73 (m, 2H, two isomers), 5.12-5.07 (m, 4H,

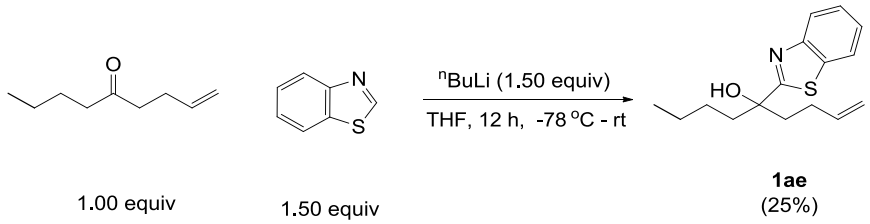
two isomers), 4.99-4.92 (m, 4H, two isomers), 3.39 (br, 2H, two isomers), 2.10-1.99 (m, 8H, two isomers) **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 153.70, 143.37, 138.42, 137.20, 128.69, 128.67, 128.62, 128.29, 127.56, 125.38, 115.00, 76.65, 75.71, 40.28, 27.84. These spectroscopic data correspond to previously reported data.[7]

(*E*)-1,3-Diphenyl-1-(2-vinylphenyl)prop-2-en-1-ol (1ad)



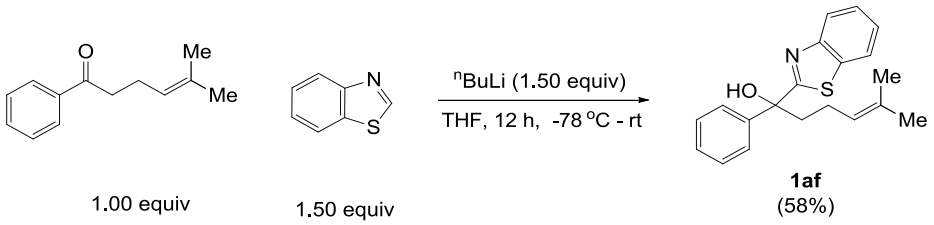
The reaction was performed according to the general procedure A using (*E*)-chalcone (625 mg, 3.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (337 mg, 1.08 mmol, 36% yield). $\mathbf{R_f}$ = 0.41 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.61 (d, *J* = 7.35 Hz, 1H), 7.51 (d, *J* = 6.16 Hz, 1H), 7.41 (d, *J* = 7.42 Hz, 2H), 7.39-7.35 (m, 2H), 7.35-7.28 (m, 7H), 7.25-7.24 (m,, 1H), 6.86-6.78 (m, 2H), 6.58 (d, *J* = 16.0 Hz, 1H), 5.49 (d, *J* = 16.8 Hz, 1H), 5.08 (d, *J* = 12.0 Hz, 1H), 2.67 (bs, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 145.96, 142.86, 137.44, 137.07, 136.93, 135.39, 129.21, 128.77, 128.53, 128.45, 128.33, 127.87, 127.63, 127.56, 127.52, 126.92, 126.86, 115.94, 80.02. These spectroscopic data correspond to previously reported data.[8]

5-(Benzo[*d*]thiazol-2-yl)non-1-en-5-ol (1ae)



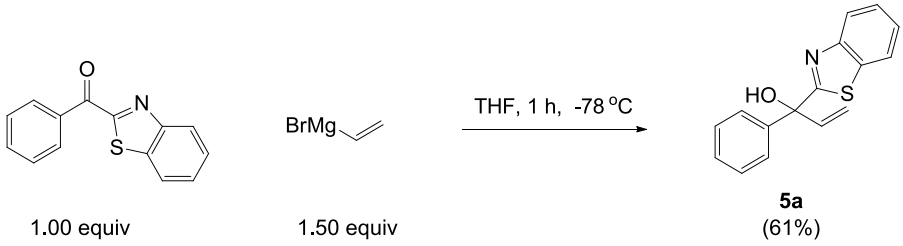
The reaction was performed according to the general procedure A using non-1-en-5-one (280 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (137 mg, 0.500 mmol, 25% yield). $\mathbf{R_f}$ = 0.50 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.00 (d, *J* = 8.10 Hz, 1H), 7.88 (d, *J* = 8.00 Hz, 1H), 7.48 (t, *J* = 7.50 Hz, 1H), 7.38 (t, *J* = 7.50 Hz, 1H), 5.81-5.76 (m, 1H), 5.00-4.91 (m, 2H), 3.44 (bs, 1H), 2.30-2.21 (m, 1H), 2.13-2.03 (m, 2H), 2.00-1.88 (m, 3H), 1.48-1.43 (m, 1H), 1.33-1.24 (m, 2H), 1.13-1.04 (m, 1H), 0.84 (t, *J* = 7.50 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 178.60, 152.95, 138.42, 135.81, 126.18, 125.06, 123.10, 121.98, 115.17, 78.43, 42.88, 41.88, 28.08, 25.58, 23.08, 14.15. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-5-methyl-1-phenylhex-4-en-1-ol (1af)



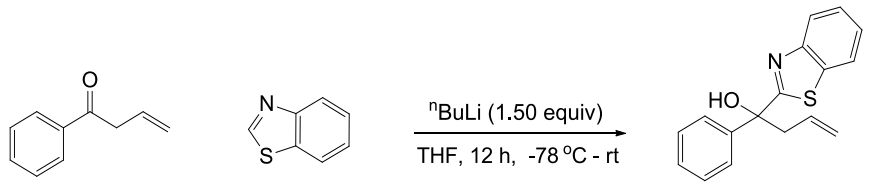
The reaction was performed according to the general procedure A using 5-methyl-1-phenylhex-4-en-1-one (188 mg, 1.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (188 mg, 0.580 mmol, 58% yield). $\mathbf{R_f}$ = 0.40 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.10 (d, *J* = 8.00 Hz, 1H), 7.83 (d, *J* = 8.00 Hz, 1H), 7.70 (d, *J* = 8.50 Hz, 2H), 7.46 (t, *J* = 7.50 Hz, 1H), 7.37-7.33 (m, 3H), 7.27 (t, *J* = 7.50 Hz, 1H), 5.22-5.19 (m, 1H), 4.03-4.01 (m, 1H), 2.59-2.49 (m, 2H), 2.21-2.10 (m, 2H), 1.67 (s, 3H), 1.50 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 178.60, 153.00, 144.17, 135.92, 133.44, 128.57, 127.74, 126.13, 125.70, 125.11, 123.85, 123.29, 121.89, 79.60, 42.46, 25.91, 22.94, 17.90. These spectroscopic data correspond to previously reported data.[5]

1-(Benzo[*d*]thiazol-2-yl)-1-phenylprop-2-en-1-ol (5a)



The reaction was performed according to the modified general procedure B using benzo[*d*]thiazol-2-yl(4-methoxyphenyl)methanone (100.0 mg, 0.418 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as an gummy solid (68.1 mg, 0.255 mmol, 61% yield). $\mathbf{R_f}$ = 0.40 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.02 (d, *J* = 8.40 Hz, 1H), 7.86 (d, *J* = 7.70 Hz, 1H), 7.58-7.56 (m, 2H), 7.48 (t, *J* = 7.00 Hz, 1H), 7.39-7.35 (m, 3H), 7.31 (t, *J* = 7.70 Hz, 1H), 6.71 (dd, *J* = 16.8 & 10.5 Hz, 1H), 5.53 (d, *J* = 17.08 Hz, 1H), 5.44 (dd, *J* = 11.2 Hz, 1H), 3.79 (s, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 176.97, 152.98, 143.44, 141.26, 135.83, 128.73, 128.46, 126.64, 126.35, 125.41, 123.49, 121.93, 115.85, 79.34. These spectroscopic data correspond to previously reported data.[5]

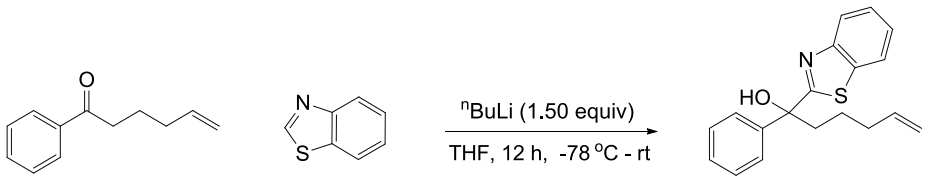
1-(Benzo[*d*]thiazol-2-yl)-1-phenylbut-3-en-1-ol (5b)



1.00 equiv 1.50 equiv **5b** (53%)

The reaction was performed according to the general procedure A using 1-phenylbut-3-en-1-one (438.6 mg, 3.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (450 mg, 1.59 mmol, 53% yield). $\mathbf{R_f}$ = 0.58 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.05-8.03 (m, 1H), 7.84 (d, *J* = 8.00 Hz, 1H), 7.74-7.72 (m, 2H), 7.47 (t, *J* = 7.50 Hz, 1H), 7.37-7.34 (m, 3H), 7.30-7.25 (m, 1H), 5.77-5.74 (m, 1H), 5.32-5.23 (m, 2H), 3.70 (bs, 1H), 3.49-3.45 (m, 1H), 3.13-3.09 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 178.08, 153.35, 143.59, 135.86, 132.73, 128.60, 127.88, 126.13, 125.66, 125.16, 123.39, 121.92, 121.49, 77.97, 47.44. These spectroscopic data correspond to previously reported data.[5]

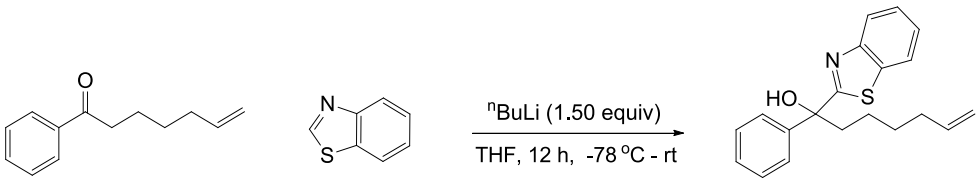
1-(Benzo[*d*]thiazol-2-yl)-1-phenylhex-5-en-1-ol (5c)



1.00 equiv 1.50 equiv **5c** (56%)

The reaction was performed according to the general procedure A using 1-phenylhex-5-en-1-one (348 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (346 mg, 1.12 mmol, 56% yield). $\mathbf{R_f}$ = 0.34 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.05 (d, *J* = 8.05 Hz, 1H), 7.85 (d, *J* = 7.63 Hz, 1H), 7.75 (d, *J* = 7.56 Hz, 2H), 7.49 (t, *J* = 8.40 Hz, 1H), 7.41 (t, *J* = 7.80 Hz, 2H), 7.38 (t, *J* = 7.14 Hz, 1H), 7.32 (t, *J* = 7.35 Hz, 1H), 5.84-5.79 (m, 1H), 5.07-5.04 (m, 1H), 5.01-4.99 (m, 1H), 4.19 (s, 1H), 2.54 (t, *J* = 8.26 Hz, 2H), 2.15 (q, *J* = 7.14 Hz, 2H), 1.60-1.53 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 178.59, 152.73, 144.05, 138.44, 135.78, 128.53, 127.73, 126.11, 125.72, 125.12, 123.20, 121.81, 115.09, 79.03, 42.12, 33.80, 22.93. These spectroscopic data correspond to previously reported data.[5]

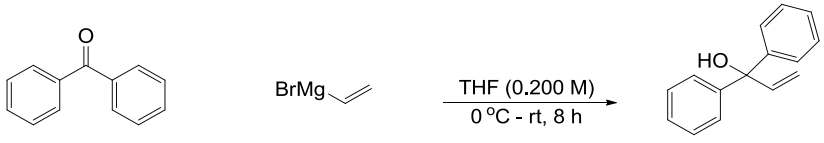
1-(Benzo[*d*]thiazol-2-yl)-1-phenylhept-6-en-1-ol (5d)



1.00 equiv 1.50 equiv **5d** (45%)

The reaction was performed according to the general procedure A using 1-phenylhept-6-en-1-one (282.4 mg, 1.50 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (220 mg, 0.675 mmol, 45% yield). $\mathbf{R_f}$ = 0.56 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 °C, δ): 8.00 (d, *J* = 8.20 Hz, 1H), 7.83 (d, *J* = 8.00 Hz, 1H), 7.68 (d, *J* = 7.50 Hz, 2H), 7.46 (t, *J* = 8.00 Hz, 1H), 7.38-7.34 (m, 3H), 7.28-7.26 (m, 1H), 5.79-5.73 (m, 1H), 4.98-4.90 (m, 2H), 3.84 (bs, 1H), 2.46 (t, *J* = 7.00 Hz, 2H), 2.05-2.01 (m, 2H), 1.47-1.38 (m, 4H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 °C, δ): 178.49, 152.77, 144.17, 138.89, 135.93, 128.61, 127.79, 126.19, 125.73, 125.19, 123.30, 121.89, 114.65, 79.12, 42.63, 33.73, 29.19, 23.20. These spectroscopic data correspond to previously reported data.[5]

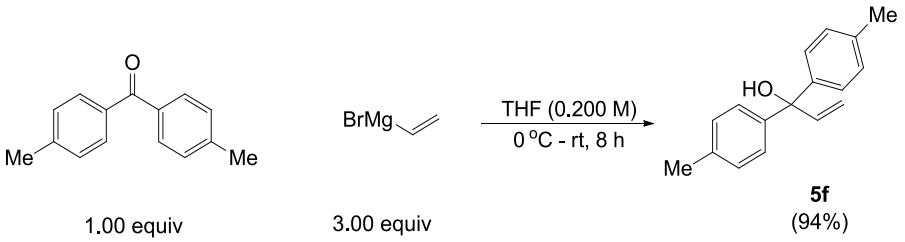
1,1-Diphenylprop-2-en-1-ol (5e)



1.00 equiv 3.00 equiv **5e** (91%)

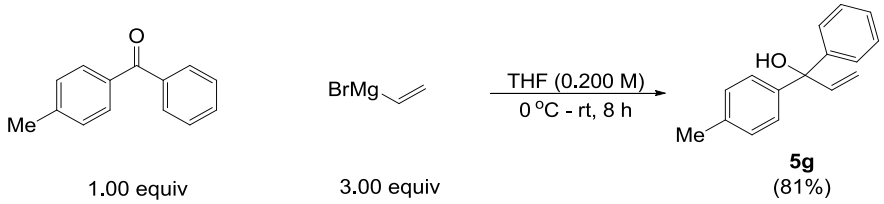
The reaction was performed according to the general procedure B using benzophenone (364.4 mg, 2.00 mmol, 2.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (382.7 mg, 1.82 mmol, 91% yield). $\mathbf{R_f}$ = 0.44 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (400 MHz, $CDCl_3$, 25 °C, δ): 7.43-7.41 (m, 4H), 7.36 (t, *J* = 7.20 Hz, 4H), 7.32-7.28 (m, 2H), 6.55 (dd, *J* = 17.28 & 10.28 Hz, 1H), 5.38-5.34 (m, 2H), 2.32 (s, 1H). **^{13}C NMR** (100 MHz, $CDCl_3$, 25 °C, δ): 145.95, 143.70, 128.36, 127.49, 127.09, 114.22, 79.60. These spectroscopic data correspond to previously reported data.[9]

1,1-Di-*p*-tolylprop-2-en-1-ol (5f)



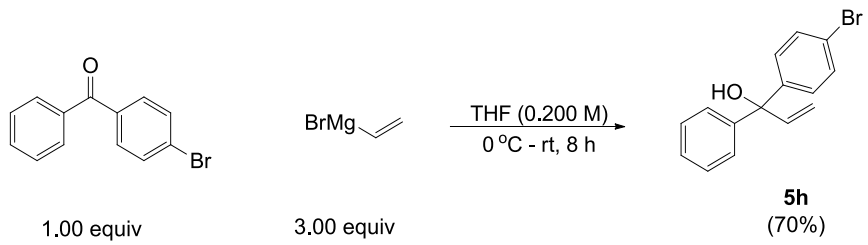
The reaction was performed according to the general procedure B using di-*p*-tolylmethanone (420.2 mg, 2.00 mmol, 2.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (450 mg, 1.88 mmol, 94% yield). $\mathbf{R_f}$ = 0.41 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.26 (d, *J* = 8.15 Hz, 4H), 7.13 (d, *J* = 8.00 Hz, 4H), 6.48 (dd, *J* = 16.95 & 10.55 Hz, 1H), 5.31 (d, *J* = 17.15 Hz, 1H), 5.28 (d, *J* = 10.6 Hz, 1H), 2.33 (s, 6H), 2.21 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 143.97, 143.25, 137.09, 129.03, 126.98, 113.72, 79.34, 21.24. These spectroscopic data correspond to previously reported data.[9]

1-Phenyl-1-(p-tolyl)prop-2-en-1-ol (5g)



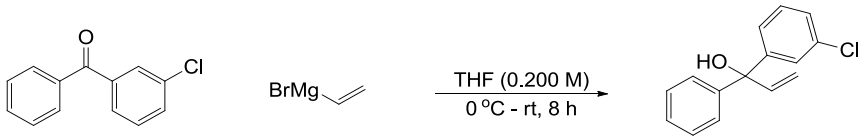
The reaction was performed according to the general procedure B using phenyl(*p*-tolyl)methanone (388.4 mg, 2.00 mmol, 2.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as an gummy solid (362 mg, 1.62 mmol, 81% yield). $\mathbf{R_f}$ = 0.34 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.38 (d, *J* = 8.00 Hz, 2H), 7.32 (t, *J* = 7.75 Hz, 2H), 7.27-7.26 (m, 3H), 7.14 (d, *J* = 7.95 Hz, 2H), 6.50 (dd, *J* = 17.50 & 10.50 Hz, 1H), 5.34-5.29 (m, 2H), 2.40 (s, 3H), 2.26 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 146.07, 143.83, 143.12, 137.18, 129.05, 128.31, 127.38, 127.03, 113.97, 79.46, 21.23. These spectroscopic data correspond to previously reported data.[9]

1-(4-Bromophenyl)-1-phenylprop-2-en-1-ol (5h)



The reaction was performed according to the general procedure B using (4-bromophenyl)(phenyl)methanone (522.2 mg, 2.00 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (405 mg, 1.40 mmol, 70% yield). $\mathbf{R_f}$ = 0.32 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.46 (d, *J* = 11.0 Hz, 2H), 7.38-7.33 (m, 4H), 7.31-7.26 (m, 3H), 6.48 (dd, *J* = 17.1 & 10.6 Hz, 1H), 5.36-5.31 (m, 2H), 2.31 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 145.49, 144.95, 143.20, 131.41, 128.91, 128.52, 127.78, 127.02, 121.54, 114.76, 79.30. These spectroscopic data correspond to previously reported data.[9]

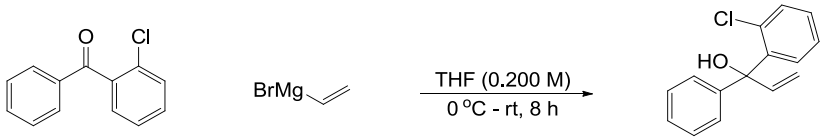
1-(3-Chlorophenyl)-1-phenylprop-2-en-1-ol (5i)



1.00 equiv 3.00 equiv **5i** (87%)

The reaction was performed according to the general procedure B using (3-chlorophenyl)(phenyl)methanone (433.2 mg, 2.00 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (425 mg, 1.74 mmol, 87% yield). $\mathbf{R_f}$ = 0.34 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.42 (s, 1H), 7.38-7.32 (m, 4H), 7.30-7.27 (m, 1H), 7.26-7.24 (m, 3H), 6.48 (dd, *J* = 17.05 & 10.6 Hz, 1H), 5.36-5.31 (m, 2H), 2.30 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 147.97, 145.37, 143.08, 134.36, 129.60, 128.55, 127.83, 127.60, 127.24, 127.04, 125.35, 114.88, 79.27. These spectroscopic data correspond to previously reported data.[9]

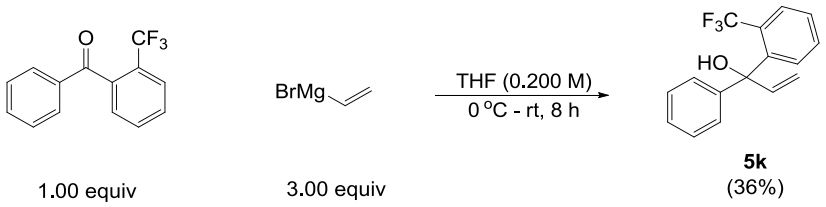
1-(2-Chlorophenyl)-1-phenylprop-2-en-1-ol (5j)



1.00 equiv 3.00 equiv **5j** (68%)

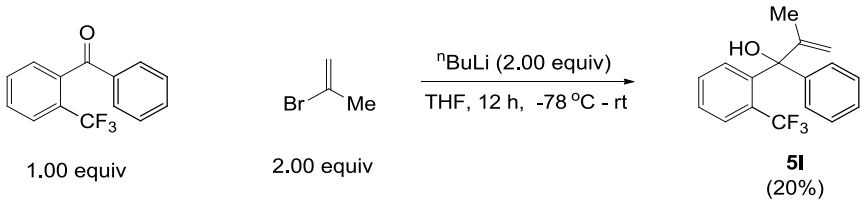
The reaction was performed according to the general procedure B using (2-chlorophenyl)(phenyl)methanone (433.2 mg, 2.00 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (335 mg, 1.36 mmol, 68% yield). $\mathbf{R_f}$ = 0.33 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.74 (dd, *J* = 7.56 & 1.50 Hz, 1H), 7.38-7.27 (m, 8H), 6.64 (dd, *J* = 16.85 & 11.0 Hz, 1H), 5.39-5.35 (m, 2H), 3.27 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 145.16, 142.56, 141.56, 132.76, 131.54, 129.38, 129.20, 128.46, 127.58, 126.90, 126.69, 115.20, 79.79. These spectroscopic data correspond to previously reported data.[9]

1-Phenyl-1-(2-(trifluoromethyl)phenyl)prop-2-en-1-ol (5k)



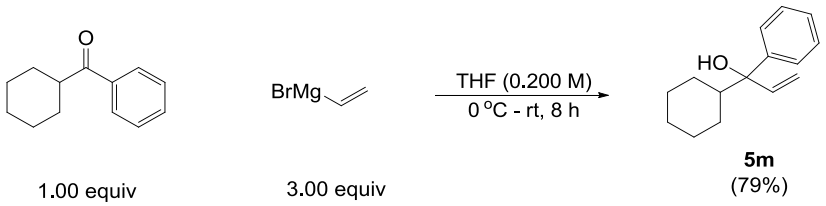
The reaction was performed according to the general procedure B phenyl(2-(trifluoromethyl)phenyl)methanone (500.4 mg, 2.00 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (200 mg, 0.72 mmol, 36% yield). $\mathbf{R_f}$ = 0.34 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.79 (d, J = 7.70 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.53 (t, J = 7.50 Hz, 1H), 7.44 (t, J = 7.50 Hz, 1H), 7.35-7.26 (m, 5H), 6.54-6.49 (m, 1H), 5.37-5.13 (m, 2H), 2.71 (s, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 145.70, 143.86, 143.74, 131.32, 130.47, 128.65 (q, J_3 = 6.57 Hz), 128.25, 128.20 (q, J_2 = 30.96 Hz), 127.91, 127.58, 126.74, 124.54 (q, J_1 = 272.50 Hz), 115.66, 80.45. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –54.60 (s). These spectroscopic data correspond to previously reported data.[9]

2-Methyl-1-phenyl-1-(2-(trifluoromethyl)phenyl)prop-2-en-1-ol (5l)



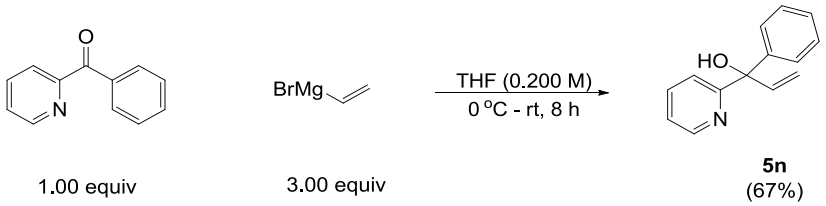
The reaction was performed according to the general procedure A using phenyl(2-(trifluoromethyl)phenyl)methanone (500 mg, 2.00 mmol, 1.00 equiv) as the substrate. After 12 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a colorless liquid (117 mg, 0.400 mmol, 20% yield). $\mathbf{R_f}$ = 0.56 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.82-7.80 (m, 1H), 7.41-7.39 (m, 2H), 7.34-7.29 (m, 5H), 7.16-7.14 (m, 1H), 5.17 (bs, 1H), 4.38 (bs, 1H), 2.90 (s, 1H), 1.87 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 149.73, 145.49, 143.67, 131.65, 130.80, 129.13 (q, J_2 = 31.19 Hz), 128.87 (q, J_1 = 6.50 Hz), 128.23, 127.81, 127.71, 127.59, 124.88 (q, J_2 = 272.6 Hz), 116.63, 84.25, 20.18. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –55.41 (s). These spectroscopic data correspond to previously reported data.[10]

1-Cyclohexyl-1-phenylprop-2-en-1-ol (5m)



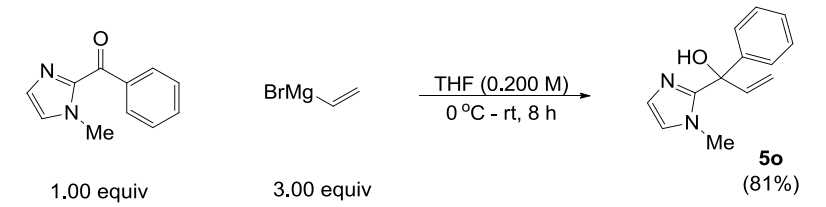
The reaction was performed according to the general procedure B cyclohexyl(phenyl)methanone (564.6 mg, 3.00 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (514 mg, 2.37 mmol, 79% yield). $\mathbf{R}_f$ = 0.44 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.43 (d, *J* = 8.15 Hz, 2H), 7.34 (t, *J* = 7.75 Hz, 2H), 7.23 (t, *J* = 7.25 Hz, 1H), 6.31 (dd, *J* = 16.50 & 10.75 Hz, 1H), 5.34-5.17 (m, 2H), 1.82-1.63 (m, 6H), 1.48-1.46 (m, 1H), 1.28-1.10 (m, 2H), 1.09-0.86 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 145.83, 143.54, 128.26, 126.73, 125.69, 112.71, 79.37, 47.90, 27.40, 26.95, 26.86, 26.75, 26.65. These spectroscopic data correspond to previously reported data.[9]

1-Phenyl-1-(pyridin-2-yl)prop-2-en-1-ol (5n)



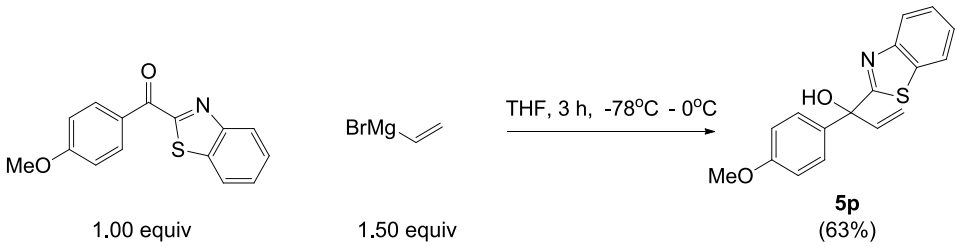
The reaction was performed according to the general procedure B phenyl(pyridin-2-yl)methanone (366.4 mg, 2.00 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (284 mg, 1.34 mmol, 67% yield). $\mathbf{R}_f$ = 0.48 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.42 (d, *J* = 4.70 Hz, 1H), 7.51 (t, *J* = 7.55 Hz, 1H), 7.30-7.28 (m, 2H), 7.18 (t, *J* = 7.25 Hz, 2H), 7.13-7.06 (m, 3H), 6.39 (dd, *J* = 17.05 & 10.50 Hz, 1H), 5.79 (s, 1H), 5.24-5.18 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 162.49, 147.75, 145.31, 142.52, 137.01, 128.41, 127.60, 127.33, 122.56, 122.03, 115.38, 78.54. These spectroscopic data correspond to previously reported data.[9]

1-(1-Methyl-1*H*-imidazol-2-yl)-1-phenylprop-2-en-1-ol (5o)



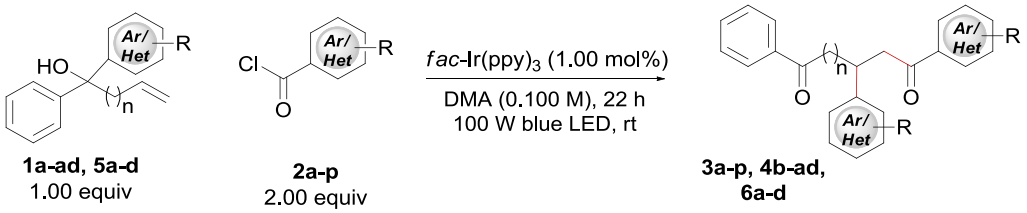
The reaction was performed according to the general procedure B (1-methyl-1*H*-imidazol-2-yl)(phenyl)methanone (372.4 mg, 2.00 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:1 (v/v)] to afford the title compound as a gummy solid (348 mg, 1.62 mmol, 81% yield). $\mathbf{R_f}$ = 0.17 EtOAc:Hexanes [1:1 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.29 (t, *J* = 7.00 Hz, 2H), 7.26-7.25 (m, 2H), 7.23 (t, *J* = 7.35 Hz, 1H), 6.84 (s, 1H), 6.76 (s, 1H), 6.74-6.72 (m, 1H), 5.22-5.19 (m, 2H), 4.47 (bs, 1H), 3.27 (s, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 149.91, 142.87, 142.18, 128.45, 127.55, 126.20, 126.02, 123.01, 113.48, 76.03, 34.30. **HRMS** (ESI-TOF) *m/z* calcd for $C_{13}H_{15}N_2O$ [$(M + H)^+$], 215.11789, found, 215.11857.

1-(Benzo[*d*]thiazol-2-yl)-1-(4-methoxyphenyl)prop-2-en-1-ol (5p)



The reaction was performed according to the modified general procedure B[11] using benzo[*d*]thiazol-2-yl(4-methoxyphenyl)methanone (100.0 mg, 0.370 mmol, 1.00 equiv) as the substrate. After completion, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as an gummy solid (69.4 mg, 0.233 mmol, 63% yield). $\mathbf{R_f}$ = 0.35 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.01 (d, *J* = 8.19 Hz, 1H), 7.84 (d, *J* = 7.98 Hz, 1H), 7.52-7.44 (m, 3H), 7.36 (t, *J* = 7.42 Hz, 1H), 6.87 (d, *J* = 8.82 Hz, 2H), 6.69 (dd, *J* = 17.08 & 10.5 Hz, 1H), 5.53 (d, *J* = 17.08 Hz, 1H), 5.41 (dd, *J* = 10.57 Hz, 1H), 4.06 (s, 1H), 3.78 (s, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 177.53, 159.54, 153.09, 141.32, 135.69, 128.05, 126.20, 125.24, 123.37, 121.83, 115.55, 113.92, 79.05, 55.42.

General Procedure C (1,4-Migration):



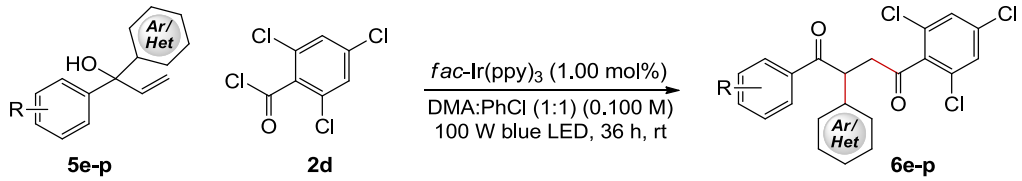
1a-ad, 5a-d
1.00 equiv

2a-p
2.00 equiv

3a-p, 4b-ad, 6a-d

In a glovebox, to an oven-dried 4 mL screw cap vial was added 1,1-aryl-heteroaryl-4-en-1-ol (1.00 equiv), and DMA (0.100 M, with respect to 1,1-aryl-heteroaryl-4-en-1-ol substrate). To this suspension was added aroyl chloride (2.00 equiv), *fac*-Ir(ppy)$_3$, (1.00 mol%), and a magnetic stir bar. Next, the vial was capped and taken out of the glovebox. The reaction vial was placed in the photoredox setup and stirred at rt with irradiation of 100W blue LED light source (450 nm, unless otherwise stated) for 22 h. After that, the reaction mixture was removed from the light source and was directly loaded on to silica column, eluting with EtOAc:Hexane (v/v) to afford the desired product.

General Procedure D (1,2-Migration):



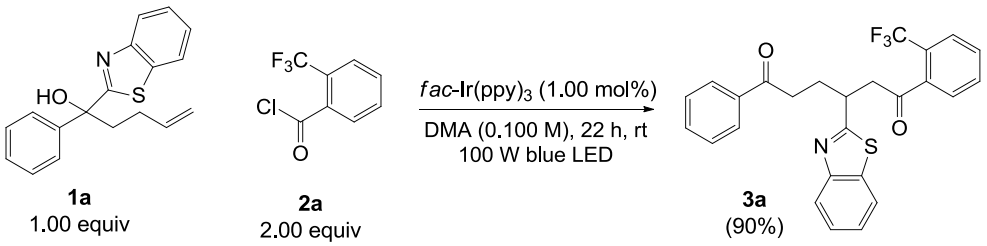
5e-p
1.00 equiv

2d
2.00 equiv

6e-p

In a glovebox, to an oven-dried 4 mL screw cap vial was added 1,1-aryl-(hetero)aryl-2-en-1-ol (1.00 equiv), and DMA:PhCl (1:1) (0.100 M, with respect to 1,1-aryl-(hetero)aryl-2-en-1-ol substrate). To this suspension was added 2,4,6-trichlorobenzoyl chloride (2.00 equiv), *fac*-Ir(ppy)$_3$, (1.00 mol%), and a magnetic stir bar. Next, the vial was capped and taken out of the glovebox. The reaction vial was placed in the photoredox setup and stirred at room temp with irradiation of 100W blue LED light source (450 nm, unless otherwise stated) for 36 h. After that, the reaction mixture was removed from the light source and was directly loaded on to silica column, eluting with EtOAc:Hexane (v/v) to afford the desired product.

3-(Benzo[*d*]thiazol-2-yl)-6-phenyl-1-(2-(trifluoromethyl)phenyl)hexane-1,6-dione (3a)



1a
1.00 equiv

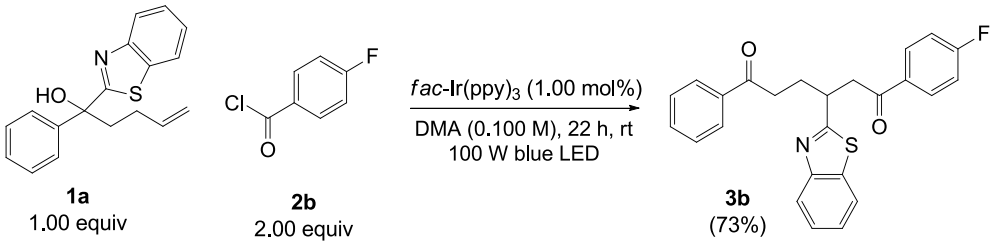
2a
2.00 equiv

3a
(90%)

The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-

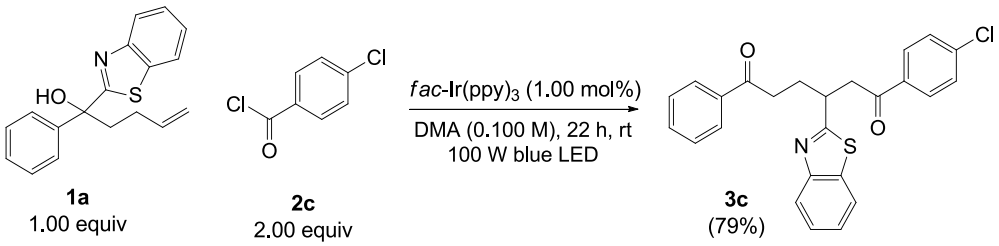
en-1-ol (29.5 mg, 0.100 mmol, 1.00 equiv) and 2-(trifluoromethyl)benzoyl chloride (41.6 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (42.3 mg, 0.0901 mmol, 90% yield). $\mathbf{R_f}$ = 0.25 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.96 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 7.21 Hz, 2H), 7.85 (d, *J* = 7.91 Hz, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.59 (t, *J* = 7.91 Hz, 1H), 7.57-7.51 (m, 3H), 7.45 (t, *J* = 8.19 Hz, 1H), 7.41 (t, *J* = 7.91 Hz, 2H), 7.36 (t, *J* = 7.98 Hz, 1H), 4.10-4.01 (m, 1H), 3.75 (dd, *J* = 18.27 & 7.77 Hz, 1H), 3.32 (dd, *J* = 18.27 & 5.81 Hz, 1H), 3.15-3.01 (m, 2H), 2.45-2.31 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 201.70, 199.17, 173.74, 153.20, 140.01, 136.85, 135.11, 133.31, 132.02, 130.42, 128.76, 128.20, 127.61, 127.16 (q, $J^2_{C\text{-}F}$ = 32.06 Hz), 126.86 (q, $J^3_{C\text{-}F}$ = 5.05 Hz), 126.19, 125.17, 123.74 (q, $J^1_{C\text{-}F}$ = 272.54 Hz), 122.92, 121.87, 48.27, 39.10, 36.07, 29.85. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –58.28 (s). **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{21}F_3NO_2S$ [$(M + H)^+$], 468.12396, found, 468.12335.

3-(Benzo[*d*]thiazol-2-yl)-1-(4-fluorophenyl)-6-phenylhexane-1,6-dione (3b)



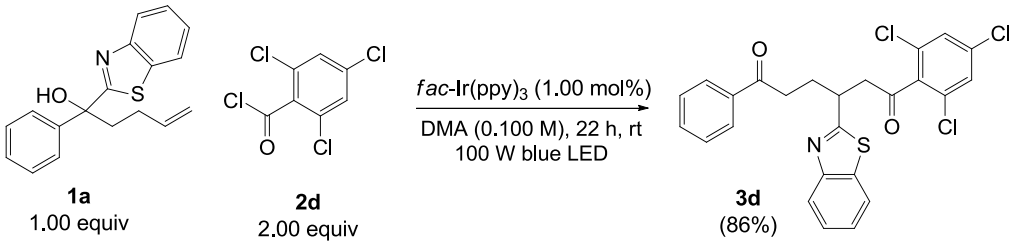
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 4-fluorobenzoyl chloride (63.4 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (60.9 mg, 0.146 mmol, 73% yield). $\mathbf{R_f}$ = 0.29 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.99 (dd, *J* = 8.61 & 5.46 Hz, 2H), 7.93 (d, *J* = 8.19 Hz, 1H), 7.87 (d, *J* = 7.49 Hz, 2H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.51 (t, *J* = 7.47 Hz, 1H), 7.43 (t, *J* = 7.42 Hz, 1H), 7.40 (t, *J* = 7.70 Hz, 2H), 7.34 (t, *J* = 7.38 Hz, 1H), 7.10 (t, *J* = 7.54 Hz, 2H), 4.08-4.04 (m, 1H), 3.80 (dd, *J* = 17.57 & 7.49 Hz, 1H), 3.44 (dd, *J* = 17.57 & 5.95 Hz, 1H), 3.12-3.03 (m, 2H), 2.39-2.36 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.29, 196.03, 174.20, 166.02 (q, $J^1_{C\text{-}F}$ = 253.6 Hz), 153.27, 136.85, 134.96, 133.28, 133.26, 130.97 (q, $J^3_{C\text{-}F}$ = 9.10 Hz), 128.73, 128.19, 126.16, 125.11, 122.92, 121.82, 115.92 (q, $J^2_{C\text{-}F}$ = 21.7 Hz), 44.24, 39.25, 36.22, 30.05. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –105.60 (m). **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{21}FNO_2S$ [$(M + H)^+$], 418.12715, found, 418.12680.

3-(Benzo[*d*]thiazol-2-yl)-1-(4-chlorophenyl)-6-phenylhexane-1,6-dione (3c)



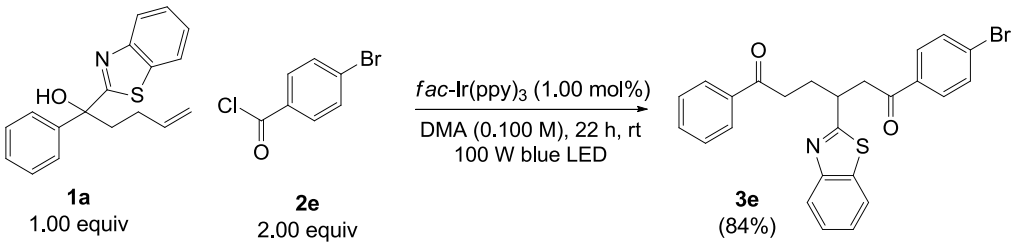
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 4-chlorobenzoyl chloride (70.0 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (67.1 mg, 0.158 mmol, 79% yield). $\mathbf{R_f}$ = 0.36 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.93 (d, *J* = 8.12 Hz, 1H), 7.90 (d, *J* = 8.54 Hz, 2H), 7.87 (d, *J* = 7.35 Hz, 2H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.51 (t, *J* = 7.42 Hz, 1H), 7.45-7.37 (m, 5H), 7.34 (t, *J* = 7.77 Hz, 1H), 4.09-4.02 (m, 1H), 3.80 (dd, *J* = 17.57 & 7.42 Hz, 1H), 3.43 (dd, *J* = 17.57 & 5.88 Hz, 1H), 3.14-3.02 (m, 2H), 2.42-2.34 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.22, 196.41, 174.07, 153.25, 139.92, 136.83, 135.12, 134.95, 133.27, 129.72, 129.11, 128.72, 128.17, 126.15, 125.10, 122.92, 121.81, 44.23, 39.20, 36.18, 30.01. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{21}ClNO_2S$ [(M + H)$^+$], 434.09760, found, 434.09674.

3-(Benzo[*d*]thiazol-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (3d)



The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:12 (v/v)] to afford the title compound as a gummy solid (84.2 mg, 0.172 mmol, 86% yield). $\mathbf{R_f}$ = 0.53 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.95 (d, *J* = 8.19 Hz, 1H), 7.87 (d, *J* = 7.49 Hz, 2H), 7.84 (d, *J* = 7.91 Hz, 1H), 7.51 (t, *J* = 7.35 Hz, 1H), 7.45 (t, *J* = 7.49 Hz, 1H), 7.39 (t, *J* = 7.70 Hz, 2H), 7.36 (t, *J* = 7.49 Hz, 1H), 7.29 (s, 2H), 4.11-4.01 (m, 1H), 3.62 (dd, *J* = 19.04 & 6.51 Hz, 1H), 3.39 (dd, *J* = 19.04 & 6.44 Hz, 1H), 3.15-2.98 (m, 2H), 2.49-2.32 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.12, 198.79, 173.29, 153.16, 137.61, 136.80, 136.05, 134.98, 133.26, 131.44, 128.71, 128.42, 128.15, 126.21, 125.18, 122.93, 121.83, 49.11, 38.43, 36.05, 29.80. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{19}Cl_3NO_2S$ [(M + H)$^+$], 502.01966, found, 502.01916.

3-(Benzo[*d*]thiazol-2-yl)-1-(4-bromophenyl)-6-phenylhexane-1,6-dione (3e)



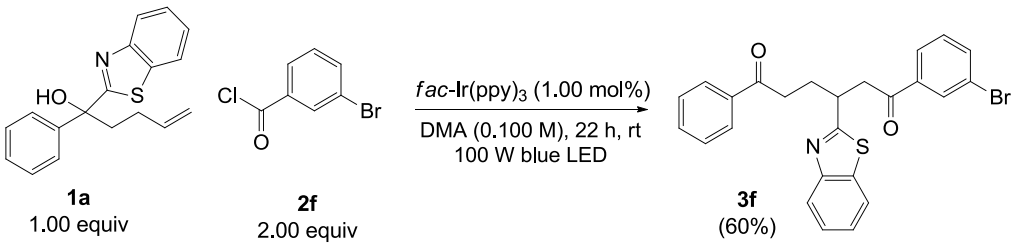
1a 1.00 equiv

2e 2.00 equiv

3e (84%)

The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (29.5 mg, 0.100 mmol, 1.00 equiv) and 4-bromobenzoyl chloride (42.8 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (40.3 mg, 0.0840 mmol, 84% yield). $\mathbf{R_f}$ = 0.36 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.96 (d, *J* = 8.12 Hz, 1H), 7.88 (d, *J* = 7.28 Hz, 2H), 7.81-7.86 (m, 3H), 7.58 (d, *J* = 8.54 Hz, 2H), 7.52 (t, *J* = 7.35 Hz, 1H), 7.44 (t, *J* = 7.42 Hz, 1H), 7.41 (t, *J* = 7.77 Hz, 2H), 7.35 (t, *J* = 7.58 Hz, 1H), 4.09-4.02 (m, 1H), 3.79 (dd, *J* = 17.64 & 7.49 Hz, 1H), 3.43 (dd, *J* = 17.64 & 5.88 Hz, 1H), 3.16-3.01 (m, 2H), 2.44-2.32 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.24, 196.64, 174.07, 153.28, 136.85, 135.55, 134.97, 133.29, 132.13, 129.84, 128.74, 128.70, 128.20, 126.17, 125.13, 122.94, 121.83, 44.24, 39.21, 36.20, 30.03. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{21}BrNO_2S$ [$(M + H)^+$], 478.04709, found, 478.04668.

3-(Benzo[*d*]thiazol-2-yl)-1-(3-bromophenyl)-6-phenylhexane-1,6-dione (3f)



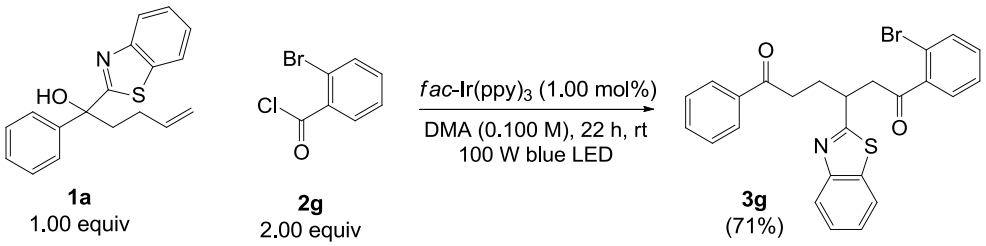
1a 1.00 equiv

2f 2.00 equiv

3f (60%)

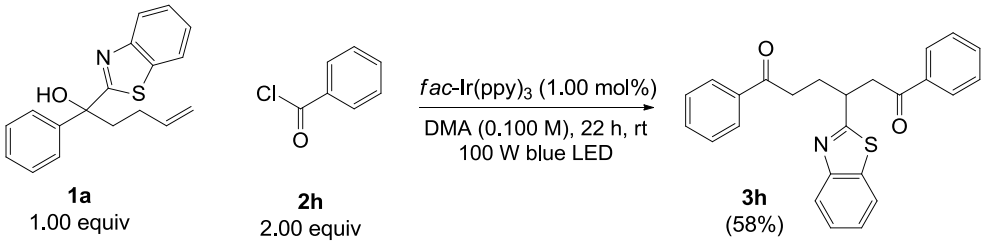
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 3-bromobenzoyl chloride (87.6 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (57.4 mg, 0.120 mmol, 60% yield). $\mathbf{R_f}$ = 0.29 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.12-8.08 (m, 1H), 7.93 (d, *J* = 8.12 Hz, 1H), 7.91-7.87 (m, 3H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.70-7.65 (m, 1H), 7.52 (t, *J* = 7.42 Hz, 1H), 7.47-7.43 (m, 3H), 7.38-7.31 (m, 2H), 4.10-4.00 (m, 1H), 3.81 (dd, *J* = 17.71 & 7.56 Hz, 1H), 3.43 (dd, *J* = 17.71 & 5.81 Hz, 1H), 3.15-3.01 (m, 2H), 2.45-2.31 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.26, 196.35, 174.00, 153.27, 138.55, 136.86, 136.34, 134.98, 133.32, 131.44, 130.43, 128.76, 128.22, 126.86, 126.19, 125.15, 123.20, 122.97, 121.84, 44.32, 39.16, 36.18, 30.03. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{21}BrNO_2S$ [$(M + H)^+$], 478.04709, found, 478.04657.

3-(Benzo[*d*]thiazol-2-yl)-1-(2-bromophenyl)-6-phenylhexane-1,6-dione (3g)



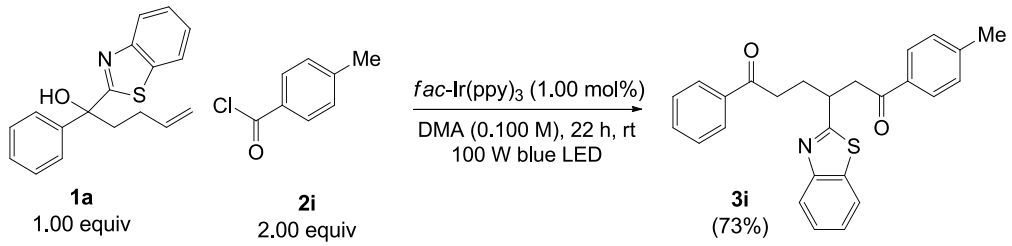
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 2-bromobenzoyl chloride (87.6 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (68.3 mg, 0.142 mmol, 71% yield). $\mathbf{R_f}$ = 0.33 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.94 (d, *J* = 8.19 Hz, 1H), 7.89 (d, *J* = 7.21 Hz, 2H), 7.84 (d, *J* = 7.98 Hz, 1H), 7.58 (d, *J* = 7.98 Hz, 1H), 7.52 (t, *J* = 7.35 Hz, 1H), 7.45 (t, *J* = 8.19 Hz, 1H), 7.42-7.39 (m, 3H), 7.38-7.31 (m, 2H), 7.31-7.26 (m, 1H), 4.08-4.04 (m, 1H), 3.80 (dd, *J* = 17.57 & 7.49 Hz, 1H), 3.44 (dd, *J* = 17.57 & 5.95 Hz, 1H), 3.12-3.03 (m, 2H), 2.39-2.36 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 201.56, 199.22, 173.81, 153.18, 141.42, 136.86, 135.11, 133.89, 133.30, 131.93, 129.01, 128.76, 128.22, 127.61, 126.18, 125.15, 122.97, 121.85, 118.90, 48.00, 39.57, 36.13, 29.94. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{21}BrNO_2S$ [$(M + H)^+$], 478.04709, found, 478.04631.

3-(Benzo[*d*]thiazol-2-yl)-1,6-diphenylhexane-1,6-dione (3h)



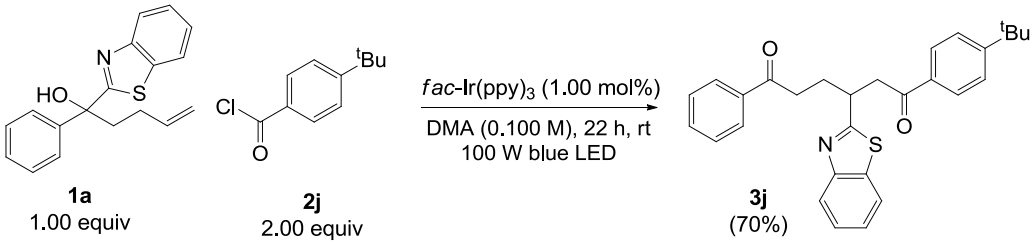
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and benzoyl chloride (56 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (46.5 mg, 0.116 mmol, 58% yield). $\mathbf{R_f}$ = 0.28 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.97 (d, *J* = 7.28 Hz, 2H), 7.94 (d, *J* = 8.19 Hz, 1H), 7.88 (d, *J* = 7.28 Hz, 2H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.55 (t, *J* = 7.42 Hz, 1H), 7.51 (t, *J* = 7.42 Hz, 1H), 7.48-7.38 (m, 5H), 7.34 (t, *J* = 7.91 Hz, 1H), 4.12-4.05 (m, 1H), 3.82 (dd, *J* = 17.64 & 7.28 Hz, 1H), 3.48 (dd, *J* = 17.64 & 6.09 Hz, 1H), 3.15-3.02 (m, 2H), 2.45-2.32 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.33, 197.57, 174.35, 153.32, 136.89, 136.82, 135.01, 133.51, 133.25, 128.83, 128.73, 128.33, 128.21, 126.13, 125.06, 122.95, 121.82, 44.40, 39.28, 36.32, 30.09. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{21}NO_2S$ [$(M + H)^+$], 400.13658, found, 400.13684.

3-(Benzo[*d*]thiazol-2-yl)-6-phenyl-1-(*p*-tolyl)hexane-1,6-dione (3i)



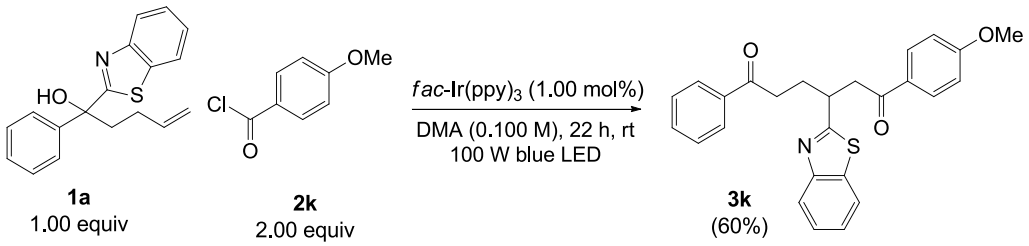
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (29.5 mg, 0.100 mmol, 1.00 equiv) and 4-methylbenzoyl chloride (30.9 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (30.2 mg, 0.0730 mmol, 73% yield). $\mathbf{R_f}$ = 0.35 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.94 (d, *J* = 8.12 Hz, 1H), 7.91-7.85 (m, 4H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.51 (t, *J* = 7.35 Hz, 1H), 7.46-7.42 (m, 1H), 7.40 (t, *J* = 7.91 Hz, 2H), 7.37-7.32 (m, 1H), 7.24 (d, *J* = 8.05 Hz, 2H), 4.13-4.02 (m, 1H), 3.78 (dd, *J* = 17.57 & 7.21 Hz, 1H), 3.46 (dd, *J* = 17.5 & 6.16 Hz, 1H), 3.14-3.01 (m, 2H), 2.39 (s, 3H), 2.39-2.33 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.36, 197.16, 174.47, 153.34, 144.33, 136.90, 135.02, 134.38, 133.23, 129.50, 128.72, 128.44, 128.21, 126.10, 125.03, 122.94, 121.81, 44.31, 39.33, 36.36, 30.10, 21.86. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{24}NO_2S$ [$(M + H)^+$], 414.15223, found, 414.15207.

3-(Benzo[*d*]thiazol-2-yl)-1-(4-(*tert*-butyl)phenyl)-6-phenylhexane-1,6-dione (3j)



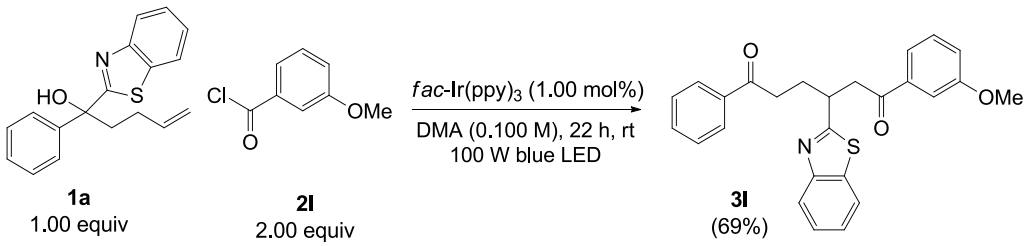
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 4-(*tert*-butyl)benzoyl chloride (78.6 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (64.3 mg, 0.140 mmol, 70% yield). $\mathbf{R_f}$ = 0.42 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.95 (d, *J* = 8.19 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 2H), 7.88 (d, *J* = 7.7 Hz, 2H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.51 (t, *J* = 7.49 Hz, 1H), 7.48-7.42 (m, 3H), 7.40 (t, *J* = 7.70 Hz, 2H), 7.34 (t, *J* = 7.70 Hz, 1H), 4.12-4.04 (m, 1H), 3.79 (dd, *J* = 17.5 & 7.28 Hz, 1H), 3.47 (dd, *J* = 17.5 & 6.09 Hz, 1H), 3.14-3.02 (m, 2H), 2.45-2.32 (m, 2H), 1.33 (s, 9H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.37, 197.20, 174.50, 157.26, 153.31, 136.90, 135.00, 134.27, 133.23, 128.71, 128.30, 128.21, 126.10, 125.77, 125.03, 122.93, 121.81, 44.35, 39.34, 36.36, 35.31, 31.25, 30.10. **HRMS** (ESI-TOF) *m/z* calcd for $C_{29}H_{30}NO_2S$ [$(M + H)^+$], 456.19918, found, 456.19879.

3-(Benzo[*d*]thiazol-2-yl)-1-(4-methoxyphenyl)-6-phenylhexane-1,6-dione (3k)



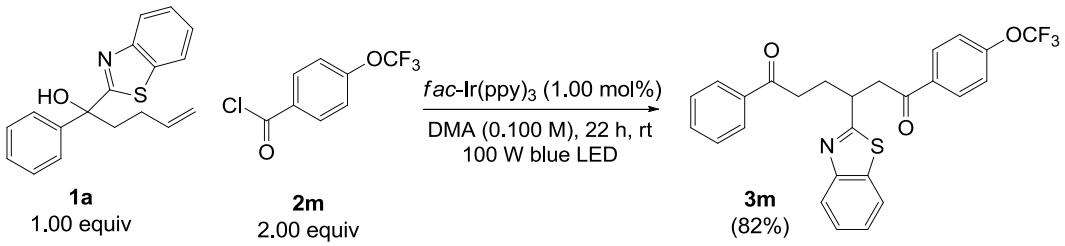
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 4-methoxybenzoyl chloride (68.2 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (51.4 mg, 0.120 mmol, 60% yield). **R$_f$** = 0.13 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.99-7.91 (m, 3H), 7.87 (d, *J* = 7.28 Hz, 2H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.51 (t, *J* = 7.35 Hz, 1H), 7.43 (t, *J* = 7.21 Hz, 1H), 7.40 (t, *J* = 7.56 Hz, 2H), 7.34 (t, *J* = 7.21 Hz, 1H), 6.91 (d, *J* = 8.82 Hz, 2H), 4.10-4.01 (m, 1H), 3.85 (s, 3H), 3.74 (dd, *J* = 17.36 & 7.21 Hz, 1H), 3.43 (dd, *J* = 17.36 & 6.23 Hz, 1H), 3.13-3.01 (m, 2H), 2.43-2.31 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.41, 196.06, 174.56, 163.84, 153.36, 136.93, 135.04, 133.24, 130.64, 129.97, 128.74, 128.23, 126.11, 125.04, 122.95, 121.83, 113.97, 55.69, 44.11, 39.44, 36.40, 30.13. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{24}NO_3S$ [(M + H)$^+$], 430.14714, found, 430.14731.

3-(Benzo[*d*]thiazol-2-yl)-1-(3-methoxyphenyl)-6-phenylhexane-1,6-dione (3l)



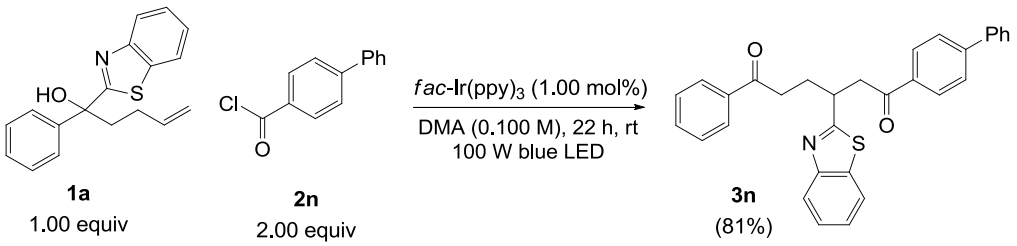
The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and 3-methoxybenzoyl chloride (68.2 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (59.3 mg, 0.138 mmol, 69% yield). **R$_f$** = 0.18 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.94 (d, *J* = 8.19 Hz, 1H), 7.88 (d, *J* = 7.28 Hz, 2H), 7.83 (d, *J* = 7.98 Hz, 1H), 7.56 (d, *J* = 7.35 Hz, 1H), 7.51 (t, *J* = 7.35 Hz, 1H), 7.47 (s, 1H), 7.46-7.42 (m, 2H), 7.40 (t, *J* = 7.84 Hz, 1H), 7.38-7.32 (m, 2H), 7.12-7.06 (m, 1H), 4.14-4.01 (m, 1H), 3.88-3.72 (m, 4H), 3.47 (dd, *J* = 17.64 & 5.95 Hz, 1H), 3.14-3.00 (m, 2H), 2.44-2.28 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.31, 197.39, 174.34, 160.01, 153.31, 138.16, 136.88, 134.99, 133.24, 129.81, 128.72, 128.20, 126.12, 125.06, 122.94, 121.81, 120.99, 120.17, 112.31, 55.62, 44.52, 39.31, 36.28, 30.07. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{24}NO_3S$ [(M + H)$^+$], 430.14714, found, 430.14618.

3-(Benzo[*d*]thiazol-2-yl)-6-phenyl-1-(4-(trifluoromethoxy)phenyl)hexane-1,6-dione (3m)



The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (29.5 mg, 0.100 mmol, 1.00 equiv) and 4-(trifluoromethoxy)benzoyl chloride (44.8 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (39.4 mg, 0.0820 mmol, 82% yield). $\mathbf{R_f}$ = 0.38 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.02 (d, *J* = 8.82 Hz, 2H), 7.93 (d, *J* = 8.19 Hz, 1H), 7.88 (d, *J* = 7.28 Hz, 2H), 7.84 (d, *J* = 7.91 Hz, 1H), 7.52 (t, *J* = 7.35 Hz, 1H), 7.47-7.43 (m, 1H), 7.41 (t, *J* = 7.77 Hz, 2H), 7.35 (t, *J* = 7.35 Hz, 1H), 7.27 (d, *J* = 7.4 Hz, 2H), 4.11-4.02 (m, 1H), 3.83 (dd, *J* = 17.64 & 7.49 Hz, 1H), 3.44 (dd, *J* = 17.64 & 5.88 Hz, 1H), 3.14-3.02 (m, 2H), 2.44-2.34 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.27, 196.16, 174.05, 153.28, 152.94, 136.86, 135.06, 134.98, 133.33, 130.39, 128.77, 128.21, 126.20, 125.16, 122.96, 121.85, 120.45 (q, $J_{C\text{-}F}$= 257.3), 120.60, 44.33, 39.23, 36.19, 30.04. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –58.19 (s). **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{21}F_3NO_3S$ [$(M + H)^+$], 484.11888, found, 484.11850.

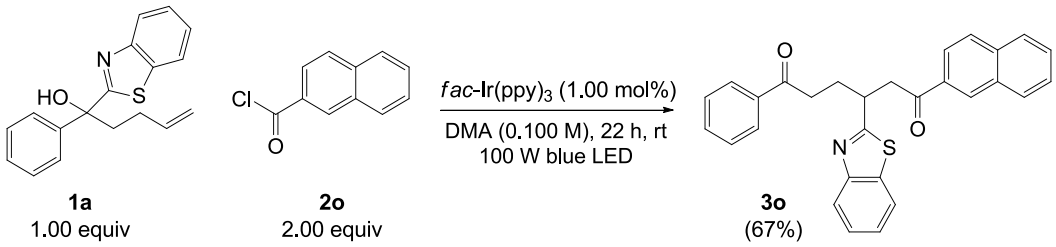
1-([1,1'-Biphenyl]-4-yl)-3-(benzo[*d*]thiazol-2-yl)-6-phenylhexane-1,6-dione (3n)



The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (29.5 mg, 0.100 mmol, 1.00 equiv) and [1,1'-biphenyl]-4-carbonyl chloride (43.3 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (31.2 mg, 0.0810 mmol, 81% yield). $\mathbf{R_f}$ = 0.31 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.05 (d, *J* = 8.4 Hz, 2H), 7.96 (d, *J* = 8.12 Hz, 1H), 7.89 (d, *J* = 7.28 Hz, 2H), 7.84 (d, *J* = 7.98 Hz, 1H), 7.67 (d, *J* = 8.33 Hz, 2H), 7.61 (d, *J* = 7.35 Hz, 2H), 7.52 (t, *J* = 7.35 Hz, 1H), 7.50-7.38 (m, 6H), 7.35 (t, *J* = 7.84 Hz, 1H), 4.15-4.05 (m, 1H), 3.86 (dd, *J* = 17.57 & 7.35 Hz, 1H), 3.51 (dd, *J* = 17.57 & 6.09 Hz, 1H), 3.16-3.03 (m, 2H), 2.46-2.35 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.36, 197.18, 174.38, 153.35, 146.18, 140.02, 136.92, 135.54, 135.04, 133.27, 129.16, 128.95, 128.75, 128.47, 128.24, 127.48, 126.15, 125.09, 122.97, 121.85, 44.45, 39.36, 36.34, 30.12. **HRMS**

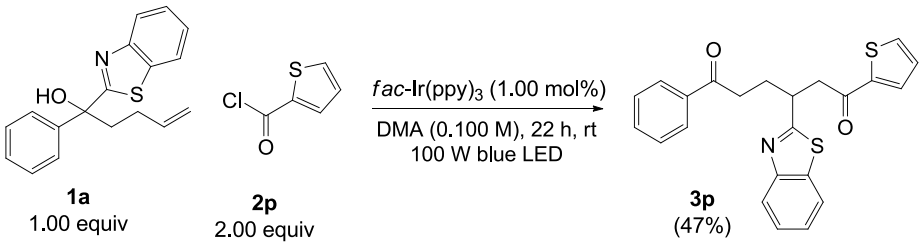
(ESI-TOF) *m/z* calcd for $C_{31}H_{26}NO_2S$ [(M + H)$^+$], 476.16788, found, 476.17760.

3-(Benzo[*d*]thiazol-2-yl)-1-(naphthalen-2-yl)-6-phenylhexane-1,6-dione (3o)



The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (29.5 mg, 0.100 mmol, 1.00 equiv) and 2-naphthoyl chloride (38.1 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (30.6 mg, 0.0670 mmol, 67% yield). $\mathbf{R_f}$ = 0.33 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.51 (s, 1H), 8.02 (dd, *J* = 8.61 & 1.68 Hz, 1H), 7.95 (d, *J* = 8.12 Hz, 2H), 7.92-7.82 (m, 5H), 7.59 (t, *J* = 8.12 Hz, 1H), 7.57-7.49 (m, 2H), 7.43 (t, *J* = 8.26 Hz, 1H), 7.41 (t, *J* = 7.98 Hz, 2H), 7.34 (t, *J* = 8.05 Hz, 1H), 4.18-4.10 (m, 1H), 3.96 (dd, *J* = 17.36 & 7.28 Hz, 1H), 3.62 (dd, *J* = 17.43 & 6.09 Hz, 1H), 3.17-3.05 (m, 2H), 2.49-2.37 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.37, 197.54, 174.41, 153.37, 136.92, 135.89, 135.04, 134.19, 133.28, 132.68, 130.18, 129.83, 128.78, 128.76, 128.72, 128.24, 127.99, 127.03, 126.16, 125.10, 123.99, 122.97, 121.85, 44.44, 39.43, 36.37, 30.17. **HRMS** (ESI-TOF) *m/z* calcd for $C_{29}H_{24}NO_2S$ [(M + H)$^+$], 450.15223, found, 450.15234.

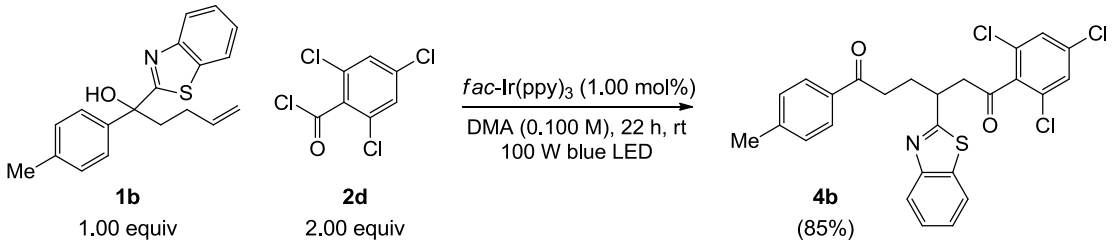
3-(Benzo[*d*]thiazol-2-yl)-6-phenyl-1-(thiophen-2-yl)hexane-1,6-dione (3p)



The reaction was performed according to the general procedure C using 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (59.0 mg, 0.200 mmol, 1.00 equiv) and thiophene-2-carbonyl chloride (58.6 mg, 0.400 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:6 (v/v)] to afford the title compound as a gummy solid (38.4 mg, 0.0940 mmol, 47% yield). $\mathbf{R_f}$ = 0.25 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.95 (d, *J* = 8.19 Hz, 1H), 7.87 (d, *J* = 7.35 Hz, 2H), 7.83 (d, *J* = 7.91 Hz, 1H), 7.79-7.75 (m, 1H), 7.64-7.61 (m, 1H), 7.51 (t, *J* = 7.42 Hz, 1H), 7.47-7.43 (m, 1H), 7.40 (t, *J* = 7.84 Hz, 2H), 7.38-7.33 (m, 1H), 7.14-7.09 (m, 1H), 4.08-4.01 (m, 1H), 3.71 (dd, *J* = 17.01 & 7.28 Hz, 1H), 3.43 (dd, *J* = 17.01 & 6.3 Hz, 1H), 3.13-3.01 (m, 2H), 2.44-2.32 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.29, 196.48, 173.97, 153.34, 144.13, 136.88, 135.02, 134.20, 133.28, 132.44, 128.75,

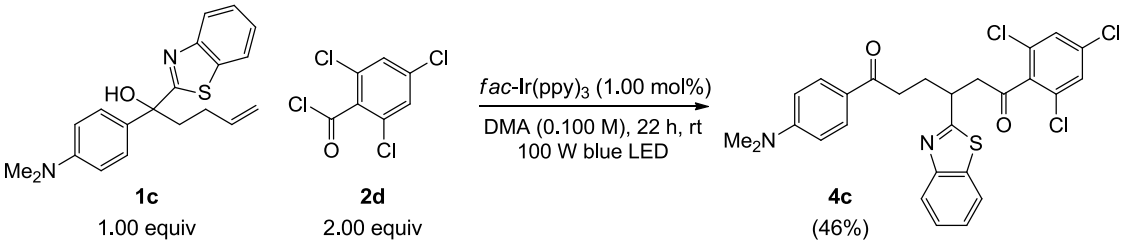
128.37, 128.22, 126.17, 125.12, 122.99, 121.85, 44.96, 39.47, 36.31, 30.01. **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{20}NO_2S_2$ [$(M + H)^+$], 406.09300, found, 406.09311.

3-(Benzo[*d*]thiazol-2-yl)-6-(*p*-tolyl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4b)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(*p*-tolyl)pent-4-en-1-ol (30.9 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (45.2 mg, 0.0850 mmol, 85% yield). $\mathbf{R_f}$ = 0.29 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.95 (d, *J* = 8.12 Hz, 1H), 7.84 (d, *J* = 7.91 Hz, 1H), 7.78 (d, *J* = 8.19 Hz, 2H), 7.45 (t, *J* = 8.12 Hz, 1H), 7.35 (t, *J* = 7.21 Hz, 1H), 7.28 (s, 2H), 7.19 (d, *J* = 8.05 Hz, 2H), 4.11-4.00 (m, 1H), 3.62 (dd, *J* = 19.11 & 6.58 Hz, 1H), 3.38 (dd, *J* = 19.11 & 6.51 Hz, 1H), 3.12-2.97 (m, 2H), 2.47-2.32 (m, 5H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.76, 198.73, 173.34, 153.15, 144.00, 137.62, 136.00, 134.99, 134.34, 131.44, 129.36, 128.39, 128.26, 126.18, 125.14, 122.91, 121.81, 49.08, 38.45, 35.91, 29.90, 21.77. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{21}Cl_3NO_2S$ [$(M + H)^+$], 516.03531, found, 516.03493.

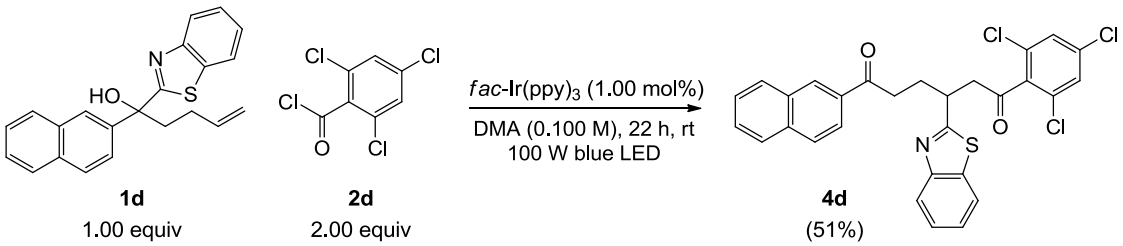
3-(Benzo[*d*]thiazol-2-yl)-6-(4-(dimethylamino)phenyl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4c)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(4-(dimethylamino)phenyl)pent-4-en-1-ol (33.8 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (25.5 mg, 0.0460 mmol, 46% yield). $\mathbf{R_f}$ = 0.26 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.96 (d, *J* = 8.05 Hz, 1H), 7.85 (d, *J* = 7.91 Hz, 1H), 7.80 (d, *J* = 9.03 Hz, 2H), 7.45 (t, *J* = 8.19 Hz, 1H), 7.36 (t, *J* = 7.98 Hz, 1H), 7.30 (s, 2H), 6.59 (d, *J* = 8.96 Hz, 2H), 4.08-4.01 (m, 1H), 3.62 (dd, *J* = 19.04 & 6.86 Hz, 1H), 3.38 (dd,

J = 19.04 & 6.16 Hz, 1H), 3.03 (s, 6H), 3.01-2.90 (m, 2H), 2.45-2.31 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.93, 197.25, 173.69, 153.56, 153.25, 137.76, 136.02, 135.13, 131.55, 130.42, 128.45, 126.16, 125.10, 124.91, 122.95, 121.86, 110.79, 49.15, 40.22, 38.71, 35.31, 30.50. **HRMS** (ESI-TOF) *m/z* calcd for $C_{27}H_{24}Cl_3N_2O_2S$ [(M + H)$^+$], 545.06186, found, 545.06127.

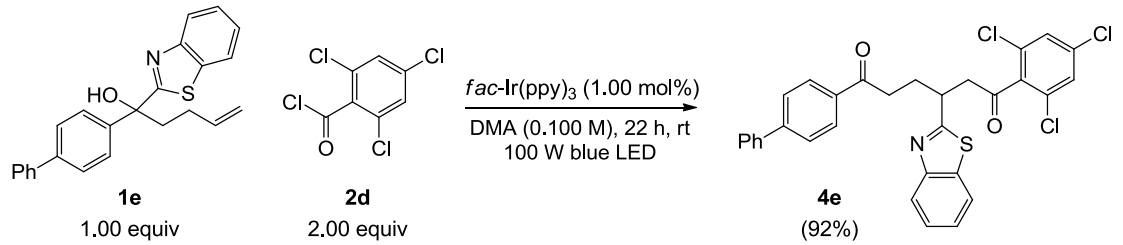
3-(Benzo[*d*]thiazol-2-yl)-6-(naphthalen-2-yl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4d)



1d 1.00 equiv | **2d** 2.00 equiv | **4d** (51%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(naphthalen-2-yl)pent-4-en-1-ol (69.0 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (56.2 mg, 0.102 mmol, 51% yield). $\mathbf{R_f}$ = 0.26 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.37 (s, 1H), 7.98-7.96 (m, 2H), 7.89-7.84 (m, 4H), 7.58 (t, *J* = 7.00 Hz, 1H), 7.52 (t, *J* = 7.00 Hz, 1H), 7.46 (t, *J* = 7.00 Hz, 1H), 7.38 (t, *J* = 7.70 Hz, 1H), 7.31 (s, 2H), 4.12-4.10 (m, 1H), 3.64 (dd, *J* = 19.11 & 6.93 Hz, 1H), 3.42 (dd, *J* = 19.11 & 6.58 Hz, 1H), 3.24-3.17 (m, 2H), 2.50-2.43 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.17, 198.87, 173.38, 153.26, 137.69, 136.13, 135.79, 135.09, 134.19, 132.66, 131.53, 129.94, 129.78, 128.65, 128.64, 128.50, 127.95, 126.94, 126.29, 125.25, 123.99, 123.02, 121.91, 49.20, 38.57, 36.16, 30.10. **HRMS** (ESI-TOF) *m/z* calcd for $C_{29}H_{21}Cl_3NO_2S$ [(M + H)$^+$], 552.03531, found, 552.03694.

6-([1,1'-Biphenyl]-4-yl)-3-(benzo[*d*]thiazol-2-yl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4e)

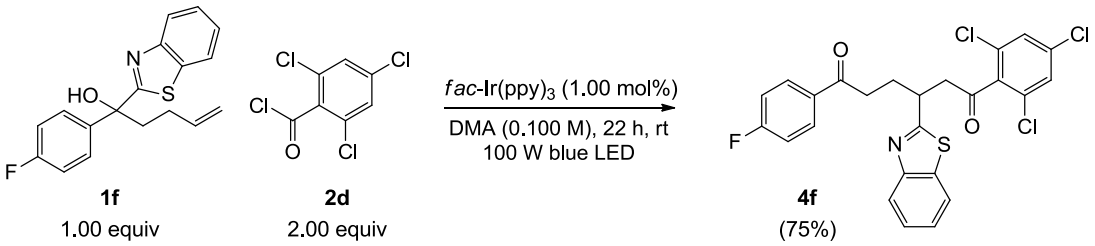


1e 1.00 equiv | **2d** 2.00 equiv | **4e** (92%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-([1,1'-biphenyl]-4-yl)-1-(benzo[*d*]thiazol-2-yl)pent-4-en-1-ol (37.1 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (53.3 mg, 0.0920 mmol, 92% yield). $\mathbf{R_f}$ = 0.21 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.99-7.94 (m, 3H), 7.86 (d, *J* = 7.98 Hz, 1H), 7.63 (d, *J* = 8.33 Hz, 2H), 7.59 (d, *J* = 7.35 Hz, 2H), 7.49-7.43 (m, 3H), 7.42-

7.35 (m, 2H), 7.30 (s, 2H), 4.16-4.02 (m, 1H), 3.63 (dd, *J* = 19.11 & 6.51 Hz, 1H), 3.40 (dd, *J* = 19.04 & 6.51 Hz, 1H), 3.19-3.01 (m, 2H), 2.55-2.32 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.84, 198.77, 173.34, 153.20, 145.92, 140.00, 137.65, 136.09, 135.53, 135.02, 131.48, 129.11, 128.80, 128.45, 128.39, 127.41, 127.37, 126.25, 125.22, 122.96, 121.87, 49.16, 38.48, 36.12, 29.91. **HRMS** (ESI-TOF) *m/z* calcd for $C_{31}H_{23}Cl_3NO_2S$ [$(M + H)^+$], 578.05096, found, 578.05060.

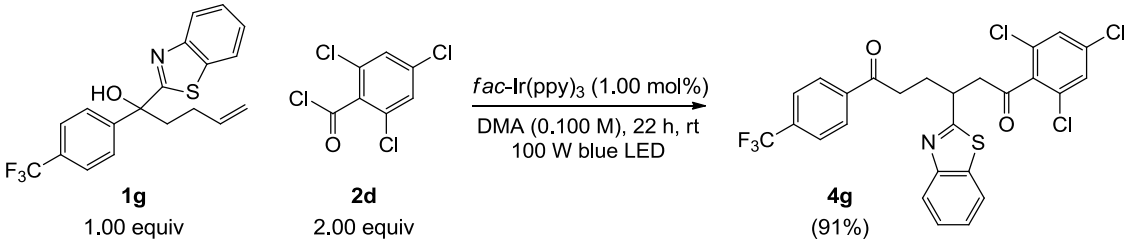
3-(Benzo[*d*]thiazol-2-yl)-6-(4-fluorophenyl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4f)



1f 1.00 equiv | **2d** 2.00 equiv | **4f** (75%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(4-fluorophenyl)pent-4-en-1-ol (62.6 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (76.9 mg, 0.150 mmol, 75% yield). $\mathbf{R_f}$ = 0.21 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.94 (d, *J* = 8.19 Hz, 1H), 7.90 (dd, *J* = 8.75 & 5.46 Hz, 2H), 7.85 (d, *J* = 7.98 Hz, 1H), 7.45 (t, *J* = 7.35 Hz, 1H), 7.36 (t, *J* = 7.35 Hz, 1H), 7.30 (s, 2H), 7.06 (t, *J* = 8.54 Hz, 2H), 4.09-4.01 (m, 1H), 3.60 (dd, *J* = 19.04 & 6.37 Hz, 1H), 3.38 (dd, *J* = 19.04 & 6.65 Hz, 1H), 3.10-2.95 (m, 2H), 2.48-2.31 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.80, 197.54, 173.21, 165.90 (d, $J^1_{C\text{-}F}$ = 253.38 Hz), 153.19, 137.62, 136.12, 135.00, 133.27, 131.47, 130.83 (q, $J^3_{C\text{-}F}$ = 9.34 Hz), 128.46, 126.28, 125.26, 122.96, 121.87, 115.83 (q, $J^2_{C\text{-}F}$ = 21.85 Hz), 49.17, 38.43, 36.02, 29.79. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): -105.50 (m). **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{18}Cl_3FNO_2S$ [$(M + H)^+$], 520.01024, found, 520.00962.

3-(Benzo[*d*]thiazol-2-yl)-1-(2,4,6-trichlorophenyl)-6-(4-(trifluoromethyl)phenyl)hexane-1,6-dione (4g)

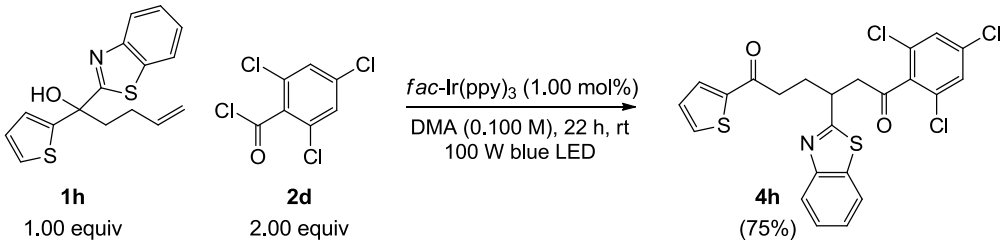


1g 1.00 equiv | **2d** 2.00 equiv | **4g** (91%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(4-(trifluoromethyl)phenyl)pent-4-en-1-ol (36.3 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography

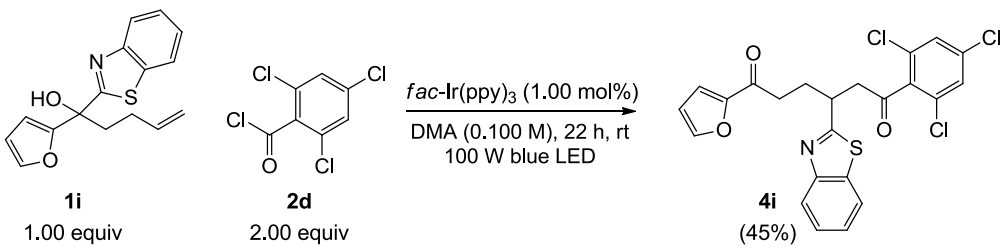
on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (52.4 mg, 0.0910 mmol, 91% yield). $\mathbf{R_f}$ = 0.21 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.97 (d, *J* = 8.12 Hz, 2H), 7.94 (d, *J* = 8.12 Hz, 1H), 7.85 (d, *J* = 7.98 Hz, 1H), 7.66 (d, *J* = 7.26 Hz, 2H), 7.46 (t, *J* = 8.12 Hz, 1H), 7.37 (t, *J* = 7.98 Hz, 1H), 7.31 (s, 2H), 4.12-3.96 (m, 1H), 3.60 (dd, *J* = 19.11 & 6.3 Hz, 1H), 3.39 (dd, *J* = 19.11 & 6.79 Hz, 1H), 3.17-3.01 (m, 2H), 2.52-2.31 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.78, 198.19, 173.04, 153.15, 139.44, 137.57, 136.16, 134.95, 134.54 (q, $J^2_{C\text{-}F}$ = 32.49 Hz), 131.44, 128.52, 128.48, 126.33, 125.82 (q, $J^3_{C\text{-}F}$ = 3.64 Hz), 125.31, 123.74 (q, $J^1_{C\text{-}F}$ = 271.05 Hz), 122.96, 121.87, 49.16, 38.34, 36.40, 29.58. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –63.20 (s). **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{18}Cl_3F_3NO_2S$ [$(M + H)^+$], 570.00704, found, 570.00640.

3-(Benzo[*d*]thiazol-2-yl)-6-(thiophen-2-yl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4h)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(thiophen-2-yl)pent-4-en-1-ol (60.2 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:15 (v/v)] to afford the title compound as a gummy solid (76.4 mg, 0.150 mmol, 75% yield). $\mathbf{R_f}$ = 0.21 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.95 (d, *J* = 8.19 Hz, 1H), 7.85 (d, *J* = 7.91 Hz, 1H), 7.62 (d, *J* = 3.78 Hz, 1H), 7.61-7.57 (m, 1H), 7.49-7.43 (m, 1H), 7.36 (t, *J* = 7.98 Hz, 1H), 7.30 (s, 2H), 7.05-7.08 (m, 1H), 4.08-4.01 (m, 1H), 3.60 (dd, *J* = 19.11 & 6.58 Hz, 1H), 3.39 (dd, *J* = 19.11 & 6.51 Hz, 1H), 3.06-2.95 (m, 2H), 2.47-2.36 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.77, 192.10, 173.15, 153.17, 144.13, 137.62, 136.10, 135.02, 133.84, 132.14, 131.48, 128.45, 128.24, 126.25, 125.23, 122.95, 121.86, 49.06, 38.45, 36.75, 30.03. **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{17}Cl_3NO_2S_2$ [$(M + H)^+$], 507.97608, found, 507.97583.

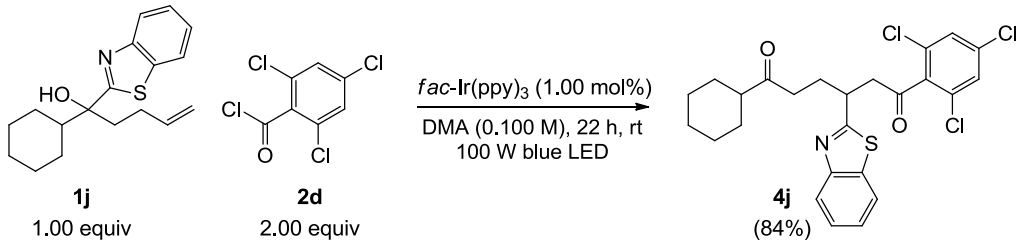
3-(Benzo[*d*]thiazol-2-yl)-6-(furan-2-yl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4i)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg,

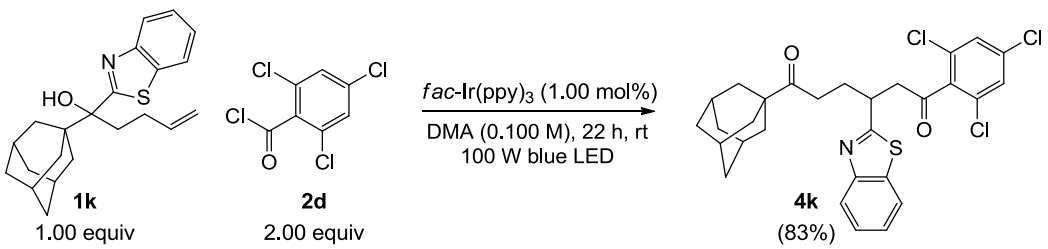
0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(furan-2-yl)pent-4-en-1-ol (57.1 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as an gummy solid (44.7 mg, 0.0900 mmol, 45% yield). $\mathbf{R}_f$ = 0.46 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.15 (d, *J* = 8.12 Hz, 1H), 7.96 (d, *J* = 7.84 Hz, 1H), 7.56 (t, *J* = 8.12 Hz, 1H), 7.51 (t, *J* = 8.05 Hz, 1H), 7.30 (s, 2H), 7.30-7.29 (m, 1H), 6.29-6.20 (m, 1H), 6.13 (d, *J* = 3.08 Hz, 1H), 3.71-3.60 (m, 1H), 3.35-3.21 (m, 3H), 3.16 (dd, *J* = 18.9 & 6.86 Hz, 1H), 2.35-2.16 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.22, 194.76, 166.44, 155.66, 153.70, 141.63, 137.98, 137.43, 135.91, 131.43, 128.42, 127.82, 127.13, 125.61, 122.62, 110.34, 106.83, 48.16, 36.52, 33.10, 27.91. **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{17}Cl_3NO_3S$ [$(M + H)^+$], 491.99892, found, 491.99837.

3-(Benzo[*d*]thiazol-2-yl)-6-cyclohexyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4j)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-cyclohexylpent-4-en-1-ol (30.1 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as an gummy solid (43.2 mg, 0.0840 mmol, 84% yield). $\mathbf{R}_f$ = 0.33 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.94 (d, *J* = 8.12 Hz, 1H), 7.85 (d, *J* = 7.91 Hz, 1H), 7.45 (t, *J* = 8.19 Hz, 1H), 7.36 (t, *J* = 8.05 Hz, 1H), 7.29 (s, 2H), 3.97-3.88 (m, 1H), 3.56 (dd, *J* = 19.11 & 6.72 Hz, 1H), 3.39 (dd, *J* = 19.11 & 5.11 Hz, 1H), 2.58-2.44 (m, 2H), 2.30-2.19 (m, 2H), 219-2.11 (m, 1H), 1.82-1.66 (m, 4H), 1.66-1.59 (m, 1H), 1.32-1.10 (m, 5H) . **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 213.02, 198.83, 173.38, 153.21, 137.69, 136.08, 135.03, 131.48, 128.45, 126.22, 125.17, 122.94, 121.86, 50.99, 49.07, 38.35, 37.93, 29.34, 28.71, 28.60, 25.98, 25.83, 25.78. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{25}Cl_3NO_2S$ [$(M + H)^+$], 508.06661, found, 508.06662.

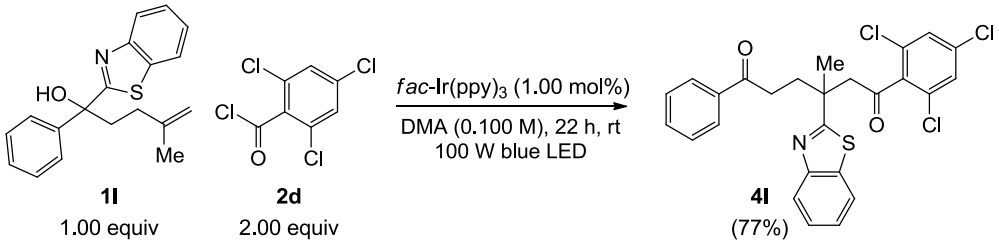
6-(Adamantan-1-yl)-3-(benzo[*d*]thiazol-2-yl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4k)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg,

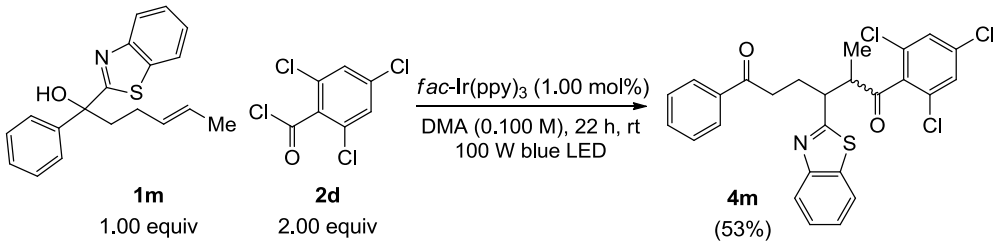
0.400 mmol, 2.00 equiv) and 1-(adamantan-1-yl)-1-(benzo[*d*]thiazol-2-yl)pent-4-en-1-ol (70.6 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (92.1 mg, 0.166 mmol, 83% yield). $\mathbf{R}_f$ = 0.38 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.94 (d, *J* = 8.12 Hz, 1H), 7.85 (d, *J* = 7.98 Hz, 1H), 7.44 (t, *J* = 8.05 Hz, 1H), 7.35 (t, *J* = 7.98 Hz, 1H), 7.29 (s, 2H), 3.97-3.88 (m, 1H), 3.56 (dd, *J* = 19.11 & 6.72 Hz, 1H), 3.31 (dd, *J* = 19.11 & 6.37 Hz, 1H), 2.62-2.46 (m, 2H), 2.25-2.10 (m, 2H), 2.02-1.93 (m, 3H), 1.78-1,72 (m, 6H), 1.69 (d, *J* = 12.18 Hz, 3H), 1.62 (d, *J* = 11.76 Hz, 3H).**^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 214.67, 198.79, 173.54, 153.17, 137.67, 136.00, 135.00, 131.45, 128.40, 126.16, 125.10, 122.89, 121.83, 49.13, 46.44, 38.39, 38.35, 36.65, 33.47, 29.45, 28.05. **HRMS** (ESI-TOF) *m/z* calcd for $C_{29}H_{29}Cl_3NO_2S$ [$(M + H)^+$], 560.09791, found, 560.09735.

3-(Benzo[*d*]thiazol-2-yl)-3-methyl-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4l)



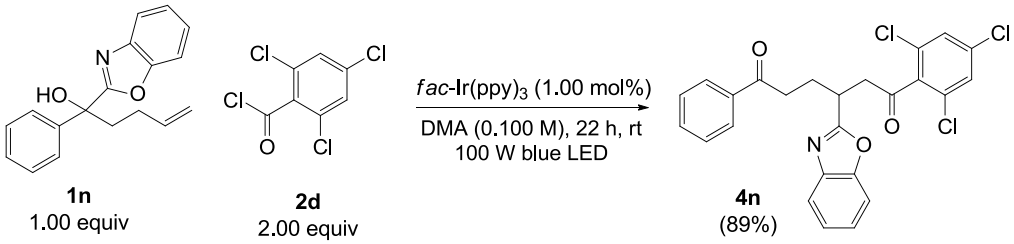
The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-4-methyl-1-phenylpent-4-en-1-ol (61.8 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (74.3 mg, 0.154 mmol, 77% yield). $\mathbf{R}_f$ = 0.48 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.92 (d, *J* = 8.12 Hz, 1H), 7.87 (d, *J* = 7.91 Hz, 1H), 7.83 (d, *J* = 7.28 Hz, 2H), 7.49 (t, *J* = 7.42 Hz, 1H), 7.43 (t, *J* = 8.12 Hz, 1H), 7.37 (t, *J* = 7.77 Hz, 2H), 7.37-7.33 (m, 1H), 7.29 (s, 2H), 3.77 (d, *J* = 19.04 Hz, 1H), 3.47 (d, *J* = 19.04 Hz, 1H), 3.03-2.91 (m, 2H), 2.63-2.53 (m, 1H), 2.44-2.33 (m, 1H), 1.85 (s, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.32, 198.25, 177.95, 153.09, 137.84, 136.79, 135.82, 135.18, 133.19, 131.45, 128.68, 128.43, 128.17, 126.05, 124.99, 122.93, 121.80, 53.14, 42.96, 36.72, 33.68, 24.97. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{21}Cl_3NO_2S$ [$(M + H)^+$], 516.03531, found, 516.03497.

3-(Benzo[*d*]thiazol-2-yl)-2-methyl-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (1:1) (4m)



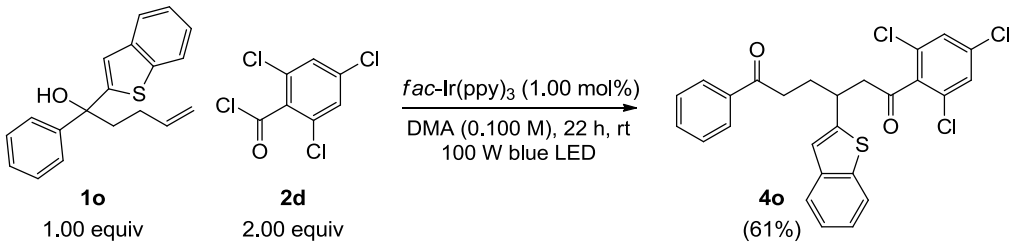
The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and (*E*)-1-(benzo[*d*]thiazol-2-yl)-1-phenylhex-4-en-1-ol (61.8 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as (1:1) ratio of a gummy solid (51.7 mg, 0.106 mmol, 53% yield). $\mathbf{R_f}$ = 0.31 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.00 (d, *J* = 8.12 Hz, 1H), 7.96 (d, *J* = 8.12 Hz, 1H), 7.89 (d, *J* = 7.98 Hz, 2H), 7.88-7.83 (m, 4H), 7.55-7.49 (m, 2H), 7.48-7.44 (m, 2H), 7.43-7.36 (m, 6H), 7.34 (s, 2H), 7.31 (s, 2H), 4.02-3.96 (m, 1H), 3.96-3.90 (m, 1H), 3.65-3.76 (m, 2H), 3.00-3.14 (m, 3H), 2.96-2.87 (m, 1H), 2.57-2.41 (m, 3H), 2.41-2.33 (m, 1H), 1.37 (d, *J* = 7.49 Hz, 3H), 1.12 (d, *J* = 7.49 Hz, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 202.23, 202.06, 199.39, 199.28, 173.06, 172.52, 153.28, 153.20, 137.03, 136.86, 136.85, 136.74, 136.26, 136.09, 135.11, 135.01, 133.23, 133.19, 132.49, 132.15, 128.81, 128.71, 128.69, 128.67, 128.29, 128.25, 128.20, 126.26, 126.24, 125.26, 125.25, 123.12, 123.04, 121.85, 121.79, 52.38, 52.12, 45.36, 43.73, 37.04, 37.00, 29.08, 24.99, 14.98, 11.61. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{21}Cl_3NO_2S$ [$(M + H)^+$], 516.03531, found, 516.03478.

3-(Benzo[*d*]oxazol-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4n)



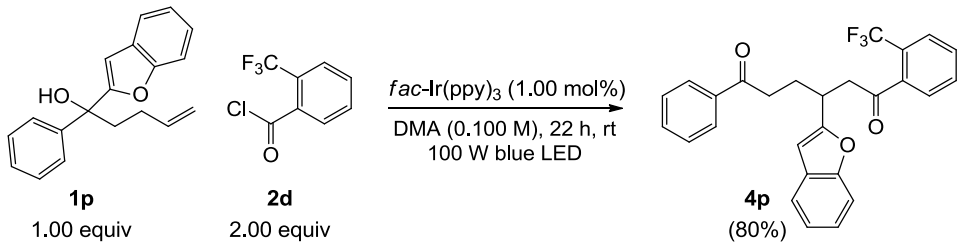
The reaction was performed according to the general procedure C using 1-(benzo[*d*]oxazol-2-yl)-1-phenylpent-4-en-1-ol (27.9 mg, 0.100 mmol, 1.00 equiv) and 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (43.3 mg, 0.089 mmol, 89% yield). $\mathbf{R_f}$ = 0.18 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.89 (d, *J* = 8.40 Hz, 2H), 7.67-7.64 (m, 1H), 7.53 (t, *J* = 7.00 Hz, 1H), 7.48-7.46 (m, 1H), 7.41 (t, *J* = 7.70 Hz, 2H), 7.32-7.30 (m, 4H), 3.91-3.89 (m, 1H), 3.61 (dd, *J* = 18.9 & 7.00 Hz, 1H), 3.38 (dd, *J* = 18.9 & 7.00 Hz, 1H), 3.16-3.06 (m, 2H), 2.44-2.33 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.93, 198.57, 167.73, 150.81, 141.17, 137.53, 136.80, 136.16, 133.30, 131.45, 128.74, 128.46, 128.17, 125.04, 124.50, 119.97, 110.72, 46.98, 36.05, 33.96, 27.67. **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{19}Cl_3NO_3$ [$(M + H)^+$], 486.04250, found, 486.04267.

3-(Benzo[*b*]thiophen-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4o)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*b*]thiophen-2-yl)-1-phenylpent-4-en-1-ol (58.8 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (61.2 mg, 0.122 mmol, 61% yield). $\mathbf{R_f}$ = 0.62 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.89-7.84 (m, 2H), 7.77 (d, *J* = 7.98 Hz, 1H), 7.67 (d, *J* = 7.84 Hz, 1H), 7.51 (t, *J* = 7.42 Hz, 1H), 7.40 (t, *J* = 8.05 Hz, 2H), 7.32 (t, *J* = 7.98 Hz, 1H), 7.29 (s, 2H), 7.29-7.26 (m, 1H), 7.16 (s, 1H), 3.94-3.87 (m, 1H), 3.33 (dd, *J* = 18.97 & 6.23 Hz, 1H), 3.27 (dd, *J* = 18.97 & 6.86 Hz, 1H), 3.11-3.02 (m, 1H), 3.02-2.94 (m, 1H), 2.45-2.37 (m, 1H), 2.17-2.09 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.54, 199.00, 147.96, 139.84, 139.22, 137.82, 136.91, 136.00, 133.22, 131.45, 128.71, 128.44, 128.17, 124.49, 124.11, 123.34, 122.52, 122.00, 51.54, 36.62, 35.92, 30.98. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{20}Cl_3O_2S$ [$(M + H)^+$], 501.02441, found, 501.02488.

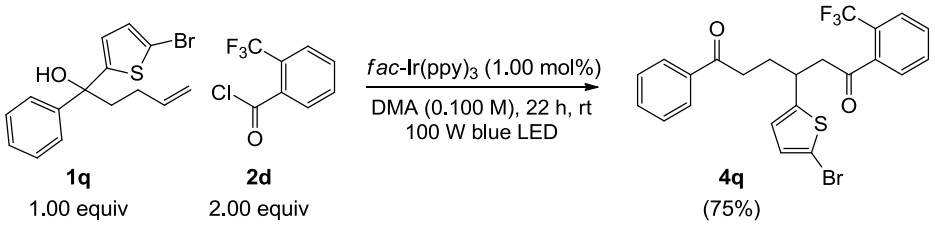
3-(Benzofuran-2-yl)-6-phenyl-1-(2-(trifluoromethyl)phenyl)hexane-1,6-dione (4p)



The reaction was performed according to the general procedure C using 2-(trifluoromethyl)benzoyl chloride (41.6 mg, 0.200 mmol, 2.00 equiv) and 1-(benzofuran-2-yl)-1-phenylpent-4-en-1-ol (27.8 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:7 (v/v)] to afford the title compound as a gummy solid (36.7 mg, 0.0800 mmol, 80% yield). $\mathbf{R_f}$ = 0.40 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.87 (d, *J* = 7.35 Hz, 2H), 7.72-766 (m, 1H), 7.56-7.52 (m, 3H), 7.48 (d, *J* = 7.49 Hz, 1H), 7.42-7.38 (m, 3H), 7.37-7.32 (m, 1H), 7.22 (t, *J* = 8.19 Hz, 1H), 7.19 (t, *J* = 7.56 Hz, 1H), 6.52 (s, 1H), 3.76-3.68 (m, 1H), 3.45 (dd, *J* = 17.99 & 6.93 Hz, 1H), 3.25 (dd, *J* = 17.99 & 6.65 Hz, 1H), 3.09-3.01 (m, 1H), 3.00-2.92 (m, 1H), 2.29-2.23 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 202.04, 199.55, 159.17, 154.86, 140.12, 136.93, 133.24, 132.01. 130.37, 128.74, 128.60, 128.19, 127.30, 127.12 (q, $J^2_{C\text{-}F}$ = 32.2 Hz), 126.90 (q, $J^3_{C\text{-}F}$ = 5.05 Hz), 123.84, 122.87, 123.74 (q, $J^1_{C\text{-}F}$= 272 Hz), 120.85, 111.11, 103.74, 47.56, 36.51, 34.47, 27.96. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –58.98 (s). **HRMS** (ESI-TOF) *m/z* calcd

for $C_{27}H_{22}F_3O_3$ [$(M + H)^+$], 451.15156, found, 451,15265.

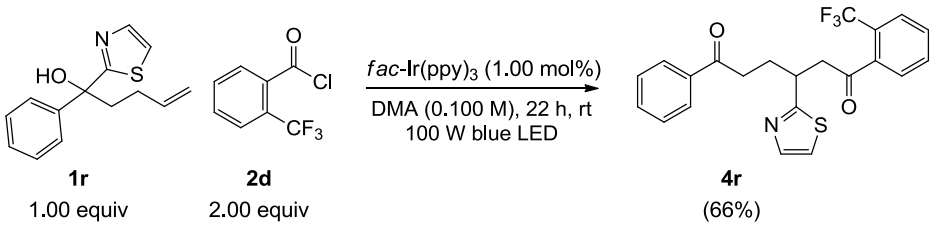
3-(5-Bromothiophen-2-yl)-6-phenyl-1-(2-(trifluoromethyl)phenyl)hexane-1,6-dione (4q)



1q 1.00 equiv | **2d** 2.00 equiv | **4q** (75%)

The reaction was performed according to the general procedure C using 2-(trifluoromethyl)benzoyl chloride (41.6 mg, 0.200 mmol, 2.00 equiv) and 1-(5-bromothiophen-2-yl)-1-phenylpent-4-en-1-ol (32.3 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (37.5 mg, 0.0750 mmol, 75% yield). $\mathbf{R_f}$ = 0.40 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.88 (d, *J* = 7.7 Hz, 2H), 7.69 (d, *J* = 7.56 Hz, 1H), 7.62-7.51 (m, 3H), 7.44 (t, *J* = 7.49 Hz, 2H), 7.31-7.26 (m, 1H), 6.86 (d, *J* = 3.15 Hz, 1H), 6.66 (d, *J* = 3.15 Hz, 1H), 3.82-3.63 (m, 1H), 3.24 (dd, *J* = 17.85 & 7.28 Hz, 1H), 3.18 (dd, *J* = 17.85 & 6.16 Hz, 1H), 3.06-2.89 (m, 2H), 2.31-2.21 (m, 1H), 2.09-1.94 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 201.87, 199.47, 149.04, 140.12, 136.92, 133.33, 132.09, 130.44, 129.76, 128.80, 128.19, 127.18, 127.00, 126.92 (q, $J^3_{C\text{-}F}$ = 4.98 Hz), 125.70, 123.72 (q, $J^1_{C\text{-}F}$ = 272.17 Hz), 110.18, 51.24, 36.59, 36.53, 31.22. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –58.56 (s). **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{19}BrF_3O_2S$ [$(M + H)^+$], 495.02357, found, 495.02249.

6-Phenyl-3-(thiazol-2-yl)-1-(2-(trifluoromethyl)phenyl)hexane-1,6-dione (4r)

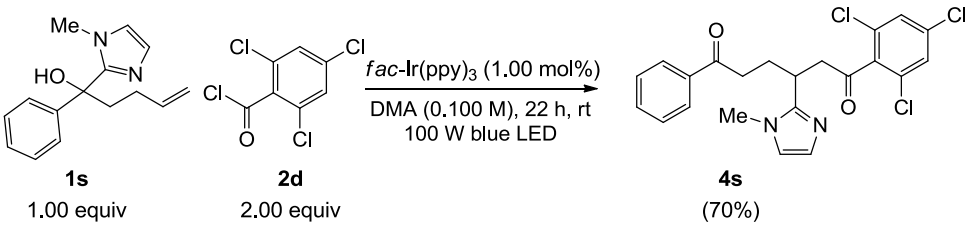


1r 1.00 equiv | **2d** 2.00 equiv | **4r** (66%)

The reaction was performed according to the general procedure C using 2-(trifluoromethyl)benzoyl chloride (41.6 mg, 0.200 mmol, 2.00 equiv) and 1-phenyl-1-(thiazol-2-yl)pent-4-en-1-ol (24.5 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (27.6 mg, 0.0660 mmol, 66% yield). $\mathbf{R_f}$ = 0.10 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.89 (d, *J* = 7.35 Hz, 2H), 7.70 (d, *J* = 3.22 Hz, 1H), 7.68 (d, *J* = 7.77 Hz, 1H), 7.58 (t, *J* = 7.49 Hz, 1H), 7.53 (t, *J* = 7.42 Hz, 2H), 7.46 (d, *J* = 7.56 Hz, 1H), 7.43 (t, *J* = 7.84 Hz, 2H), 7.22 (d, *J* = 3.29 Hz, 1H), 4.07-3.93 (m, 1H), 3.64 (dd, *J* = 18.2 & 7.98 Hz, 1H), 3.25 (dd, *J* = 18.2 & 5.6 Hz, 1H), 3.11-2.93 (m, 2H), 2.38-2.21 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 201.86, 199.29, 172.70, 142.52, 140.07, 136.91, 133.31, 132.02, 130.40, 128.78, 128.21, 127.54, 127.17 (q, $J^2_{C\text{-}F}$ = 32.18 Hz), 126.87 (q, $J^3_{C\text{-}F}$ = 5.06 Hz), 122.17 (q, $J^1_{C\text{-}F}$ = 272.51 Hz), 118.68, 48.62, 38.13, 36.10, 30.23. **^{19}F NMR**

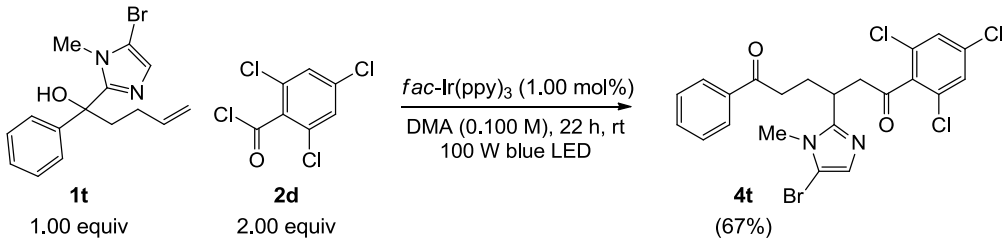
(376 MHz, $CDCl_3$, 25 ºC, δ): –58.80 (s). **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{19}F_3NO_2S$ [$(M + H)^+$], 418.10831, found, 418.10815.

3-(1-Methyl-1*H*-imidazol-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4s)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(1-methyl-1*H*-imidazol-2-yl)-1-phenylpent-4-en-1-ol (48.4 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (62.6 mg, 0.140 mmol, 70% yield). $\mathbf{R}_f$ = 0.15 EtOAc:Hexanes [3:7 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.86 (d, *J* = 7.21 Hz, 2H), 7.53 (d, *J* = 7.42 Hz, 1H), 7.42 (d, *J* = 7.91 Hz, 2H), 7.28 (s, 2H), 6.93 (s, 1H), 6.74-6.71 (m, 1H), 3.79-3.72 (m, 1H), 3.68 (s, 3H), 3.52 (dd, *J* = 19.04 & 8.47 Hz, 1H), 3.23 (dd, *J* = 19.04 & 4.69 Hz, 1H), 3.00-2.92 (m, 1H), 2.85-2.77 (m, 1H), 2.31-2.19 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 200.27, 199.86, 149.39, 137.87, 136.90, 135.92, 133.32, 131.34, 128.80, 128.38, 128.22, 127.45, 120.47, 49.25, 35.44, 32.91, 29.94, 29.17. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{20}Cl_3N_2O_2$ [$(M + H)^+$], 449.05849, found, 449.05797

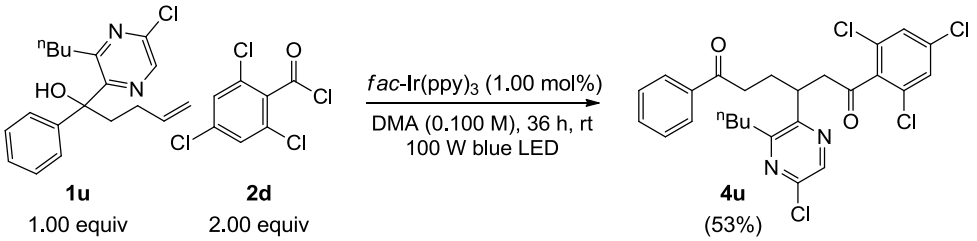
3-(5-Bromo-1-methyl-1*H*-imidazol-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4t)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(5-bromo-1-methyl-1*H*-imidazol-2-yl)-1-phenylpent-4-en-1-ol (32.1 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (35.3 mg, 0.067 mmol, 67% yield). $\mathbf{R}_f$ = 0.12 EtOAc:Hexanes [3:7 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.86 (d, *J* = 7.35 Hz, 2H), 7.54 (t, *J* = 7.35 Hz, 1H), 7.43 (t, *J* = 7.84 Hz, 2H), 7.29 (s, 2H), 6.92 (s, 1H), 3.79-3.72 (m, 1H), 3.62 (s, 3H), 3.50 (dd, *J* = 18.97 & 8.47 Hz, 1H), 3.20 (dd, *J* = 19.04 & 4.69 Hz, 1H), 3.01-2.94 (m, 1H), 2.85-2.80 (m, 1H), 2.29-2.15 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 200.04, 199.68, 150.31, 137.72, 136.82, 136.01, 133.40, 131.34, 128.83, 128.41, 128.19, 127.96, 103.04, 48.83, 35.23, 31.65, 31.18, 28.92. **HRMS** (ESI-TOF) *m/z* calcd for

$C_{22}H_{29}BrCl_3N_2O_2$ [(M + H)$^+$], 526.96900, found, 526.96882.

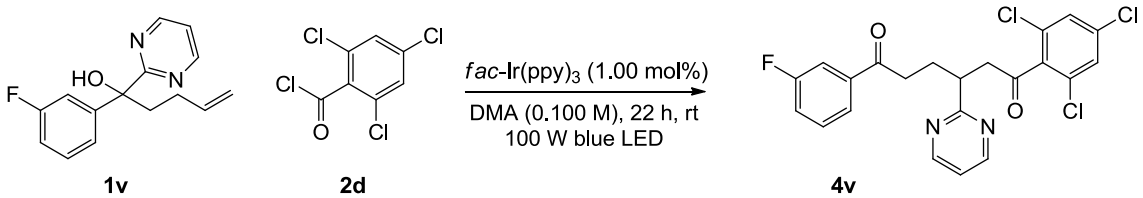
3-(3-Butyl-5-chloropyrazin-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4u)



1u 1.00 equiv **2d** 2.00 equiv **4u** (53%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(3-butyl-5-chloropyrazin-2-yl)-1-phenylpent-4-en-1-ol (66.2 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (56.5 mg, 0.106 mmol, 53% yield). $\mathbf{R_f}$ = 0.60 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.39 (s, 1H),7.87 (d, *J* = 7.21 Hz, 2H), 7.55 (t, *J* = 7.42 Hz, 1H), 7.44 (t, *J* = 7.91 Hz, 2H), 7.29 (s, 2H), 3.68-3.57 (m, 1H), 3.52 (dd, *J* = 18.97 & 8.75 Hz, 1H), 3.21 (dd, *J* = 18.97 & 4.62 Hz, 1H), 2.97-2.81 (m, 4H), 2.27-2.17 (m, 2H), 1.77-1.66 (m, 2H), 1.48-1.36 (m, 2H), 0.96 (t, *J* = 7.35 Hz, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.55, 199.19, 155.07, 154.45, 148.36, 142.50, 137.71, 136.79, 136.00, 133.40, 131.34, 128.83, 128.43, 128.18, 48.50, 37.73, 36.00, 34.58, 30.07, 29.28, 22.71, 14.08. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{25}Cl_4N_2O_2$ [(M + H)$^+$], 537.06647, found, 537.06617.

6-(3-Fluorophenyl)-3-(pyrimidin-2-yl)-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4v)

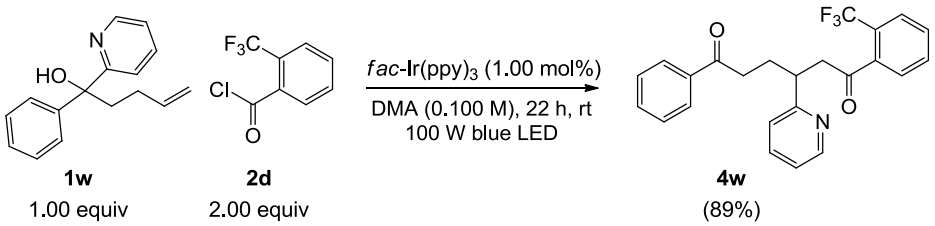


1v 1.00 equiv **2d** 2.00 equiv **4v** (90%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(3-fluorophenyl)-1-(pyrimidin-2-yl)pent-4-en-1-ol (25.8 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as an colorless oil (42.0 mg, 0.0900 mmol, 90% yield). $\mathbf{R_f}$ = 0.30 EtOAc:Hexanes [1:2 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.68 (d, *J* = 4.90 Hz, 2H), 7.66 (dt, *J* = 8.00 & 1.20 Hz, 1H), 7.55 (dt, *J* = 9.50 & 3.90 & 1.90 Hz, 1H), 7.40 (td, *J* = 8.00 & 5.50 Hz, 1H), 7.30 (s, 2H), 7.22 (dt, *J* = 8.00 & 2.50 Hz, 1H), 7.16 (t, *J* = 4.90 Hz, 1H), 3.79-3.74 (m, 1H), 3.64 (dd, *J* = 18.80 & 7.30 Hz, 1H), 3.29 (dd, *J* = 18.80 & 5.80 Hz, 1H), 3.07-3.04 (m, 1H), 2.93-2.86 (m, 1H), 2.34-2.21 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 199.72, 198.25 (d, $J^4_{C\text{-}F}$ = 1.30 Hz), 171.88, 163.00 (d, $J^1_{C\text{-}F}$ = 248.00

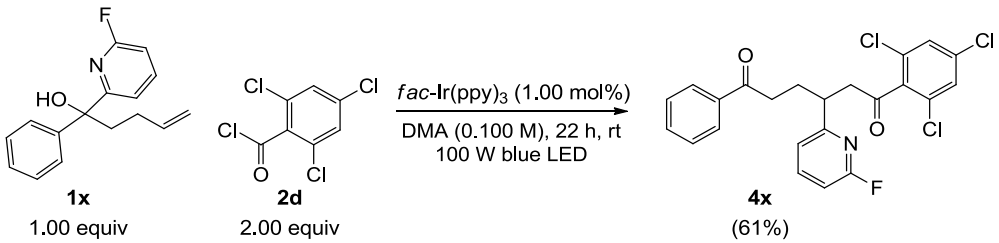
Hz), 157.25, 139.10 (d, $J^{3'}_{C\text{-}F}$ = 5.00 Hz), 138.02, 135.86, 131.49, 130.39 (d, $J^{3}_{C\text{-}F}$ = 7.50 Hz), 128.43, 123.96 (d, $J^{4}_{C\text{-}F}$ = 2.50 Hz), 120.16 (d, $J^{2'}_{C\text{-}F}$ = 20.0 Hz), 119.27, 114.95 (d, $J^{2}_{C\text{-}F}$ = 22.5 Hz), 48.13, 42.80, 36.52, 29.11. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –114.91 (m). **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{17}Cl_3FN_2O_2$ [(M + H)$^+$], 465.03342, found, 465.03388.

6-Phenyl-3-(pyridin-2-yl)-1-(2-(trifluoromethyl)phenyl)hexane-1,6-dione (4w)



The reaction was performed according to the general procedure C using 2-(trifluoromethyl)benzoyl chloride (41.6 mg, 0.200 mmol, 2.00 equiv) and 1-phenyl-1-(pyridin-2-yl)pent-4-en-1-ol (23.9 mg, 0.100 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (39.4 mg, 0.0890 mmol, 89% yield). **R_f** = 0.07 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.54 (d, *J* = 4.76 Hz, 1H), 7.85 (d, *J* = 7.14 Hz, 2H), 7.66 (d, *J* = 7.7 Hz, 1H), 7.63-7.57 (m, 1H), 7.58-7.48 (m, 3H), 7.44-7.39 (m, 3H), 7.27 (d, *J* = 7.77 Hz, 1H), 7.16-7.10 (m, 1H), 3.68 (dd, *J* = 17.78 & 8.82 Hz, 1H), 3.65-3.57 (m, 1H), 3.16 (dd, *J* = 17.85 & 4.69 Hz, 1H), 2.95-2.86 (m, 1H), 2.86-2.78 (m, 1H), 2.28-2.13 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 203.02, 199.81, 162.57, 149.62, 140.48, 137.00, 136.61, 133.19, 131.88, 130.17, 128.74, 128.21, 127.49, 127.09 (q, $J^{2}_{C\text{-}F}$ = 32.2 Hz), 126.79 (q, $J^{1}_{C\text{-}F}$ = 5.00 Hz), 124.43, 123.72 (q, $J^{3}_{C\text{-}F}$ = 271.74 Hz), 121.94, 48.27, 41.86, 36.37, 29.91. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –58.91 (s). **HRMS** (ESI-TOF) *m/z* calcd for $C_{24}H_{21}F_3NO_2$ [(M + H)$^+$], 412.15189, found, 412.15392.

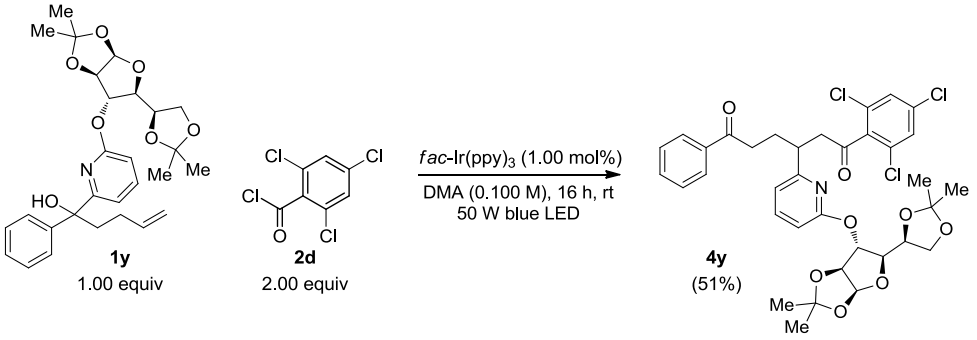
3-(6-Fluoropyridin-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4x)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(6-fluoropyridin-2-yl)-1-phenylpent-4-en-1-ol (51.4 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:4 (v/v)] to afford the title compound as a gummy solid (56.5 mg, 0.122 mmol, 61% yield). **R_f** = 0.07 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.85 (d, *J* = 7.21 Hz, 2H), 7.69 (dd,

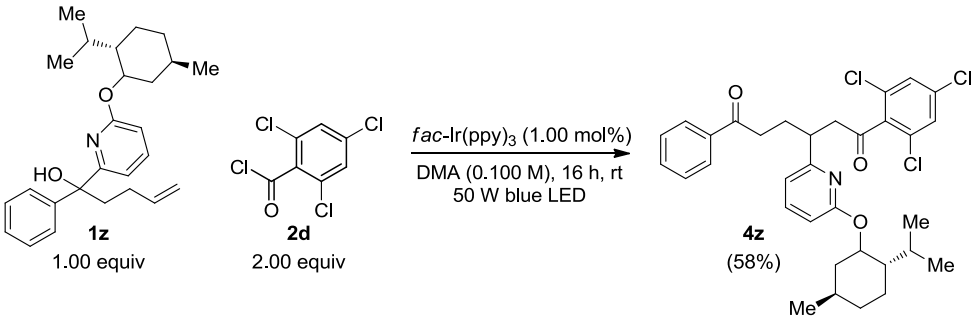
J = 15.68 & 8.12 Hz, 1H), 7.52 (t, *J* = 7.42 Hz, 1H), 7.41 (t, *J* = 7.98 Hz, 2H), 7.27 (s, 2H), 7.17 (dd, *J* = 7.28 & 2.10 Hz, 1H), 6.76 (dd, *J* = 8.12 & 2.66 Hz, 1H), 3.65-3.57 (m, 1H), 3.48 (dd, *J* = 19.04 & 8.19 Hz, 1H,), 3.19 (dd, *J* = 19.04 & 5.04 Hz, 1H), 2.90-2.81 (m, 2H), 2.24-2.18 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.78, 199.52, 163.66 (d, $J^1_{C\text{-}F}$ = 237.82 Hz), 161.63 (d, $J^3_{C\text{-}F}$ = 12.09 Hz), 141.50 (d, $J^3_{C\text{-}F}$ = 7.52 Hz), 137.94, 136.90, 135.83, 133.24, 131.32, 128.75, 128.37, 128.15, 121.60 (d, $J^3_{C\text{-}F}$ = 3.92 Hz), 107.59 (d, $J^2_{C\text{-}F}$ = 37.22 Hz), 48.86, 40.44, 36.13, 29.36. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –68.59 (d). **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{18}Cl_3FNO_2$ [(M + H)$^+$], 464.03817, found, 464.03775.

3-(6-(((3a*S*,5*R*,6*R*,6a*S*)-5-((*S*)-2,2-Dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl)oxy)pyridin-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4y)



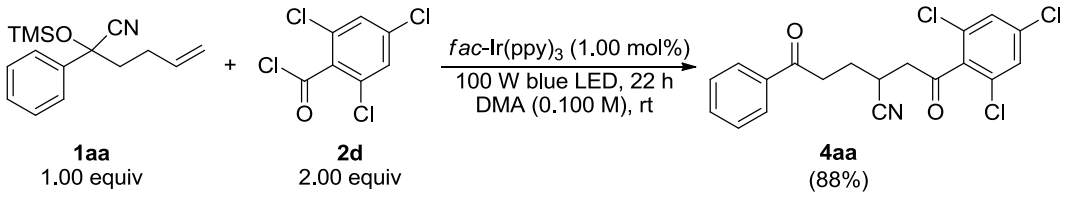
The reaction was performed according to the modified general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(6-(((3a*R*,5*S*,6*S*,6a*R*)-5-((*R*)-2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl)oxy)pyridin-2-yl)-1-phenylpent-4-en-1-ol (49.7 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 16 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (35.9 mg, 0.0510 mmol, 51% yield). $\mathbf{R}_f$ = 0.15 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.87-7.83 (m, 2H), 7.54-7.50 (m, 2H), 7.44-7.41 (m, 2H), 7.28 (s, 2H), 6.90 (t, *J* = 7.00 Hz, 1H), 6.59 (d, *J* = 7.70 Hz, 1H), 5.87-5.85 (m, 1H), 5.51-5.46 (m, 1H), 4.60-4.56 (m, 1H), 4.41-4.39 (m, 1H), 4.34-4.32 (m, 1H), 4.11-4.10 (m, 2H), 3.56-3.52 (m, 2H), 3.26-3.16 (m, 1H), 3.04-2.93 (m, 2H), 2.87-2.81 (m, 1H), 2.24-2.19 (m, 1H), 1.52 (s, 3H), 1.41-1.38 (m, 3H), 1.29-1.25 (m, 3H), 1.19-1.16 (m, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 200.12, 199.84, 199.67, 162.28, 159.97, 159.94, 139.58, 138.27, 138.15, 137.04, 137.02, 135.83, 135.80, 133.21, 131.46, 131.37, 128.82, 128.77, 128.59, 128.54, 128.49, 128.41, 128.39, 128.20, 128.18, 117.71, 117.66, 112.14, 112.00, 109.58, 109.53, 109.25, 109.23, 105.22, 105.15, 83.58, 83.37, 80.20, 80.15, 72.93, 72.87, 67.13, 66.96, 49.19, 49.15, 40.91, 40.83, 36.48, 36.36, 29.65, 27.03, 27.01, 26.99, 26.97, 26.50, 26.29, 26.22, 25.54, 25.50. **HRMS** (ESI-TOF) *m/z* calcd for $C_{35}H_{37}Cl_3NO_8$ [(M + H)$^+$], 704.15793, found, 704.15713.

3-(6-(((2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl)oxy)pyridin-2-yl)-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4z)



The reaction was performed according to the modified general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(6-(((2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl)oxy)pyridin-2-yl)-1-phenylpent-4-en-1-ol (39.3 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 16 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as an gummy solid (34.8 mg, 0.0580 mmol, 58% yield). $\mathbf{R}_f$ = 0.50 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.84 (d, *J* = 7.00 Hz, 2H), 7.52 (t, *J* = 7.70 Hz, 1H), 7.45-7.40 (m, 3H), 7.29-7.28 (m, 2H), 6.78 (bs, 1H), 6.51 (bs, 1H), 5.01-4.92 (m, 1H), 3.52-3.42 (m, 2H), 3.15-3.13 (m, 1H), 2.92-2.89 (m, 1H), 2.80 (bs, 1H), 2.26-2.17 (m, 1H), 2.11-1.99 (m, 2H), 1.70-1.67 (m, 2H), 1.49-1.46 (m, 2H), 1.10-1.06 (m, 1H), 1.01-0.93 (m, 2H), 0.89-0.81 (m, 6H), 0.72-0.66 (m, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 200.21, 199.95, 199.93, 163.87, 159.63, 159.56, 139.08, 138.26, 137.10, 137.05, 135.77, 133.15, 131.44, 131.40, 128.73, 128.39, 128.20, 128.16, 116.29, 109.40, 109.30, 74.77, 74.43, 49.63, 49.45, 47.90, 47.72, 41.30, 41.11, 40.93, 36.52, 36.40, 34.70, 31.74, 31.63, 29.39, 26.43, 26.41, 23.91, 23.83, 22.44, 21.00, 20.91, 16.95, 16.74. **HRMS** (ESI-TOF) *m/z* calcd for $C_{33}H_{37}Cl_3NO_3$ [$(M + H)^+$], 600.18335, found, 600.18241.

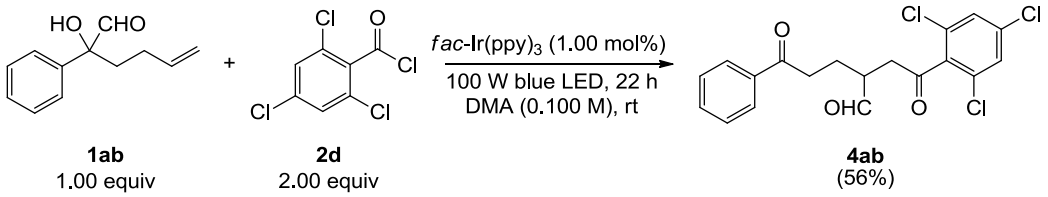
5-Oxo-2-(2-oxo-2-(2,4,6-trichlorophenyl)ethyl)-5-phenylpentanenitrile (4aa)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 2-phenyl-2-((trimethylsilyl)oxy)hex-5-enenitrile (27.8 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (69.1 mg, 0.176 mmol, 88 % yield). $\mathbf{R}_f$ = 0.30 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.98 (d, *J* = 7.84 Hz, 2H), 7.58 (t, *J* = 7.35 Hz, 1H), 7.48 (t, *J* = 7.63 Hz, 2H), 7.37 (s, 2H), 3.46-3.39 (m, 1H), 3.35-3.23 (m, 3H), 3.14 (dd, *J* = 19.04 & 6.02 Hz, 1H), 2.29-2.21 (m, 1H), 2.12-2.05 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.10, 196.83,

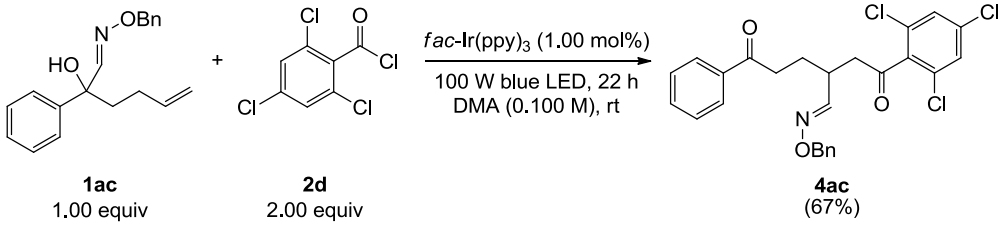
136.79, 136.75, 136.53, 133.76, 131.52, 128.98, 128.63, 128.24, 120.71, 45.77, 35.85, 26.13, 25.58. **HRMS** (ESI-TOF) *m/z* calcd for $C_{19}H_{15}Cl_3NO_2$ [(M + H)$^+$], 394.0163, found, 394.0170.

5-Oxo-2-(2-oxo-2-(2,4,6-trichlorophenyl)ethyl)-5-phenylpentanal (4ab)



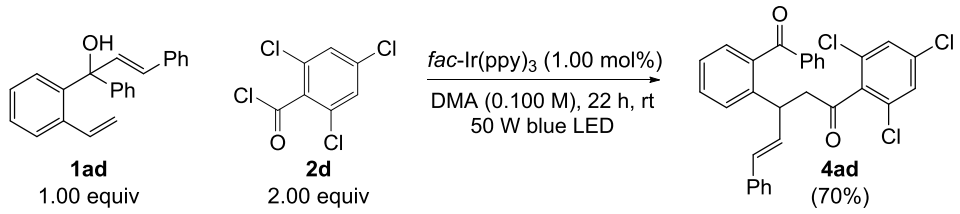
The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (55.6 mg, 0.230 mmol, 2.00 equiv) and 2-hydroxy-2-phenylhex-5-enal (21.8 mg, 0.115 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:10 (v/v)] to afford the title compound as a colorless oil (25.0 mg, 0.064 mmol, 56% yield). R_f = 0.20 EtOAc:Hexanes [1:10 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 9.86 (d, *J* = 0.89 Hz, 1H), 7.95 (d, *J* = 7.80 Hz, 2H), 7.57 (t, *J* = 7.33 Hz, 1H), 7.47 (t, *J* = 7.80 Hz, 2H), 7.38-7.33 (m, 2H), 3.37 (dd, *J* = 19.40 & 6.60 Hz, 1H), 3.19-3.06 (m, 3H), 3.02 (dd, *J* = 19.40 & 5.32 Hz, 1H), 2.33-2.24 (m, 1H), 2.08-1.99 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 202.22, 199.26, 199.04, 137.48, 136.77, 136.30, 133.54, 131.41, 128.91, 128.57, 128.21, 45.51, 43.22, 35.74, 23.06. **HRMS** (ESI-TOF) *m/z* calcd for $C_{19}H_{16}Cl_3O_3$ [(M + H)$^+$], 397.0160, found, 397.0049.

5-Oxo-2-(2-oxo-2-(2,4,6-trichlorophenyl)ethyl)-5-phenylpentanal *O*-benzyl oxime (4ac)



The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (50.7 mg, 0.210 mmol, 2.00 equiv) and 2-hydroxy-2-phenylhex-5-enal *O*-benzyl oxime (30.9 mg, 0.105 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:10 (v/v)] to afford the title compound as a white solid (34.7 mg, 0.072 mmol, 67% yield, mixture of *Z*/*E* oxime, major isomer). R_f = 0.37 EtOAc:Hexanes [1:10 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.89 (d, *J* = 8.40 Hz, 2H), 7.57 (t, *J* = 7.40 Hz, 1H), 7.50 (d, *J* = 6.18 Hz, 1H), 7.45 (t, *J* = 7.83 Hz, 2H), 7.33 (s, 2H), 7.33-7.29 (m, 4H), 7.27-7.24 (m, 1H), 5.02 (s, 2H), 3.15 (dd, *J* = 18.53 & 6.60 Hz, 1H,), 3.11-3.06 (m, 1H), 3.04-2.95 (m, 3H), 2.10-1.97 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.53, 199.15, 152.11, 137.85, 137.84, 136.96, 136.06, 133.30, 131.45, 128.79, 128.57, 128.50, 128.40, 128.25, 128.02, 75.93, 46.69, 35.99, 34.53, 26.58. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{23}Cl_3NO_3$ [(M + H)$^+$], 502.0738, found, 502.0751.

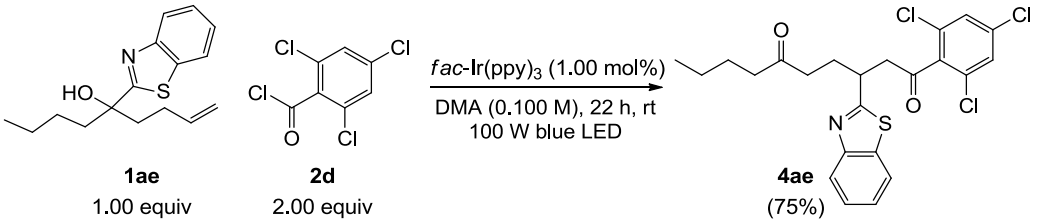
(*E*)-3-(2-Benzoylphenyl)-5-phenyl-1-(2,4,6-trichlorophenyl)pent-4-en-1-one (4ad)



1ad 1.00 equiv | **2d** 2.00 equiv | **4ad** (70%)

The reaction was performed according to the general procedure C using (*E*)-1,3-diphenyl-1-(2-vinylphenyl)prop-2-en-1-ol (31.2 mg, 0.100 mmol, 1.00 equiv) and 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (36.0 mg, 0.0700 mmol, 70% yield). $\mathbf{R_f}$ = 0.38 EtOAc:Hexanes [1:19 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.73 (d, *J* = 8.00 Hz, 2H), 7.58-7.54 (m, 2H), 7.48-7.45 (m, 1H), 7.40 (t, *J* = 8.00 Hz, 2H), 7.27-7.26 (m, 2H), 7.24 (s, 2H), 7.11-7.09 (m, 2H), 7.05 (t, *J* = 7.50 Hz, 3H), 6.44 (d, *J* = 11.5 Hz, 1H), 5.96 (dd, *J* = 11.50 & 9.50 Hz, 1H), 4.88-4.83 (m, 1H), 3.50-3.45 (m, 1H), 3.30-3.25 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.80, 198.16, 143.60, 138.24, 138.03, 137.64, 136.74, 135.67, 133.33, 133.22, 131.52, 131.00, 130.81, 130.68, 129.37, 128.89, 128.65, 128.50, 128.31, 128.24, 127.09, 125.90, 52.01, 35.97. **HRMS** (ESI-TOF) *m/z* calcd for $C_{30}H_{22}Cl_3O_2$ [$(M + H)^+$], 519.0680, found, 519.0705.

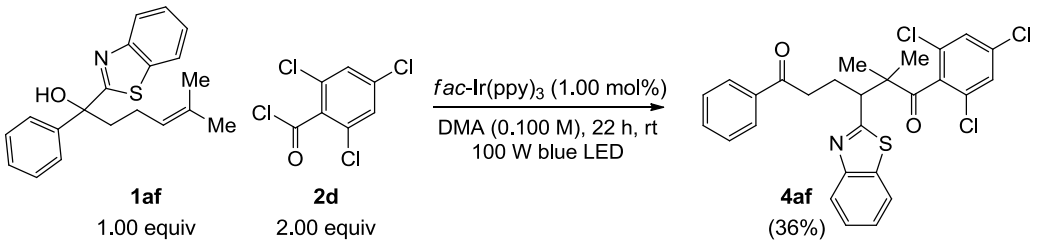
3-(Benzo[*d*]thiazol-2-yl)-1-(2,4,6-trichlorophenyl)decane-1,6-dione (4ae)



1ae 1.00 equiv | **2d** 2.00 equiv | **4ae** (75%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 5-(benzo[*d*]thiazol-2-yl)non-1-en-5-ol (55.0 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (72.4 mg, 0.150 mmol, 75% yield). $\mathbf{R_f}$ = 0.48 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.95 (d, *J* = 8.00 Hz, 1H), 7.85 (d, *J* = 8.00 Hz, 1H), 7.46 (t, *J* = 7.50 Hz, 1H), 7.37 (t, *J* = 7.50 Hz, 1H), 7.30 (s, 2H), 3.95-3.90 (m, 1H), 3.56 (dd, *J* = 19.0 & 6.50 Hz, 1H), 3.32 (dd, *J* = 19.0 & 6.50 Hz, 1H), 2.53-2.42 (m, 2H), 2.34 (t, *J* = 7.50 Hz, 2H), 2.28-2.13 (m, 2H), 1.52-1.46 (m, 2H), 1.29-1.21 (m, 2H), 0.860 (t, *J* = 7.50 Hz, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 210.12, 198.82, 173.27, 153.19, 137.65, 136.09, 135.00, 131.47, 128.47, 126.24, 125.20, 122.94, 121.85, 49.01, 42.80, 39.99, 38.31, 29.35, 26.02, 22.49, 14.02. **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{23}Cl_3NO_2S$ [$(M + H)^+$], 482.0510, found, 482.0512.

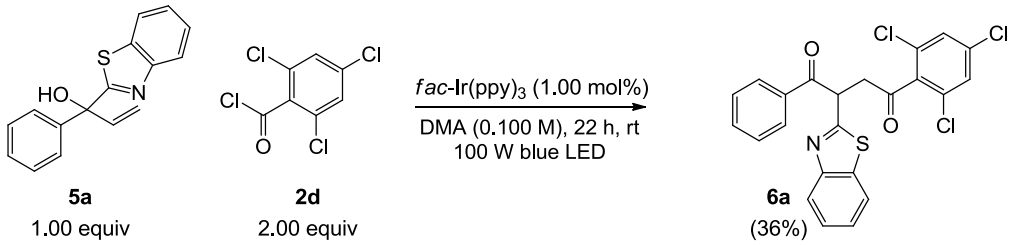
3-(Benzo[*d*]thiazol-2-yl)-2,2-dimethyl-6-phenyl-1-(2,4,6-trichlorophenyl)hexane-1,6-dione (4af)



1af 1.00 equiv | **2d** 2.00 equiv | **4af** (36%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-5-methyl-1-phenylhex-4-en-1-ol (64.7 mg, 0.200 mmol, 1.00 equiv) as the substrates. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (38.2 mg, 0.072 mmol, 36% yield). $\mathbf{R_f}$ = 0.41 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.82 (d, *J* = 7.70 Hz, 2H), 7.80 (d, *J* = 8.40 Hz, 1H), 7.77 (d, *J* = 7.70 Hz, 1H), 7.51 (t, *J* = 7.70 Hz, 1H), 7.41-7.37 (m, 3H), 7.30 (t, *J* = 7.00 Hz, 1H), 7.02 (s, 2H), 4.52-4.50 (m, 1H), 3.05-2.95 (m, 2H), 2.48-2.42 (m, 1H), 2.20-2.15 (m, 1H), 1.68 (s, 3H), 1.60 (s, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 201.82, 199.56, 179.49, 152.71, 137.36, 136.70, 135.69, 134.75, 133.23, 132.81, 128.75, 128.70, 128.13, 126.09, 125.13, 122.81, 121.52, 60.01, 45.14, 37.40, 27.93, 24.84, 21.64. **HRMS** (ESI-TOF) *m/z* calcd for $C_{27}H_{23}Cl_3NO_2S$ [(M + H)$^+$], 530.0510, found, 530.0537.

2-(Benzo[*d*]thiazol-2-yl)-1-phenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6a)



5a 1.00 equiv | **2d** 2.00 equiv | **6a** (36%)

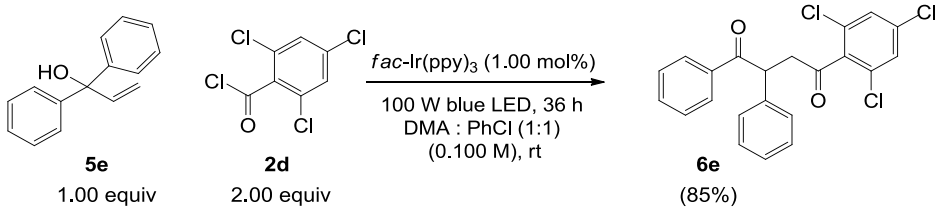
The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-phenylprop-2-en-1-ol (26.7 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (17.1 mg, 0.0360 mmol, 36% yield). $\mathbf{R_f}$ = 0.35 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.18 (d, *J* = 7.70 Hz, 2H), 7.99 (d, *J* = 8.40 Hz, 1H), 7.81 (d, *J* = 7.70 Hz, 1H), 7.57 (t, *J* = 7.70 Hz, 1H), 7.48 (t, *J* = 7.70 Hz, 2H), 7.45 (t, *J* = 8.40 Hz, 1H), 7.36-7.35 (m, 1H), 7.34 (s, 2H), 5.89 (dd, *J* = 9.10 & 4.20 Hz, 1H), 4.19 (dd, *J* = 19.6 & 9.10 Hz, 1H), 3.63 (dd, *J* = 19.1 & 4.20 Hz, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 198.48, 195.10, 166.59, 153.04, 137.11, 136.33, 135.86, 135.65, 133.97, 131.73, 129.47, 129.01, 128.52, 126.49, 125.63, 123.47, 121.83, 47.04, 46.80. **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{15}Cl_3NO_2S$ [(M + H)$^+$], 473.98836, found, 473.98846.

3-(Benzo[*d*]thiazol-2-yl)-7-phenyl-1-(2,4,6-trichlorophenyl)heptane-1,7-dione (6c)

5c 1.00 equiv | **2d** 2.00 equiv | **6c** (67%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-phenylhex-5-en-1-ol (61.8 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (68.1 mg, 0.134 mmol, 67% yield). $\mathbf{R_f}$ = 0.24 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.94 (d, *J* = 8.12 Hz, 1H), 7.90 (d, *J* = 7.21 Hz, 2H), 7.84 (d, *J* = 7.98 Hz, 1H), 7.52 (t, *J* = 7.42 Hz, 1H), 7.47-7.43 (m, 1H), 7.41 (t, *J* = 7.84 Hz, 2H), 7.34 (t, *J* = 7.14 Hz, 1H), 7.29 (s, 2H), 4.03-3.92 (m, 1H), 3.57 (dd, *J* = 19.11 & 6.37 Hz, 1H), 3.36 (dd, *J* = 19.11 & 6.72 Hz, 1H), 3.11-2.93 (m, 2H), 2.12-2.01 (m, 2H), 1.89-1.76 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.74, 199.05, 173.69, 153.18, 137.69, 136.97, 136.00, 134.96, 133.16, 131.43, 128.71, 128.41, 128.15, 126.13, 125.06, 122.85, 121.78, 48.80, 38.93, 38.22, 35.02, 21.77. **HRMS** (ESI-TOF) *m/z* calcd for $C_{26}H_{21}Cl_3NO_2S$ [$(M + H)^+$], 516.03531, found, 516.03468.

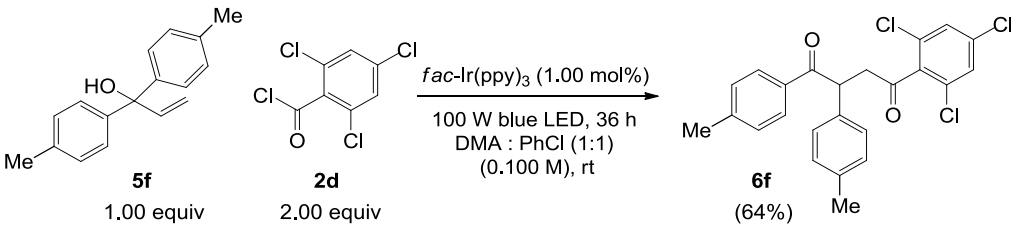
1,2-Diphenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6e)



5e 1.00 equiv | **2d** 2.00 equiv | **6e** (85%)

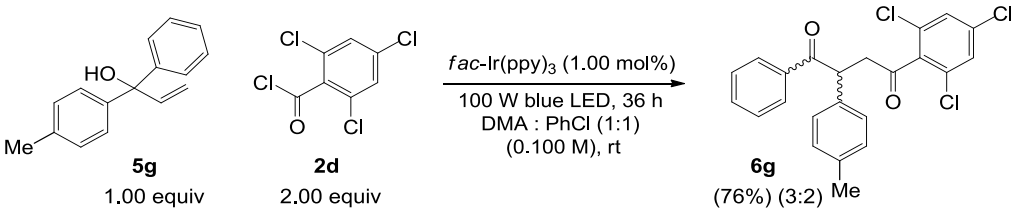
The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1,1-diphenylprop-2-en-1-ol (27.8 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (36.4 mg, 0.0850 mmol, 85% yield). $\mathbf{R_f}$ = 0.60 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.03 (d, *J* = 7.28 Hz, 2H), 7.49 (d, *J* = 7.28 Hz, 1H), 7.40 (d, *J* = 7.98 Hz, 2H), 7.36-7.32 (m, 2H), 7.31 (s, 2H), 7.28 (t, *J* = 7.49 Hz, 2H), 7.23-7.17 (m, 1H), 5.29 (dd, *J* = 8.82 & 4.34 Hz, 1H), 3.99 (dd, *J* = 19.18 & 8.82 Hz, 1H), 3.25 (dd, *J* = 19.18 & 4.34 Hz, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.56, 198.08, 138.16, 137.65, 136.39, 135.99, 133.23, 131.59, 129.35, 129.15, 128.73, 128.49, 128.43, 127.70, 48.32, 47.99. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{16}Cl_3O_2$ [$(M + H)^+$], 417.02104, found, 417.02108.

1,2-Di-*p*-tolyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6f)



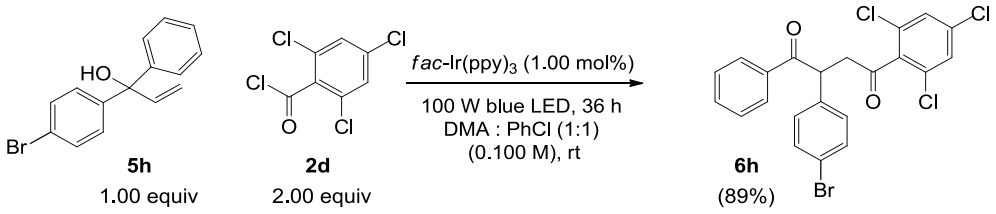
The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1,1-di-p-tolylprop-2-en-1-ol (47.6 mg, 0.200 mmol, 1,00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (56.7 mg, 0.128 mmol, 64% yield). $\mathbf{R_f}$ = 0.62 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.93 (d, *J* = 8.26 Hz, 2H), 7.30 (s, 2H), 7.23-7.17 (m, 4H), 7.07 (d, *J* = 7.91 Hz, 2H), 5.23 (dd, *J* = 8.82 & 4.27 Hz, 1H), 3.96 (dd, *J* = 19.11 & 8.82 Hz, 1H), 3.20 (dd, *J* = 19.11 & 4.27 Hz, 1H), 2.35 (s, 3H), 2.26 (s, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.72, 197.76, 143.98, 137.78, 137.31, 135.92, 135.40, 133.86, 131.62, 130.00, 129.42, 129.29, 128.42, 128.32, 48.27, 47.45, 21.83, 21.23. **HRMS** (ESI-TOF) *m/z* calcd for $C_{24}H_{20}Cl_3O_2$ [$(M + H)^+$], 445.05234, found, 445.05161.

1-Phenyl-2-(*p*-tolyl)-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6g)



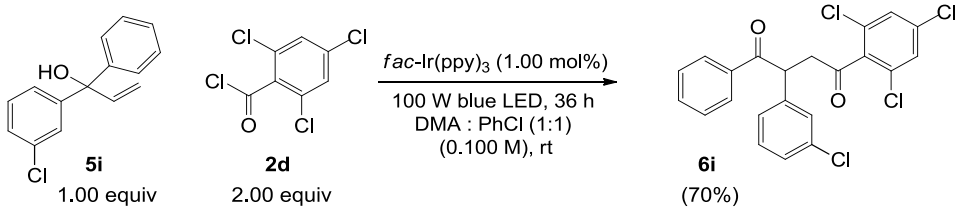
The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-phenyl-1-(*p*-tolyl)prop-2-en-1-ol (22.4 mg, 0.100 mmol, 1 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (33.7 mg, 0.076 mmol, 76% yield). $\mathbf{R_f}$ = 0.60 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.06 (d, *J* = 7.00 Hz, 1.30H), 7.97 (d, *J* = 8.40 Hz, 1.80H), 7.51 (t, *J* = 7.00 Hz, 0.99H), 7.43 (t, *J* = 7.70 Hz, 1.72H), 7.36-7.35 (m, 2.05H), 7.34-7.33 (m, 2.60H), 7.31-7.28 (m, 2.40H), 7.25-7.22 (m, 4.02H), 7.12 (d, *J* = 7.70 Hz, 1.42H), 5.32-5.28 (m, 1.50H), 4.03-3.99 (m, 1.53H), 3.28-3.25 (m, 1.53H), 2.38 (s, 3.00H), 2.29 (s, 1.89H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.65, 199.56, 198.19, 197.63, 144.04, 138.48, 137.72, 135.95, 133.83, 133.14, 131.60, 130.04, 129.43, 129.29, 129.13, 128.70, 128.47, 128.41, 128.33, 127.59, 48.26, 47.85, 47.60, 21.81, 21.21. **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{18}Cl_3O_2$ [$(M + H)^+$], 431.03669, found, 431.03588.

2-(4-Bromophenyl)-1-phenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6h)



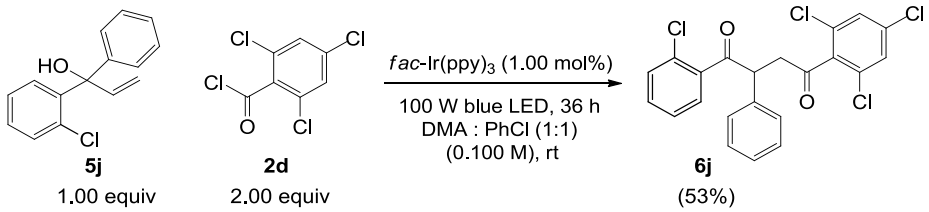
The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (48.6 mg, 0.200 mmol, 2.00 equiv) and 1-(4-bromophenyl)-1-phenylprop-2-en-1-ol (28.8 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (45.2 mg, 0.0890 mmol, 89% yield). $\mathbf{R_f}$ = 0.58 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.00 (d, *J* = 7.35 Hz, 2H), 7.51 (t, *J* = 7.42 Hz, 1H), 7.45-7.39 (m, 4H), 7.31 (s, 2H), 7.22 (d, *J* = 8.47 Hz, 2H), 5.27 (dd, *J* = 8.4 & 4.76 Hz, 1H), 3.94 (dd, *J* = 19.18 & 8.4 Hz, 1H), 3.23 (dd, *J* = 19.18 & 4.76 Hz, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.27, 197.72, 137.46, 137.16, 136.12, 136.09, 133.47, 132.47, 131.55, 130.22, 129.10, 128.84, 128.46, 121.80, 48.00, 47.29. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{15}BrCl_3O_2$ [(M + H)$^+$], 494.93155, found, 494.93239.

2-(3-Chlorophenyl)-1-phenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6i)



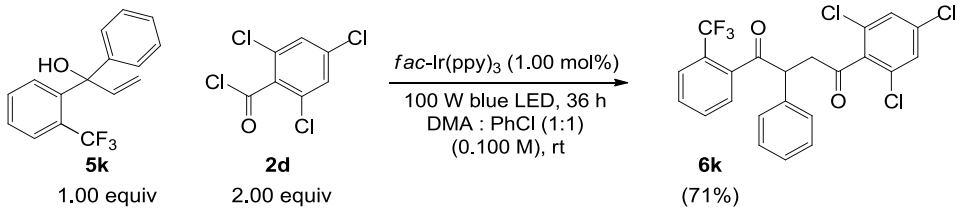
The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(3-chlorophenyl)-1-phenylprop-2-en-1-ol (48.8 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (63.4 mg, 0.140 mmol, 70% yield). $\mathbf{R_f}$ = 0.56 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.02 (d, *J* = 7.25 Hz, 2H), 7.52 (t, *J* = 7.40 Hz, 1H), 7.43 (t, *J* = 7.85 Hz, 2H), 7.33 (s, 1H), 7.31 (s, 2H), 7.25-7.17 (m, 3H), 5.27 (dd, *J* = 8.65 & 4.55 Hz, 1H), 3.96 (dd, *J* = 19.1 & 8.65 Hz, 1H), 3.24 (dd, *J* = 19.1 & 4.55 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 199.20, 197.55, 140.07, 137.45, 136.13, 135.12, 133.50, 131.58, 130.58, 129.13, 128.87, 128.56, 128.47, 128.01, 126.76, 48.13, 47.48. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{15}Cl_4O_2$ [(M + H)$^+$], 450.98207, found, 450.98264.

2-(2-Chlorophenyl)-1-phenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6j)



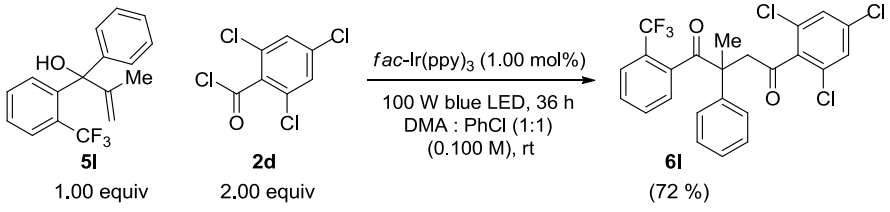
The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (48.6 mg, 0.200 mmol, 2.00 equiv) and 1-(2-chlorophenyl)-1-phenylprop-2-en-1-ol (24.4 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (24.7 mg, 0.0530 mmol, 53% yield). $\mathbf{R_f}$ = 0.56 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.74-7.69 (m, 1H), 7.38-7.32 (m, 4H), 7.31-7.21 (m, 6H), 5.13 (dd, *J* = 8.68 & 4.41 Hz, 1H), 4.05 (dd, *J* = 19.18 & 8.68 Hz, 1H,), 3.39 (dd, *J* = 19.18 & 4.41 Hz, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 199.95, 199.59, 138.61, 137.58, 136.09, 131.83, 131.70, 131.64, 130.77, 129.48, 129.18, 128.97, 128.47, 127.98, 126.74, 51.87, 47.02. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{15}Cl_4O_2$ [$(M + H)^+$], 450.98207, found, 450.98219.

1-Phenyl-4-(2,4,6-trichlorophenyl)-2-(2-(trifluoromethyl)phenyl)butane-1,4-dione (6k)



The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (48.6 mg, 0.200 mmol, 2.00 equiv) and 1-phenyl-1-(2-(trifluoromethyl)phenyl)prop-2-en-1-ol (27.8 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (34.4 mg, 0.0710 mmol, 71% yield). $\mathbf{R_f}$ = 0.46 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.81 (d, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 7.77 Hz, 1H), 7.54 (t, *J* = 7.49 Hz, 1H), 7.49 (t, *J* = 7.63 Hz, 1H), 7.28 (s, 2H), 7.21 (t, *J* = 7.35 Hz, 2H), 7.20-7.16 (m, 3H), 5.02 (dd, *J* = 8.19 & 4.83 Hz, 1H), 4.02 (dd, *J* = 19.25 & 8.19 Hz, 1H), 3.29 (dd, *J* = 19.25 & 4.83 Hz, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 200.64, 199.64, 138.66, 137.53, 136.13, 135.86, 131.74, 131.59, 130.85, 129.14, 129.09, 128.99, 128.46, 128.34 (q, $J^2_{C\text{-}F}$ = 32.07 Hz), 128.07, 127.22 (q, $J^3_{C\text{-}F}$ = 5.16 Hz), 123.39 (q, $J^1_{C\text{-}F}$ = 272.03 Hz), 52.06, 42.73. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –58.95 (s). **HRMS** (ESI-TOF) *m/z* calcd for $C_{23}H_{15}Cl_3F_3O_2$ [$(M + H)^+$], 485.00842, found, 485.00867.

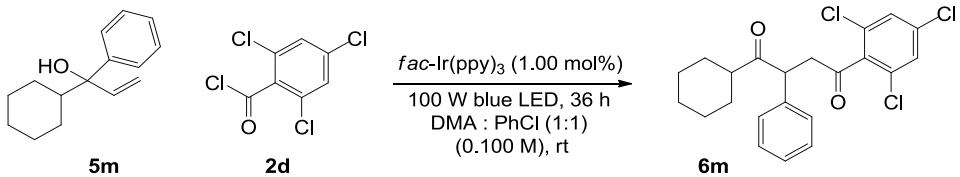
2-Methyl-2-phenyl-4-(2,4,6-trichlorophenyl)-1-(2-(trifluoromethyl)phenyl)butane-1,4-dione (6l)



The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (48.6 mg, 0.200 mmol, 2.00 equiv) and 2-methyl-1-phenyl-1-(2-(trifluoromethyl)phenyl)prop-2-en-1-ol (29.2 mg, 0.100

mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (36.2 mg, 0.0720 mmol, 72% yield). $\mathbf{R_f}$ = 0.46 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.71 (d, *J* = 7.91 Hz, 1H), 7.55 (d, *J* = 7.91 Hz, 2H), 7.46 (t, *J* = 7.63 Hz, 1H), 7.42 (t, *J* = 7.63 Hz, 2H), 7.36 (t, *J* = 6.86 Hz, 1H), 7.31 (m, 2H), 7.29-7.26 (m, 1H), 6.45 (d, *J* = 7.77 Hz, 1H), 4.10 (d, *J* = 19.53 Hz, 1H), 3.47 (d, *J* = 19.53 Hz, 1H), 1.86 (s, 3H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 205.29, 197.79, 139.29, 137.91, 137.75, 135.83, 131.47, 131.11, 129.76, 129.03, 128.43, 128.29 (q, $J^2_{C\text{-}F}$ = 32.00 Hz), 127.92, 127.41, 127.25 (q, $J^3_{C\text{-}F}$ = 4.91 Hz), 127.10, 123.69 (q, $J^1_{C\text{-}F}$ = 271.88 Hz), 53.60, 52.39, 20.36. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –57.54 (s).

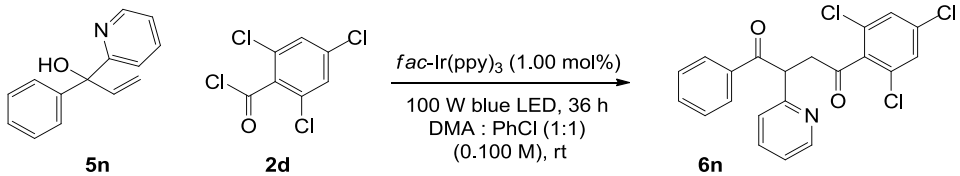
1-Cyclohexyl-2-phenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6m)



5m 1.00 equiv | **2d** 2.00 equiv | **6m** (77%)

The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-cyclohexyl-1-phenylprop-2-en-1-ol (43.2 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:19 (v/v)] to afford the title compound as a gummy solid (65.4 mg, 0.154 mmol, 77% yield). $\mathbf{R_f}$ = 0.44 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.33-7.26 (m, 4H), 7.24 (t, *J* = 7.56 Hz, 1H), 7.21 (d, *J* = 7.07 Hz, 2H), 4.50 (dd, *J* = 9.1 & 3.99 Hz, 1H), 3.79 (dd, *J* = 19.18 & 9.17 Hz, 1H), 3.00 (dd, *J* = 19.25 & 4.06 Hz, 1H), 2.54-2.45 (m, 1H), 2.15-2.07 (m, 1H), 1.75-1.82 (m, 1H), 1.56-1.66 (m, 2H), 1.43-1.40 (m, 1H), 1.3-1.4 (m, 2H), 1.29-1.2 (m, 1H), 1.19-1.05 (m, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 211.42, 199.67, 137.72, 137.68, 135.92, 131.56, 129.24, 128.66, 128.41, 127.77, 51.06, 50.12, 47.37, 29.65, 28.54, 26.12, 25.97, 25.52. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{22}Cl_3O_2$ [$(M + H)^+$], 423.06799, found, 423.06808.

1-Phenyl-2-(pyridin-2-yl)-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6n)

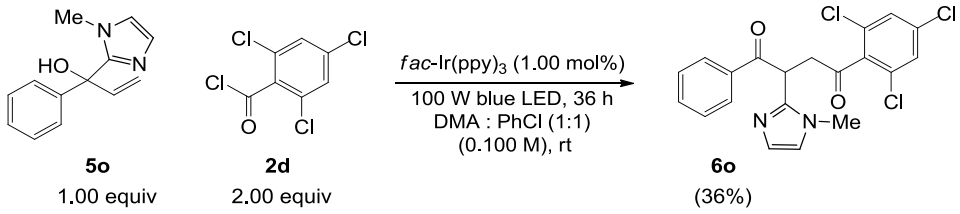


5n 1.00 equiv | **2d** 2.00 equiv | **6n** (41%)

The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-phenyl-1-(pyridin-2-yl)prop-2-en-1-ol (42.2 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (34.6 mg, 0.0820 mmol, 41% yield). $\mathbf{R_f}$

= 0.22 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 8.60-8.51 (m, 1H), 8.09 (d, *J* = 7.35 Hz, 2H), 7.65-7.56 (m, 1H), 7.50 (t, *J* = 7.49 Hz, 1H), 7.41 (t, *J* = 7.85 Hz, 2H), 7.36 (d, *J* = 7.90 Hz, 1H), 7.30 (s, 2H), 7.18-7.09 (m, 1H), 5.61-5.50 (m, 1H), 4.00 (dd, *J* = 19.2 & 8.35 Hz, 1H), 3.46 (dd, *J* = 19.15 & 4.4 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 199.24, 197.30, 157.87, 150.22, 137.58, 137.42, 136.39, 136.03, 133.39, 131.65, 129.33, 128.79, 128.43, 123.53, 122.61, 50.48, 46.82. **HRMS** (ESI-TOF) *m/z* calcd for $C_{21}H_{15}Cl_3NO_2$ [$(M + H)^+$], 418.01629, found, 418.01579.

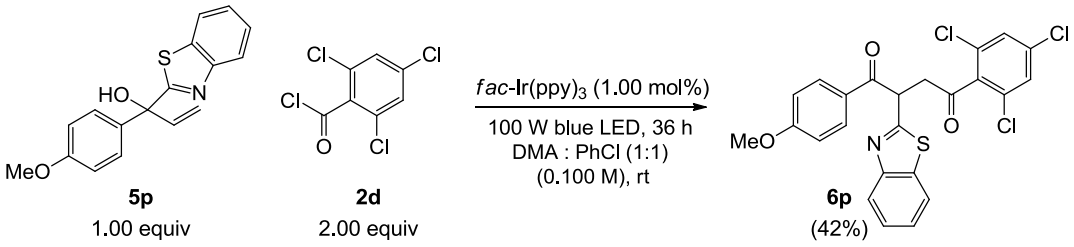
2-(1-Methyl-1*H*-imidazol-2-yl)-1-phenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6o)



5o 1.00 equiv | **2d** 2.00 equiv | **6o** (36%)

The reaction was performed according to the general procedure D using 2,4,6-trichlorobenzoyl chloride (97.5 mg, 0.400 mmol, 2.00 equiv) and 1-(1-methyl-1*H*-imidazol-2-yl)-1-phenylprop-2-en-1-ol (42.8 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 36 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (30.4 mg, 0.0720 mmol, 36% yield). $\mathbf{R_f}$ = 0.09 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.47 (d, *J* = 7.25 Hz, 2H), 7.31 (s, 2H), 7.30-7.26 (m, 2H), 7.24-7.18 (m, 1H), 7.18-7.16 (m, 1H), 6.98 (s, 1H), 5.75 (dd, *J* = 10.35 & 3.80 Hz, 1H), 4.02-3.92 (m, 4H), 3.27 (dd, *J* = 19.05 & 3.80 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 199.33, 190.23, 142.49, 137.97, 137.68, 135.93, 131.64, 129.73, 128.95, 128.88, 128.40, 127.52, 127.42, 47.41, 47.33, 36.35. **HRMS** (ESI-TOF) *m/z* calcd for $C_{20}H_{16}Cl_3N_2O_2$ [$(M + H)^+$], 421.02719, found, 421.02724.

2-(Benzo[*d*]thiazol-2-yl)-1-(4-methoxyphenyl)-4-(2,4,6-trichlorophenyl)butane-1,4-dione (6p)

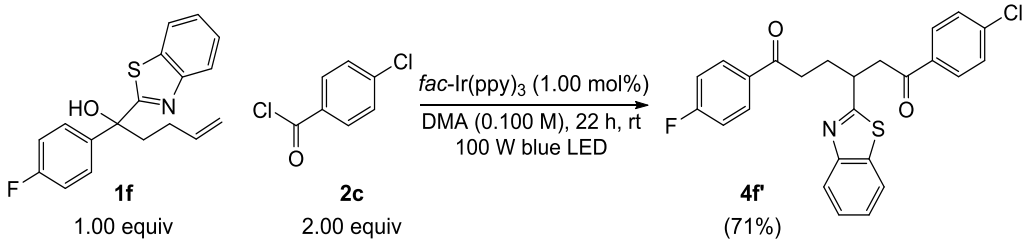


5p 1.00 equiv | **2d** 2.00 equiv | **6p** (42%)

The reaction was performed according to the general procedure C using 2,4,6-trichlorobenzoyl chloride (48.7 mg, 0.200 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(4-methoxyphenyl)prop-2-en-1-ol (29.7 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (21.2 mg, 0.0420 mmol, 42% yield). $\mathbf{R_f}$ = 0.19 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.17 (d, *J* = 8.89 Hz,

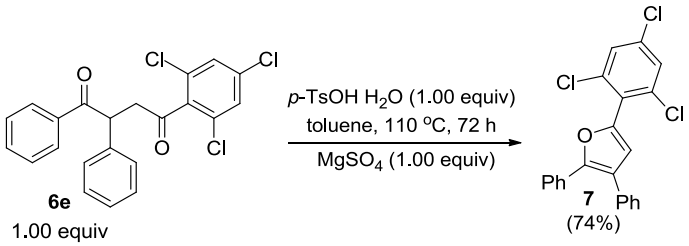
2H), 7.99 (d, *J* = 8.19 Hz, 1H), 7.80 (d, *J* = 7.98 Hz, 1H), 7.44 (t, *J* = 7.49 Hz, 1H), 7.38-7.33 (m, 1H), 7.33 (s, 2H), 6.95 (t, *J* = 8.89 Hz, 2H), 5.86 (dd, *J* = 8.89 & 3.99 Hz, 1H), 4.16 (dd, *J* = 19.11 & 8.96 Hz, 1H), 3.85 (s, 3H), 3.60 (dd, *J* = 19.18 & 4.06 Hz, 1H). **^{13}C NMR** (175 MHz, CD_3CN, 25 ºC, δ): 200.30, 194.48, 168.64, 165.57, 154.10, 138.47, 137.20, 136.63, 132.72, 132.41, 129.86, 129.80, 127.75, 126.85, 124.03, 123.36, 115.51, 56.79, 47.41, 47.38. **HRMS** (ESI-TOF) *m/z* calcd for $C_{24}H_{17}Cl_3NO_3S$ [(M + H)$^+$], 503.99892, found, 503.99873.

3-(Benzo[*d*]thiazol-2-yl)-1-(4-chlorophenyl)-6-(4-fluorophenyl)hexane-1,6-dione (4f')



The reaction was performed according to the general procedure C using 4-chlorobenzoyl chloride (70.0 mg, 0.400 mmol, 2.00 equiv) and 1-(benzo[*d*]thiazol-2-yl)-1-(4-fluorophenyl)pent-4-en-1-ol (62.6 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 22 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:14 (v/v)] to afford the title compound as a gummy solid (64.2 mg, 0.142 mmol, 71% yield). $\mathbf{R_f}$ = 0.26 EtOAc:Hexanes [1:4 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.97-7.87 (m, 5H), 7.83 (d, *J* = 7.90 Hz, 1H), 7.48-7.39 (m, 3H), 7.35 (t, *J* = 7.95 Hz, 1H), 7.07 (t, *J* = 8.55 Hz, 2H), 4.12-3.97 (m, 1H), 3.79 (dd, *J* = 17..65 & 7.30 Hz, 1H), 3.43 (dd, *J* = 17.65 & 6.05 Hz, 1H,), 3.13-2.96 (m, 2H), 2.44-2.30 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 197.64, 196.38, 174.04, 165.91 (d, $J^1_{C\text{-}F}$ =253.25 Hz), 153.25, 135.13, 134.95, 133.31, 133.29, 130.84 (d, $J^3_{C\text{-}F}$ = 9.42 Hz), 129.74, 129.16, 126.23, 125.19, 122.94, 121.85, 115.82 (d, $J^2_{C\text{-}F}$ = 21.7 Hz), 44.30, 39.20, 36.13, 30.01. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –106.15 (m). **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{20}ClFNO_2S$ [(M + H)$^+$], 452.08818, found, 452.08787.

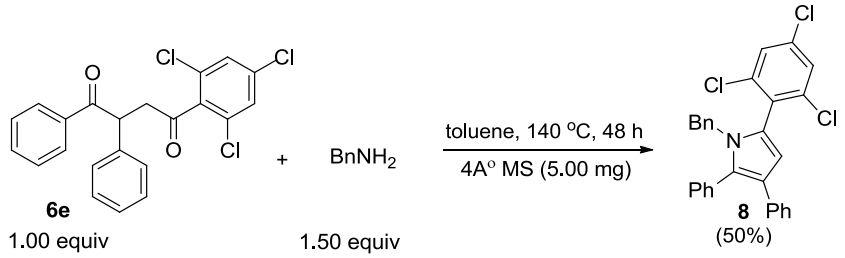
2,3-Diphenyl-5-(2,4,6-trichlorophenyl)furan (7)



The reaction was performed according to the modified literature procedure[12] using 1,2-piphenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (83.5 mg, 0.200 mmol, 1.00 equiv) as the substrate. After 72 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (59.0 mg, 0.148 mmol, 74% yield). $\mathbf{R_f}$ = 0.65 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.59 (d, *J* = 8.61 Hz, 2H), 7.49 (d, *J* = 8.33 Hz, 2H), 7.46 (s, 2H),

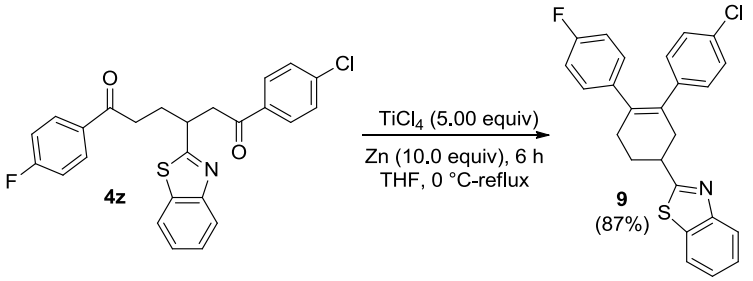
7.39 (t, *J* = 7.35 Hz, 2H), 7.33 (t, *J* = 7.42 Hz, 1H), 7.30 (t, *J* = 7.63 Hz, 2H), 7.27-7.25 (m, 1H), 6.79 (s, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 149.22, 145.41, 136.55, 135.22, 134.08, 130.97, 128.96, 128.89, 128.80, 128.65, 128.31, 128.08, 127.57, 126.58, 123.46, 117.00. **HRMS** (ESI-TOF) *m/z* calcd for $C_{22}H_{14}Cl_3O$ [$(M + H)^+$], 399.01047, found, 399.01061.

1-Benzyl-2,3-diphenyl-5-(2,4,6-trichlorophenyl)-1*H*-pyrrole (8)



The reaction was performed according to the modified literature procedure[12] using 1,2-piphenyl-4-(2,4,6-trichlorophenyl)butane-1,4-dione (41.8 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 48 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (24.4 mg, 0.0500 mmol, 50% yield). $\mathbf{R}_f$ = 0.70 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 7.34 (s, 2H), 7.32-7.31 (m, 3H), 7.29-7.28 (m, 2H), 7.22-7.21 (m, 2H), 7.16 (t, *J* = 7.91 Hz, 2H), 7.09-7.06 (m, 4H), 6.68 (d, *J* = 7.70 Hz, 2H), 6.51 (s, 1H), 4.83 (s, 2H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 138.09, 138.04, 136.18, 134.82, 133.15, 132.35, 131.68, 130.69, 128.77, 128.30, 128.26, 128.10, 127.69, 127.19, 126.93, 126.78, 125.35, 122.82, 111.28, 48.95. **HRMS** (ESI-TOF) *m/z* calcd for $C_{29}H_{21}Cl_3N$ [$(M + H)^+$], 488.07341, found, 488.07492.

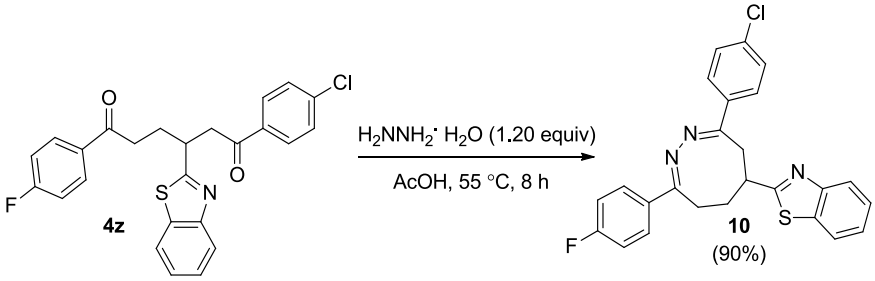
2-(4''-Chloro-4-fluoro-3',4',5',6'-tetrahydro-[1,1':2',1''-terphenyl]-4'-yl)benzo[*d*]thiazole (9)



The reaction was performed according to the modified literature procedure[13] using 3-(benzo[*d*]thiazol-2-yl)-1-(4-chlorophenyl)-6-(4-fluorophenyl)hexane-1,6-dione (45.2 mg, 0.100 mmol, 1.00 equiv) as the substrate. After 6 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a gummy solid (36.5 mg, 0.0870 mmol, 87% yield). $\mathbf{R}_f$ = 0.32 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.01 (d, *J* = 7.00 Hz, 1H), 7.88 (d, *J* = 7.70 Hz, 1H), 7.48 (t, *J* = 7.70 Hz, 1H), 7.38 (t, *J* = 7.70 Hz, 1H), 7.10 (d, *J* = 8.40 Hz, 2H), 6.95 (t, *J* = 8.40 Hz, 4H), 6.83 (t, *J* = 8.40 Hz, 2H), 3.67 (bs, 1H), 2.99-2.87 (m, 2H), 2.65-2.60 (m, 2H), 2.45-2.44 (m, 1H), 2.24-2.17 (m, 1H). **^{13}C NMR** (175

MHz, $CDCl_3$, 25 ºC, δ): 175.96, 161.50 (d, $J^1_{C\text{-}F}$ = 244.11 Hz), 153.13, 141.15, 138.51 (d, $J^3_{C\text{-}F}$ = 3.46 Hz), 135.01, 134.75, 132.79, 132.23, 130.67, 130.62, 128.33, 126.32, 125.10, 122.89, 121.86, 115.06 (d, $J^2_{C\text{-}F}$ = 21.05 Hz), 39.88, 37.95, 31.77, 29.65. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –116.46 (m). **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{20}ClFNS$ [$(M + H)^+$], 420.09835, found, 420.09804

2-((1*E*,2*E*)-3-(4-Chlorophenyl)-8-(4-fluorophenyl)-4,5,6,7-tetrahydro-1,2-diazocin-5-yl)benzo[*d*]thiazole (10)



The reaction was performed according to the modified literature procedure[14] using 3-(benzo[*d*]thiazol-2-yl)-1-(4-chlorophenyl)-6-(4-fluorophenyl)hexane-1,6-dione (45.2 mg, 0.100 mmol, 1.00 equiv) and hydrazine monohydrate (6.00 mg, 0.120 mmol, 1.20 equiv) as the substrate. After 8 h, the reaction mixture was purified by flash column chromatography on silica gel, eluting with EtOAc:Hexanes [1:9 (v/v)] to afford the title compound as a white solid (40.3 mg, 0.0900 mmol, 90% yield). $\mathbf{R}_f$ = 0.50 EtOAc:Hexanes [1:9 (v/v)]. **^{1}H NMR** (700 MHz, $CDCl_3$, 25 ºC, δ): 8.00 (d, *J* = 8.40 Hz, 1H), 7.97-7.94 (m, 4H), 7.87 (d, *J* = 7.70 Hz, 1H), 7.49 (t, *J* = 7.70 Hz, 1H), 7.44 (d, *J* = 8.40 Hz, 2H), 7.39 (t, *J* = 7.70 Hz, 1H), 7.14 (t, *J* = 8.40 Hz, 2H), 3.40 (d, *J* = 13.6 Hz, 1H), 3.24-3.20 (m, 1H), 3.06-3.03 (m, 1H), 2.81-2.77 (m, 1H), 2.56-2.52 (m, 1H), 2.42 (t, *J* = 13.3 Hz, 1H), 1.87-1.82 (m, 1H). **^{13}C NMR** (175 MHz, $CDCl_3$, 25 ºC, δ): 173.84, 164.01 (d, $J^1_{C\text{-}F}$ = 248.95 Hz), 153.19, 151.30, 150.26, 136.24, 134.82, 134.19, 132.04 (d, $J^3_{C\text{-}F}$ = 3.38 Hz), 129.24, 129.11 (d, $J^3_{C\text{-}F}$ = 8.64 Hz), 128.40, 126.55, 125.46, 123.14, 121.85, 115.89 (d, $J^2_{C\text{-}F}$ = 21.09 Hz), 41.09, 31.95, 31.04, 25.50. **^{19}F NMR** (376 MHz, $CDCl_3$, 25 ºC, δ): –111.50 (m). **HRMS** (ESI-TOF) *m/z* calcd for $C_{25}H_{20}ClFN_3S$ [$(M + H)^+$], 448.10450, found, 448.10463.

Mechanistic Studies

DFT Calculation

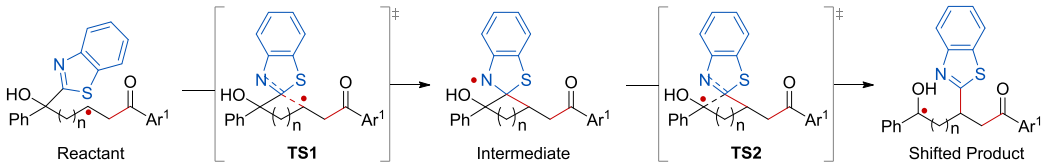
Computational Details: Geometries were optimized and harmonic vibrational frequencies were determined at the UMN15[15]/def2-SVP[16] level of theory in the presence of the SMD[17] continuum solvation model (*N*,*N*-diemthylacetamide). Each transition state structure was confirmed via IRC calculations. Single-point energies were determined at the UMN15/def2-TZVP + SMD level. Energies discussed are relative Gibbs free energies at 298 K and 1 M determined by adding the MN15/def2-SVP + SMD free energy correction to the UMN15/def2-TZVP + SMD electronic energy. All calculations were performed using Gaussian 16 Revision A.03.[18]

We have modeled the *ipso*-heteroaryl migration from initial radical intermediates **5a**/**5b**/**1a**/**5c**/**5d** toward the shifted products at the UMN15/def2-TZVP//UMN15-SVP + SMD (*N*,*N*-dimethyladetamide) level of theory (Figure S1). We determined relative Gibbs free energies compared to both folded conformations of radicals **1a** and **5a-d** as predicted by IRC calculations as well as more extended conformations. In the case of **5d**, the extended conformation was found to be substantially more stable, indicating an unfavorable folding event prior to reaction. For the other radicals, folding is favorable or energetically negligible.

In every case, we predict a two-step reaction with a cyclic intermediate. The cyclic intermediates for **1a** and **5d** are notably more stable than the others, however, this has no particular consequence. Opening of the cyclic intermediate to the shifted radicals has a negligible barrier relative to the first step with the exception of **1a**, for which the two barriers are isoenergetic.

The calculated barrier for the radical shift reaction is measured from the lower-energy conformation of **1a**/**5a-d** to the first (closure) TS. We find a good correlation between the predicted barrier heights and observed experimental yields. We can understand the correlation by considering the geometries of each closure TS. The best (**1a**, barrier 9 kcal/mol, 86% yield) forms a 5-membered ring TS while the second best (**5c**, barrier 10 kcal/mol, 66% yield) forms a 6-membered ring TS. The third best (**5a**, barrier 12 kcal/mol, 36% yield) forms a 3-membered ring TS which should not be stable. However, the ease of this shift can be understood by considering the TS to exist as a resonance structure where the π electrons of the alkene and the radical are delocalized within the ring. Finally, radical **5b** must form a strained 4-membered ring while **5d** must form a distorted 7-membered ring. Neither is a favorable proposition, resulting in high barriers (16 and 22 kcal/mol, respectively) and no observed product.

a. Relative Gibbs free energies (kcal/mol) for the ipso-heteroaryl migration reaction



Compound	5a	5b	1a	5c	5d
Reactant (extended conformation)	3	1	-1	5	-11
Reactant (folded conformation)	0	0	0	0	0
TS1	12	16	8	10	11
Intermediate	5	3	-11	2	-12
TS2	4	9	-2	2	-1
Shifted product (folded conformation)	-14	-13	-17	-15	-23
***Ipso*-heteroaryl migration barrier**	**12**	**16**	**9**	**10**	**22**
Experimental yield	36%	0%	86%	67%	0%

b. Activation energy barrier for competitive aryl group transfer

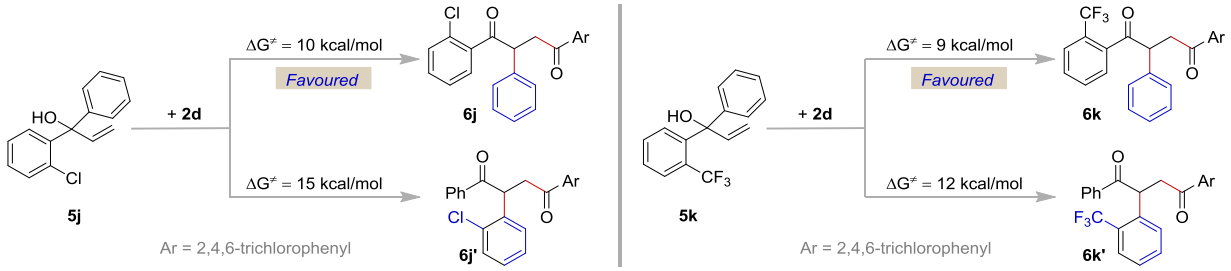


Figure S1. a) Relative Gibbs free energies (kcal/mol) for the ipso-heteroaryl migration reaction. b) Relative Gibbs free energies (kcal/mol) relative to the lowest-energy reactant conformation for each species. Activation energy barriers were calculated relative to lowest-energy reactant conformation. All Gibbs free energy were calculated on UMN15/def2-TZVP//UMN15-SVP + SMD (N,N-dimethyladetamide) level of theory.

Radical Trapping Experiment

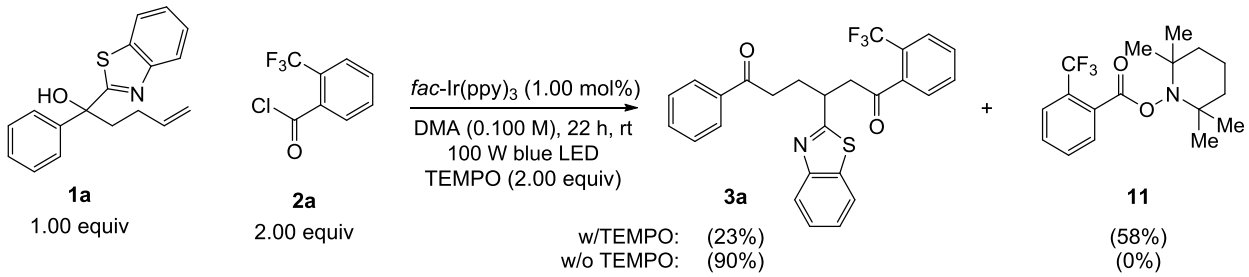


Figure S2. Radical trap experiment using TEMPO.

In a glovebox, to an oven-dried 4 mL screw cap vial was added 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (**1a**) (59.1 mg, 0.200 mmol, 1.00 equiv), TEMPO, (2,2,6,6-Tetramethylpiperidin-1-yl)oxyl (62.0 mg, 0.400 mmol, 2.00 equiv), and DMA (0.100 M, with respect to 1,1-aryl-heteroaryl-4-en-1-ol substrate). To this suspension was added 2-(trifluoromethyl)benzoyl chloride (83.2 mg, 0.400 mmol, 2.00 equiv) (**2a**), *fac*-Ir(ppy)$_3$, (1.00 mol%), and a magnetic stir bar. Next, the vial was capped and taken out of the glovebox. The reaction vial was placed in the photoredox setup and stirred at rt with an irradiation of 100W blue LED light source (450 nm, unless otherwise stated) for 22 h. After that, the reaction mixture was removed from the light source and was directly loaded on to silica column, eluting with Hexane:EtOAc [6:1 (v/v)] to afford the desired coupling product (**3a**) as a gummy solid (21.5 mg, 0.0460 mmol, 23% yield) and 2,2,6,6-Tetramethylpiperidin-1-yl 2-(trifluoromethyl)benzoate (**11**) as white solid (38.2 mg, 0.116 mmol, 58% yield). $\mathbf{R_f}$ (**11**) = 0.58 Hexane:EtOAc [9:1 (v/v)]. **^{1}H NMR** (500 MHz, $CDCl_3$, 25 ºC, δ): 7.82-7.77 (m, 2H), 7.63-7.61 (m, 2H), 1.80-1.66 (m, 3H), 1.58 (d, J = 12.8 Hz, 2H), 1.44 (d, J = 13.0 Hz, 1H), 1.22 (s, 6H), 1.18 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$, 25 ºC, δ): 166.68, 131.88, 131.33, 130.98, 130.30, 129.24 (q, $J^2_{C\text{-}F}$ = 32.2 Hz), 127.14 (q, $J^3_{C\text{-}F}$ = 5.41 Hz), 123.41 (q, $J^1_{C\text{-}F}$ = 272.0 Hz), 60.90, 39.63, 32.01, 20.87, 17.15. **^{19}F NMR** (470 MHz, $CDCl_3$, 25 ºC, δ): –59.61 (s).[19]

Quantum Yield Experiment

Quantum yield experiments suggest that an extended radical chain propagation is unlikely under our reaction conditions. The following quantum yield measurements are adapted from the procedure developed by Yoon et al.[20]

Determination of Fraction of Light Absorbed at 450 nm:

The fraction of light absorbed (*f*) by ferrioxalate solution was calculated as shown below, where the absorbance of this solution at 450 nm was measured to be 1.75006, indicating $f = 0.98226$.

1 Fraction of light absorbed at 450 nm

$f = 1\text{-}10^{(-A)}$ A= absorbance at 450 nm

$f = 1\text{-}10^{(-1.75006)}$ A= 1.75006 (*Measure absorbance of ferrioxalate solution at 450 nm*)

$= 0.98226$

Determination of the Light Intensity at 450 nm:

The photon flux of the 100 W Blue LEDs (λ_{max} = 450 nm) was determined by standard ferrioxalate actinometry.[21] A 0.150 M solution of ferrioxalate was prepared by dissolving 2.21 g of potassium ferrioxalate hydrate ($K_3[Fe(C_2O_4)_3] \cdot 3\ H_2O$) in 30.0 mL of 0.05 M H_2SO_4 (aq). Next, a buffered solution of phenanthroline was prepared by dissolving 50.0 mg of phenanthroline and 11.25 g of sodium acetate in 50.0 mL of 0.500 M H_2SO_4. Both solutions were stored in an amber vial in the dark. To determine the photon flux of the 100 W Blue LEDs, 0.500 mL of the ferrioxalate solution was placed in a cuvette and irradiated for 5.00 seconds at $\lambda = 450$ nm. After irradiation, 1.000 mL of the phenanthroline solution was added to the cuvette. The solution was then rested for 1 h in the dark to allow the ferrous ions to completely coordinate to the phenanthroline. A non-irradiated sample was also prepared and developed in the dark as well *(note: after developing the non/irradiated samples they were diluted with a dilution factor of 10 to prevent deviation from the Beer-Lambert law at high concentrations A = >2. Thus, to obtain the actual mol of Fe^{2+} they were multiplied by ten. The values of the optical difference are the average of two trials*).

1 **Ferrioxalate Actinometry**

$$\text{mol of } Fe^{2+} = 10 \times \left[\frac{V \times \Delta A_{510}}{l \times \varepsilon_{510}}\right]$$

$$\text{mol of } Fe^{2+} = 10 \times \left[\frac{0.00150 \times 1.34859}{1 \times 11{,}100}\right] \text{ mol}$$

$= 1.8224 \times 10^{-6}$ mol

V= 0.00150L *(total volume)*
$\Delta A_{510} = 1.34859$ *(difference in absorption at 510 nm)*
l = 1.00 cm *(path length)*
$\varepsilon_{510} = 11{,}100$ L $mol^{-1}cm^{-1}$ *(molar absorptivity at 510 nm)*

2 **Determination of photon flux of 100W Blue Led**

$$\text{photon flux} = \left[\frac{\text{mol of } Fe^{2+}}{\phi \times t \times f}\right]$$

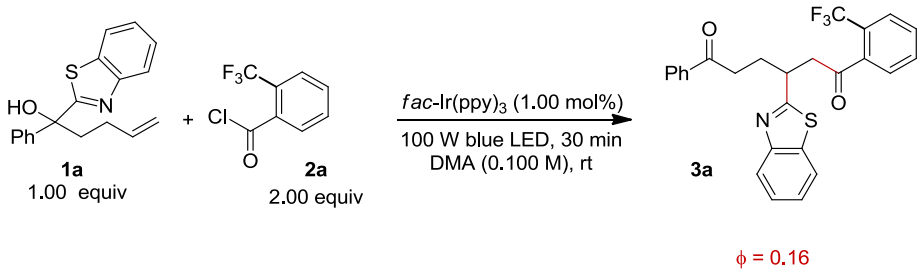
$$\text{photon flux} = \left[\frac{1.8224 \times 10^{-6}}{1.01 \times 5.00 \times 0.98226}\right] \text{einstein } s^{-1}$$

$= 3.674 \times 10^{-7}$ einstein s^{-1}

$\phi = 1.01$ *(quantum yield of ferrioxalate actiometer)*
t = 5.00s *(time)*
f = 0.98226 *(Fraction of light absorbed)*

Afterward, the absorbance of both solutions was measured at 510 nm and with mol of Fe^{2+} known, next, the photon flux determined to be 3.674×10^{-7} einstein s^{-1}. We can obtain the quantum yield of our reaction provided if it is irradiated using the same geometry (*note: although $\Phi = 1.01$ at 436 nm was used for the calculation of the photon flux it known that the ferrioxalate system varied little with the wavelength as the Φ remained between 0.9 and 1.1 at wavelength between 400–480 nm*).

Determination of Quantum Yield:



To determine the photon flux, in a glovebox, the same cuvette used flux was charged with 1-(benzo[*d*]thiazol-2-yl)-1-phenylpent-4-en-1-ol (**1a**) (0.300 mmol, 1.00 equiv), and DMA (0.100 M, with respect to substrate **1a**). To this suspension was added aroyl chloride (0.600 mmol, 2.00 equiv), *fac*-$Ir(ppy)_3$, (1.00 mol%). Afterward the cuvette was capped with a PTFE stopper and taken out of the glovebox. The reaction mixture was irradiated (λ_{max} = 450 nm) for 1800 s (30 min) with the same 100 W Blue LEDs. To determine the yield of the product, an internal standard, trifluorotoluene ($PhCF_3$) (43.8 mg, 0.300 mmol,) was added to the cuvette. Then, a 200 μL of the reaction mixture was taken and then diluted with 500 μL $CDCl_3$ followed by 19F NMR. The quantum yield was determined using the equation shown below. (Here, $f = 1 - 10^{-A} = 1 - 10^{-2.943} = 0.998$, meaning $Ir(ppy)_3$ absorbs 99.8% of incident light.)

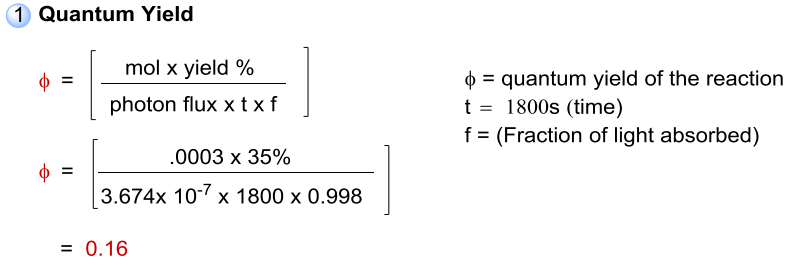


Figure S3. *Quantum yield determination.*

Stern–Volmer Luminescence Quenching Experiments

Emission intensities were recorded using a Perkin Elmer LS50B Luminescence spectrometer. All quenching data was recorded in the dark using a 1.00 cm screw-top quartz cuvette at 23 °C in the presence of $Ir(ppy)_3$ (3.00 μM) and varying concentration of quencher in degassed DMA. Excitation of the sample was performed at 420 nm with a slit width of 10.0 nm, and emission was detected at 510 nm. After the acquisition, the data were plotted according to the Stern-Volmer equation shown below.

$$\mathbf{I_o/I = 1+K_{SV}[Q]}$$

$$\boldsymbol{K_{SV} = k_q\tau_o}$$

Where I_o is the luminescence intensity in the absence of the quencher, I is the intensity in the presence of the quencher, K_{SV} is the Stern−Volmer constant, k_q is the quenching rate, τ_o is the life-time of the photoredox catalyst ($\tau_o = 1.90 \times 10^{-6}$ s for $Ir(ppy)_3$),[22] and [Q] is the concentration of the quencher.

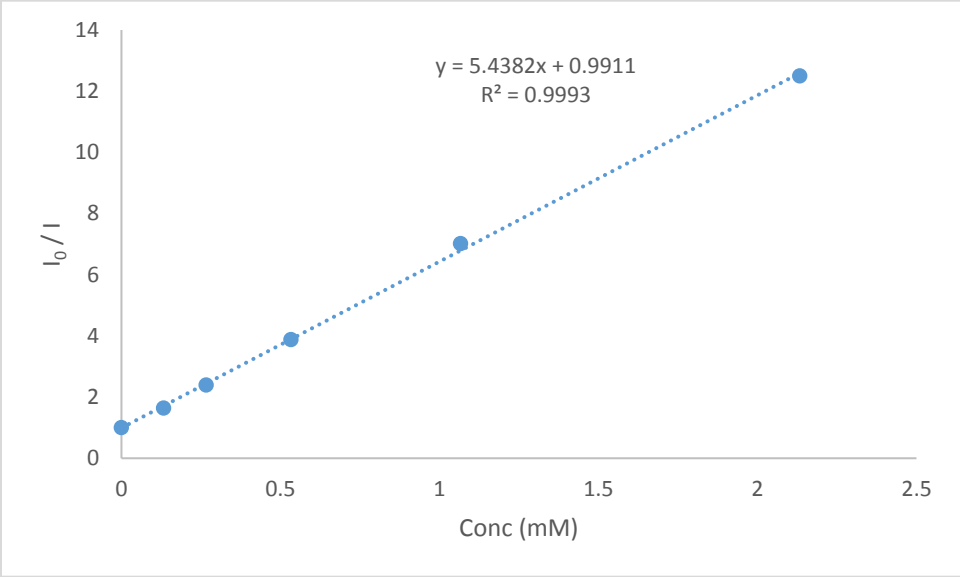
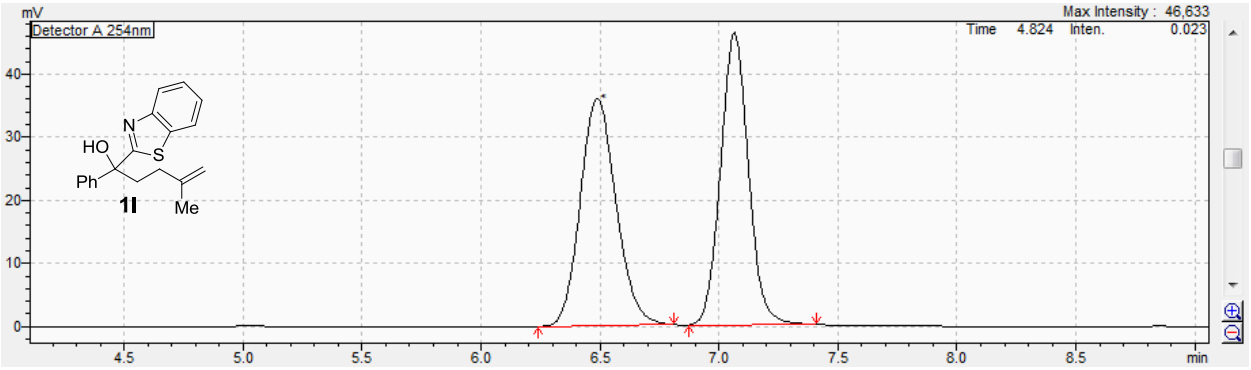


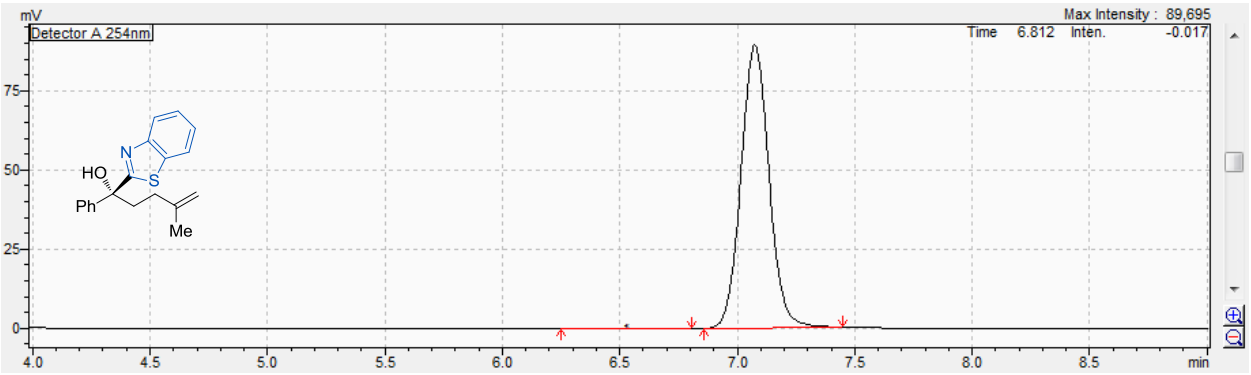
Figure S4: Quenching of excited *fac* $Ir(ppy)_3$ by 2-CF_3-benzoyl chloride at 420 nm

Chirality Transfer Experiments

The ee of **1l** was determined by HPLC analysis: Lux® 3µm Cellulose-4 (4.6 mm i.d. x 250 mm); hexane/2-propanol = 90/10; flow rate 1.0 mL/min; 25 °C; 254 nm; retention time: 6.5 min (minor) and 7.1 min (major).

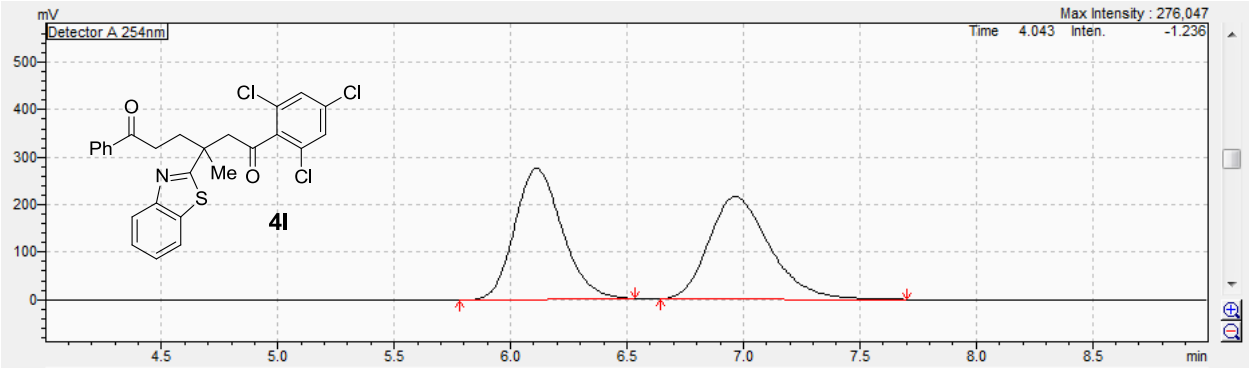


Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	6.488	376162	50.013	35947	0.349
2	7.065	375969	49.987	46355	0.274

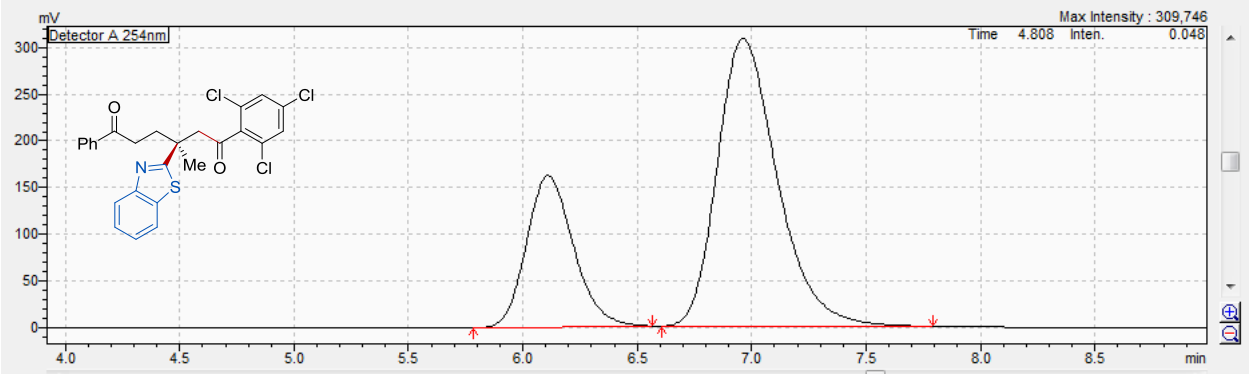


Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	6.506	484	0.065	56	0.286
2	7.075	742324	99.935	89543	0.278

The ee of **4l** was determined by HPLC analysis: Lux® 3µm Cellulose-4 (4.6 mm i.d. x 250 mm); hexane/2-propanol = 95/5; flow rate 0.5 mL/min; 25 °C; 254 nm; retention time: 6.1 min (minor) and 6.9 min (major).

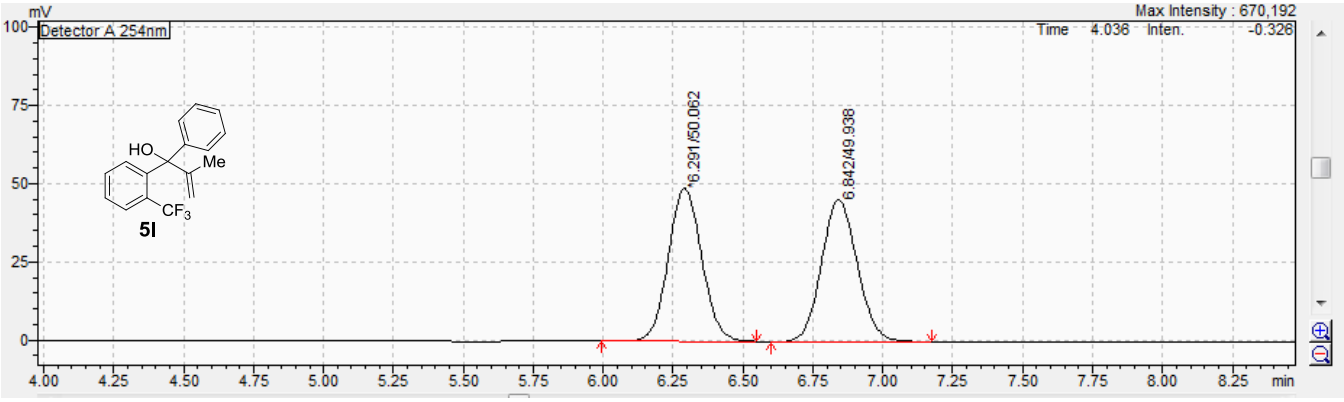


Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	6.111	3919356	50.051	275774	0.479
2	6.966	3911373	49.949	215990	0.624

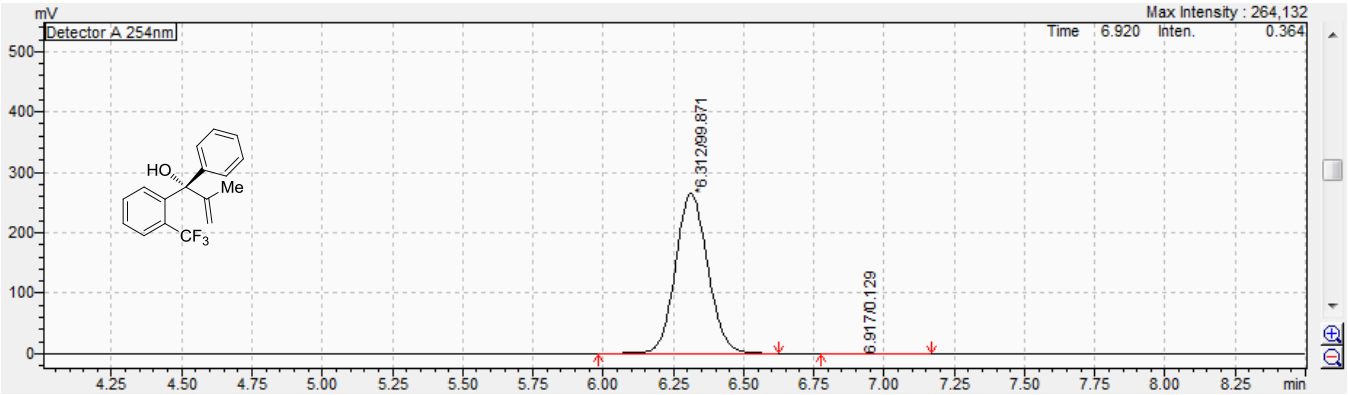


Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	6.110	2318527	29.168	162155	0.483
2	6.963	5630252	70.832	308075	0.632

The ee of **5l** was determined by HPLC analysis: Lux® 3µm Cellulose-1 (4.6 mm i.d. x 250 mm); hexane/2-propanol = 100/2; flow rate 1.0 mL/min; 25 °C; 254 nm; retention time: 6.31 min (minor) and 6.91 min (major)

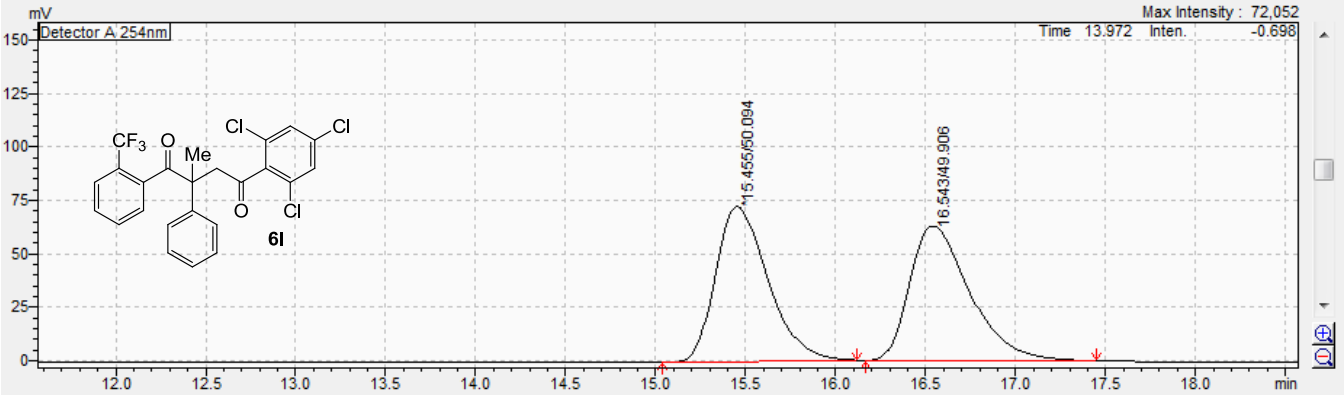


Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	6.291	405365	50.062	48886	0.276
2	6.842	404367	49.938	45532	0.293
Total		809732	100.000	94418	

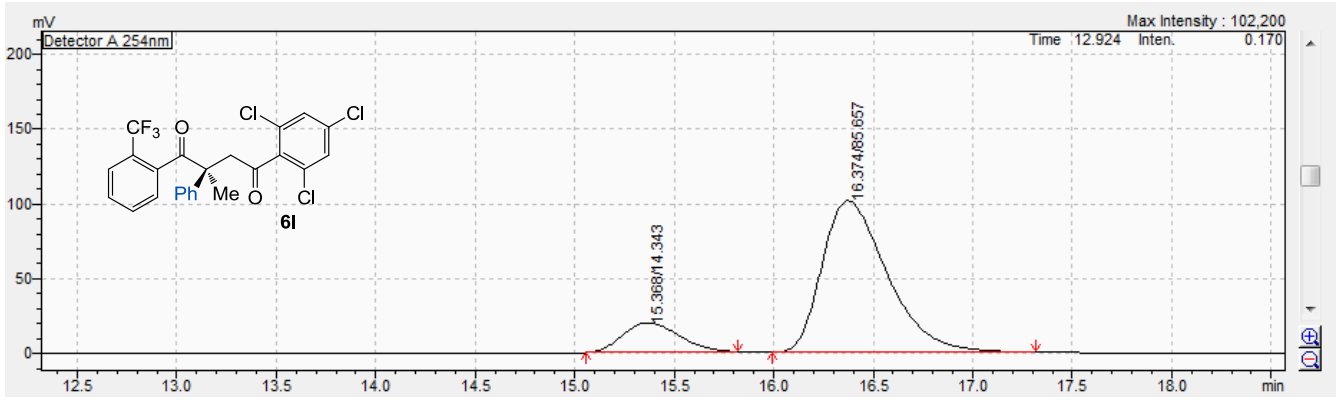


Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	6.312	2114178	99.871	263856	0.266
2	6.917	2732	0.129	367	0.240
Total		2116910	100.000	264222	

The ee of **6l** was determined by HPLC analysis: Lux® 3µm i-Cellulose-5 (4.6 mm i.d. x 250 mm); hexane/2-propanol = 100/2; flow rate 0.5 mL/min; 25 °C; 254 nm; retention time: 15.36 min (minor) and 16.37 min (major)



Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	15.455	1464525	50.094	72417	0.684
2	16.543	1459025	49.906	62767	0.803
Total		2923550	100.000	135184	



Peak#	Ret. Time	Area	Area%	Height	Width(5%)
1	15.368	387617	14.343	19691	0.630
2	16.374	2314945	85.657	101519	0.776
Total		2702562	100.000	121210	

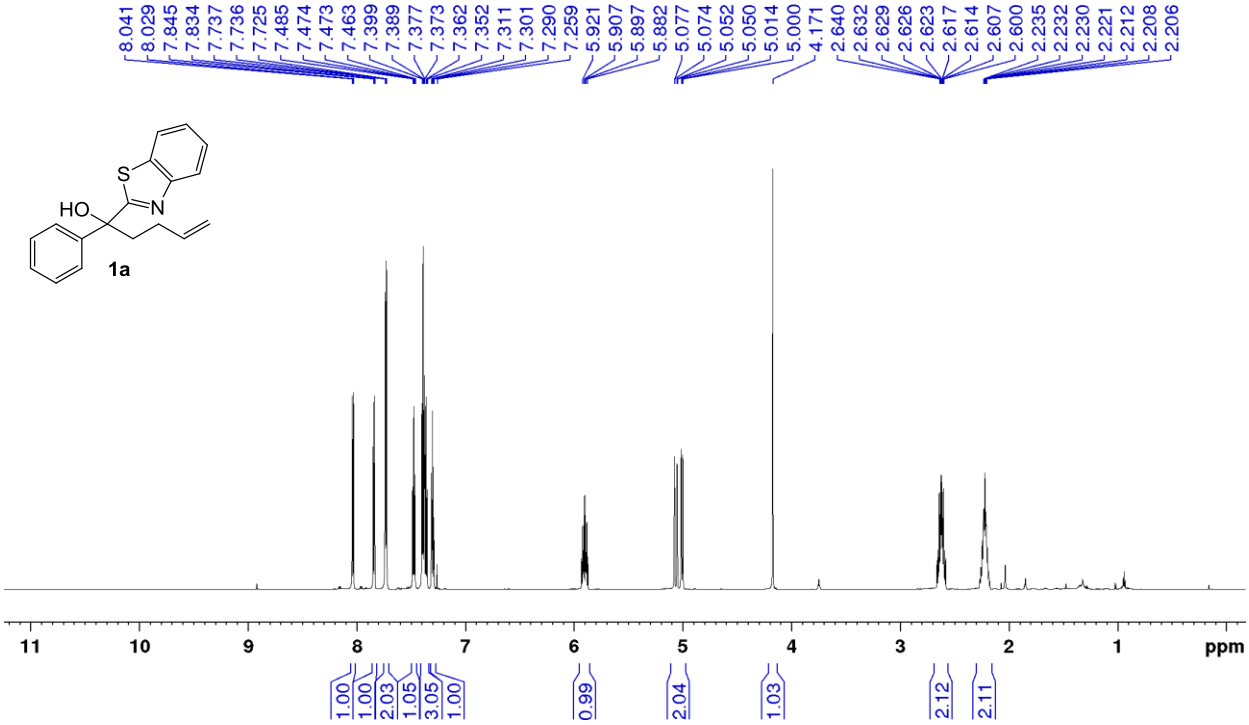
Reference

1. Still, W. C.; Kahn, M.; Mitra, A., Rapid Chromatographic Technique for Preparative Separations with Moderate Resolution. *J. Org. Chem.* **1978,** *43*, 2923-2925.
2. Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I., NMR Chemical Shifts of Trace Impurities: Common Laboratory Solvents, Organics, and Gases in Deuterated Solvents Relevant to the Organometallic Chemist. *Organometallics* **2010,** *29*, 2176-2179.
3. Wang, X.; Xu, Y.; Mo, F.; Ji, G.; Qiu, D.; Feng, J.; Ye, Y.; Zhang, S.; Zhang, Y.; Wang, J., Silver-Mediated Trifluoromethylation of Aryldiazonium Salts: Conversion of Amino Group into Trifluoromethyl Group. *J. Am. Chem. Soc.* **2013,** *135*, 10330-10333.
4. Fujimoto, T.; Ritter, T., PhenoFluorMix: Practical Chemoselective Deoxyfluorination of Phenols. *Org. Lett.* **2015,** *17*, 544-547.
5. Wu, Z.; Wang, D.; Liu, Y.; Huan, L.; Zhu, C., Chemo- and Regioselective Distal Heteroaryl ipso-Migration: A General Protocol for Heteroarylation of Unactivated Alkenes. *J. Am. Chem. Soc.* **2017,** *139*, 1388-1391.
6. Keenan, M.; Abbott, M. J.; Alexander, P. W.; Armstrong, T.; Best, W. M.; Berven, B.; Botero, A.; Chaplin, J. H.; Charman, S. A.; Chatelain, E.; von Geldern, T. W.; Kerfoot, M.; Khong, A.; Nguyen, T.; McManus, J. D.; Morizzi, J.; Ryan, E.; Scandale, I.; Thompson, R. A.; Wang, S. Z.; White, K. L., Analogues of Fenarimol Are Potent Inhibitors of Trypanosoma Cruzi and Are Efficacious in a Murine Model of Chagas Disease. *J. Med. Chem.* **2012,** *55*, 4189-4204.
7. Wang, N.; Wang, J.; Guo, Y.-L.; Li, L.; Sun, Y.; Li, Z.; Zhang, H.-X.; Guo, Z.; Li, Z.-L.; Liu, X.-Y., Oximinotrifluoromethylation of Unactivated Alkenes Under Ambient Conditions. *Chem. Commun. (Cambridge, U. K.)* **2018,** *54*, 8885-8888.
8. Li, L.; Li, Z.-L.; Gu, Q.-S.; Wang, N.; Liu, X.-Y., A Remote C-C Bond Cleavage-Enabled Skeletal Reorganization: Access to Medium-/Large-Sized Cyclic Alkenes. *Sci. Adv.* **2017,** *3*, e1701487/1-e1701487/8.
9. Liu, X.; Xiong, F.; Huang, X.; Xu, L.; Li, P.; Wu, X., Copper-Catalyzed Trifluoromethylation-Initiated Radical 1,2-Aryl Migration in α,α-Diaryl Allylic Alcohols. *Angew. Chem. Int. Ed.* **2013,** *52*, 6962-6966.
10. Weng, W. Z.; Sun, J. G.; Li, P.; Zhang, B., α-Quaternary Mannich Bases through Copper-Catalyzed Amination-Induced 1, 2-Rearrangement of Allylic Alcohols. *Chem. - Eur. J.* **2017,** *23*, 9752-9755.
11. Boga, C.; Stengel, R.; Abdayem, R.; Del Vecchio, E.; Forlani, L.; Todesco, P. E., Regioselectivity in the Addition of Vinylmagnesium Bromide to Heteroarylic Ketones: C- versus O-Alkylation. *J. Org. Chem.* **2004,** *69*, 8903-8909.
12. Mortensen, D. S.; Rodriguez, A. L.; Carlson, K. E.; Sun, J.; Katzenellenbogen, B. S.; Katzenellenbogen, J. A., Synthesis and Biological Evaluation of a Novel Series of Furans: Ligands Selective for Estrogen Receptor α. *J. Med. Chem.* **2001,** *44*, 3838-3848.
13. Fuerstner, A.; Hupperts, A.; Ptock, A.; Janssen, E., "Site Selective" Formation of Low-Valent Titanium Reagents: An "Instant" Procedure for the Reductive Coupling of Oxo Amides to Indoles. *J. Org. Chem.* **1994,** *59*, 5215-29.
14. Shi, Y.-C.; Duan, H.-Y., Two Seven-Membered Heterocycles with 1,2-Diaza Ring N Atoms: 3,5,7-Triphenyl-1,2-Diazacyclohepta-1(7),2-Diene And 3,7-Bis(2-Hydroxyphenyl)-5-Phenyl-1,2-Diazacyclohepta-1(7),2-Diene. *Acta Crystallogr., Sect. C: Cryst. Struct. Commun.* **2013,** *69*, 1177-1180.
15. Haoyu, S. Y.; He, X.; Li, S. L.; Truhlar, D. G., MN15: A Kohn–Sham Global-Hybrid Exchange–Correlation Density Functional with Broad Accuracy for Multi-Reference and Single-Reference Systems and Noncovalent Interactions. *Chem. Sci.* **2016,** *7*, 5032-5051.

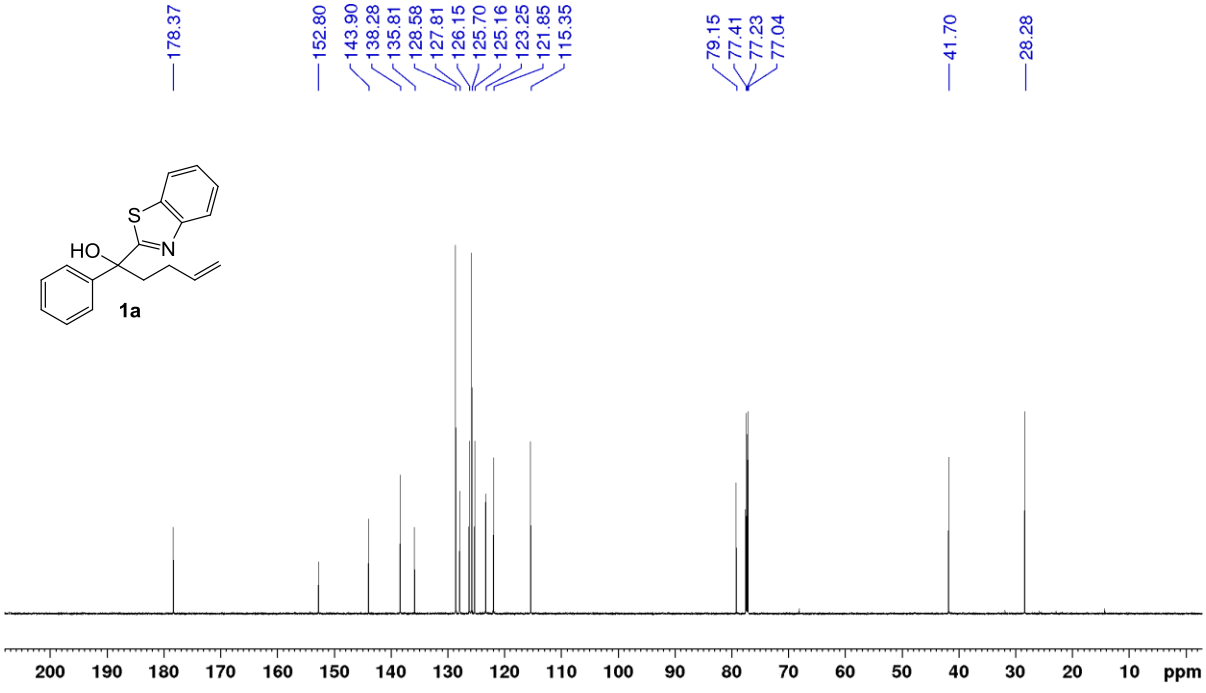
16. Weigend, F.; Ahlrichs, R., Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005,** *7*, 3297-3305.
17. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G., Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009,** *113*, 6378-6396.
18. Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.
19. Guin, J.; De Sarkar, S.; Grimme, S.; Studer, A., Biomimetic carbene-catalyzed oxidations of aldehydes using TEMPO. *Angew. Chem. Int. Ed.* **2008,** *47*, 8727-8730.
20. Cismesia, M. A.; Yoon, T. P., Characterizing Chain Processes in Visible Light Photoredox Catalysis. *Chem. Sci.* **2015,** *6*, 5426-5434.
21. (a) Hatchard, C. G.; Parker, C. A., A New Sensitive Chemical Actinometer. II. Potassium Ferrioxalate As a Standard Chemical Actinometer. *Proc. R. Soc. London, Ser. A* **1956,** *235*, 518-36; (b) Montalti, M.; Credi, A.; Prodi, L.; Gandolfi, M. T.; Editors, *Handbook of Photochemistry - Third Edition*. CRC Press LLC: 2006; p 650 pp.
22. Flamigni, L.; Barbieri, A.; Sabatini, C.; Ventura, B.; Barigelletti, F., Photochemistry and Photophysics of Coordination Compounds: Iridium. *Top. Curr. Chem.* **2007,** *281*, 143-203.

Spectroscopic Data

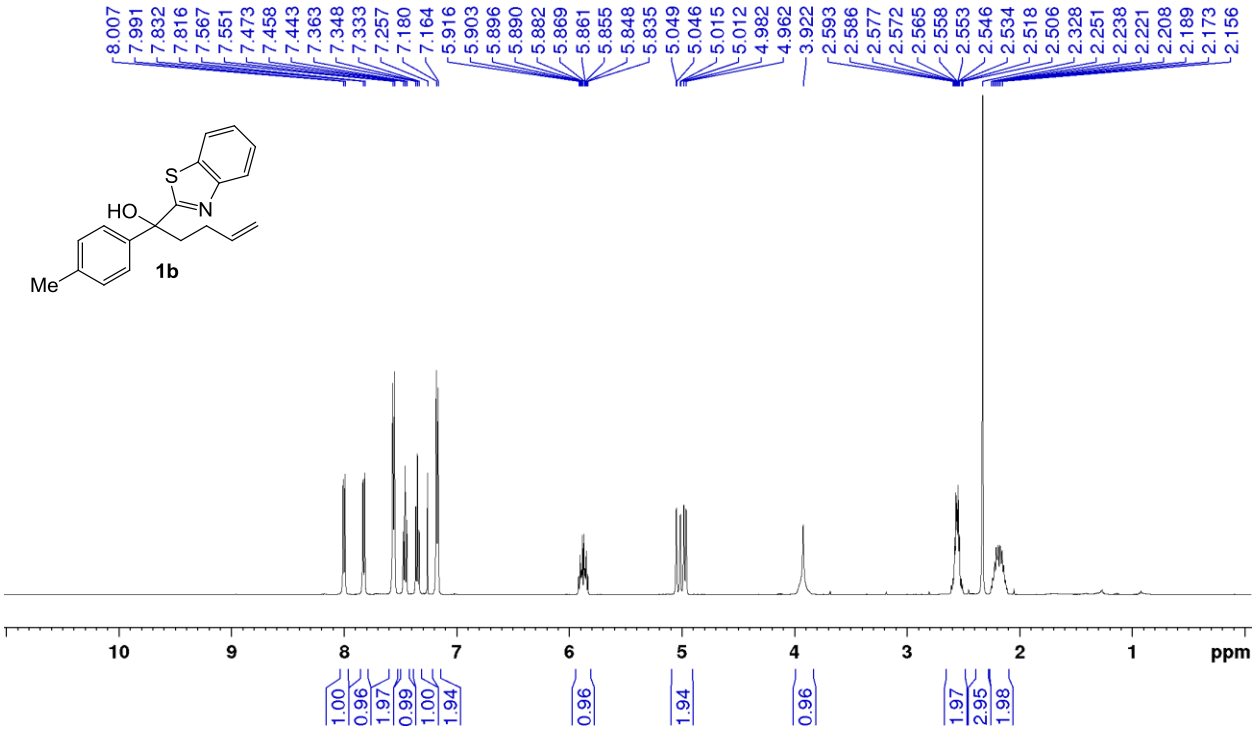
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1a)



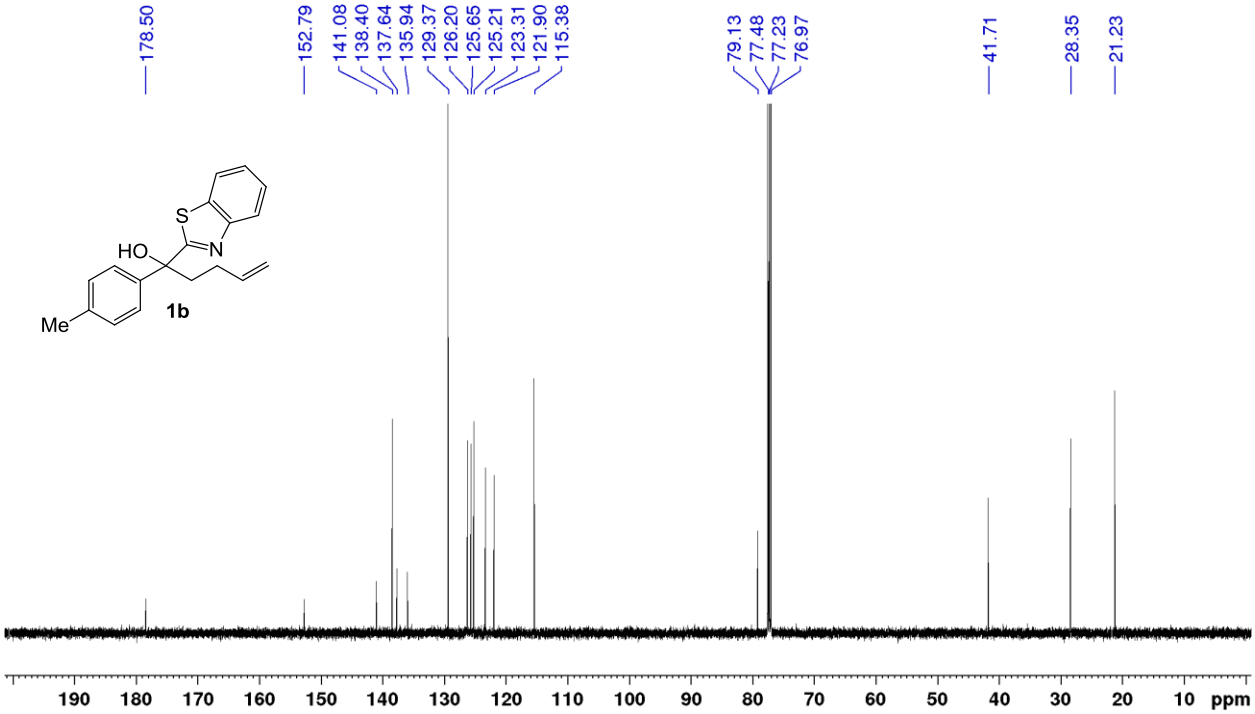
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1a)



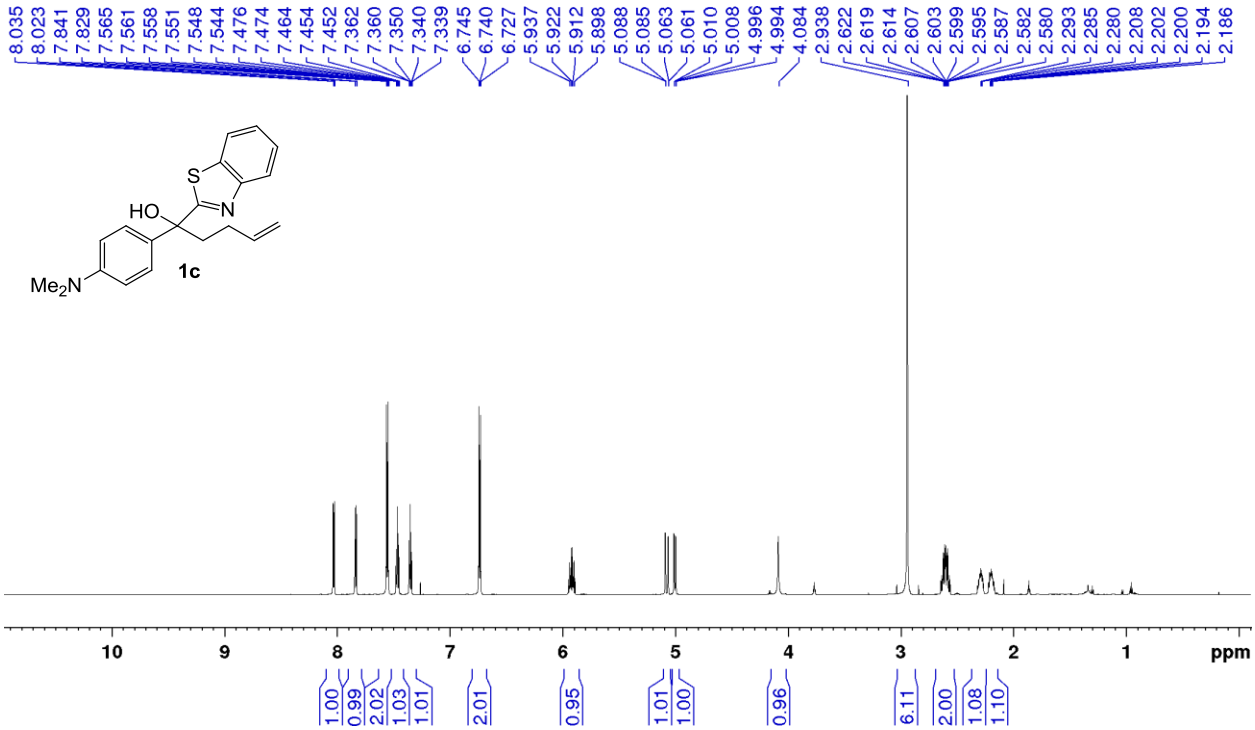
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1b)



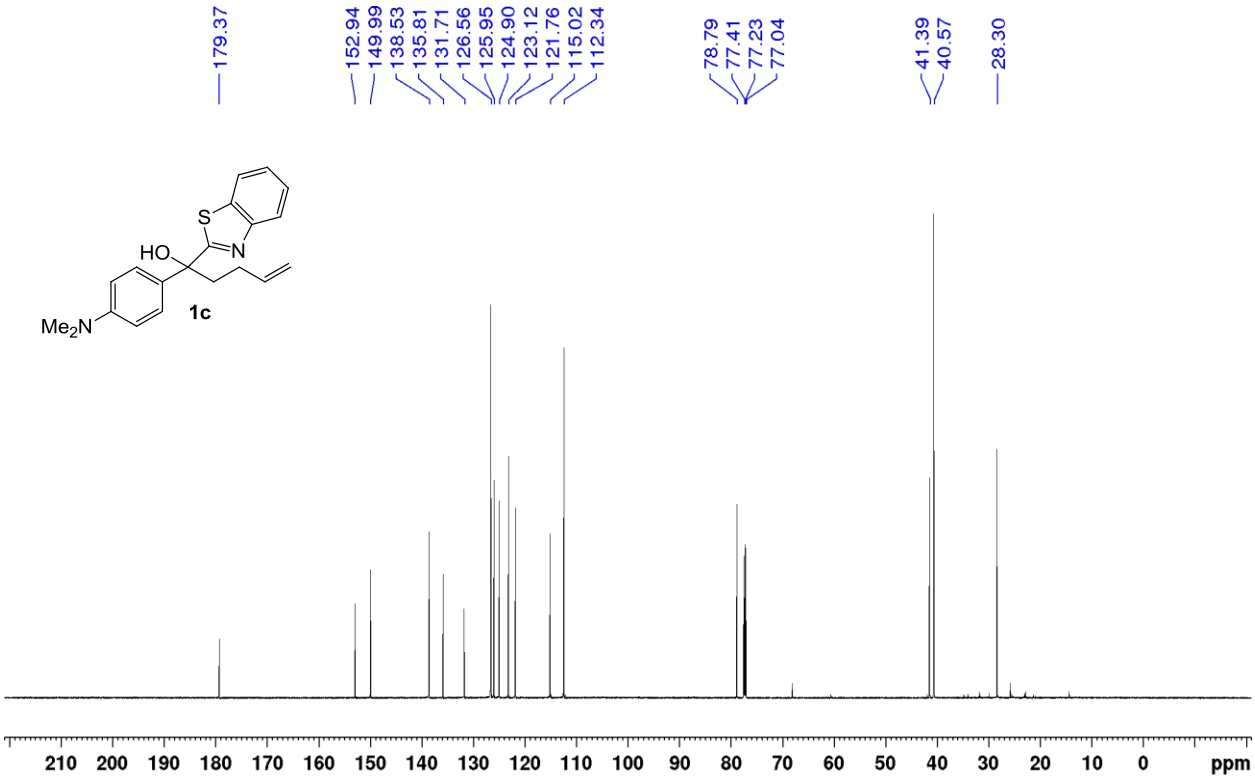
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1b)



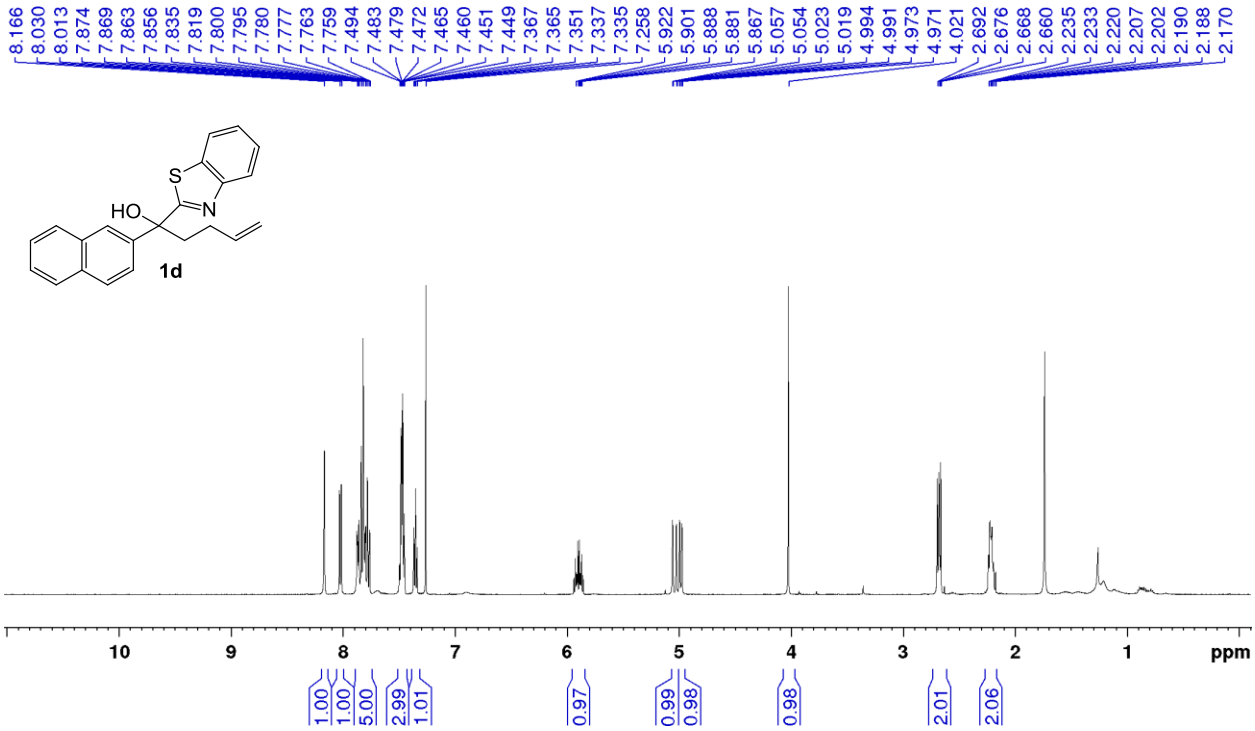
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1c)



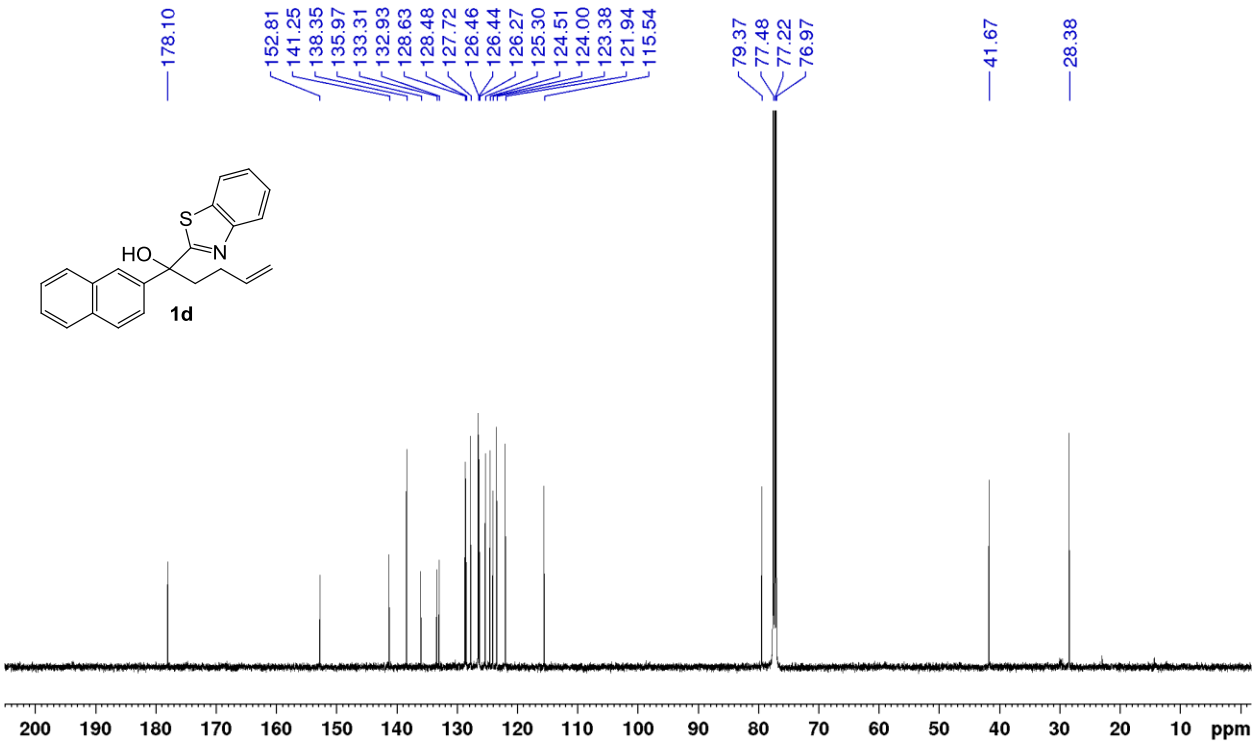
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1c)



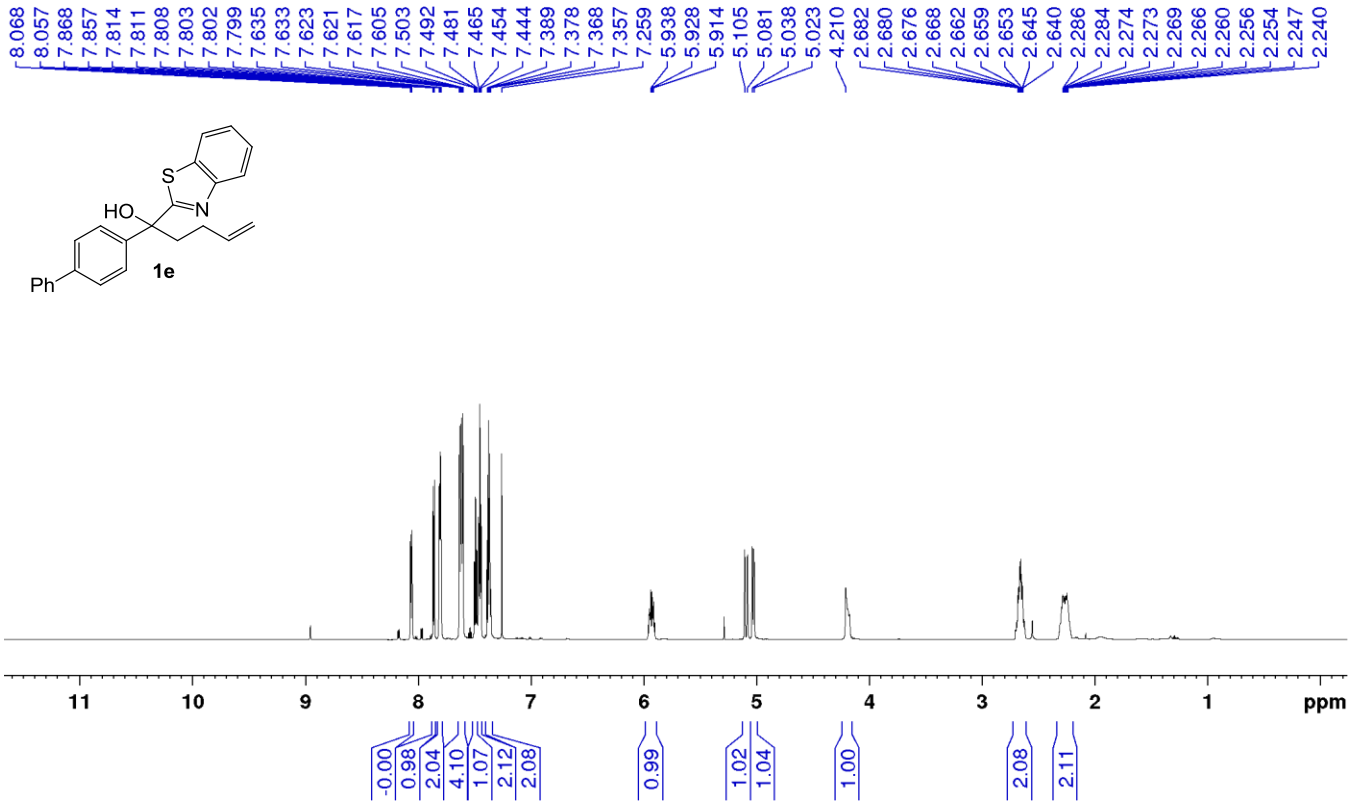
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1d)



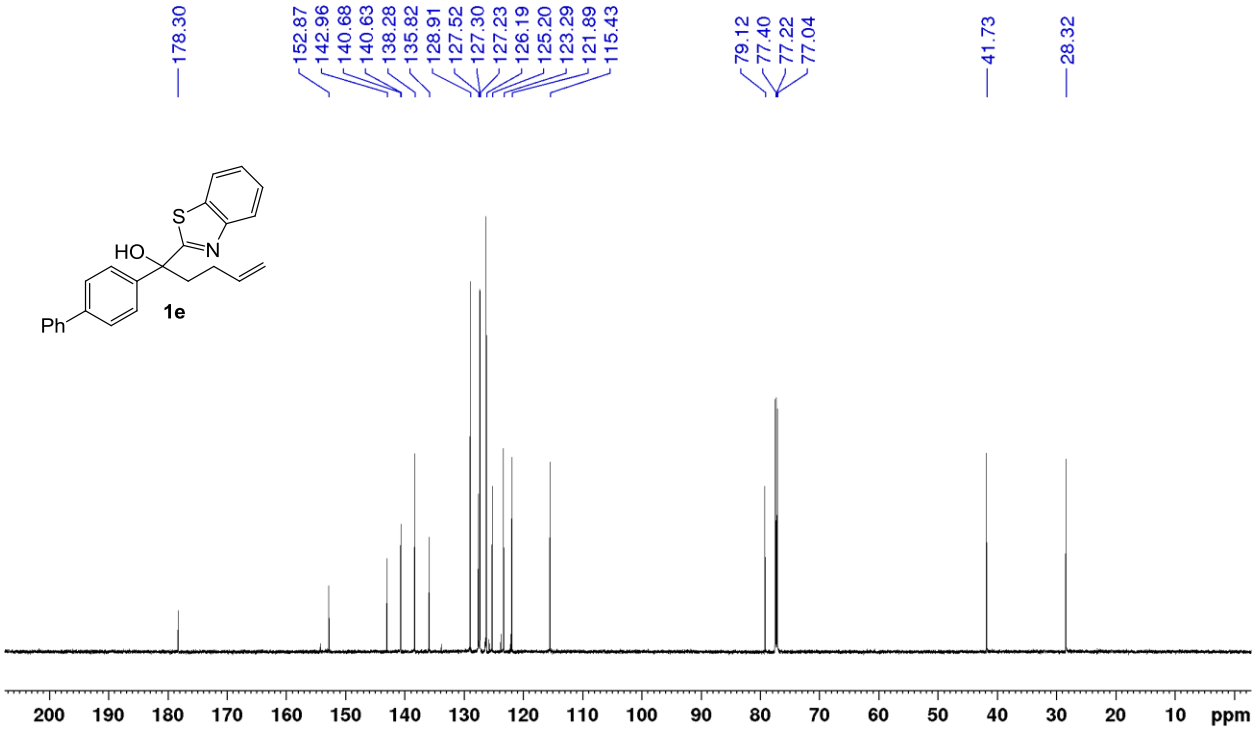
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1d)



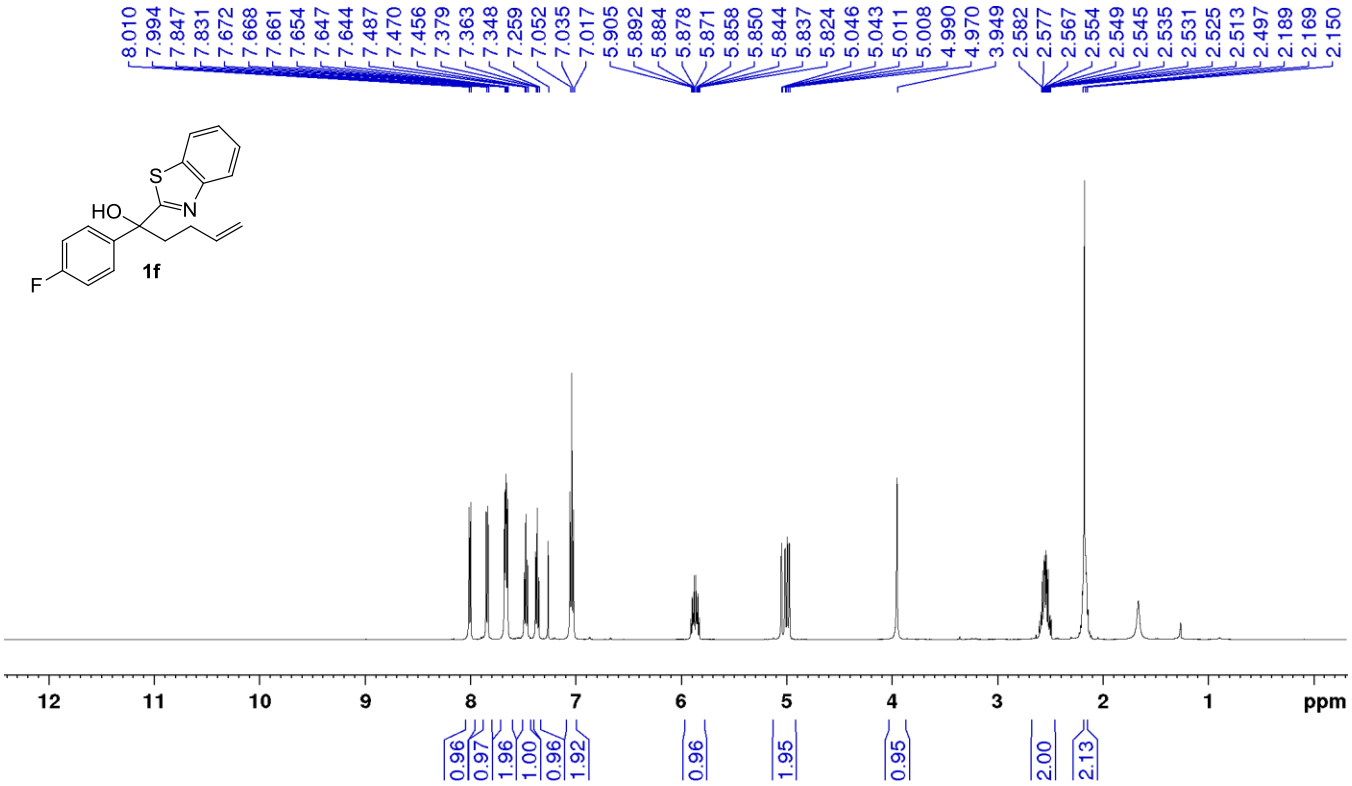
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1e)



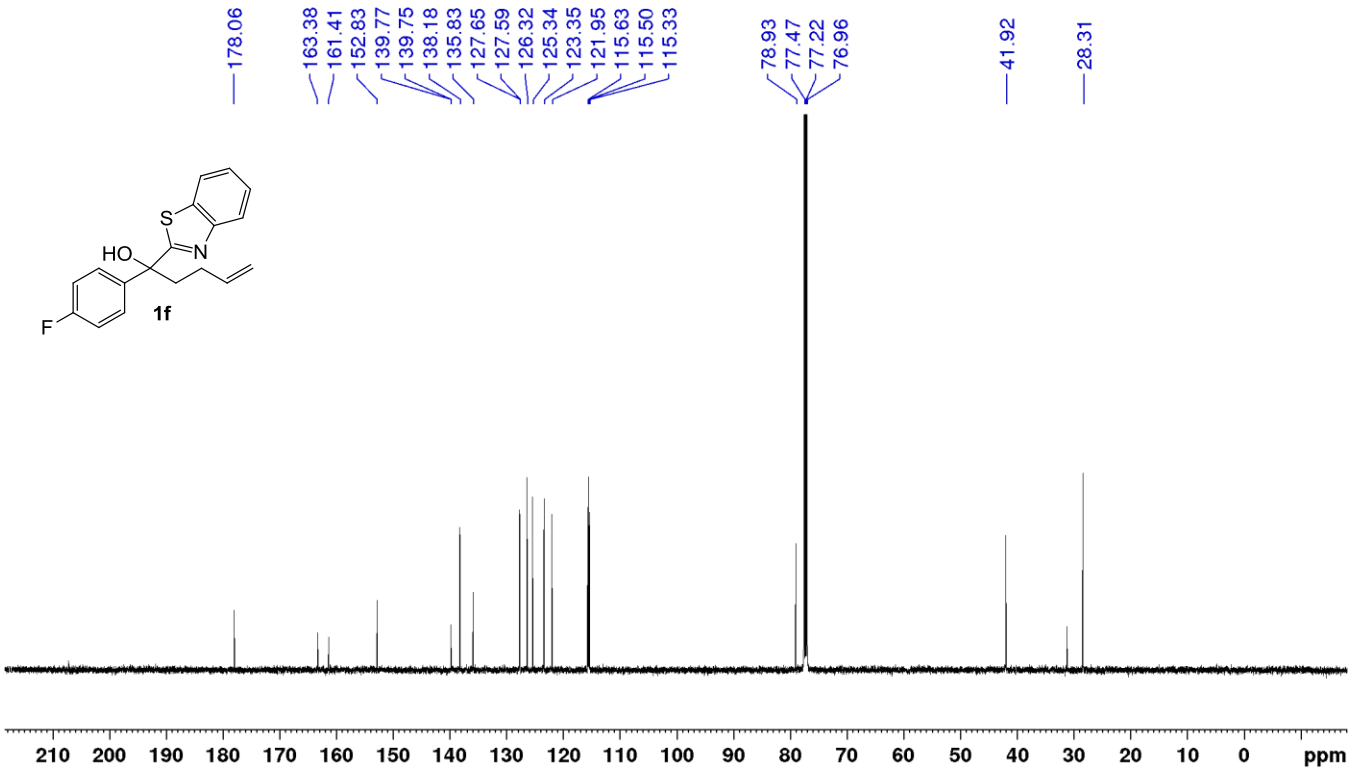
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1e)



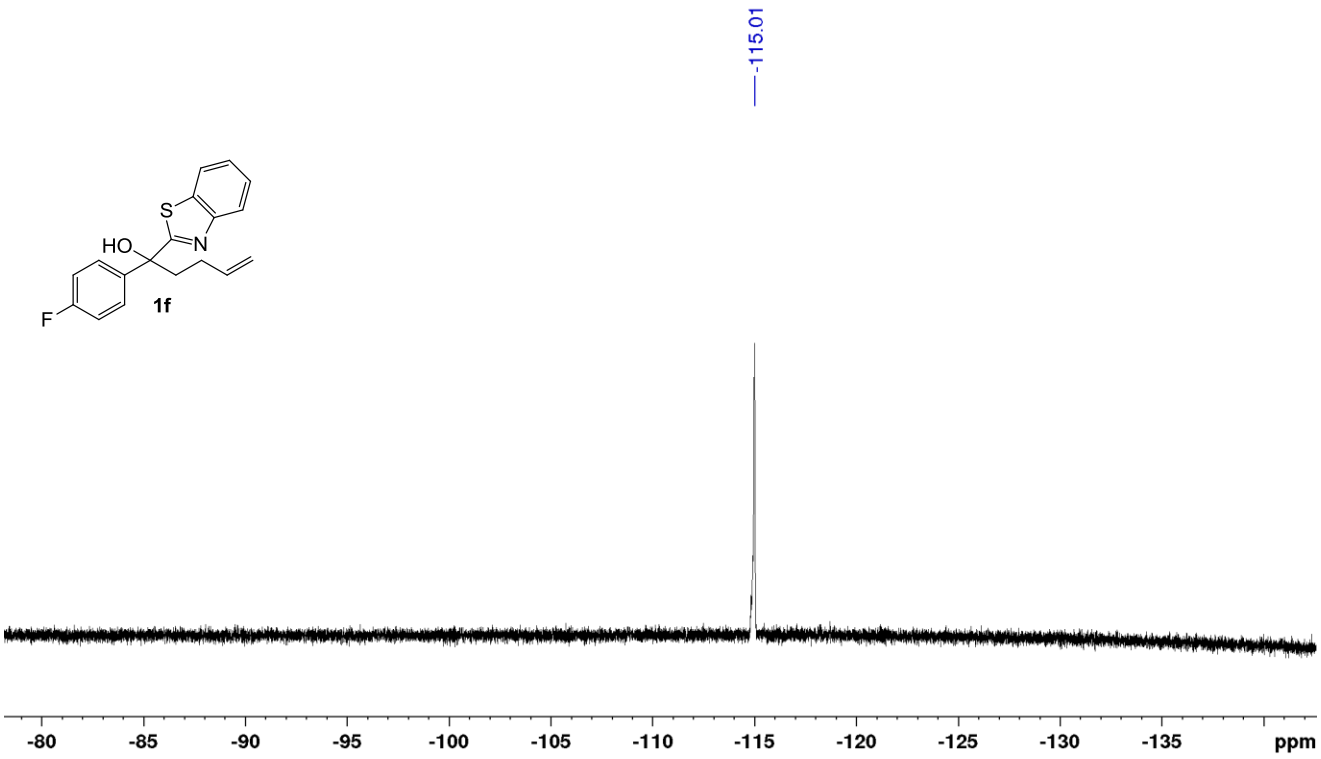
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1f)



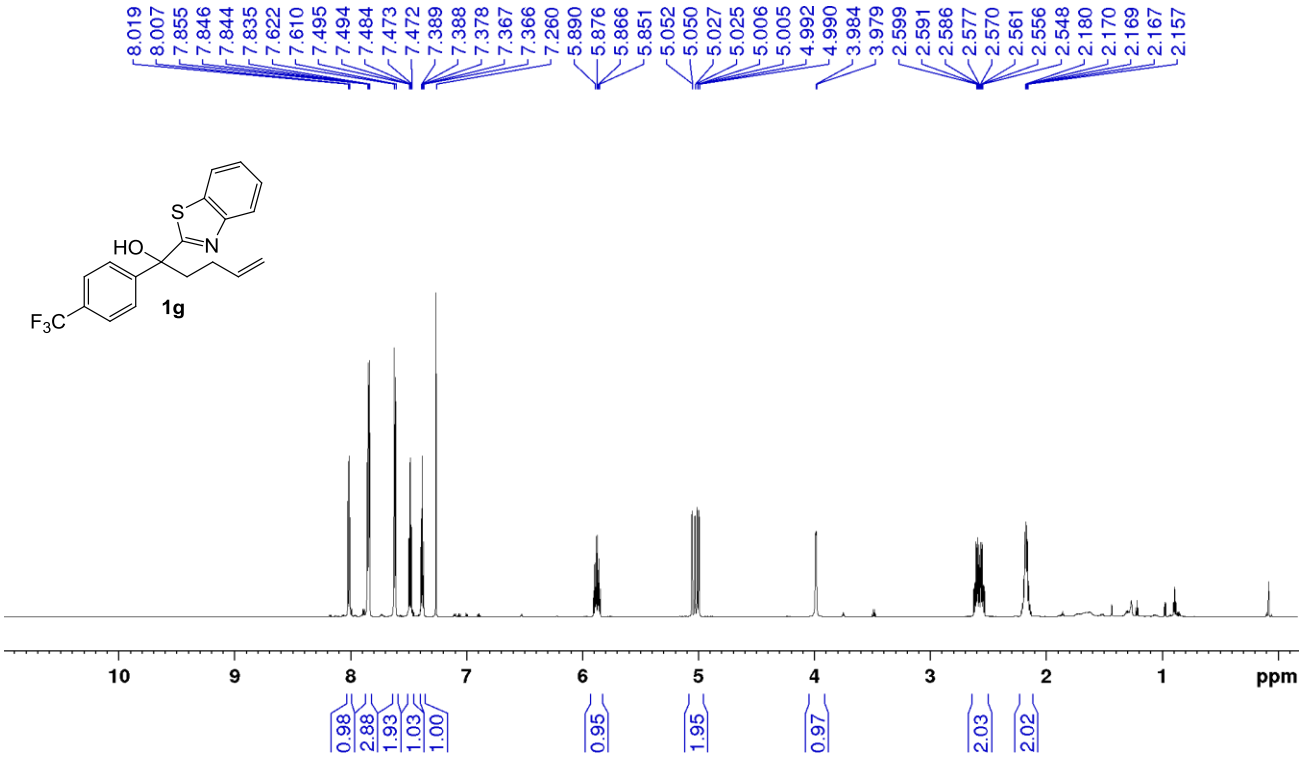
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1f)



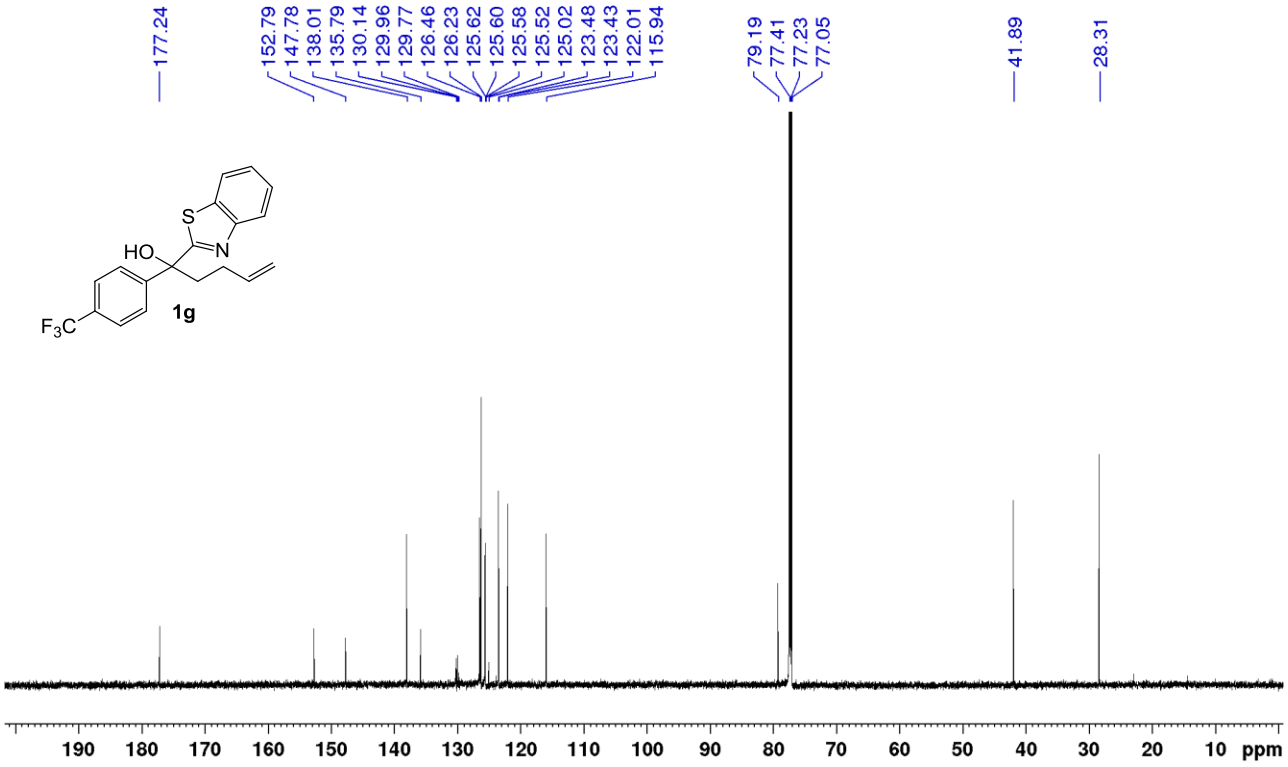
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (1f)



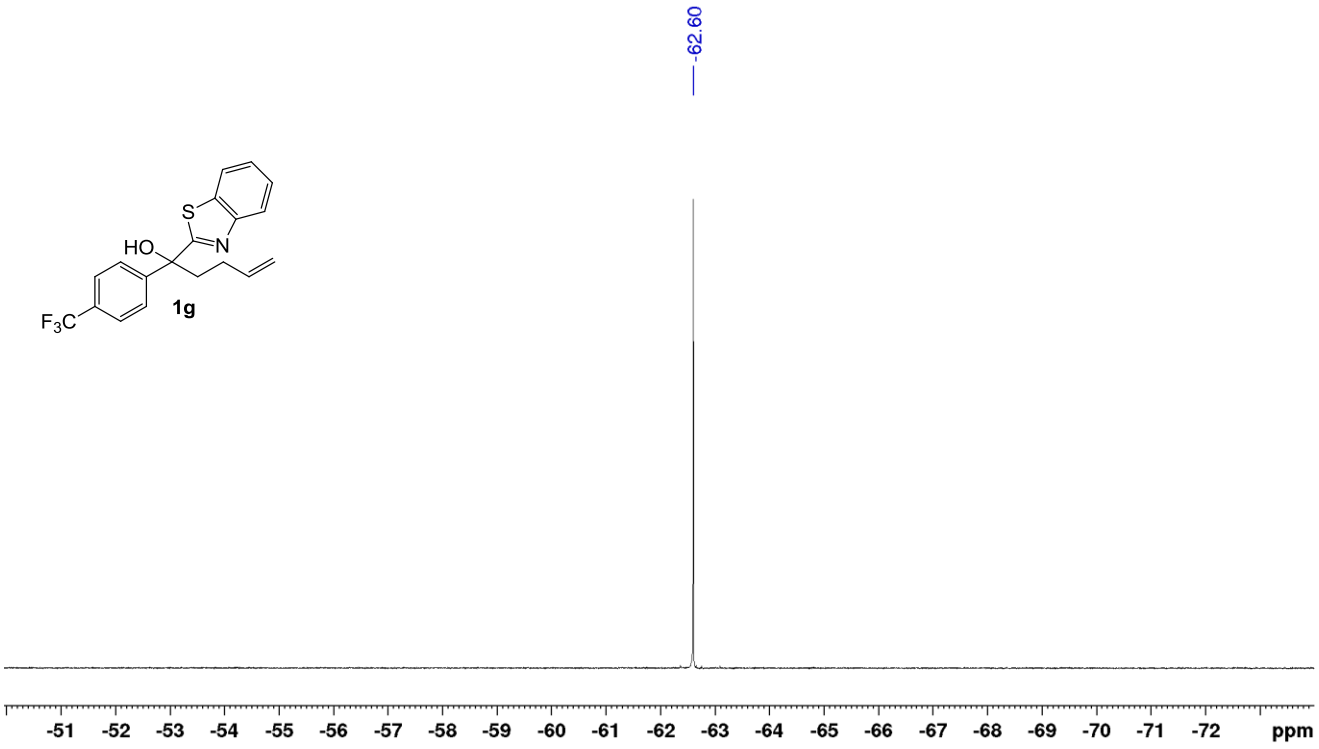
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (1g)



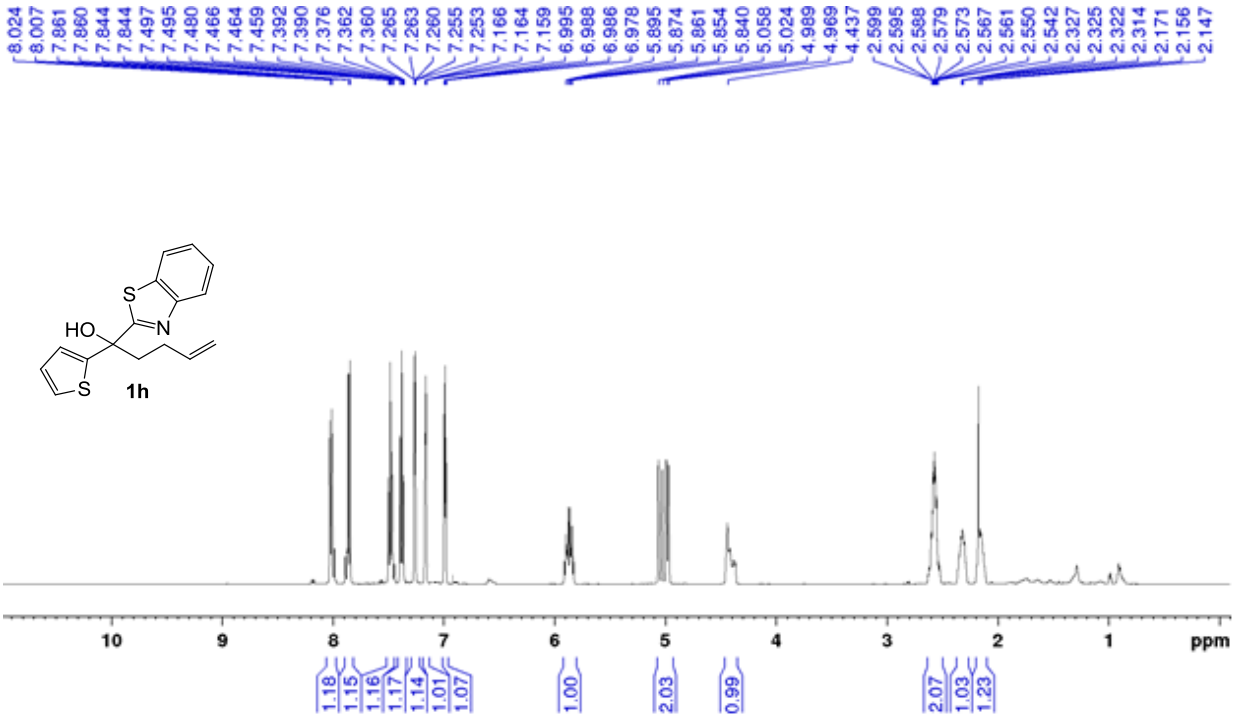
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (1g)



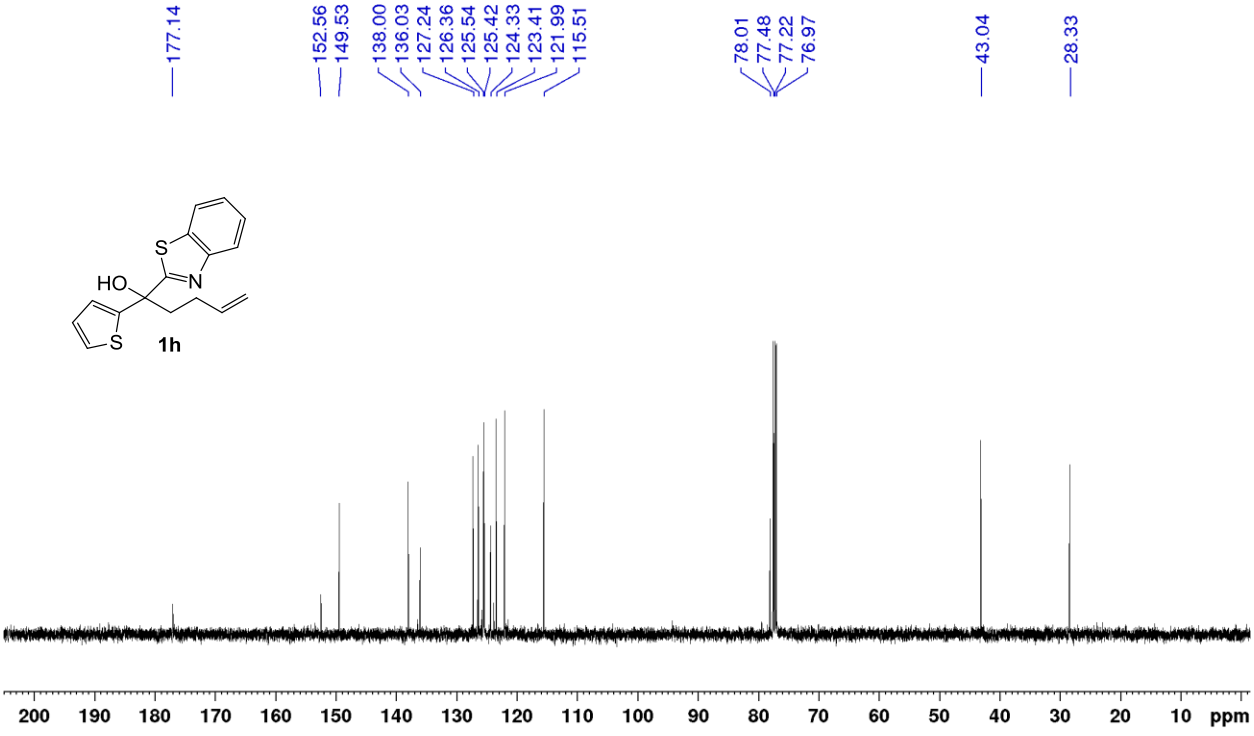
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (1g)



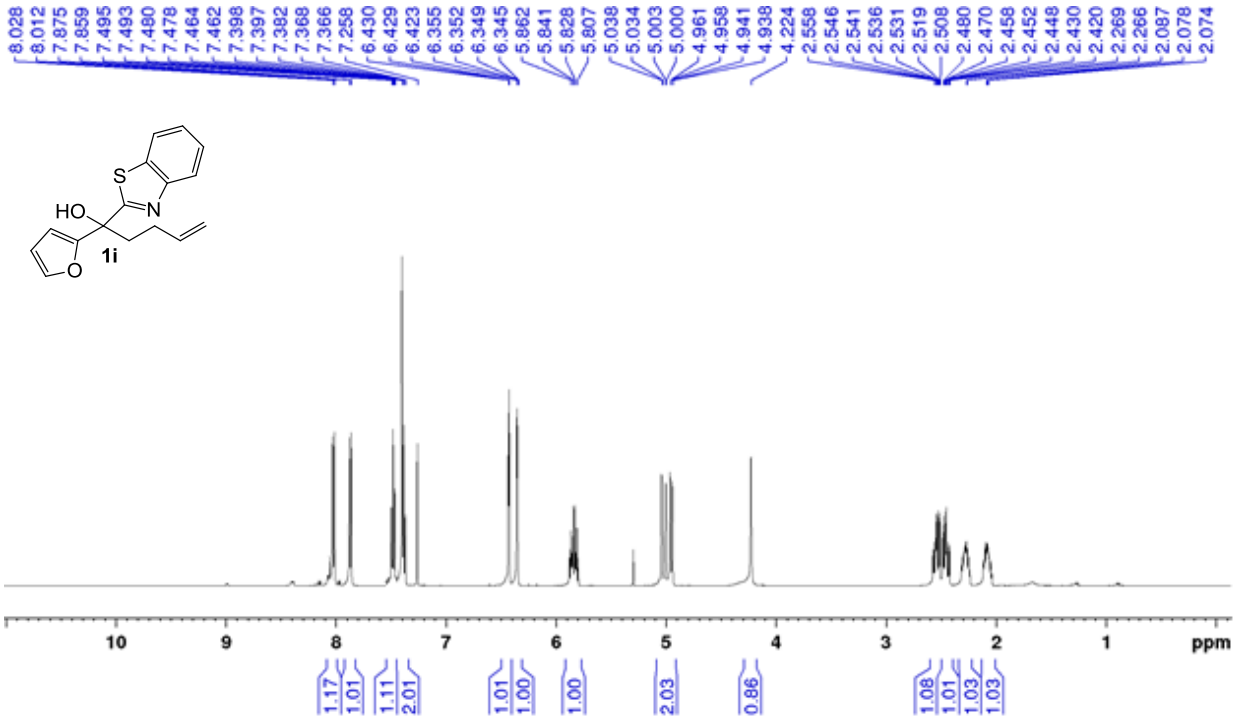
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1h)



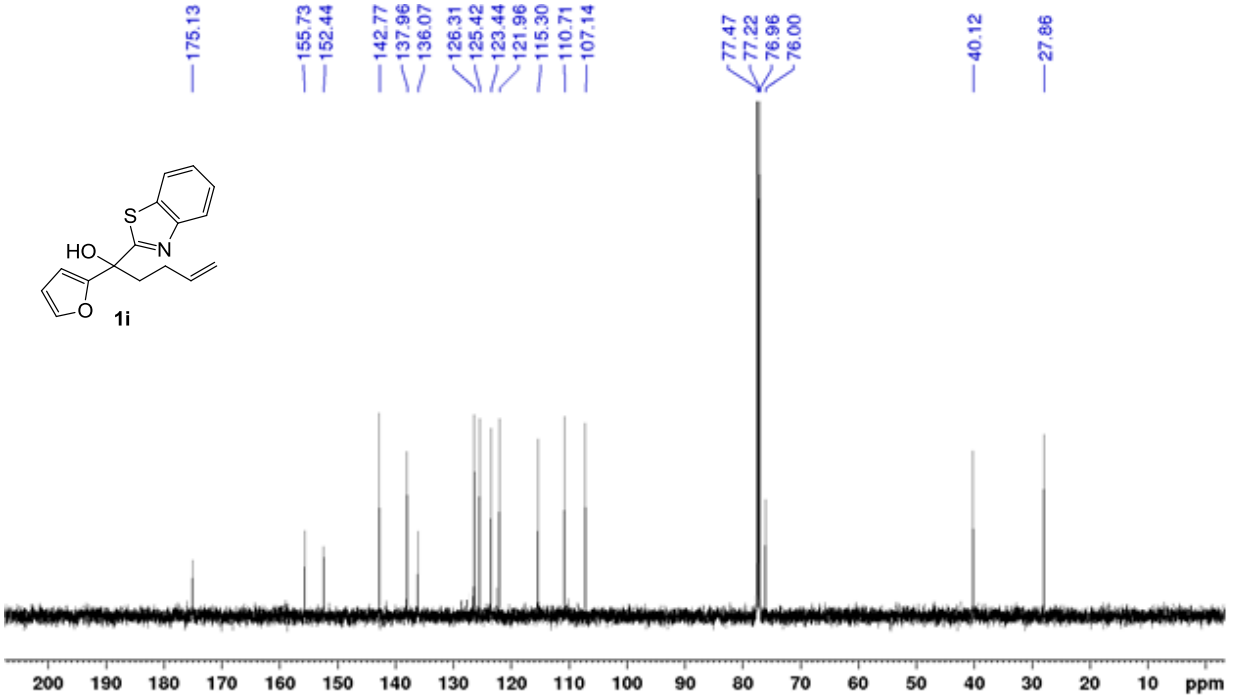
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1h)



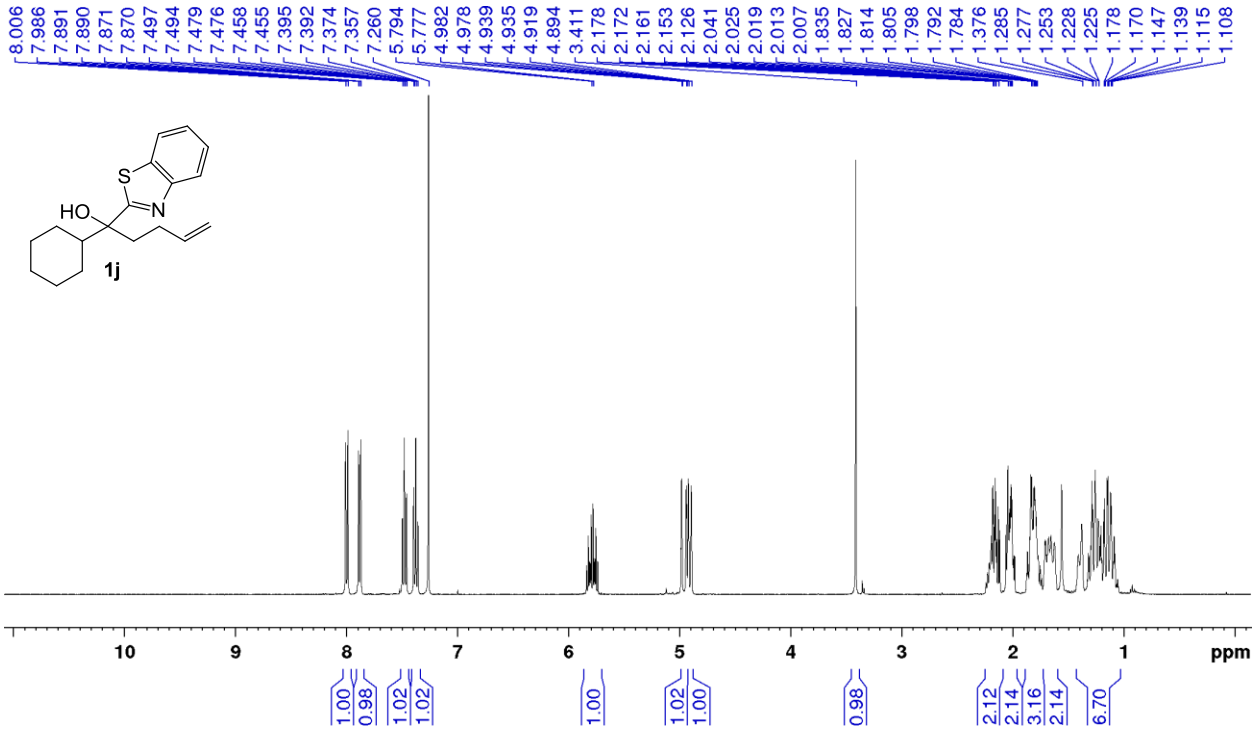
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1i)



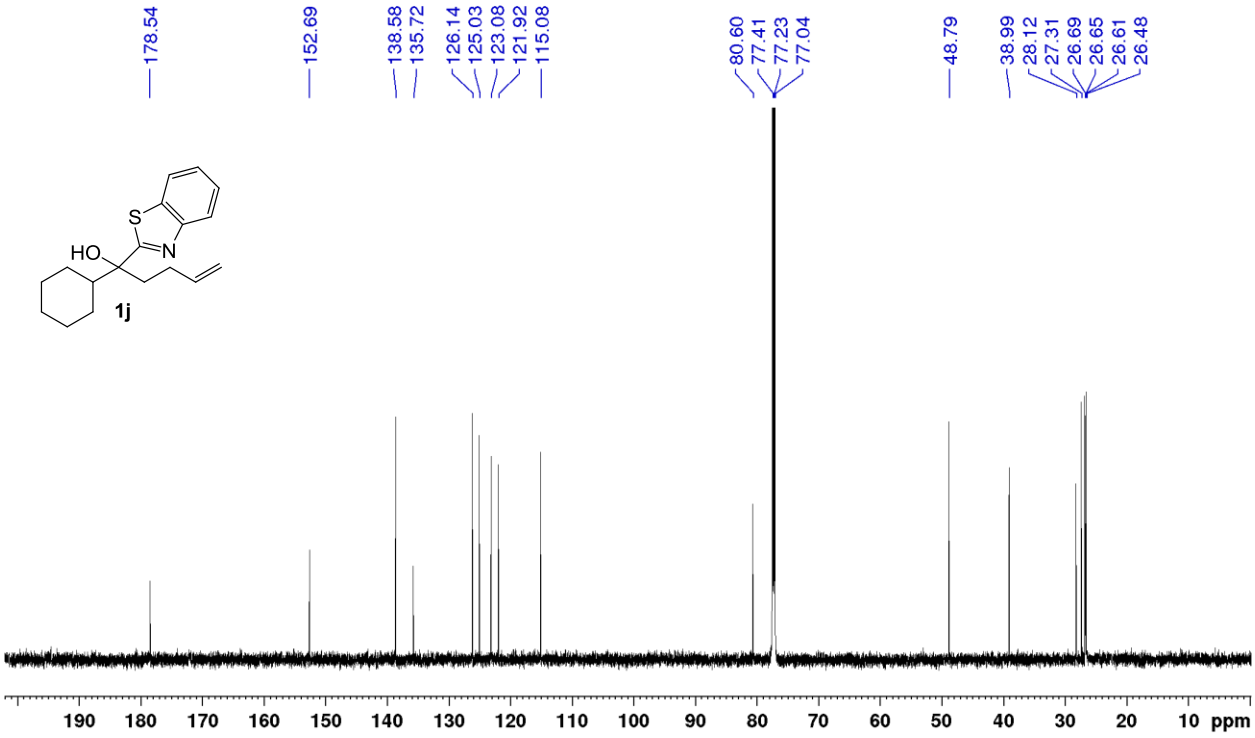
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1i)



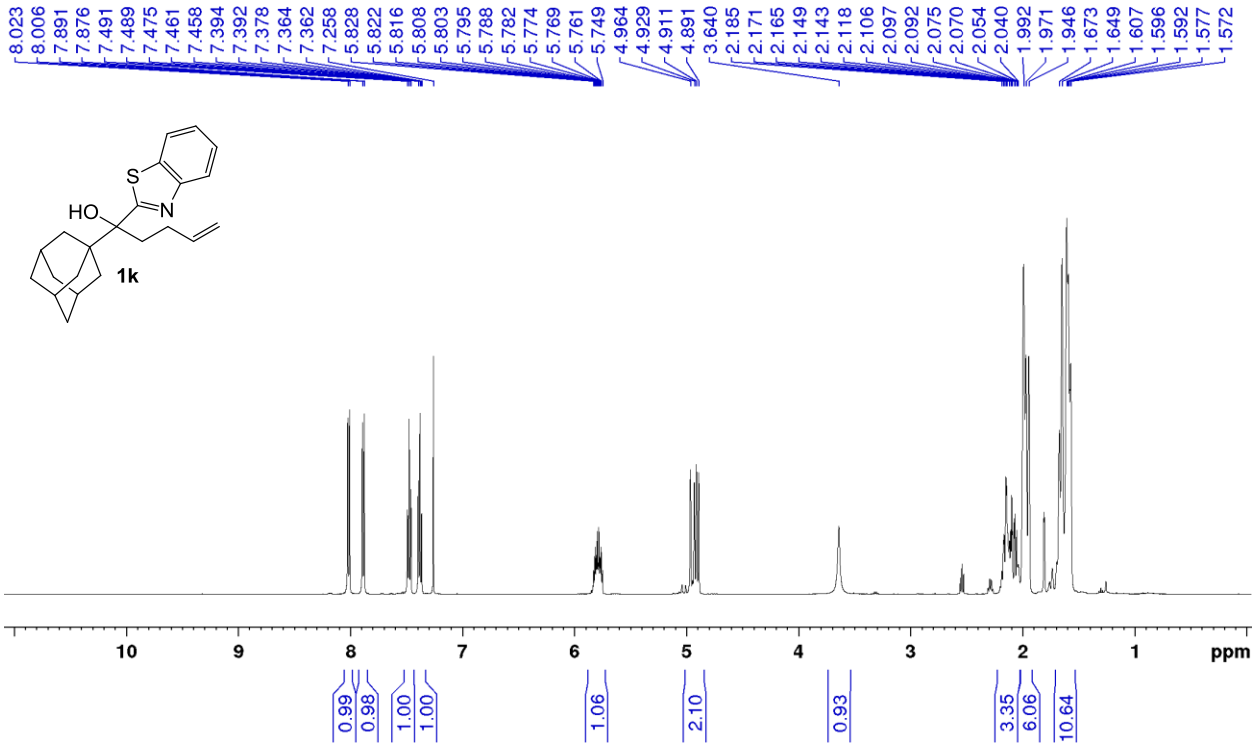
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) of (1j)



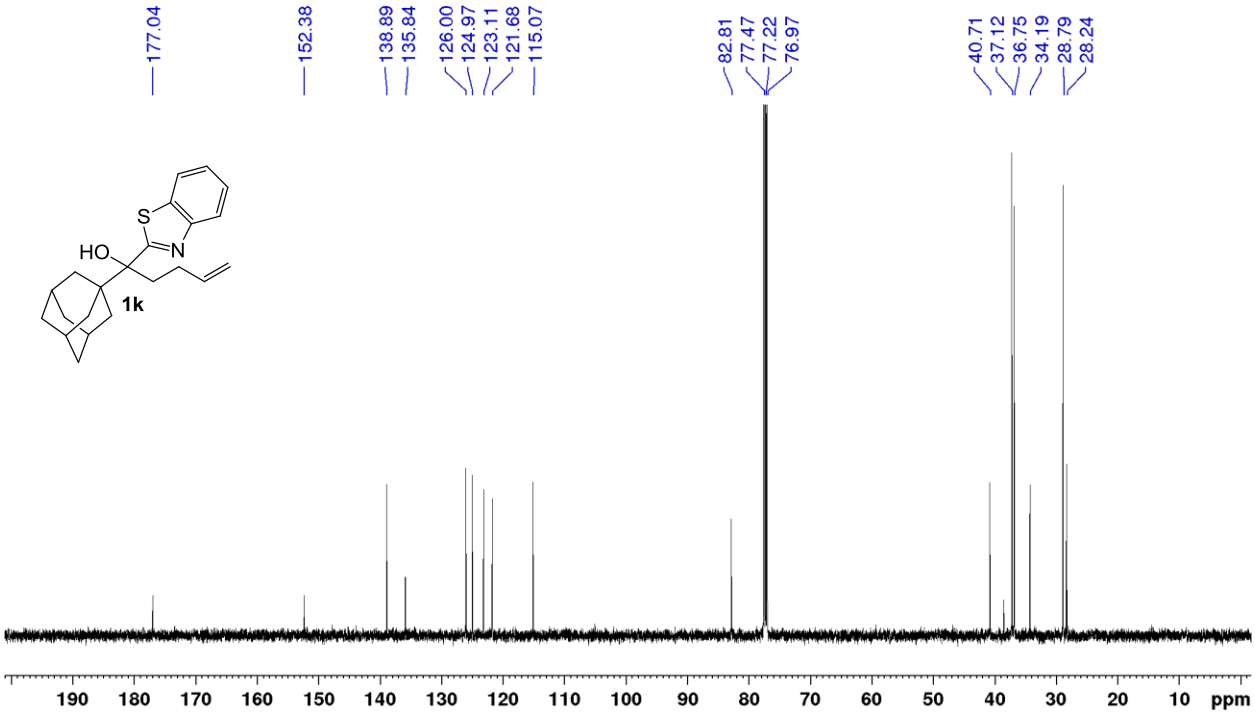
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1j)



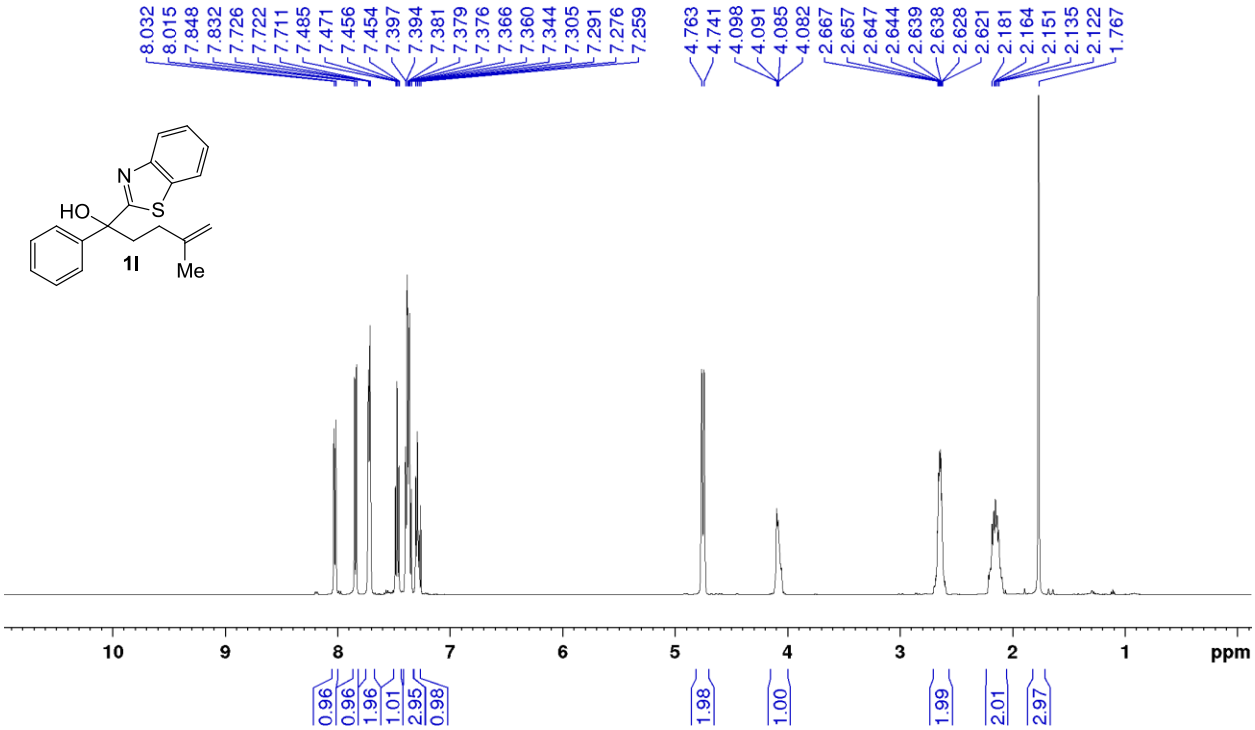
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1k)



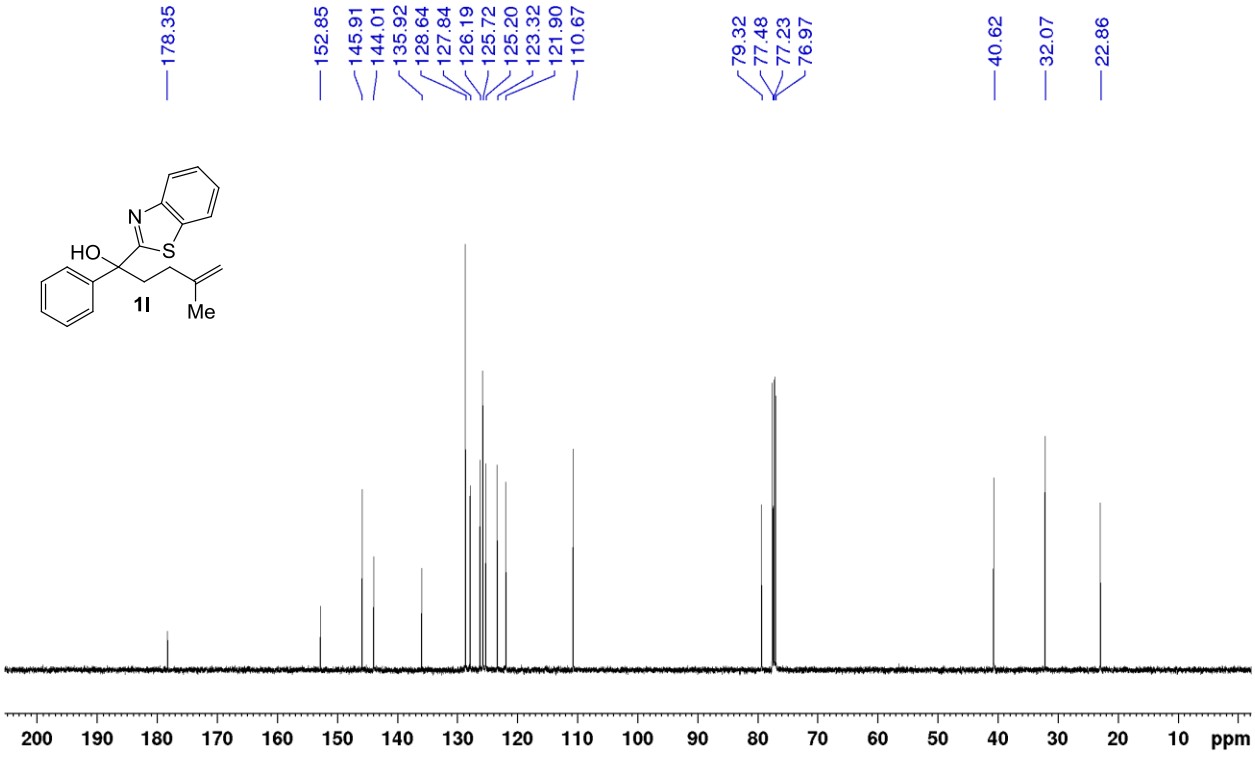
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1k)



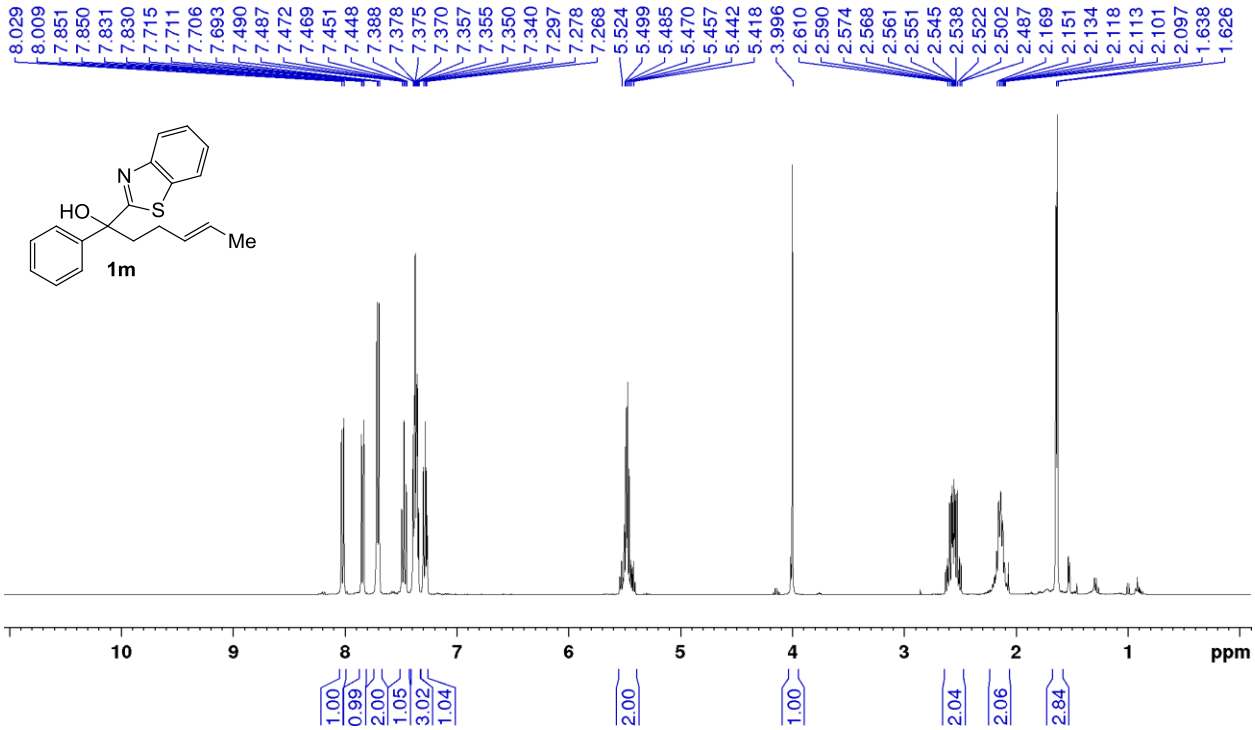
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1l)



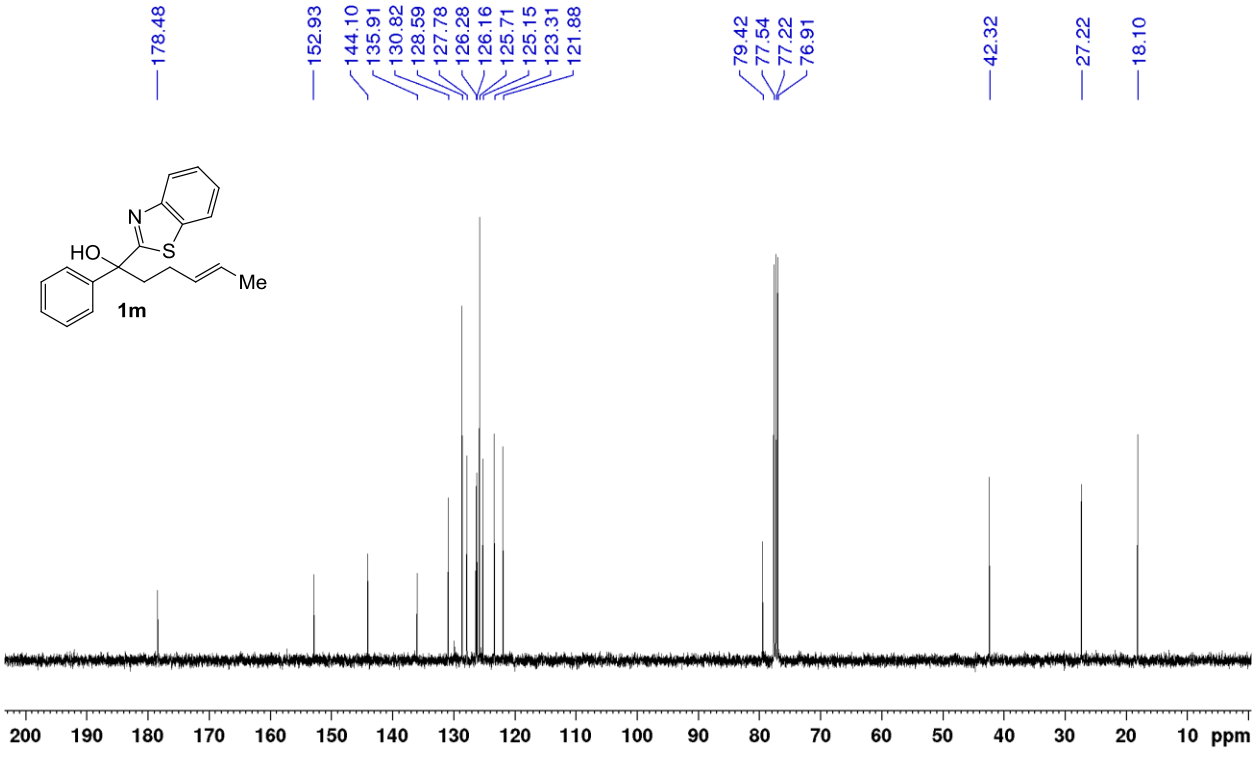
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1l)



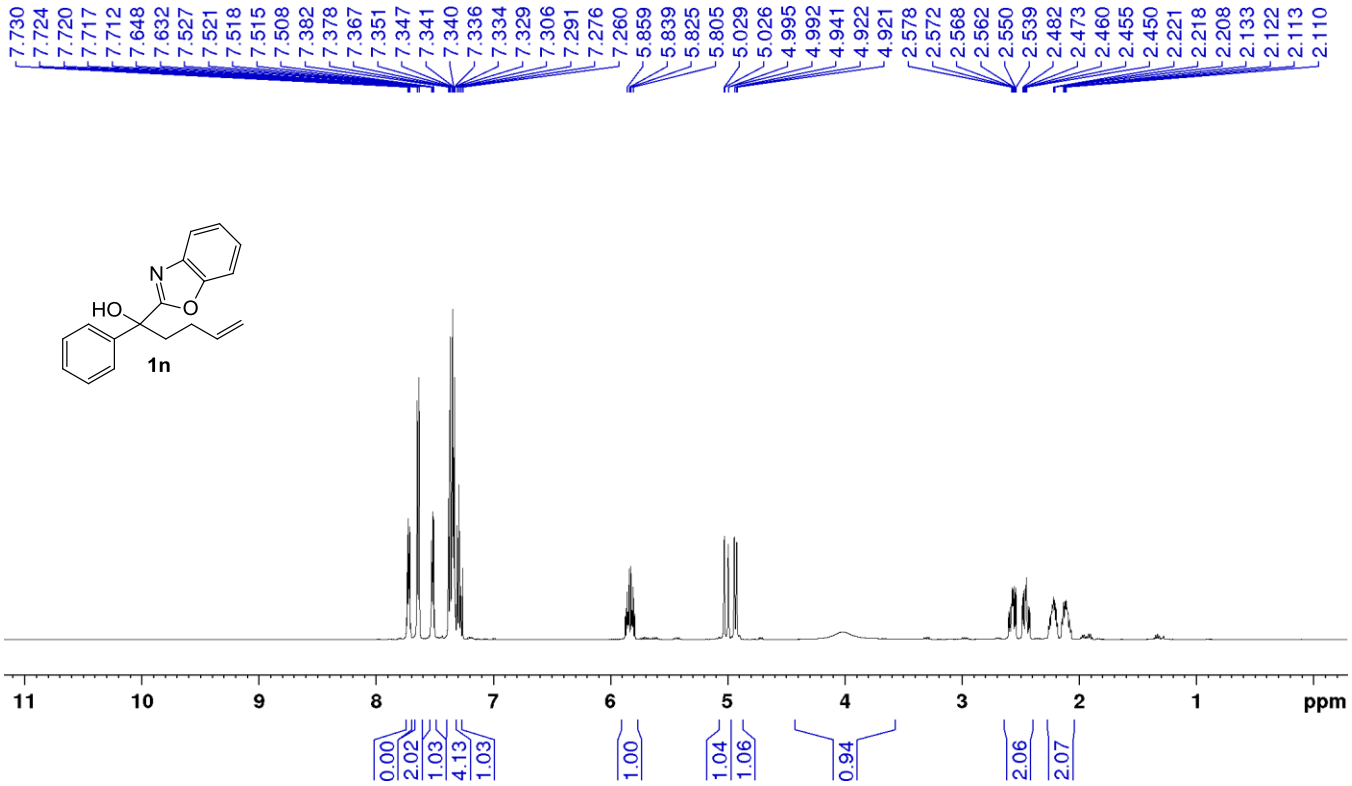
^{1}H NMR (400 MHz, $CDCl_3$, 25 °C) of (1m)



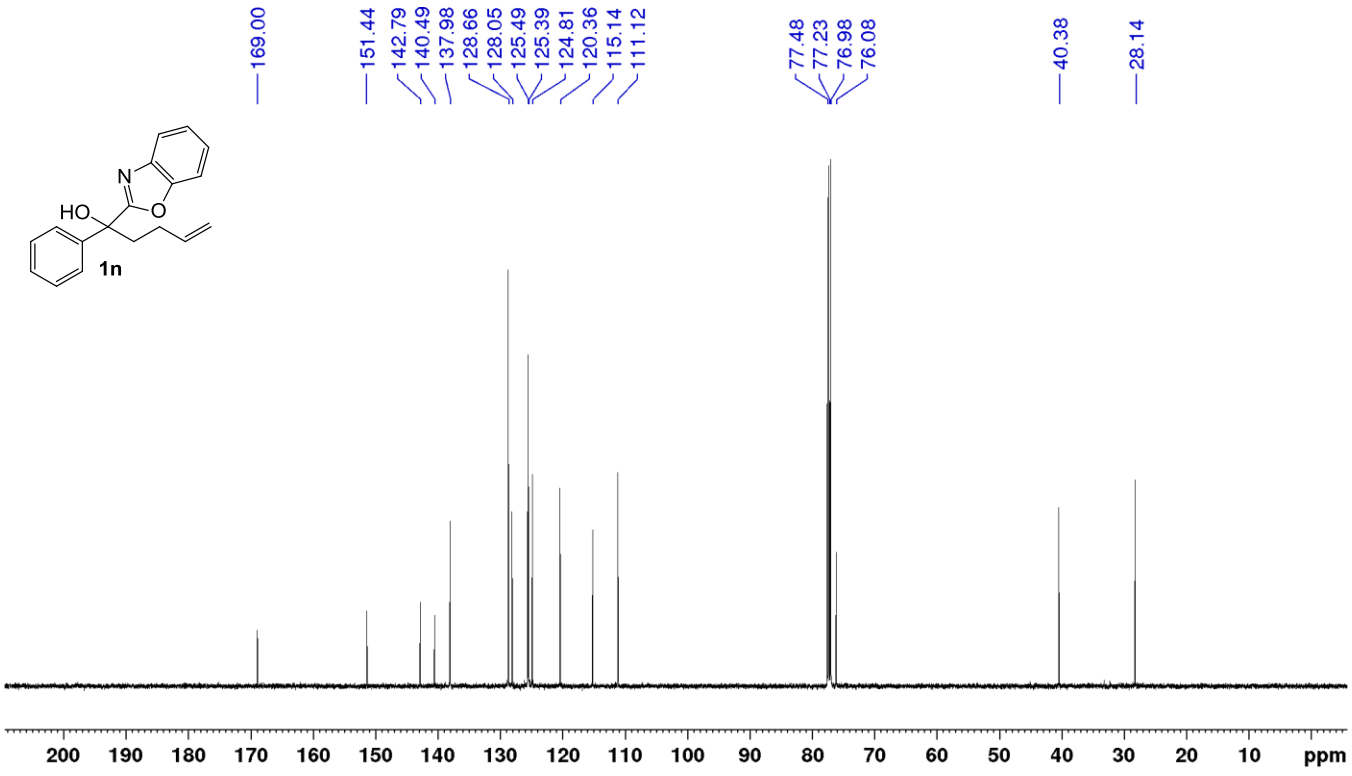
^{13}C NMR (100 MHz, $CDCl_3$, 25 °C) of (1m)



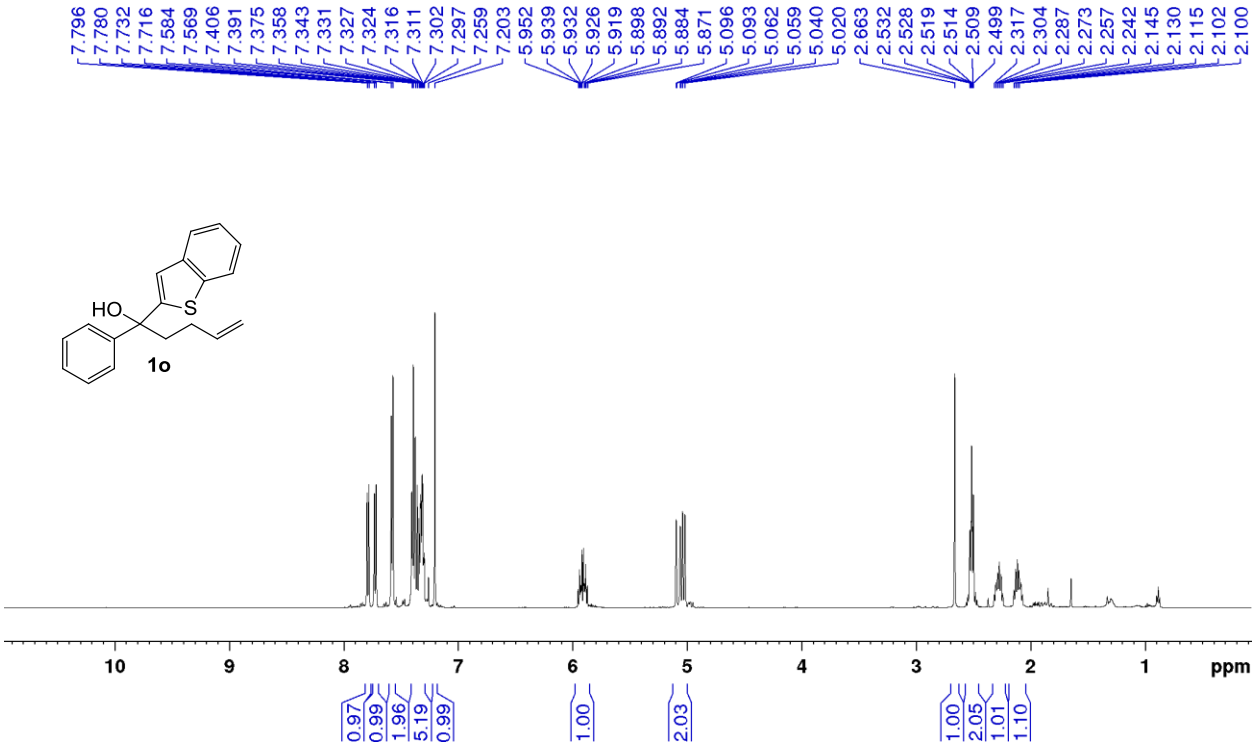
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1n)



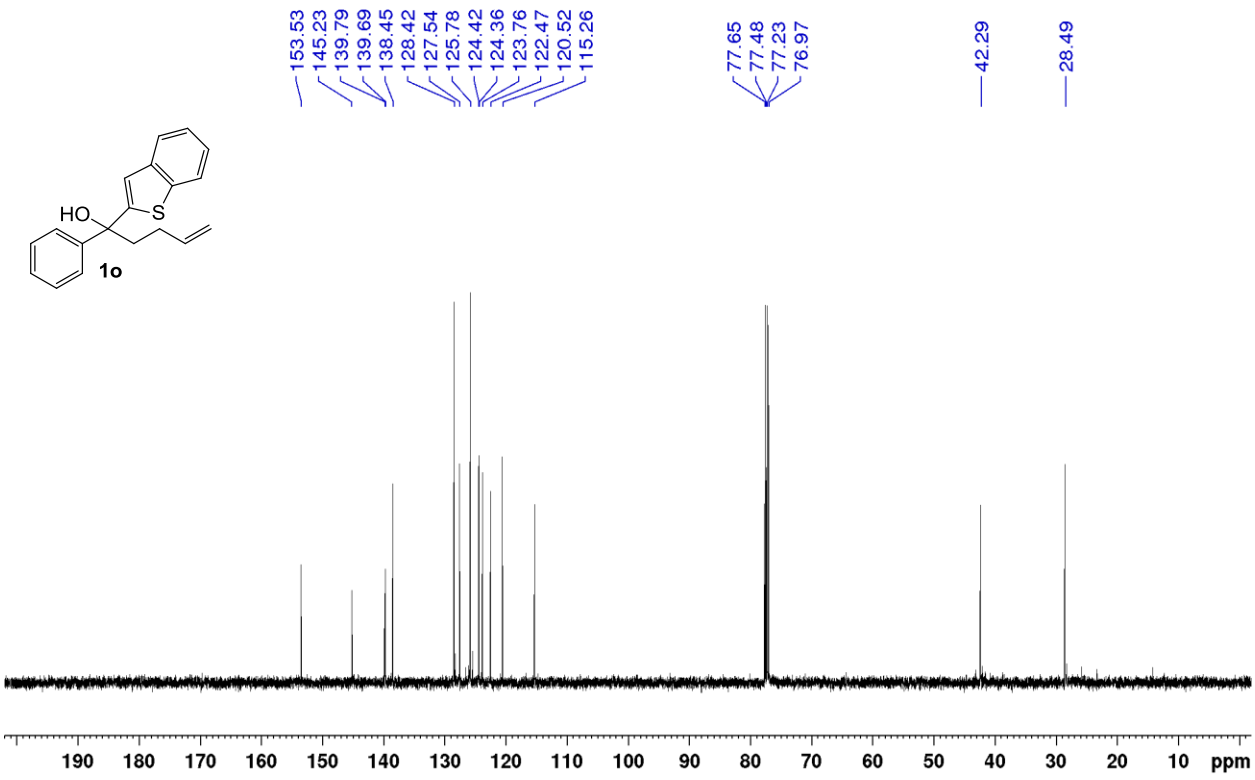
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1n)



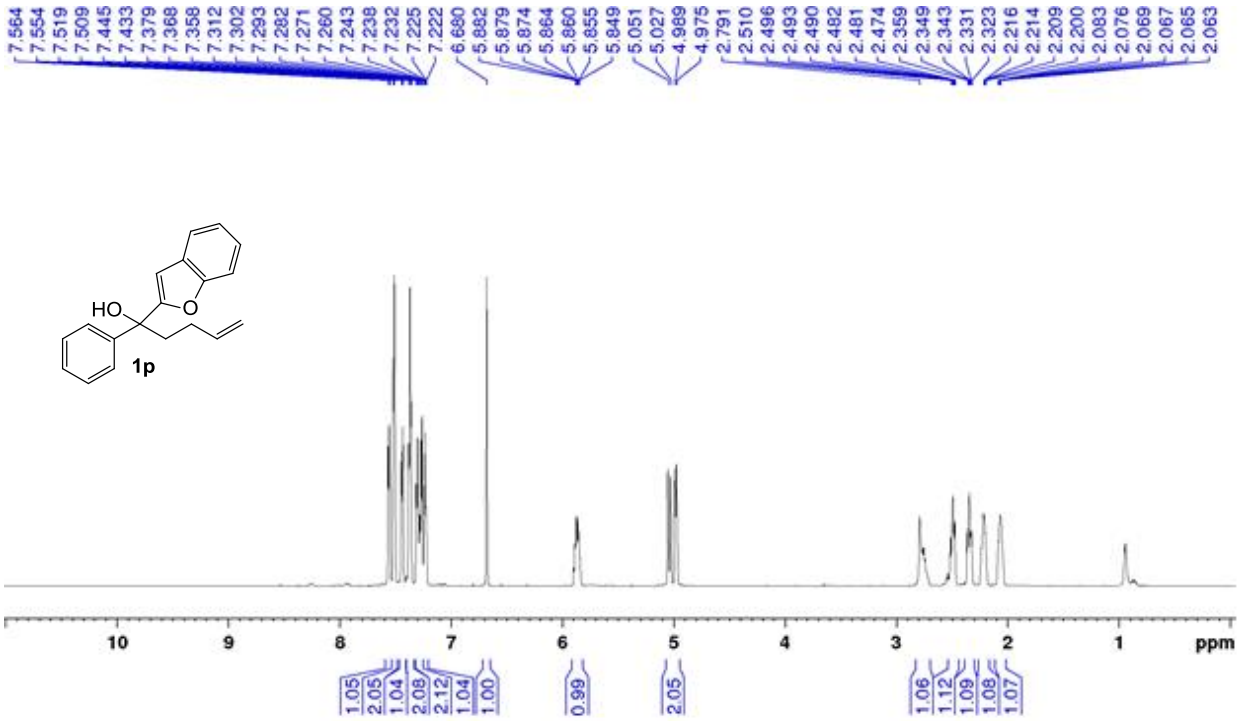
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1o)



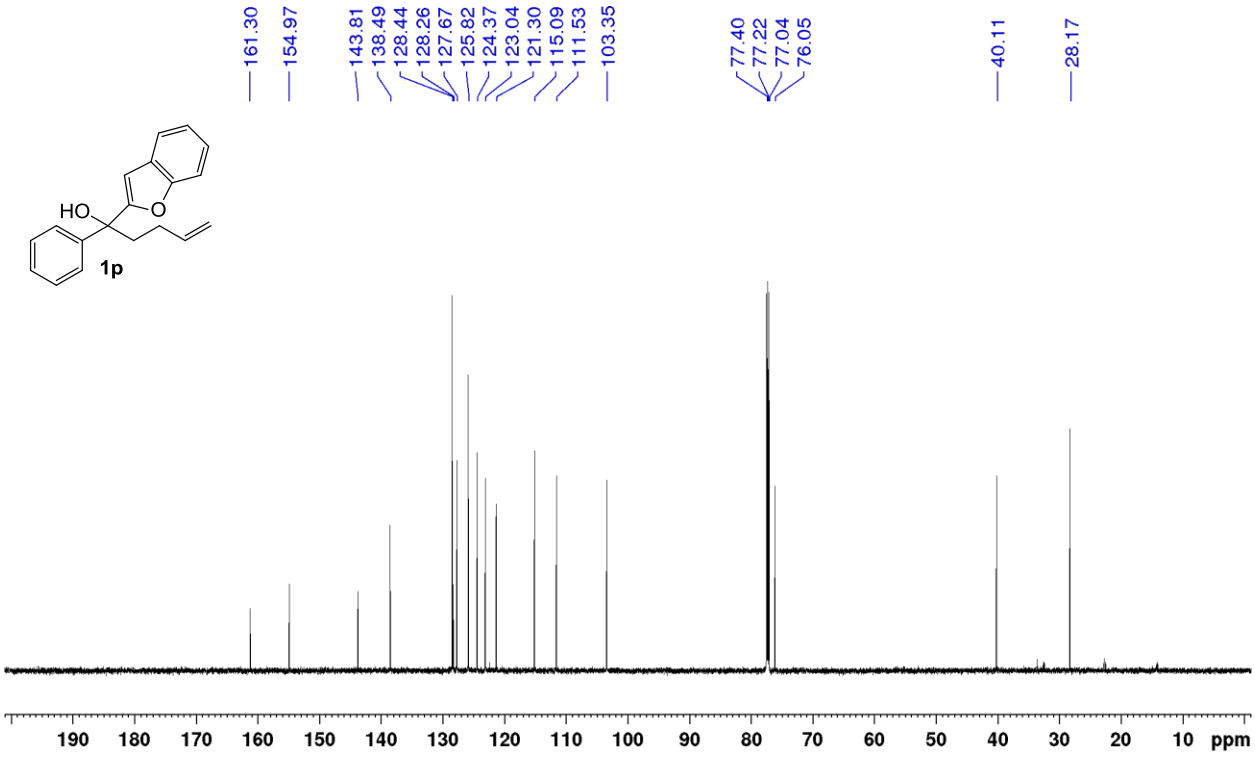
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1o)



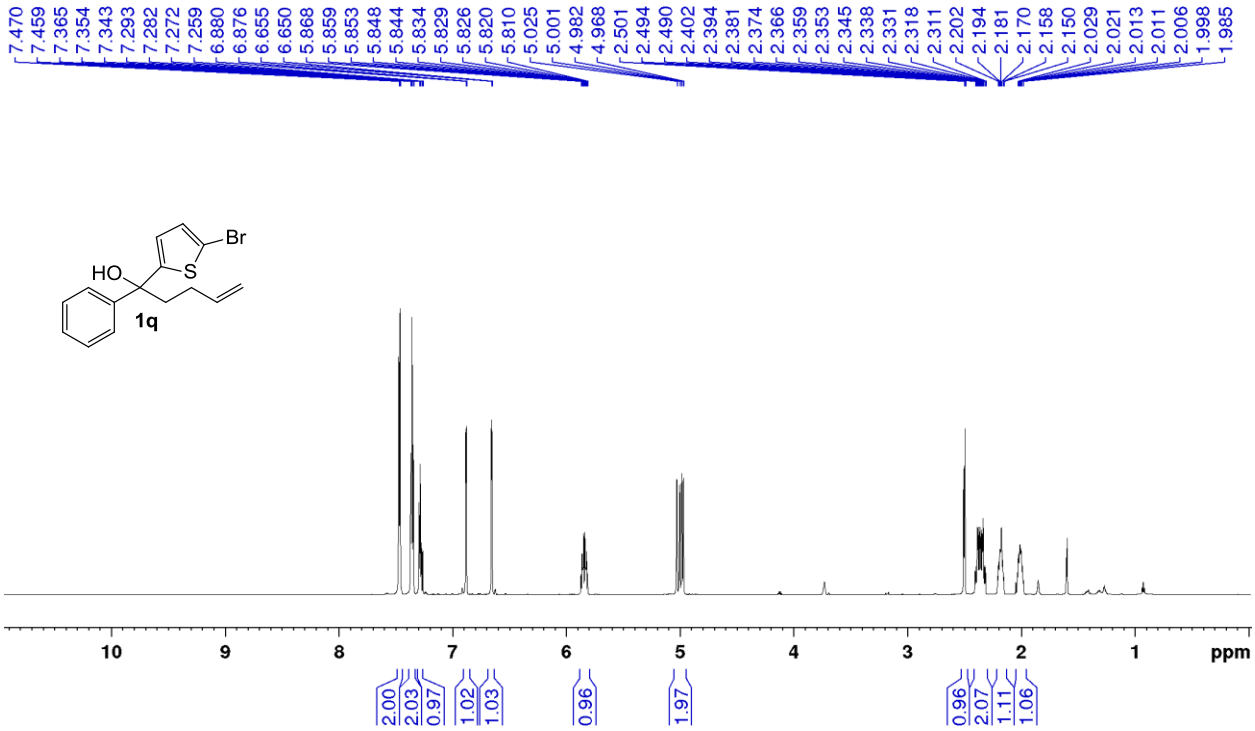
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (1p)



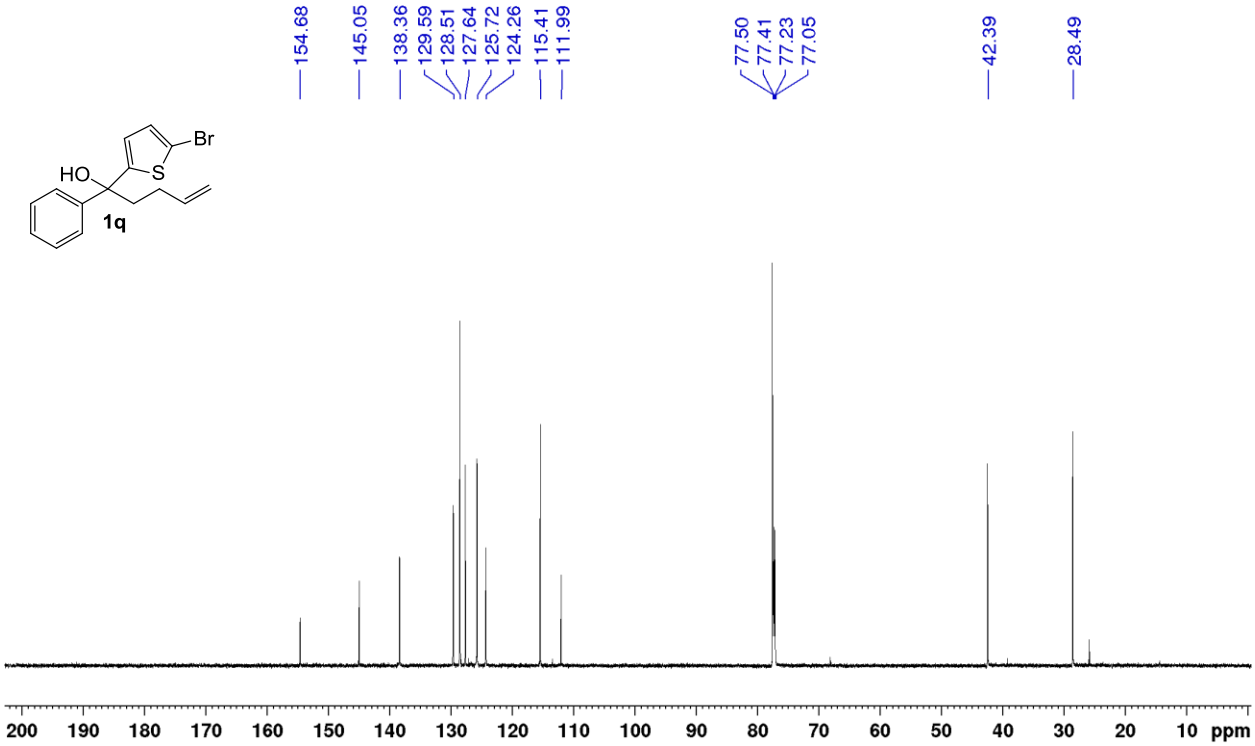
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (1p)



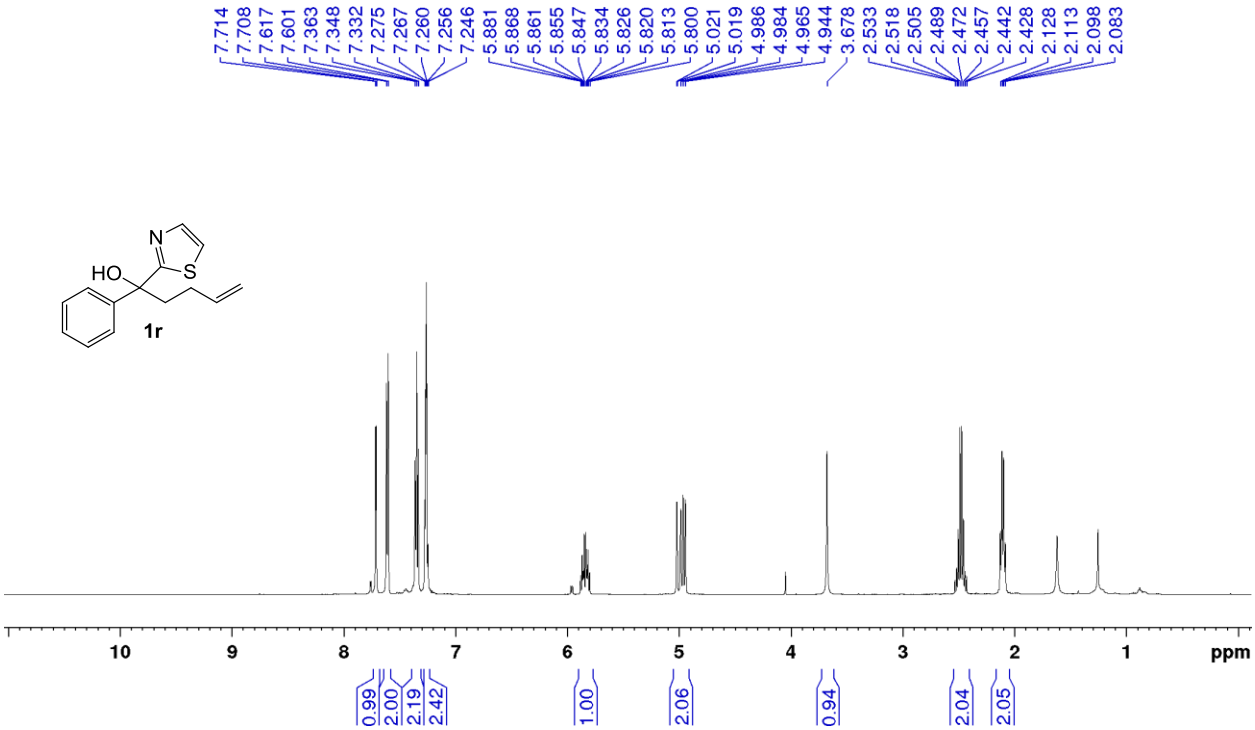
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1q)



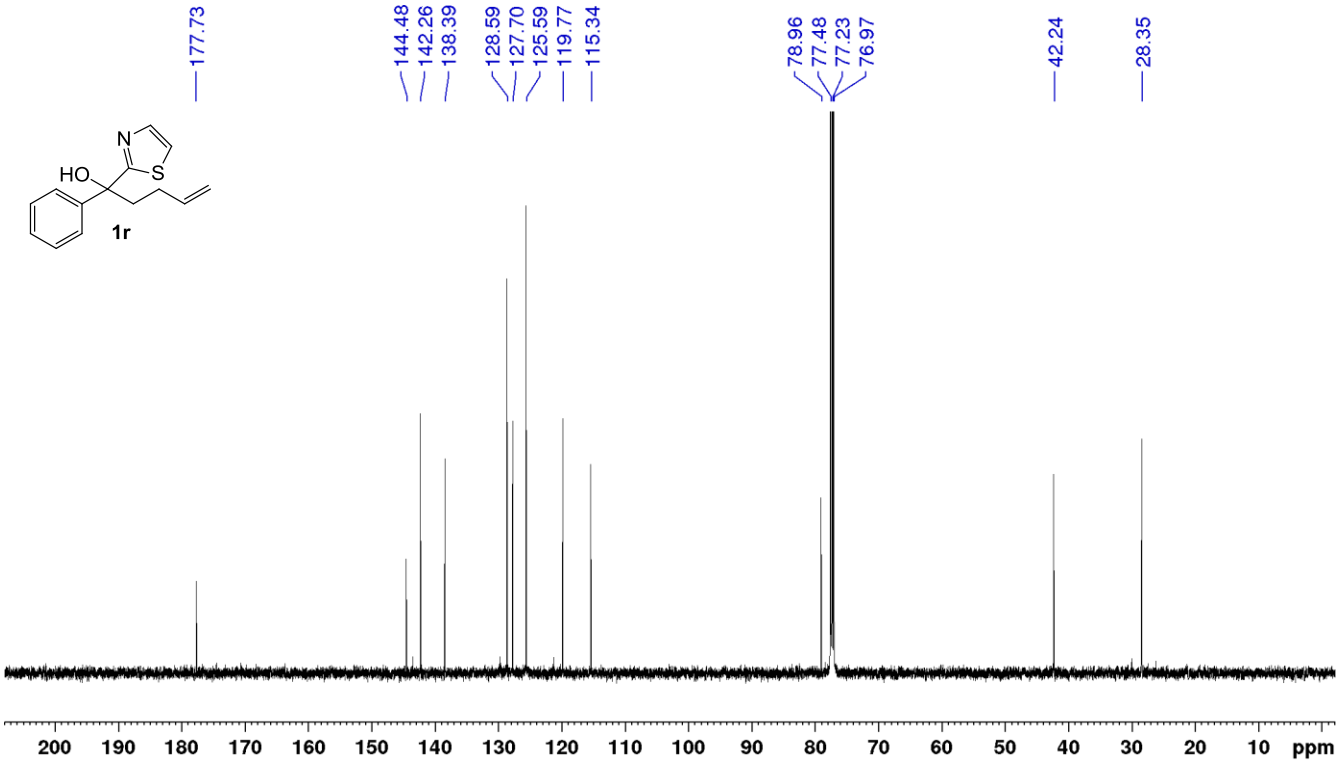
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1q)



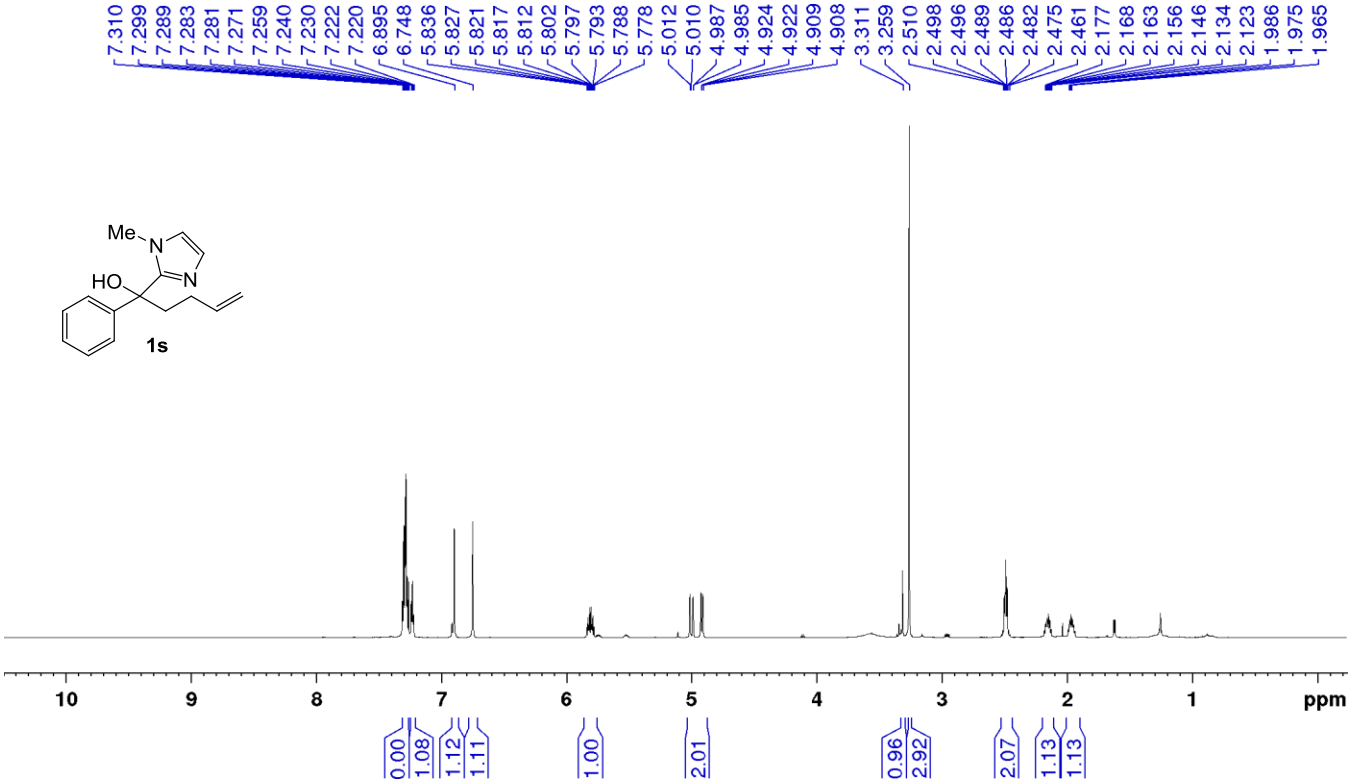
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1r)



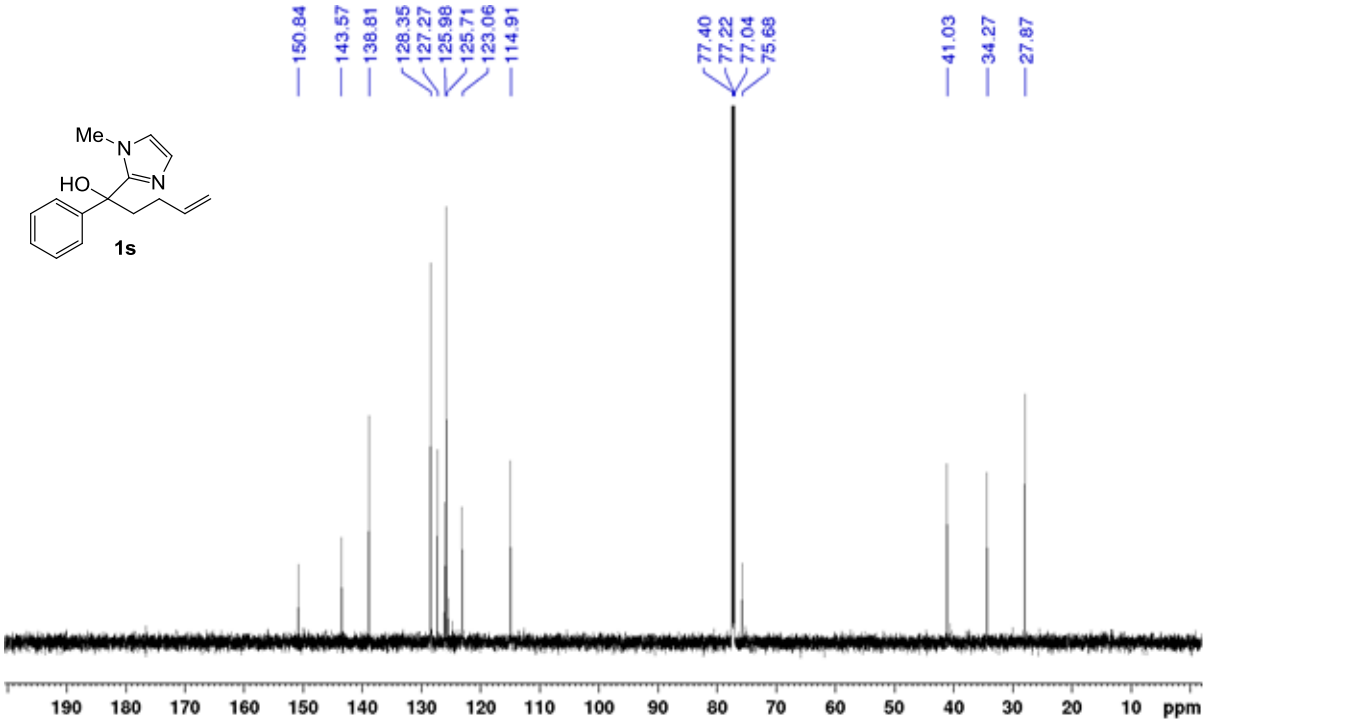
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1r)



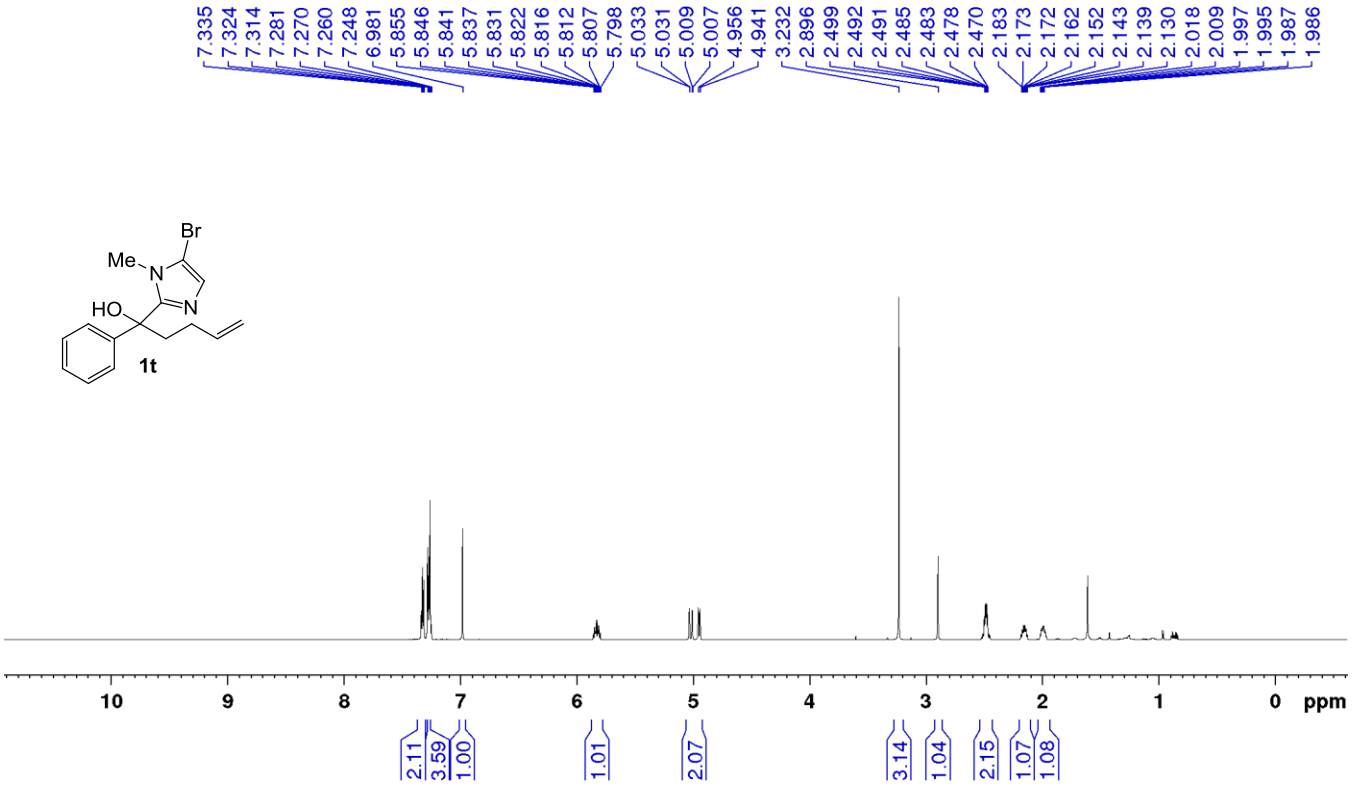
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1s)



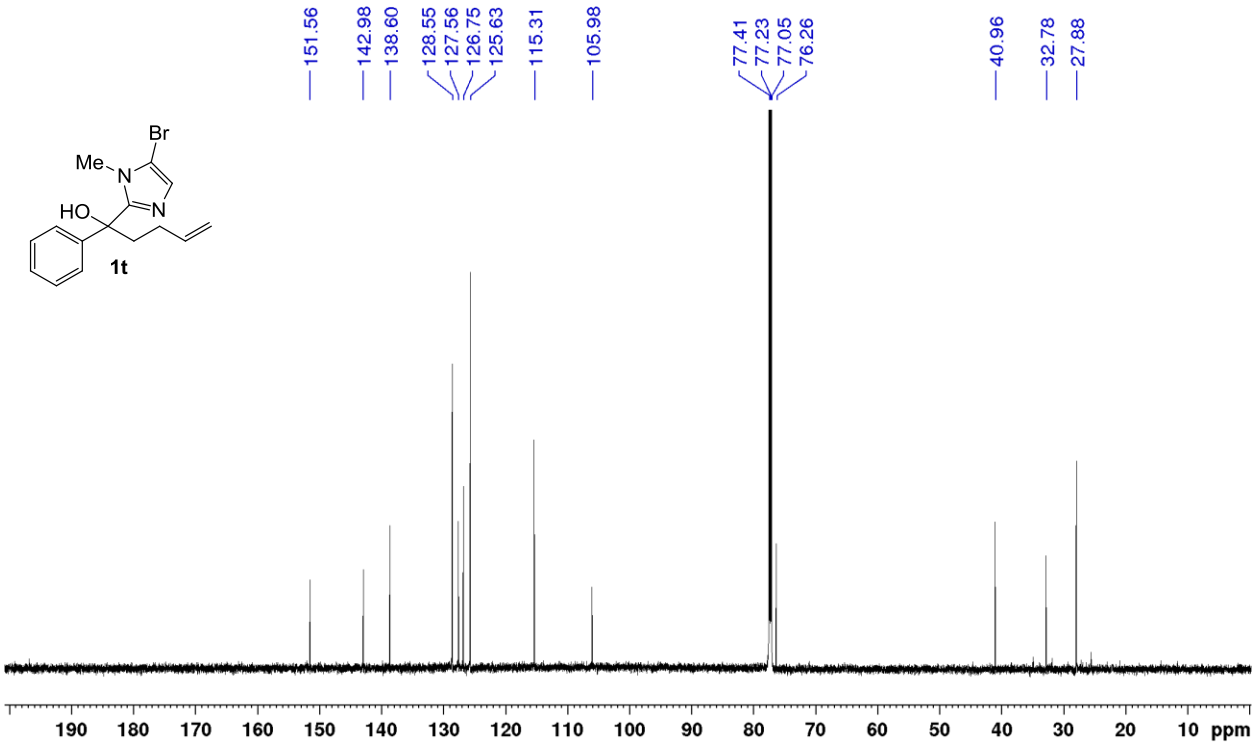
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1s)



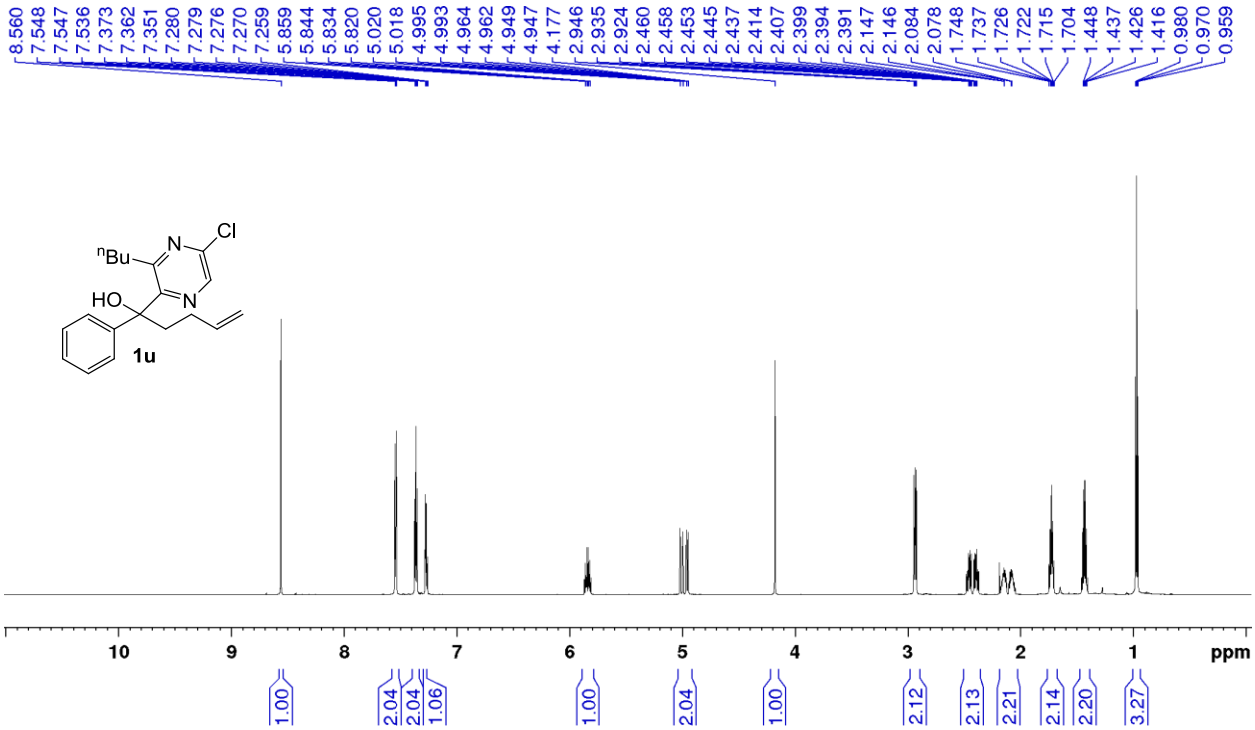
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1t)



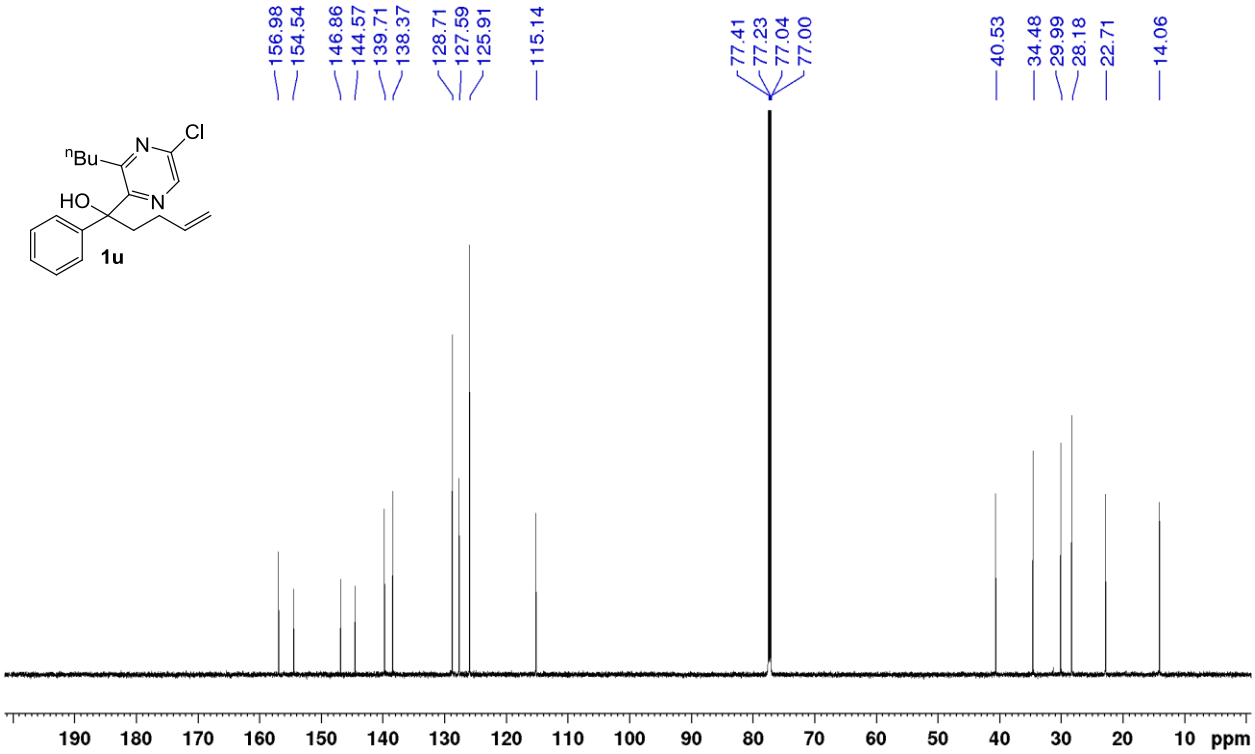
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1t)



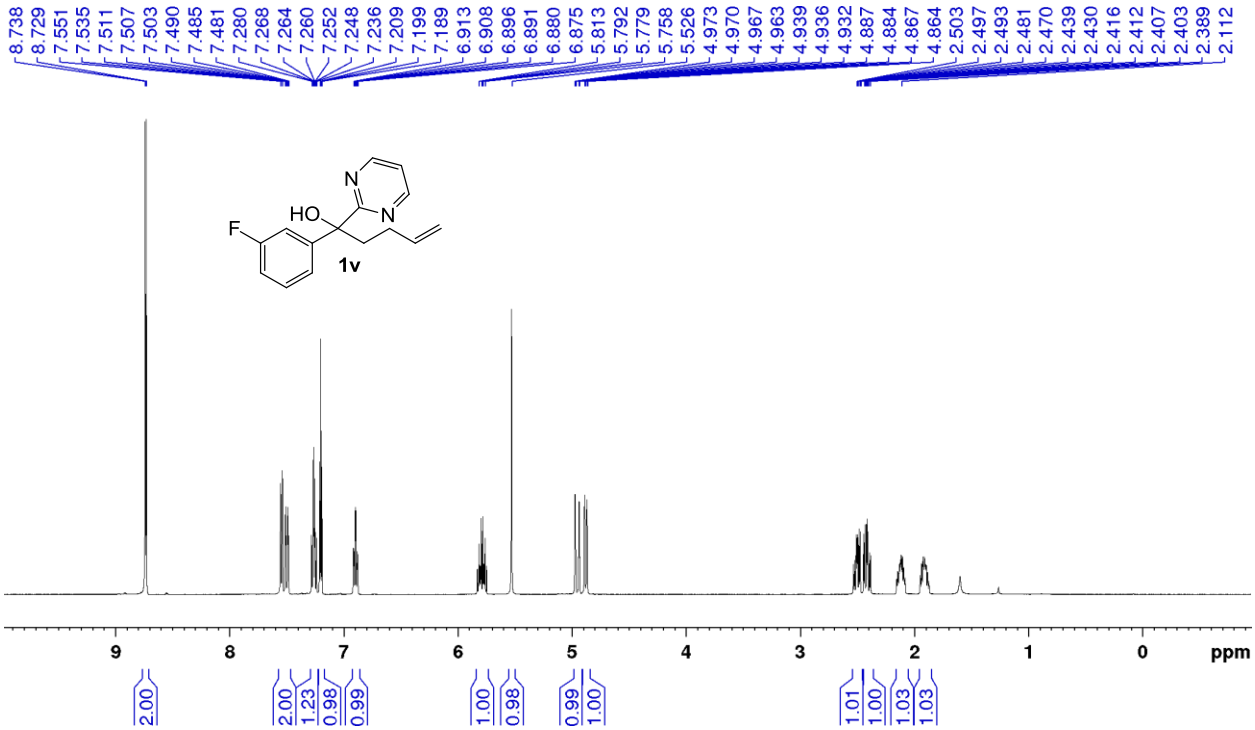
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (1u)



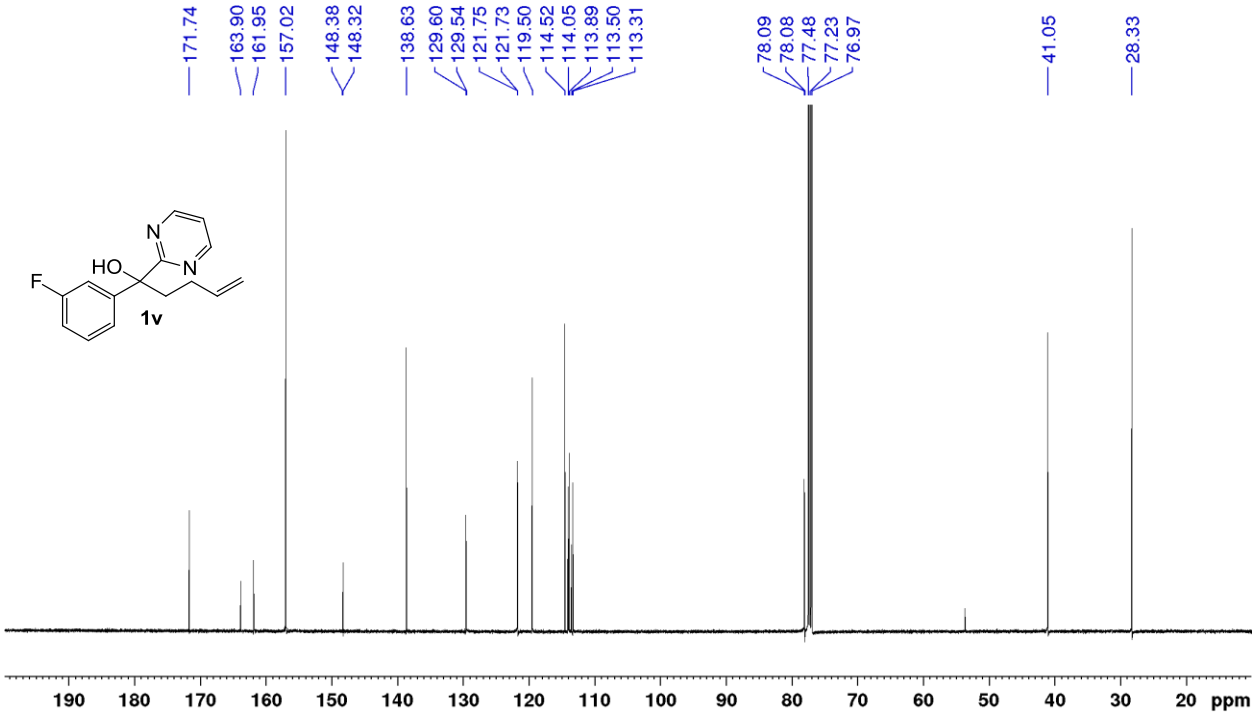
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (1u)



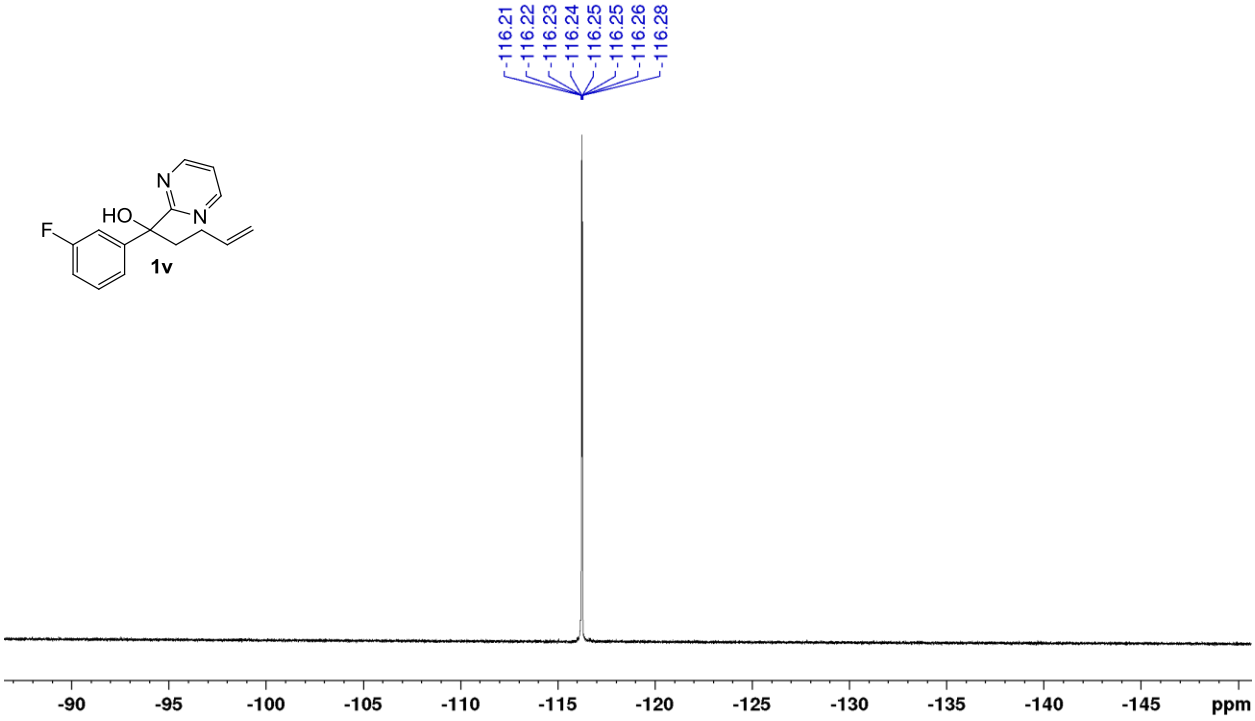
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (1v)



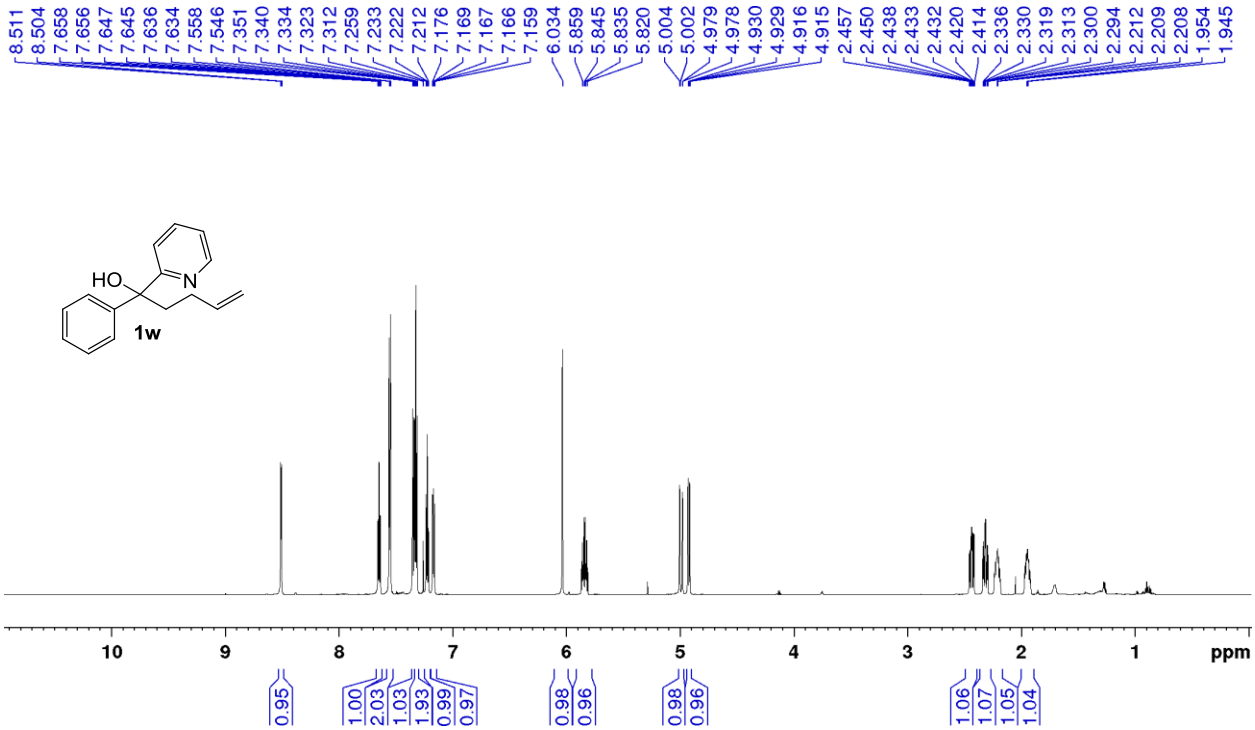
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (1v)



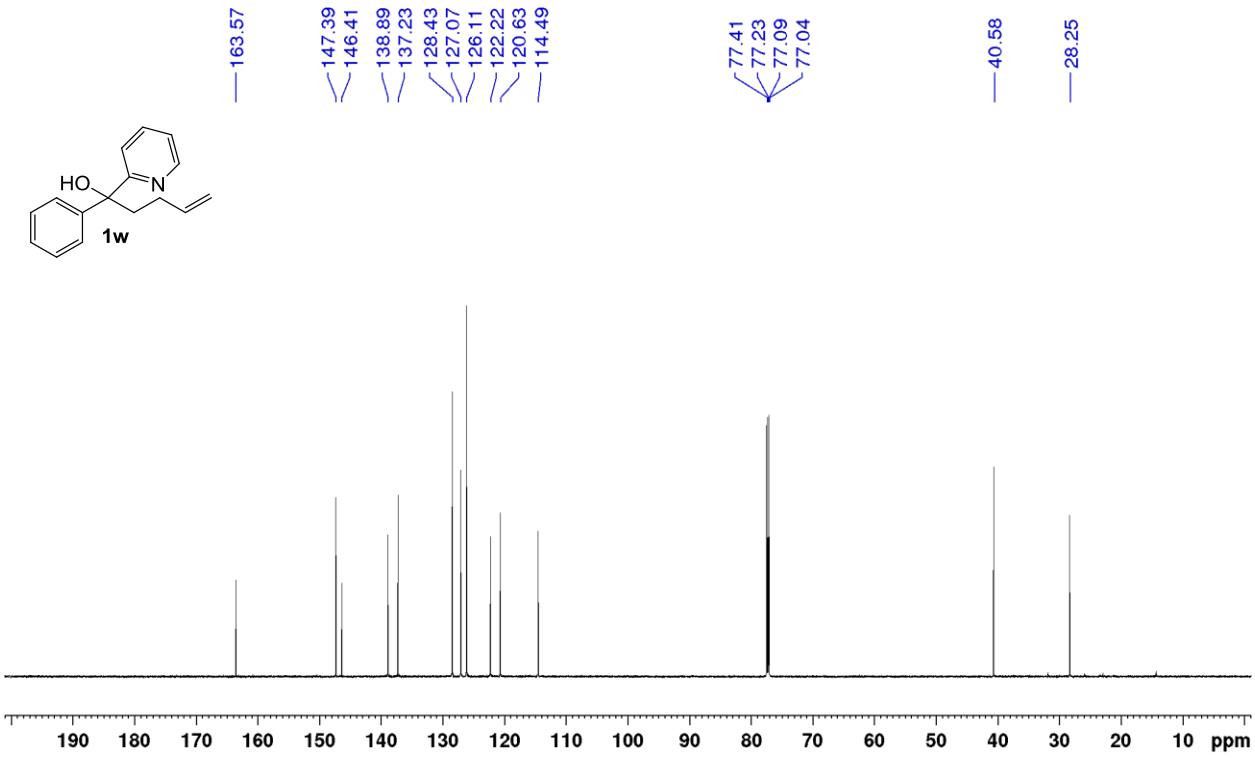
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (1v)



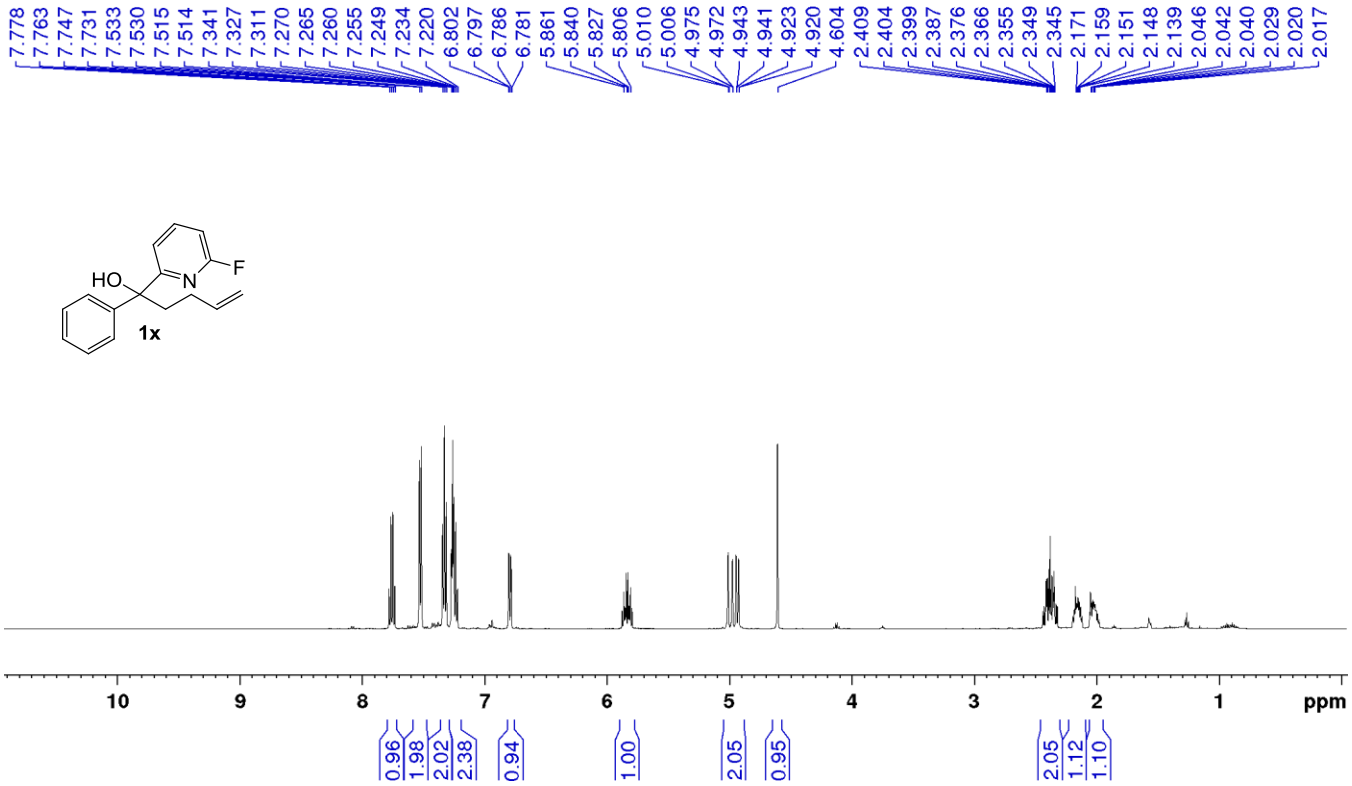
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1w)



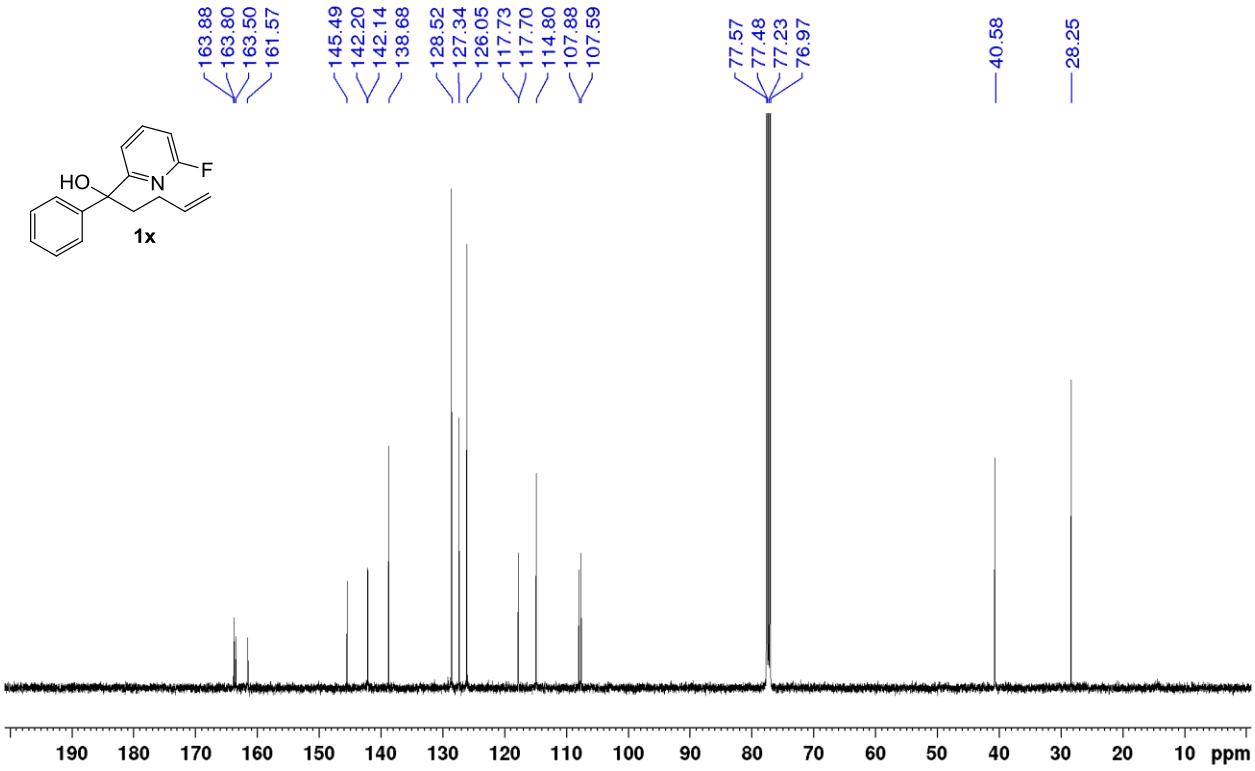
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1w)



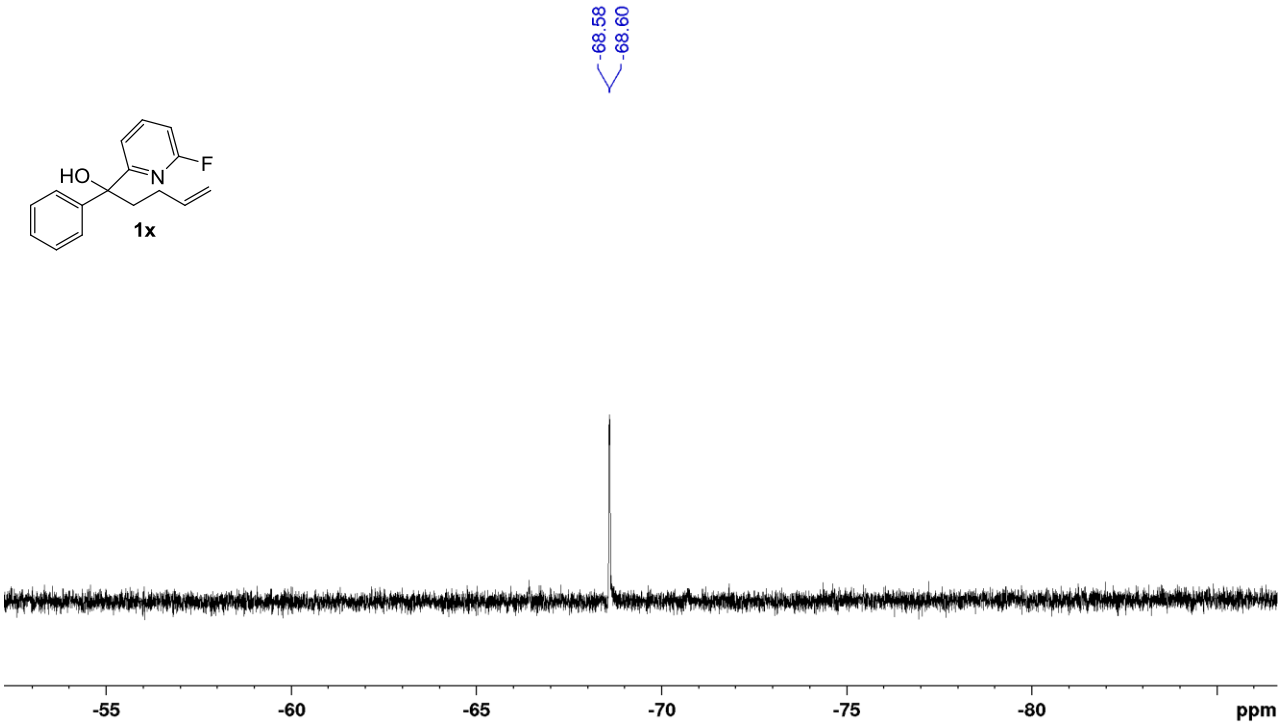
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (1x)



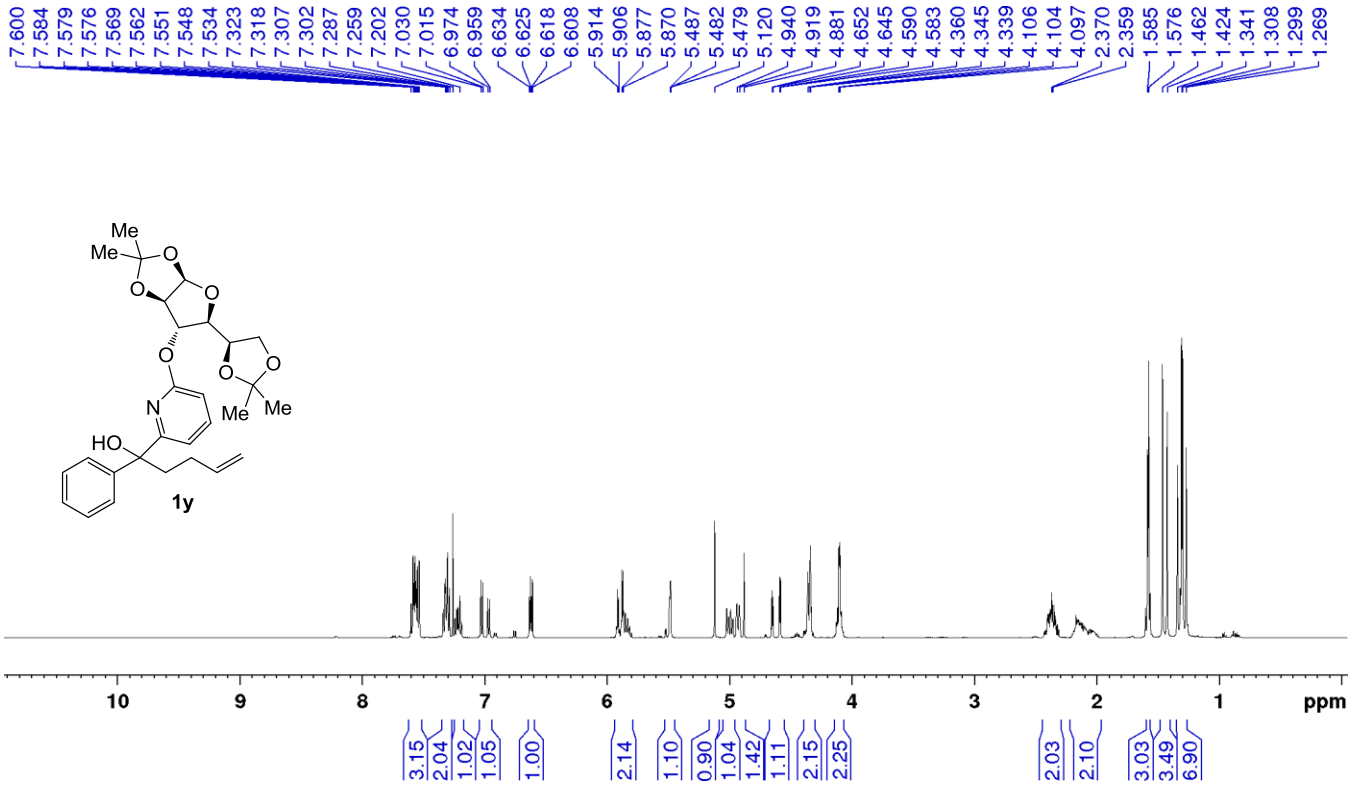
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (1x)



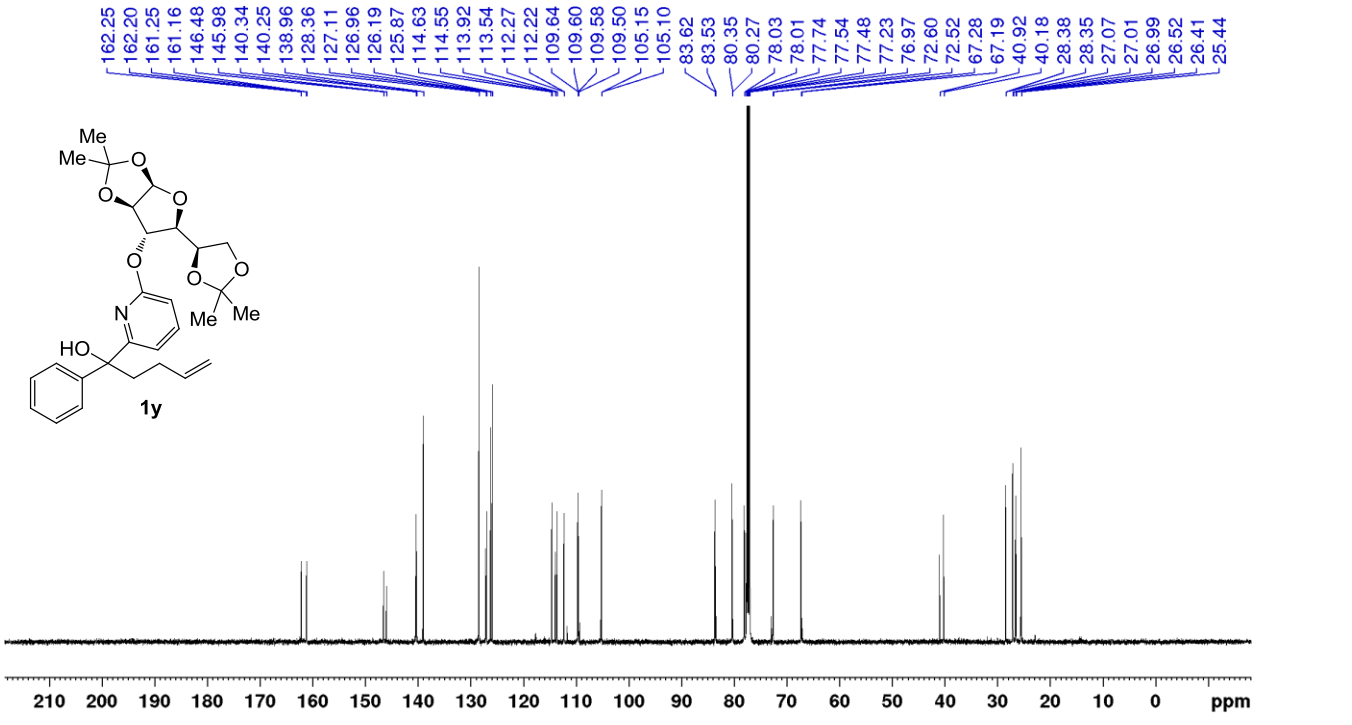
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (1x)



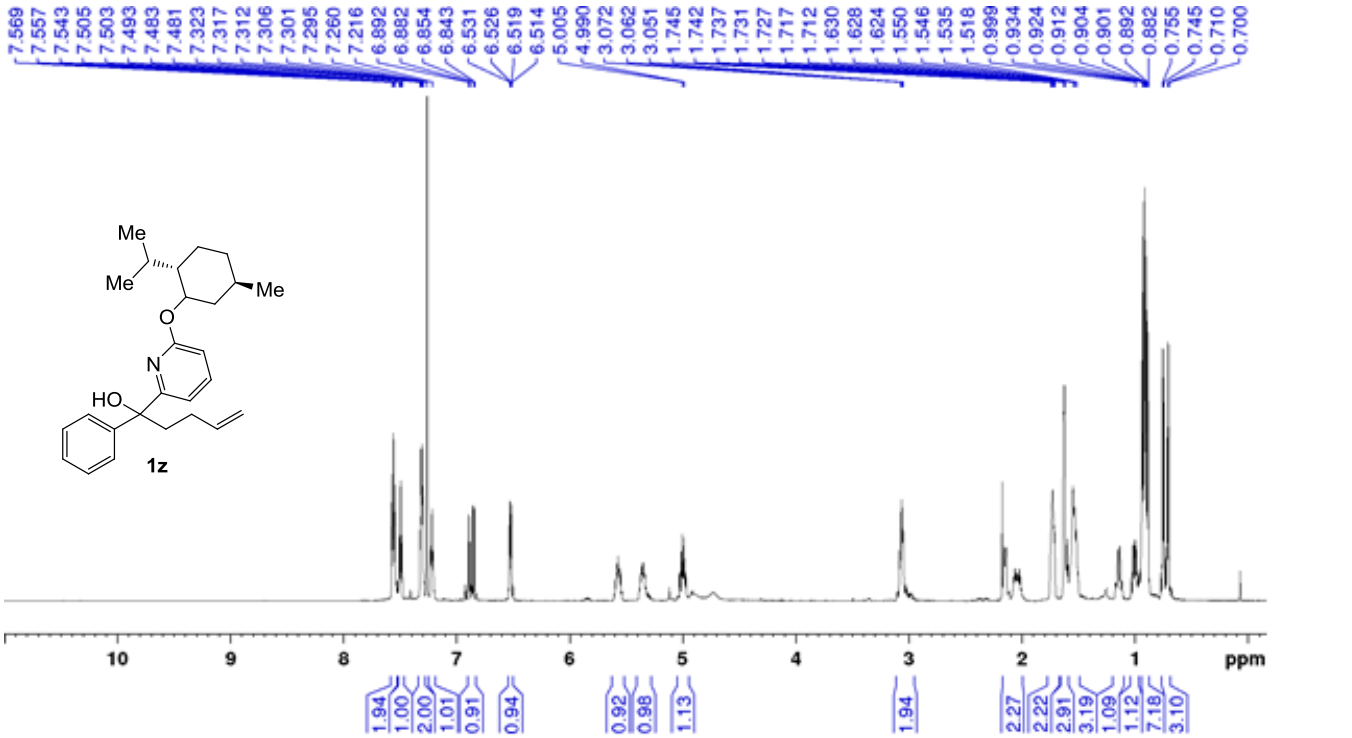
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (1y)



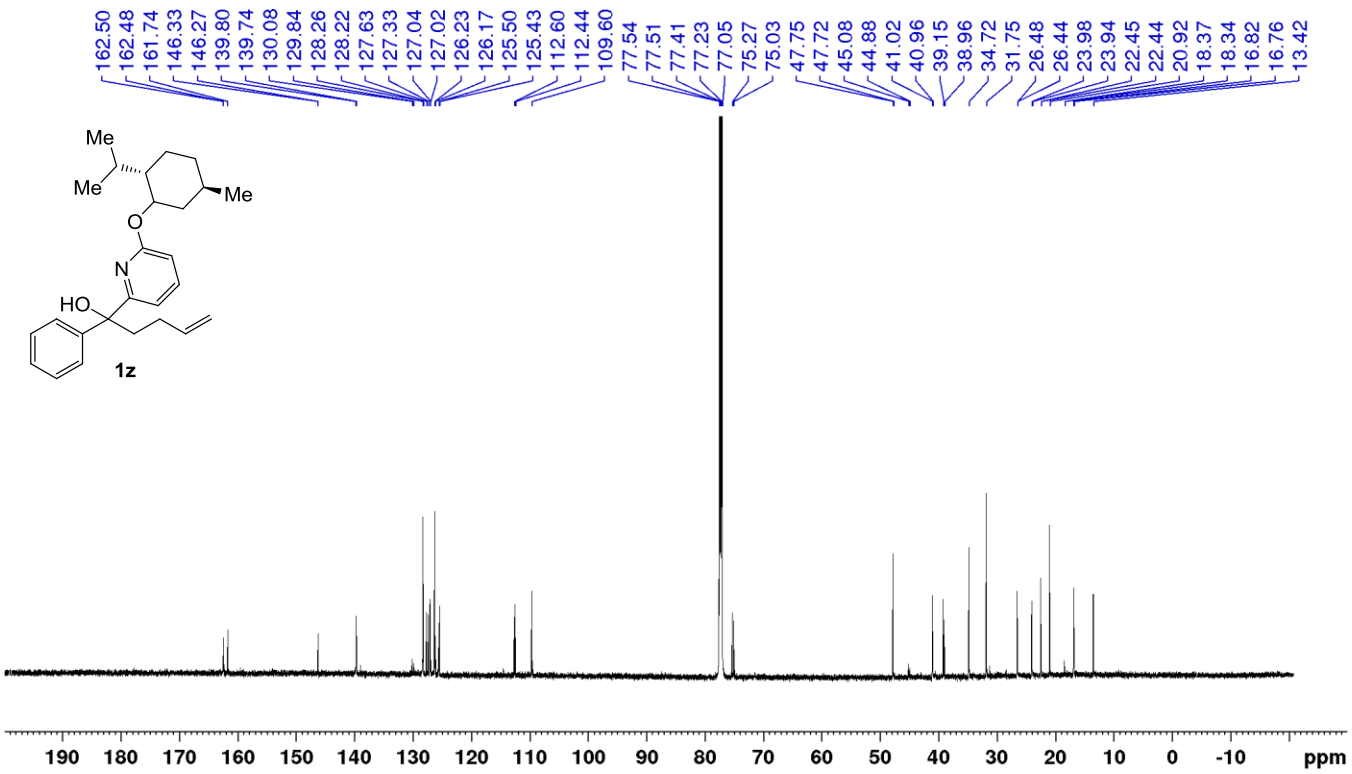
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (1y)



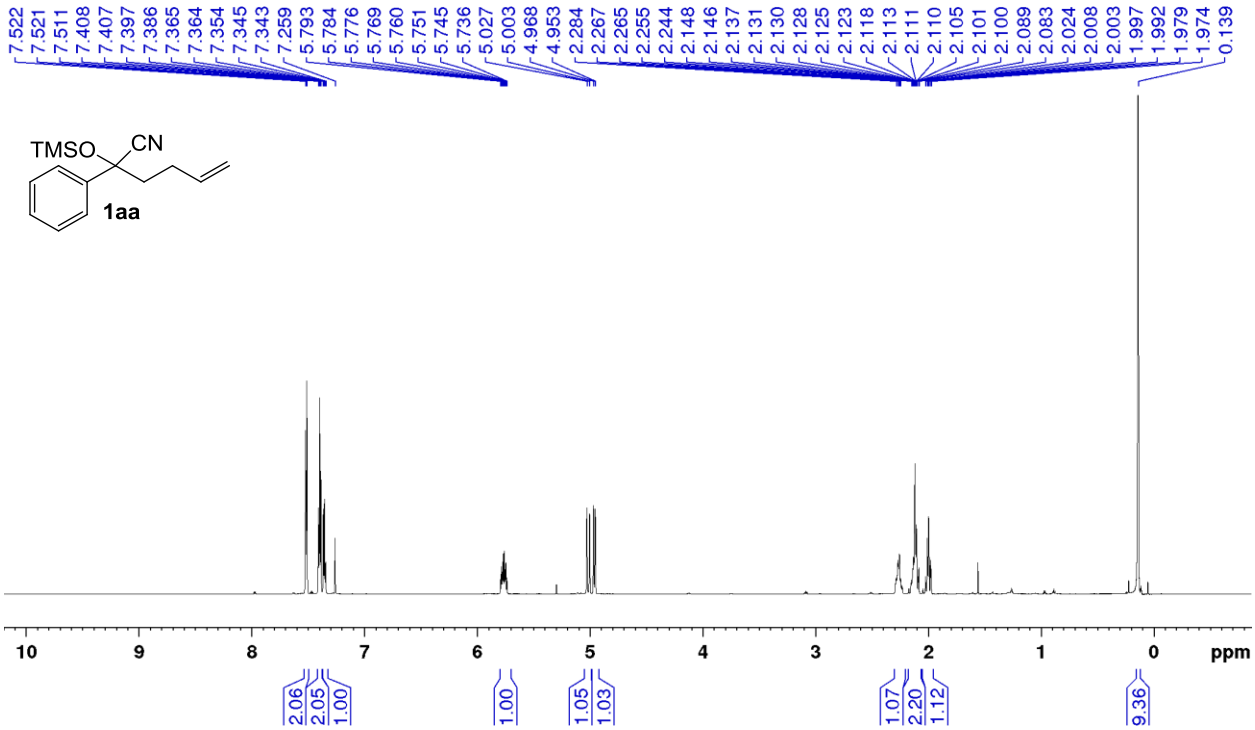
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (1z)



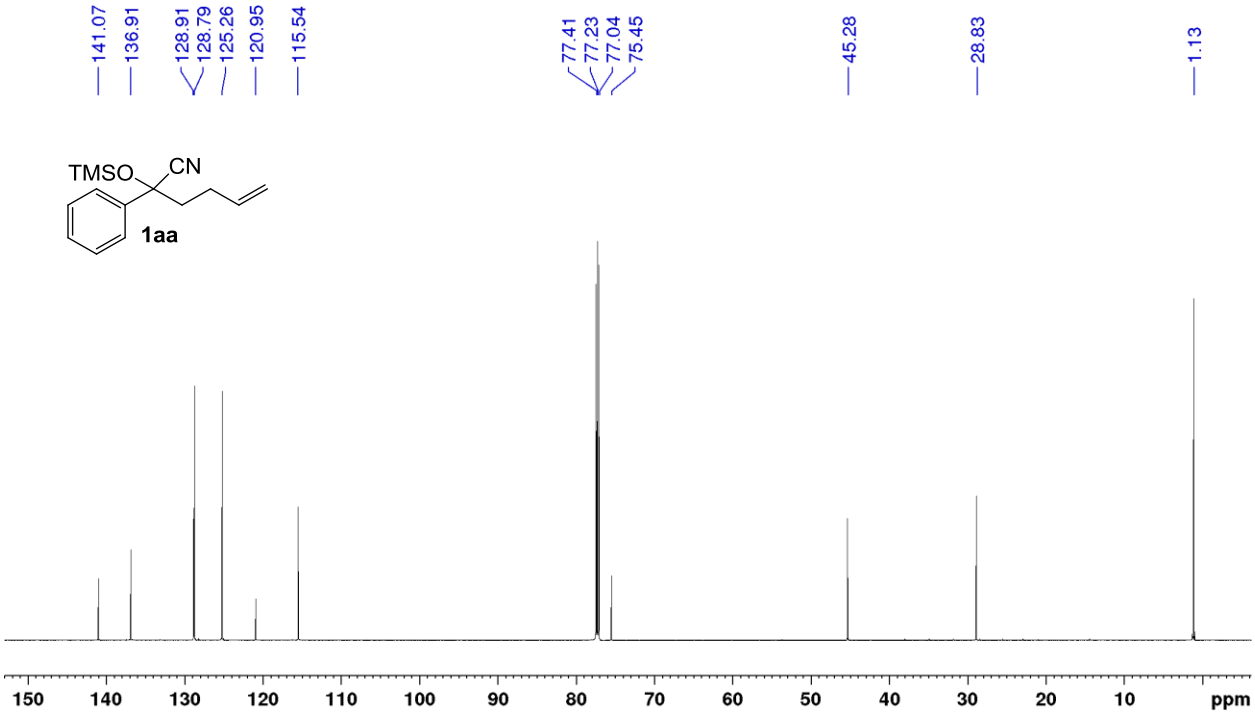
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (1z)



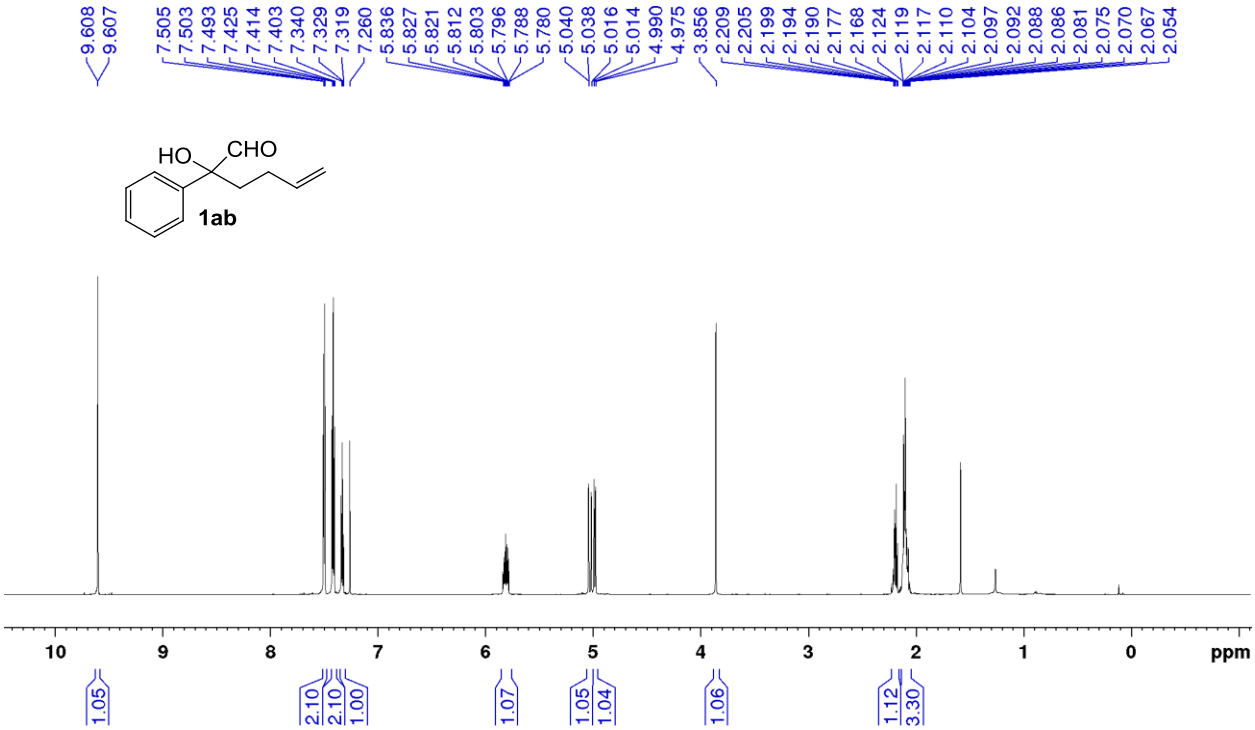
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1aa)



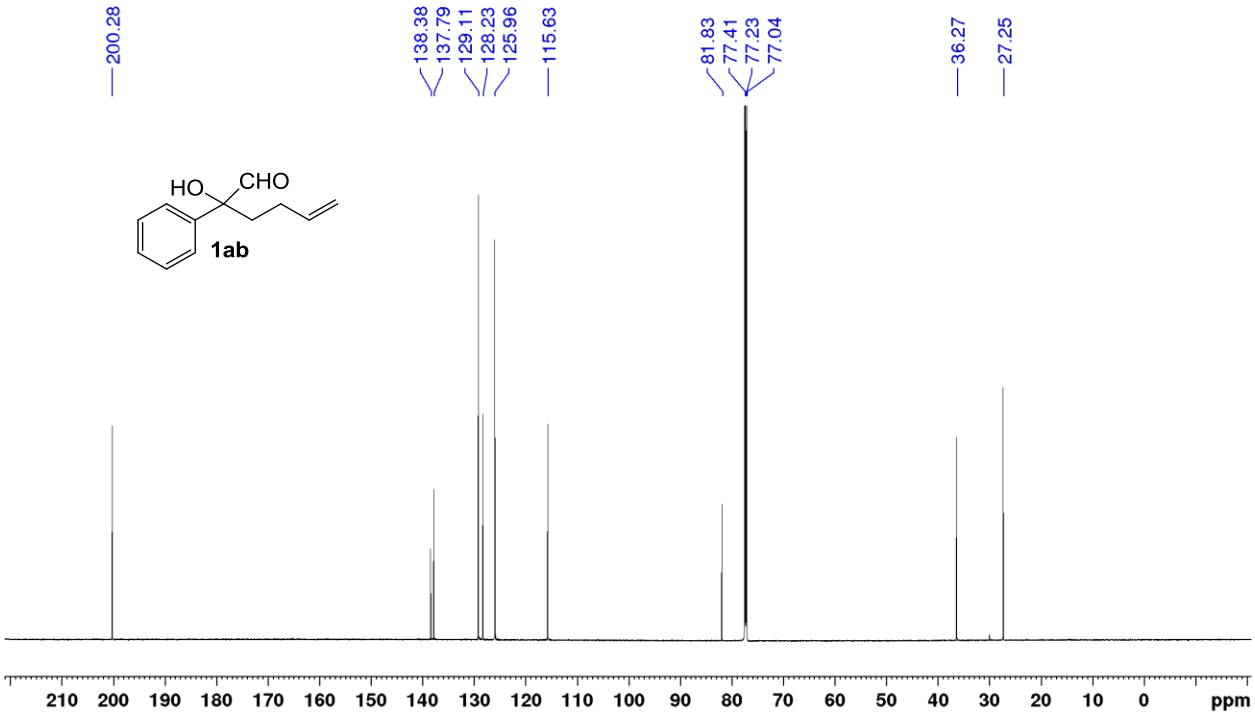
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1aa)



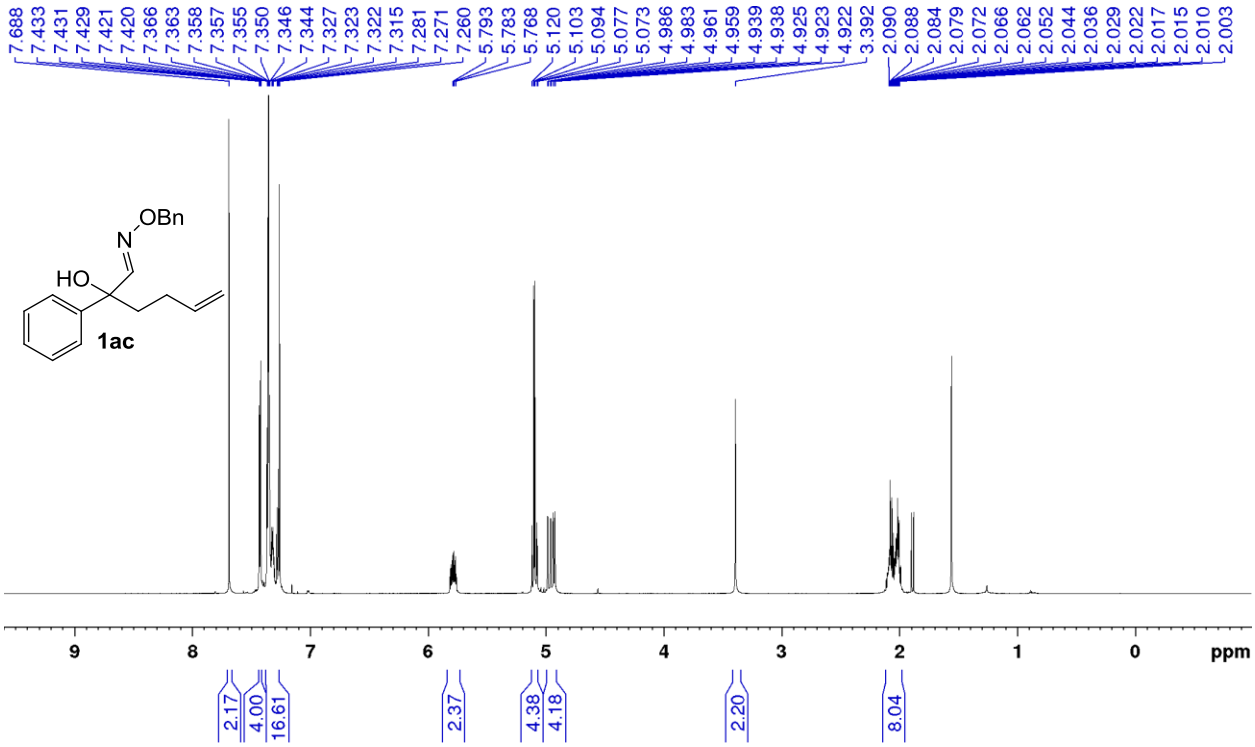
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1ab)



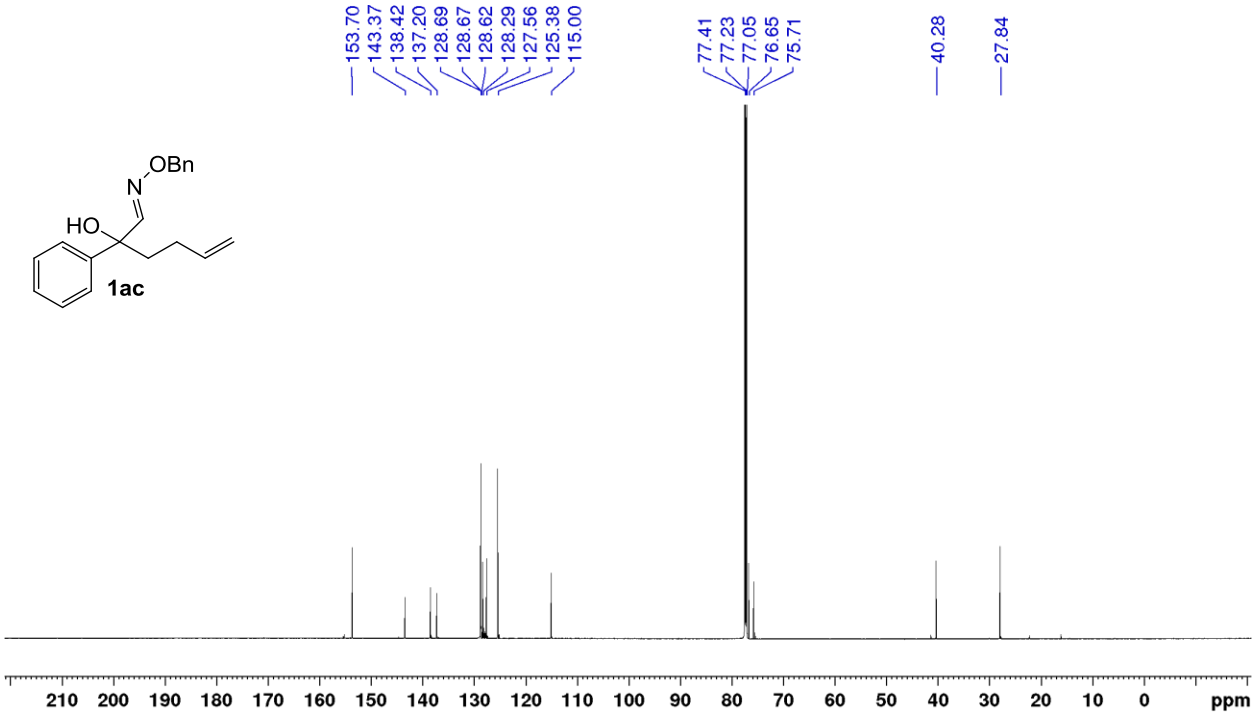
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1ab)



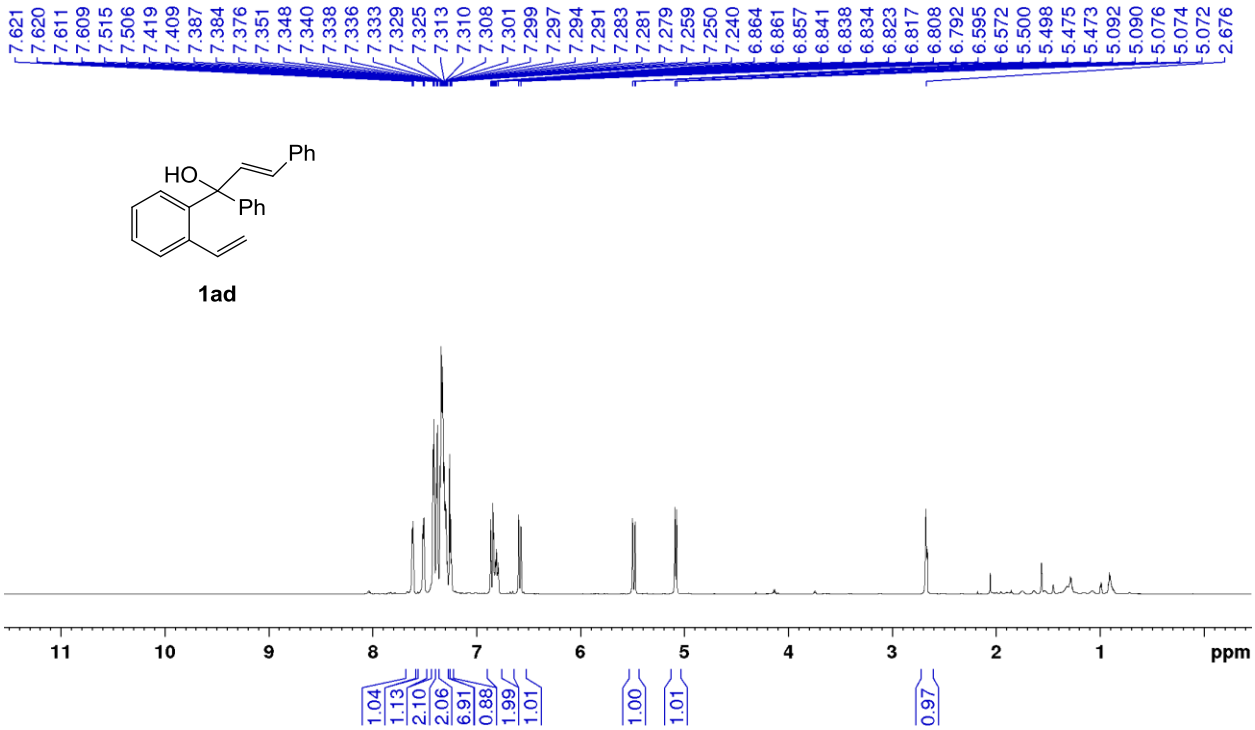
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1ac)



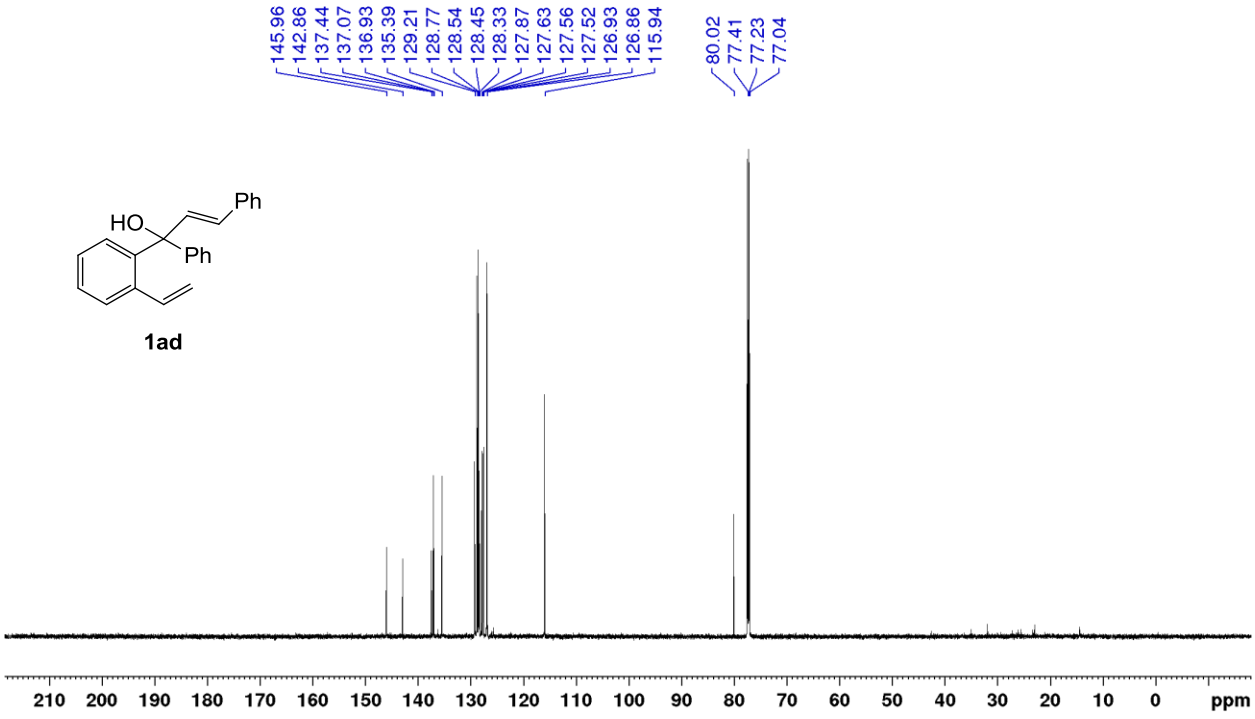
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1ac)



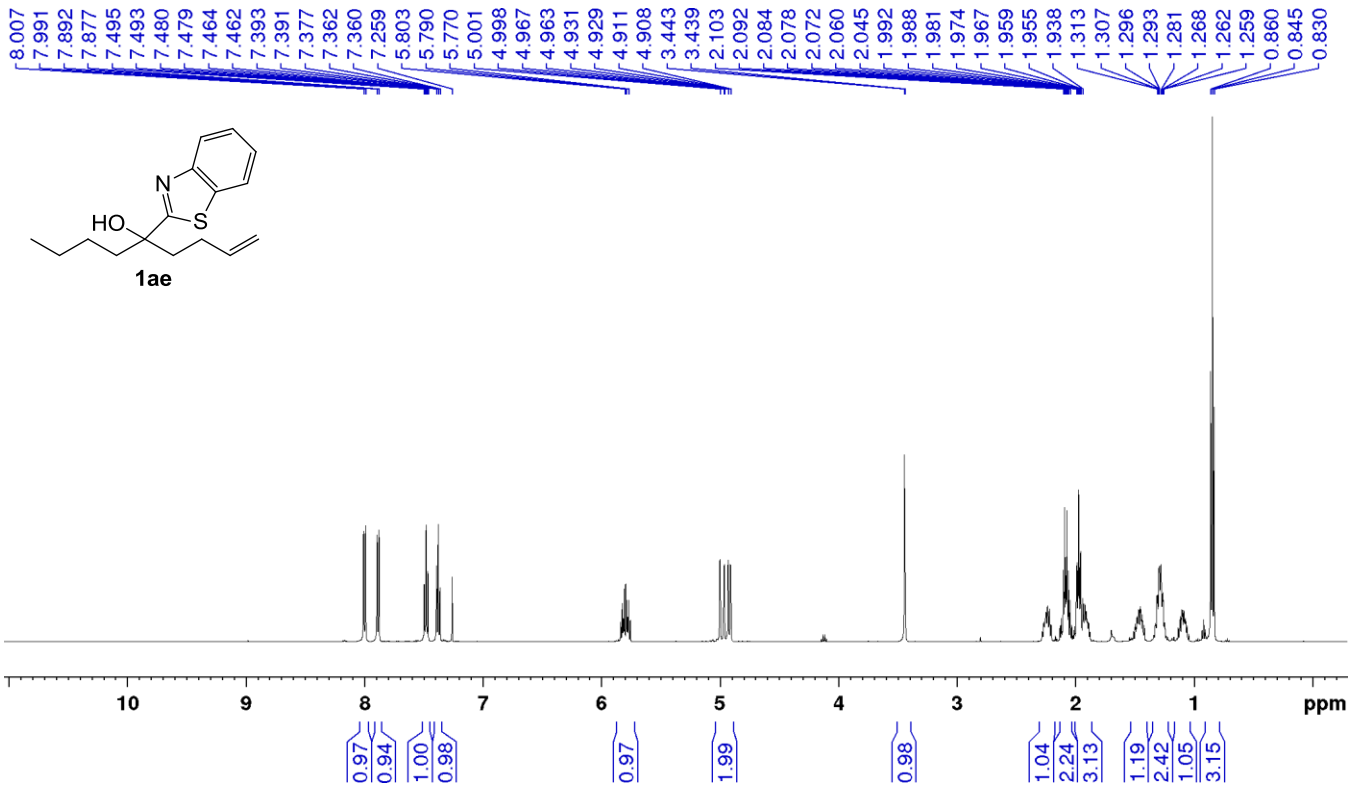
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (1ad)



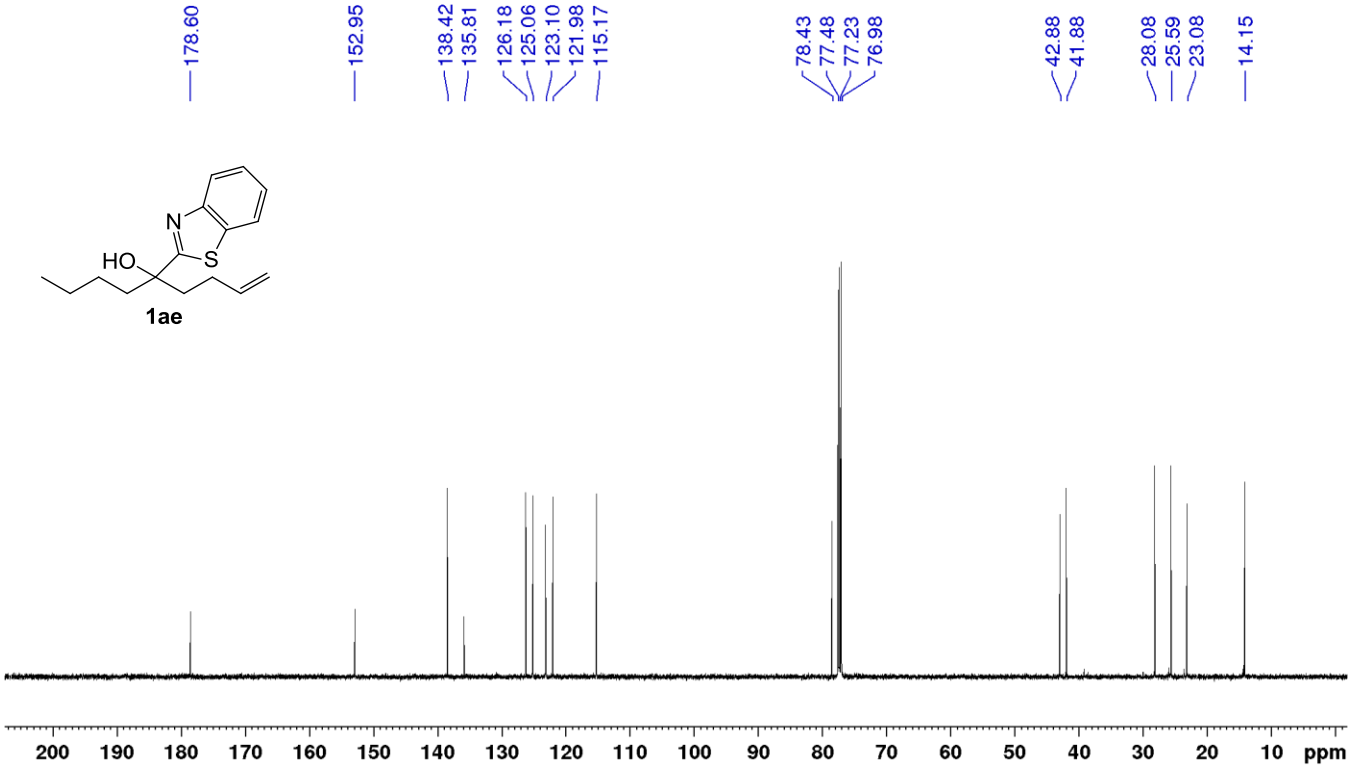
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (1ad)



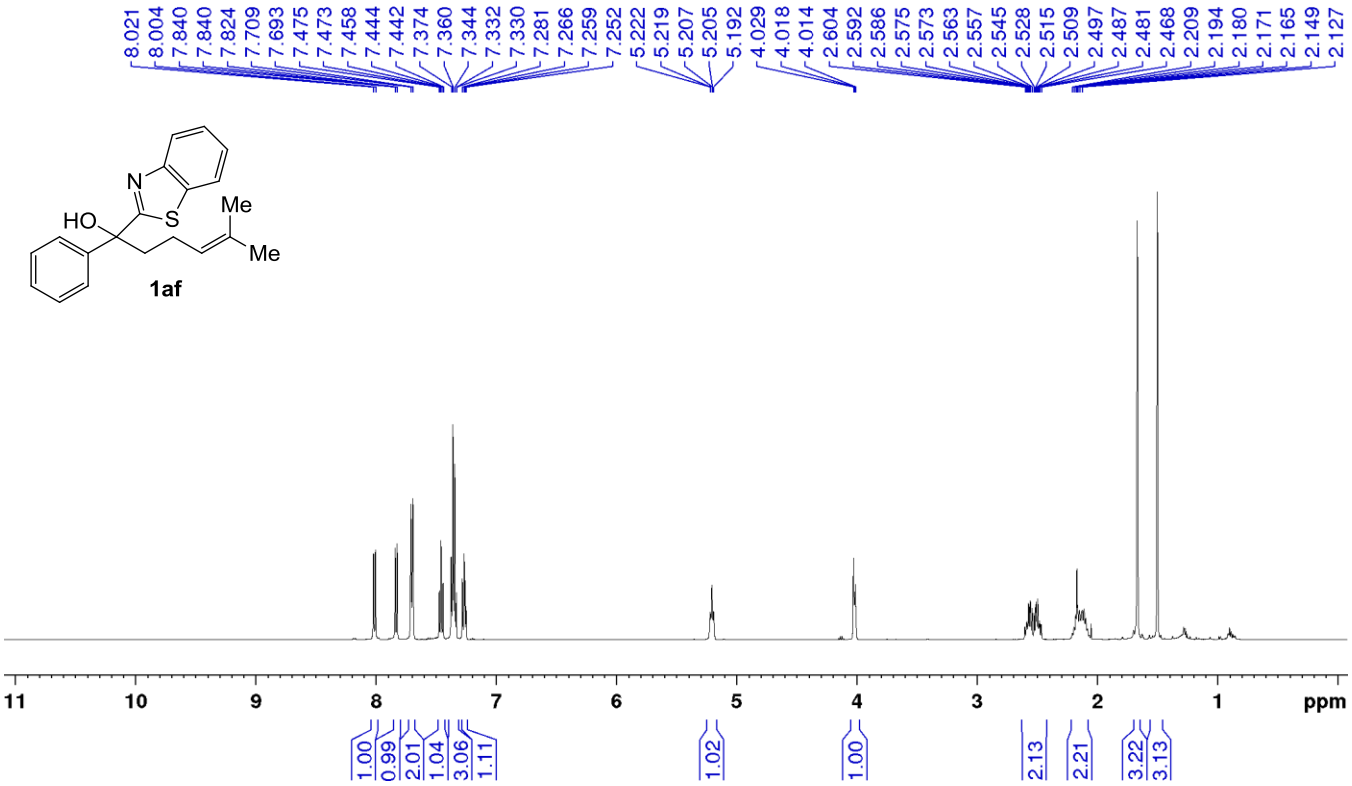
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1ae)



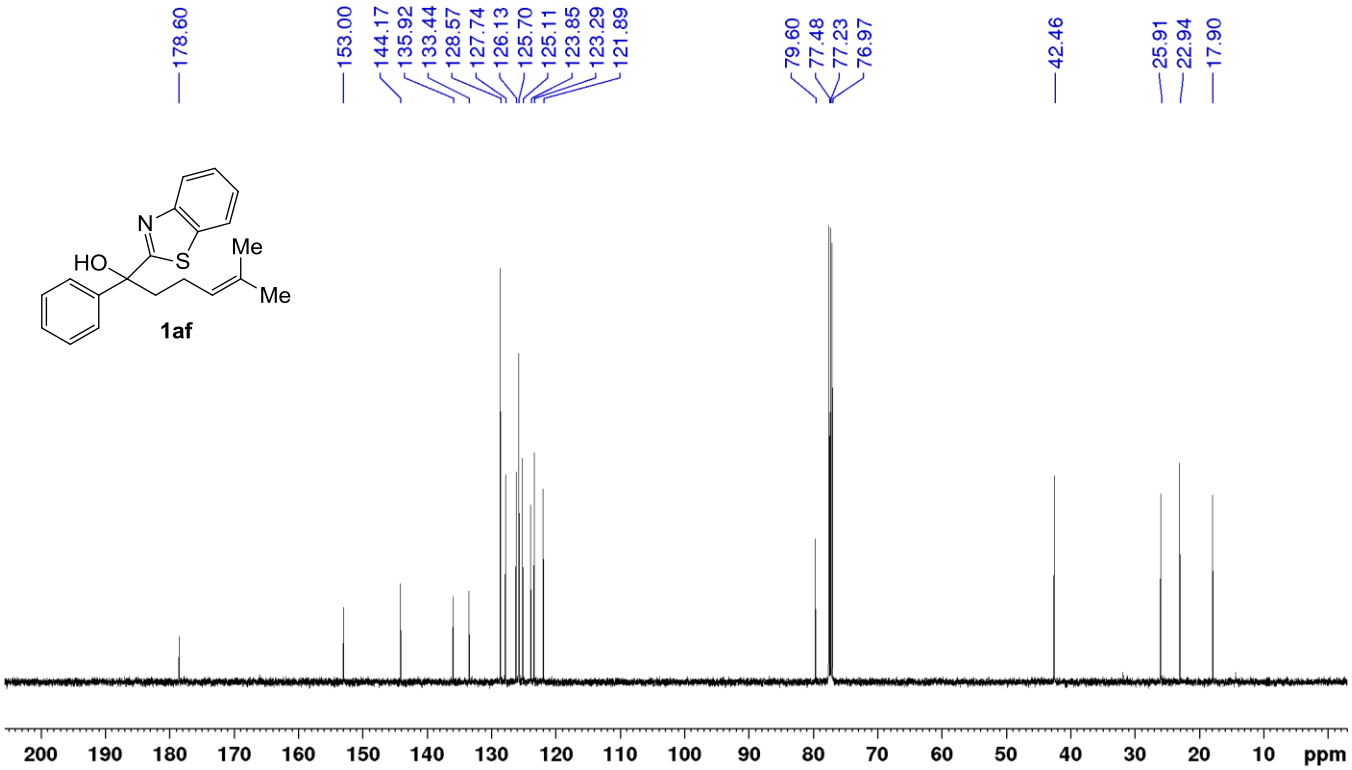
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1ae)



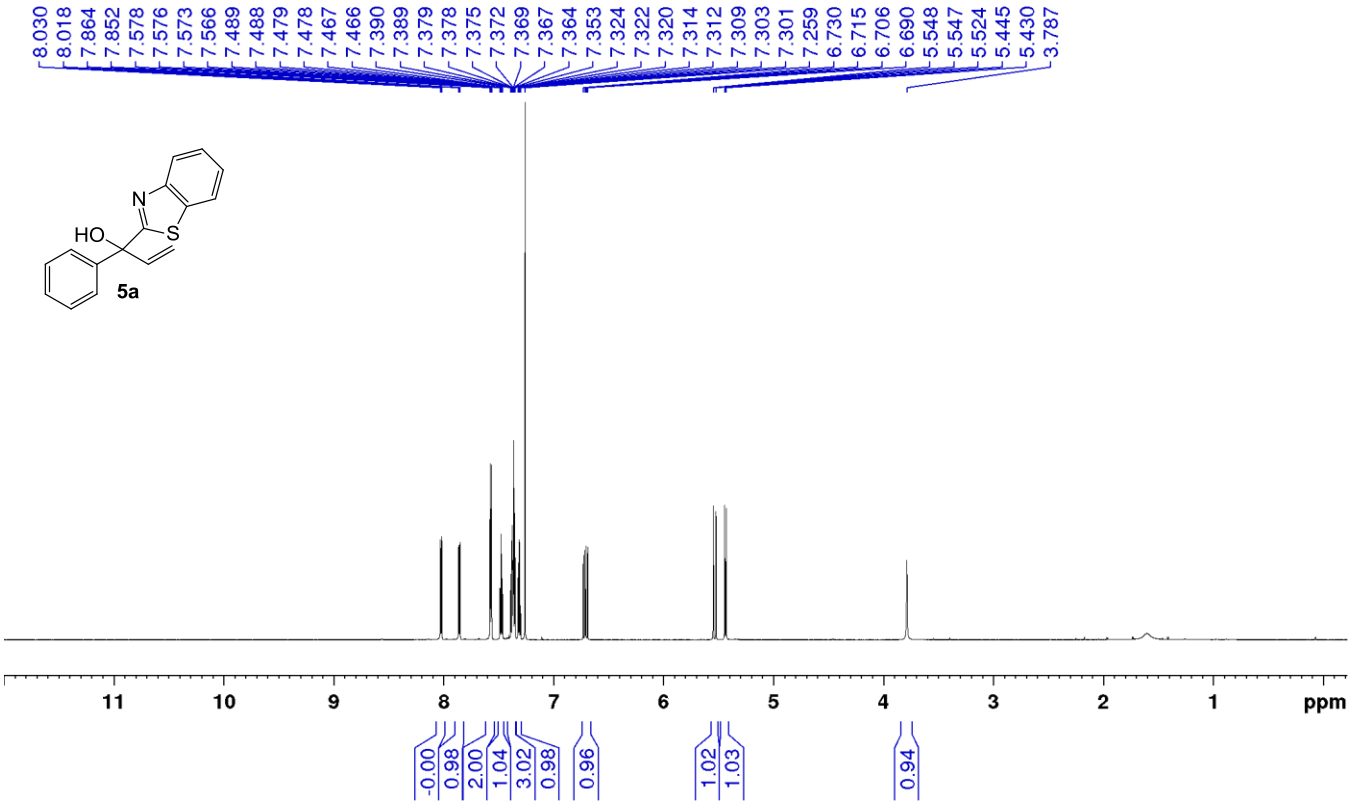
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (1af)



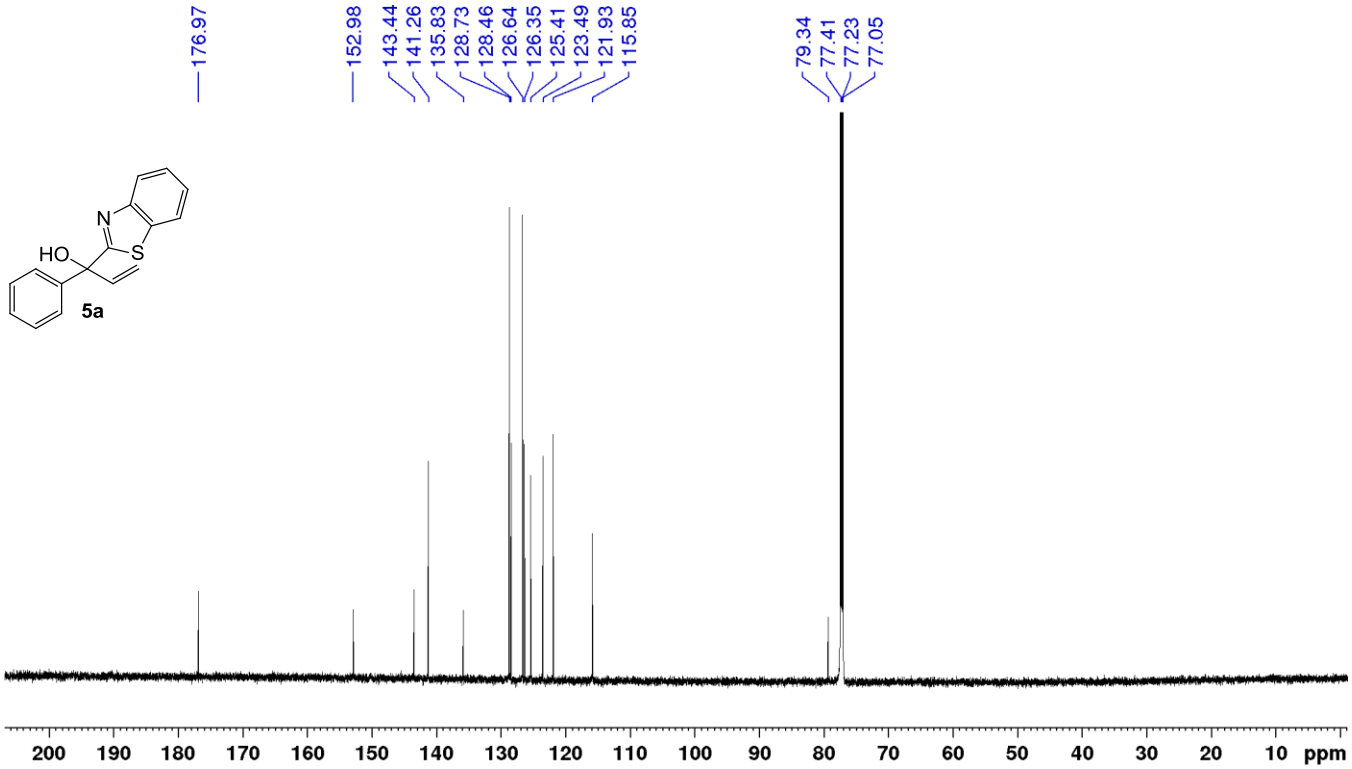
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (1af)



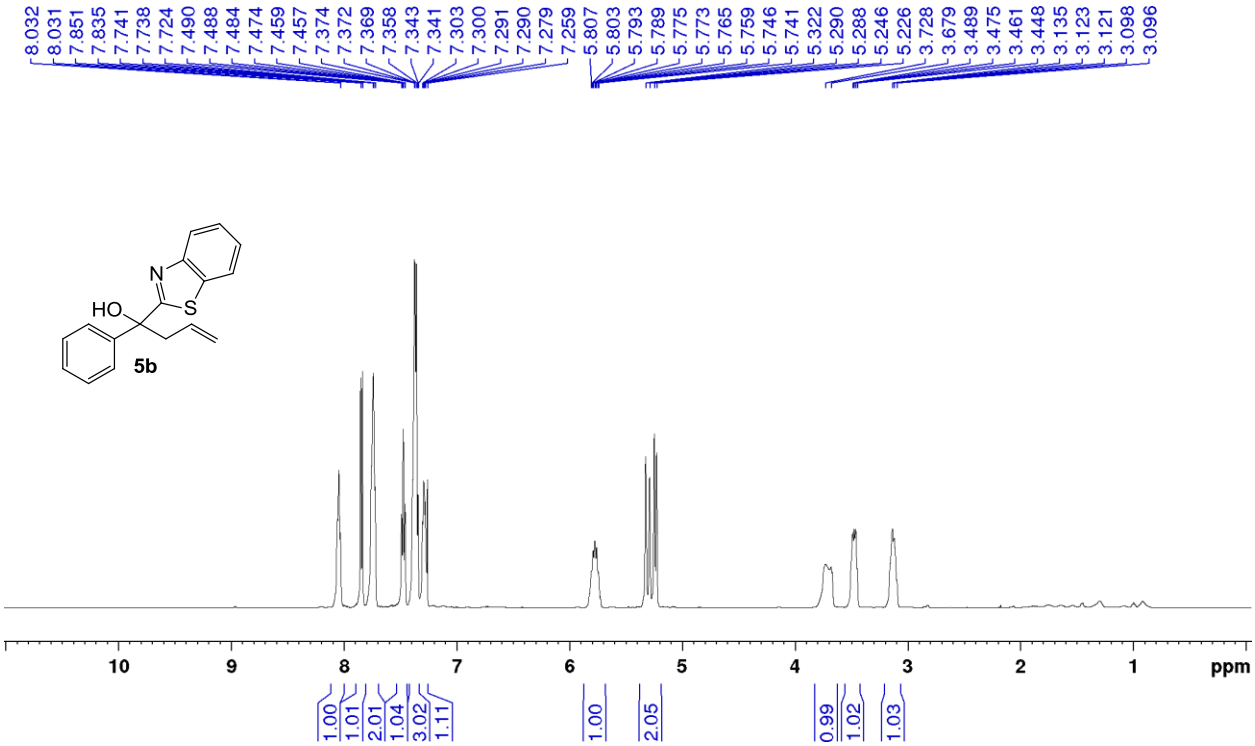
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (5a)



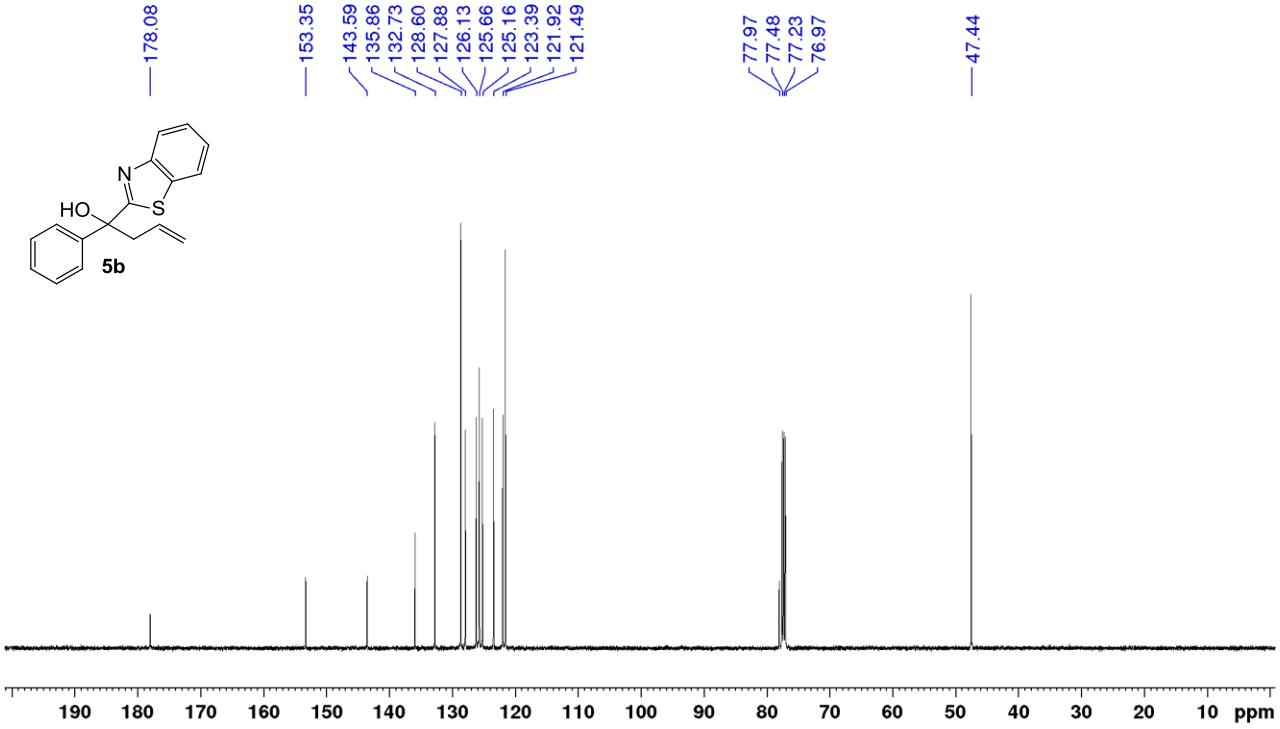
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (5a)



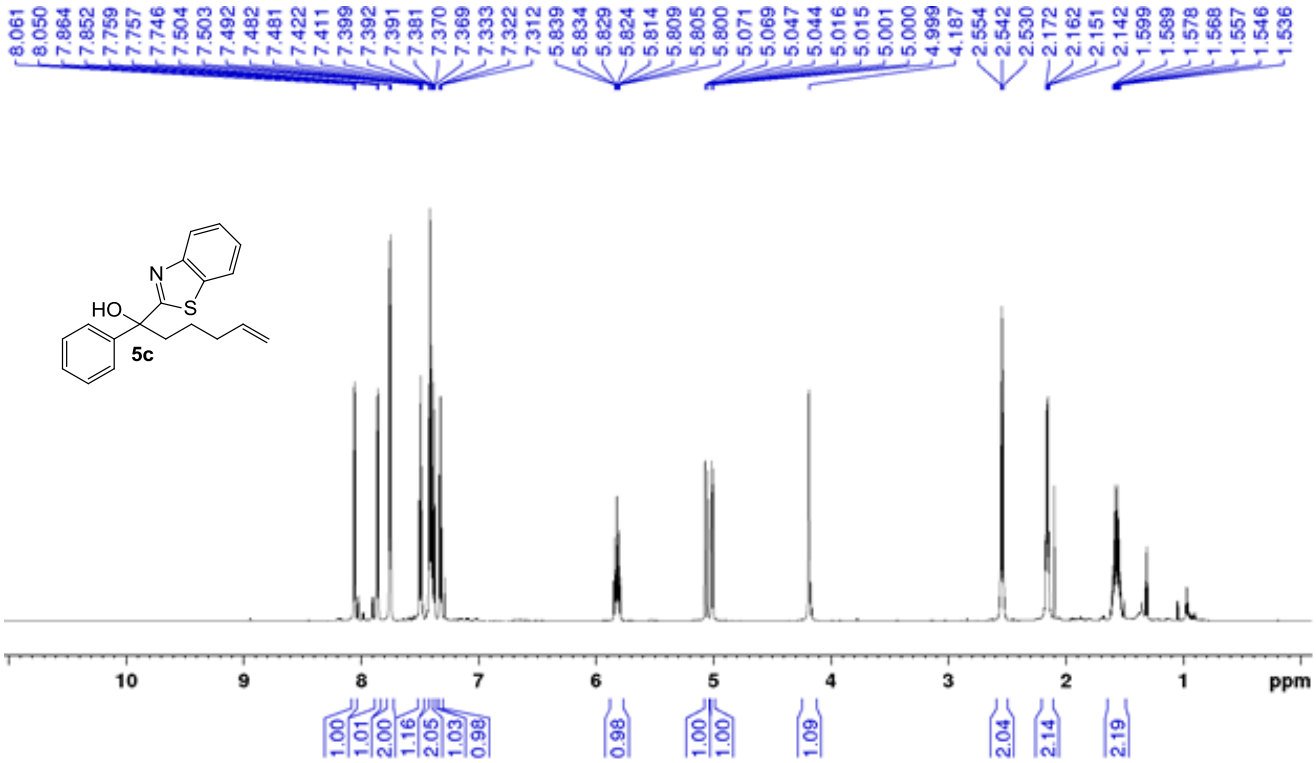
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5b)



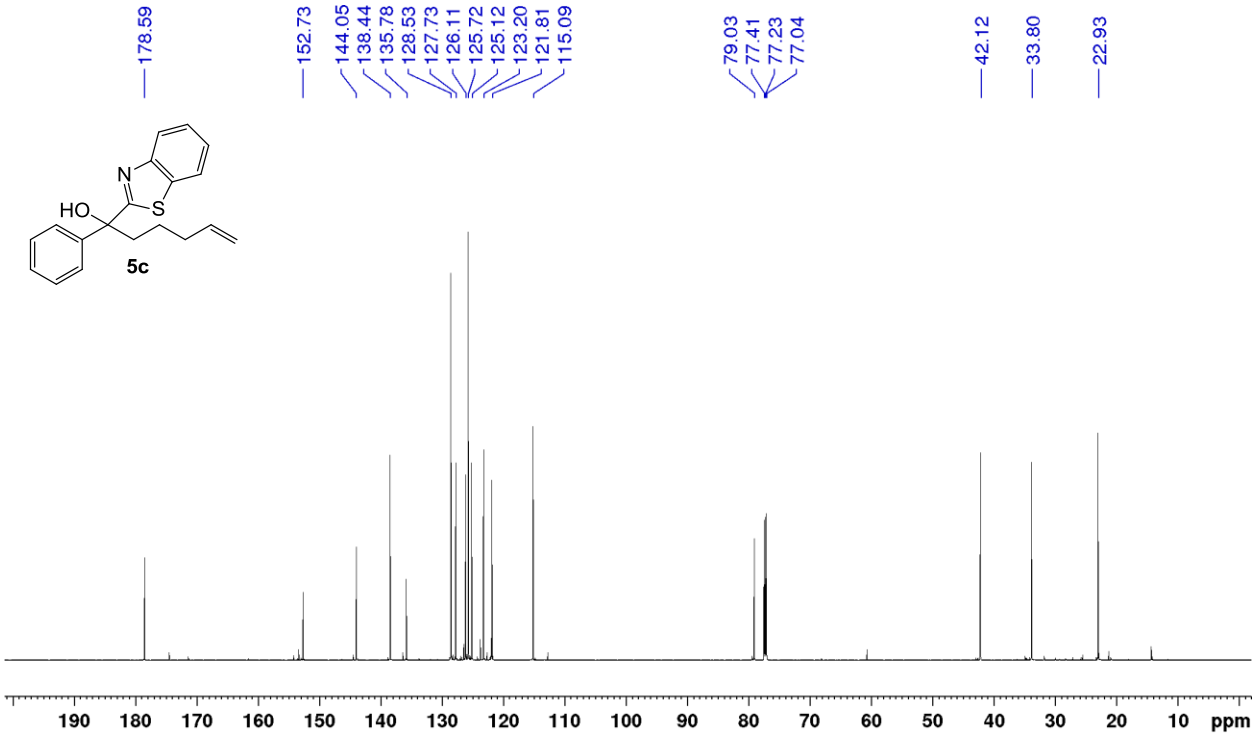
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5b)



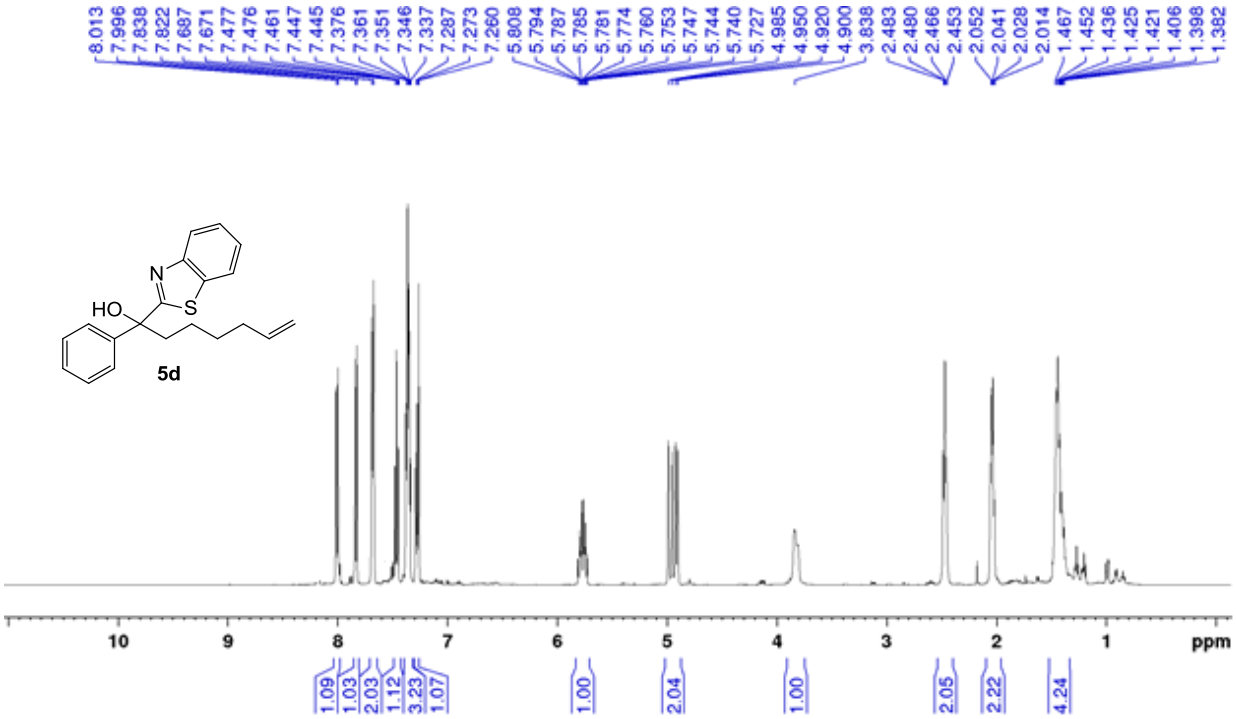
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (5c)



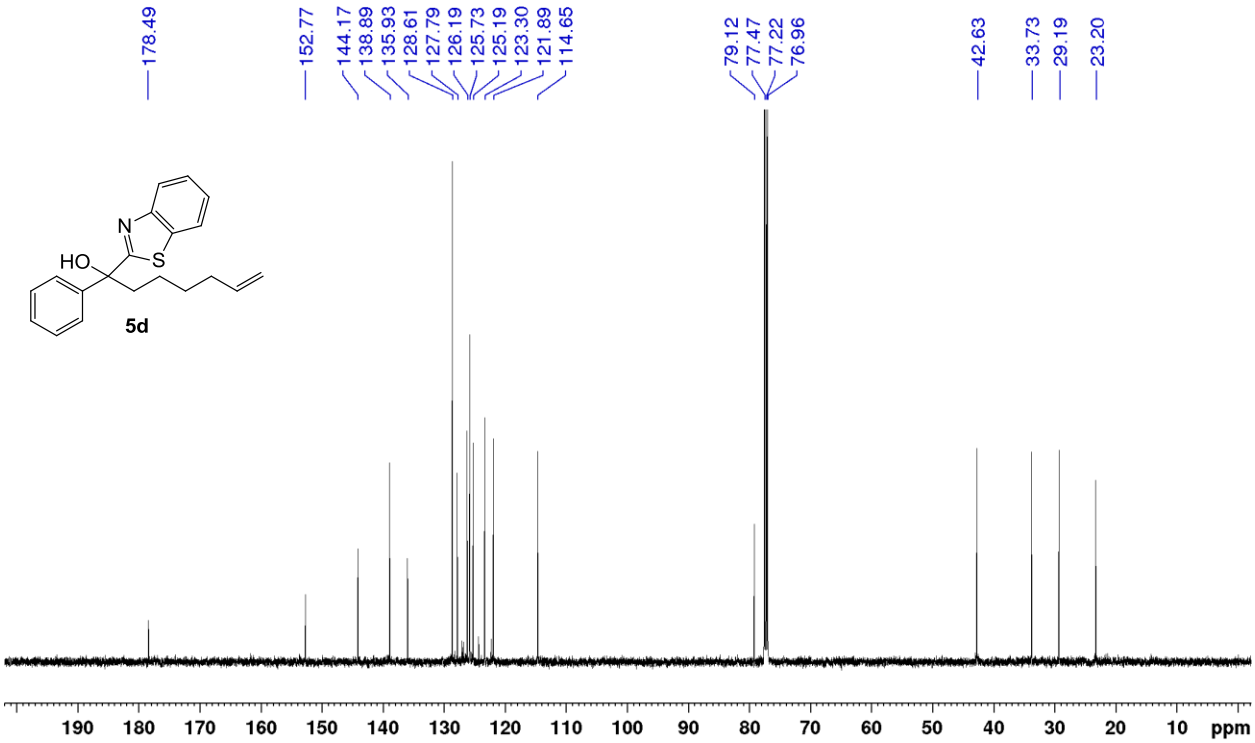
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (5c)



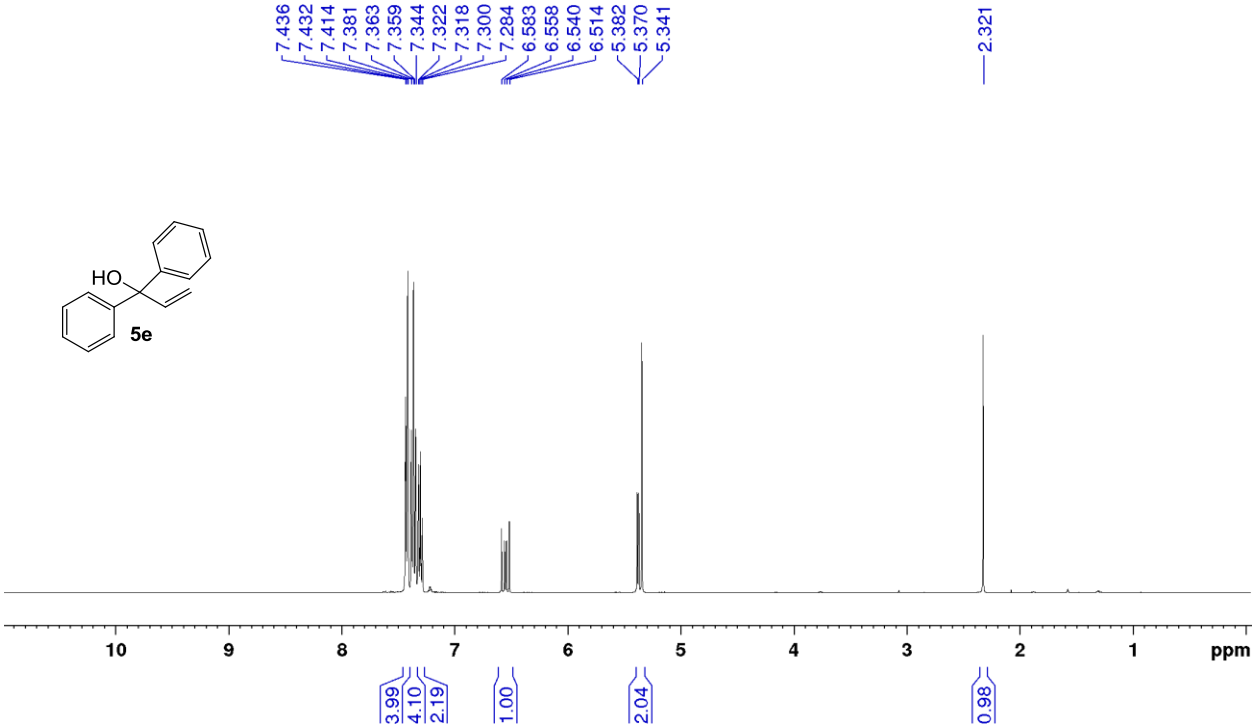
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (5d)



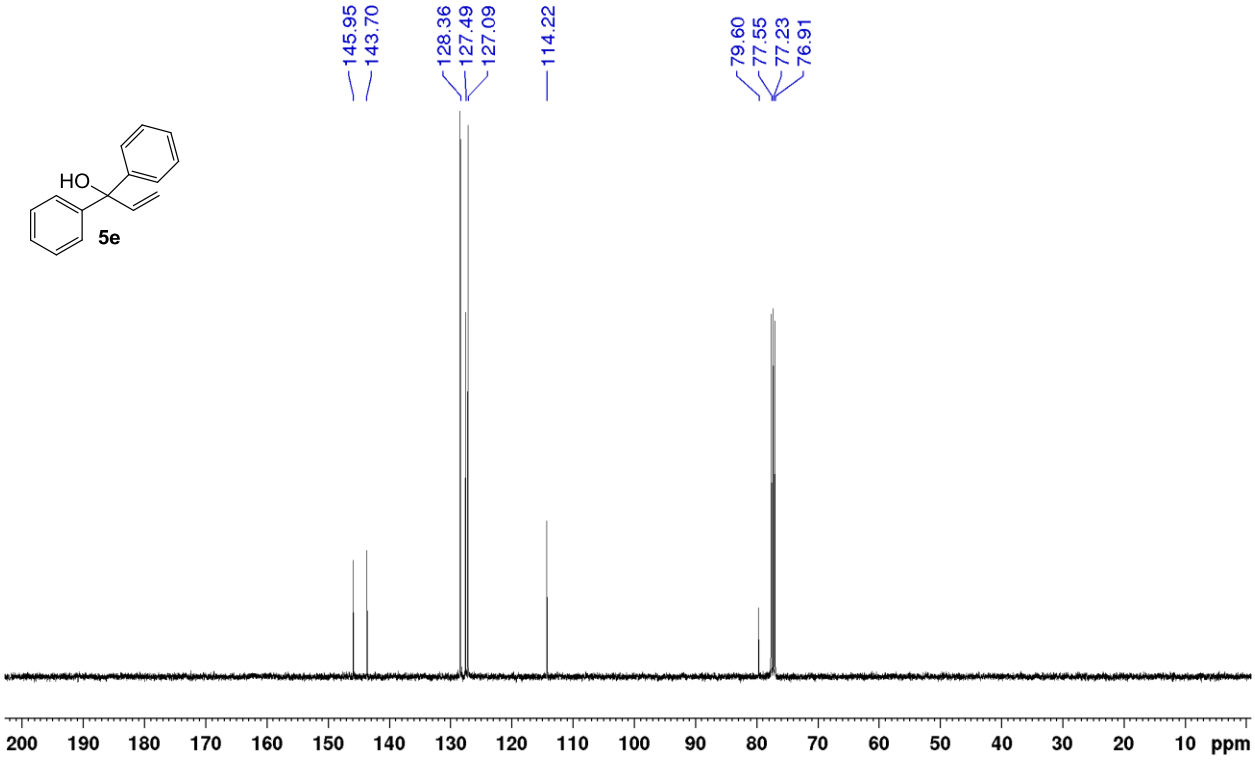
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (5d)



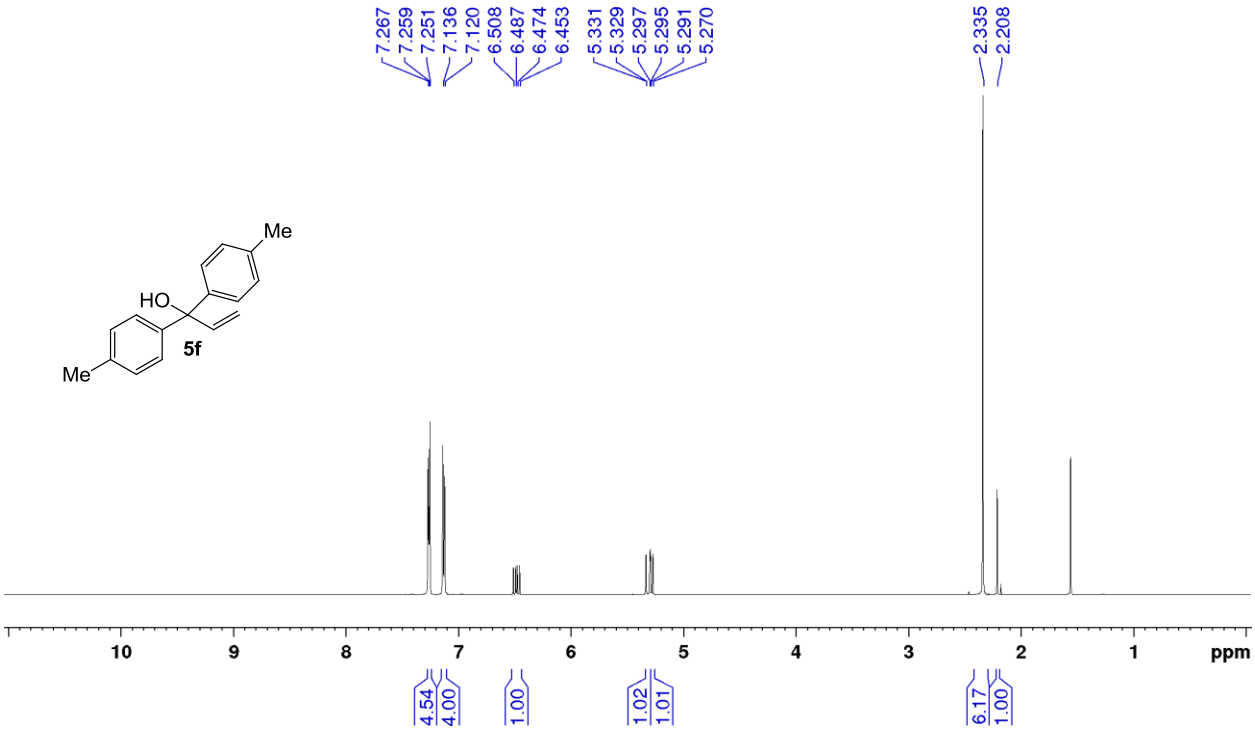
^{1}H NMR (400 MHz, $CDCl_3$, 25 ºC) of (5e)



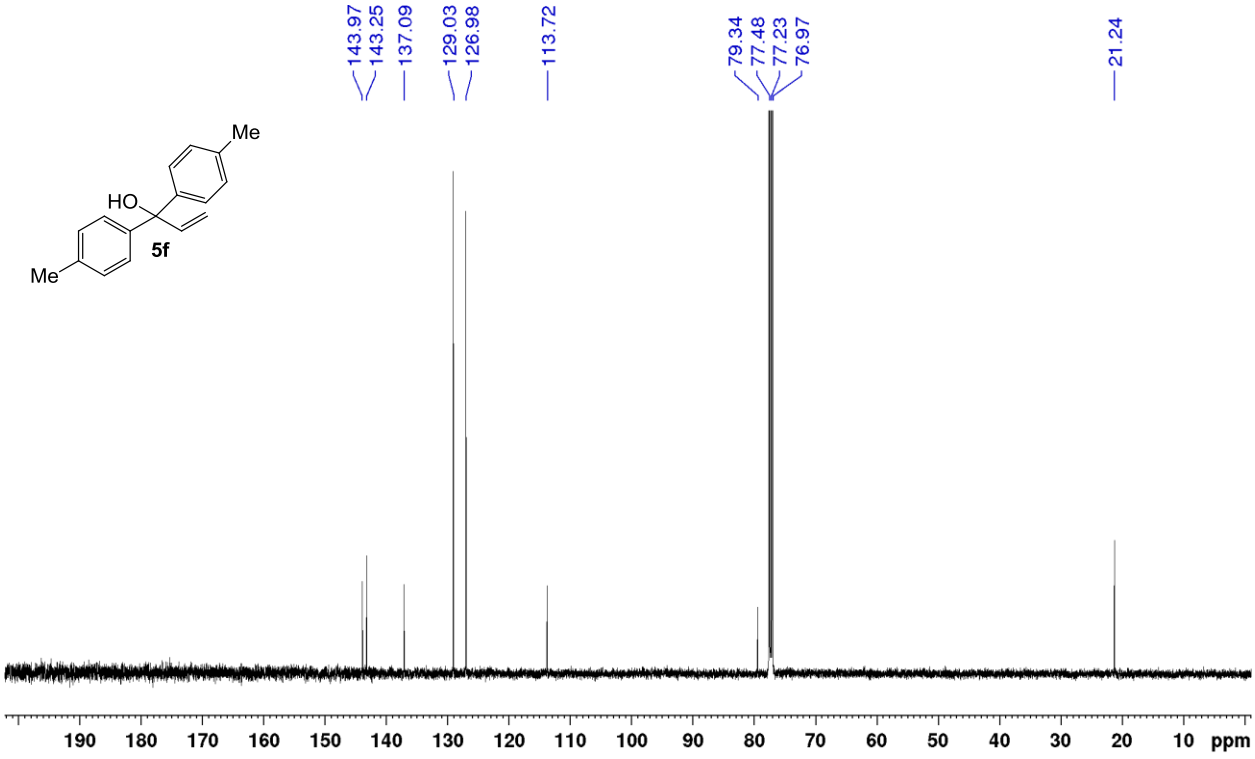
^{13}C NMR (100 MHz, $CDCl_3$, 25 ºC) of (5e)



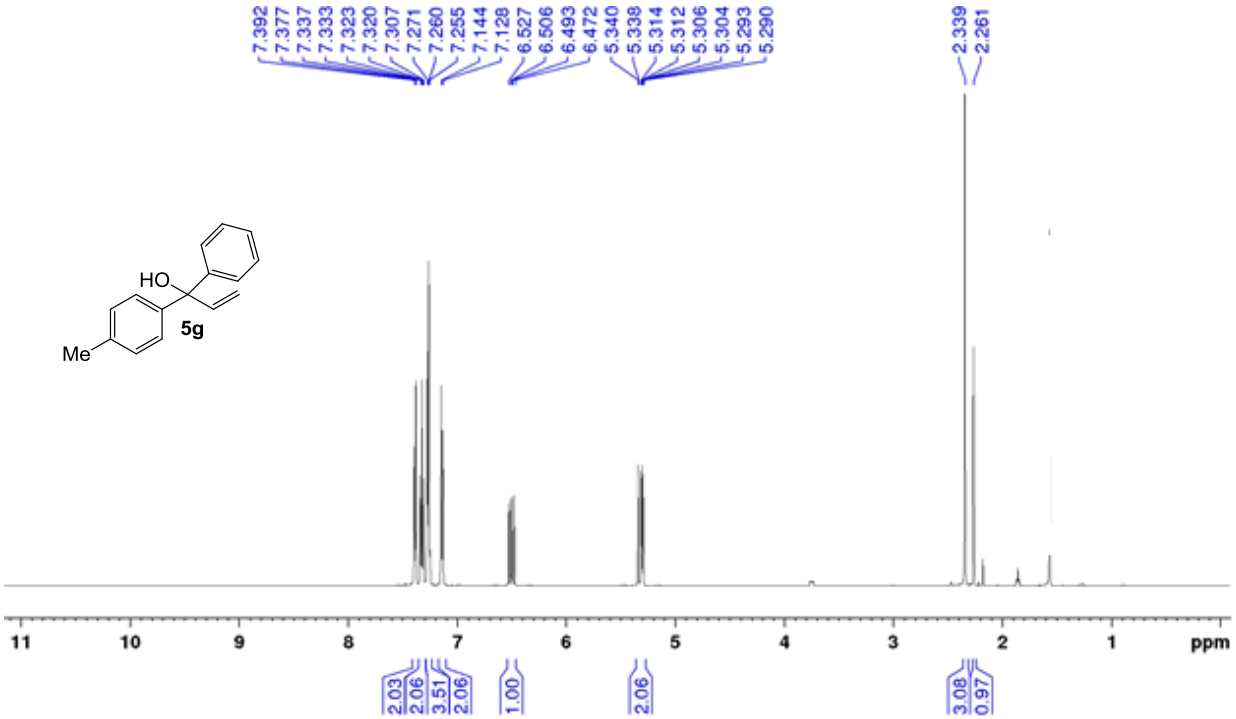
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5f)



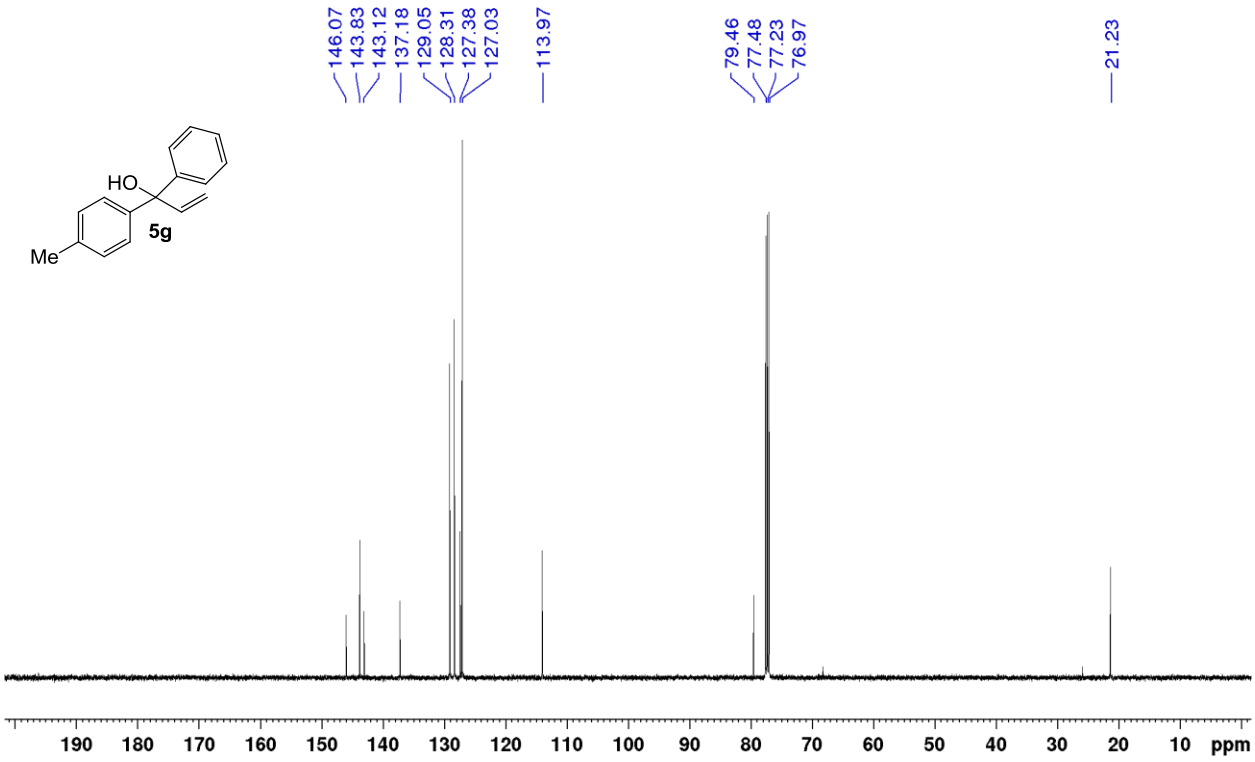
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5f)



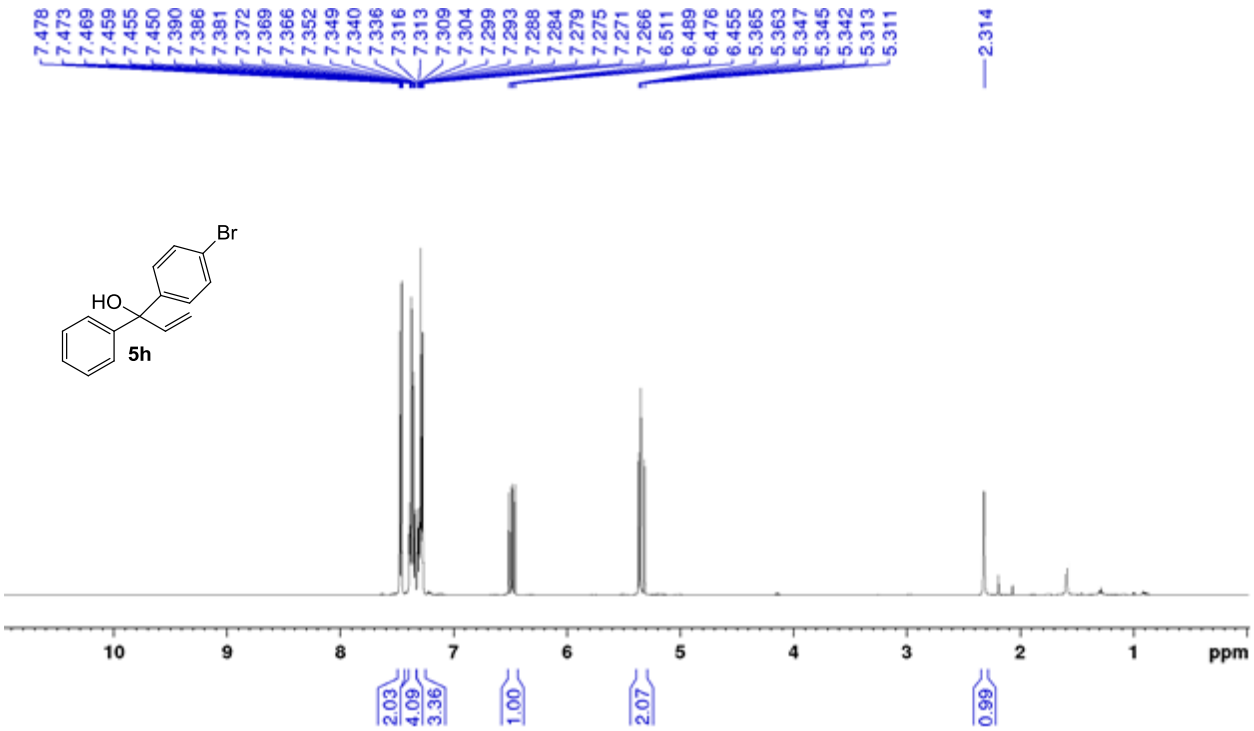
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5g)



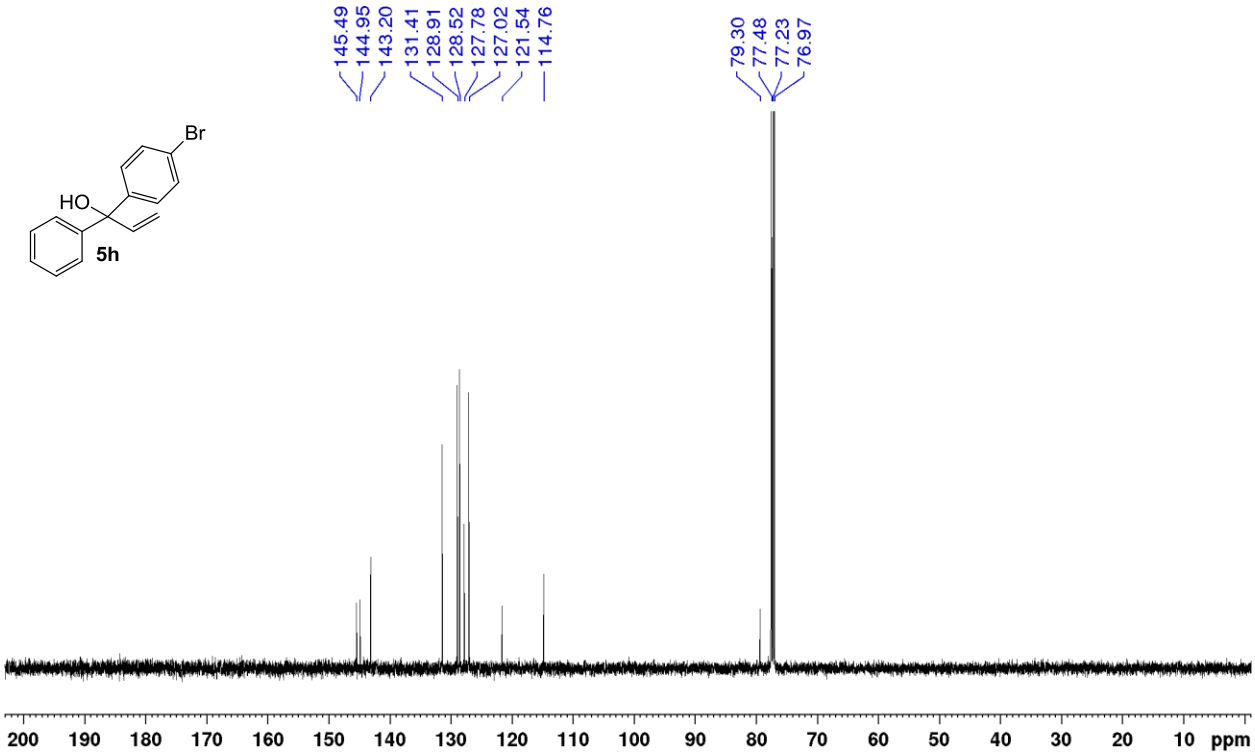
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5g)



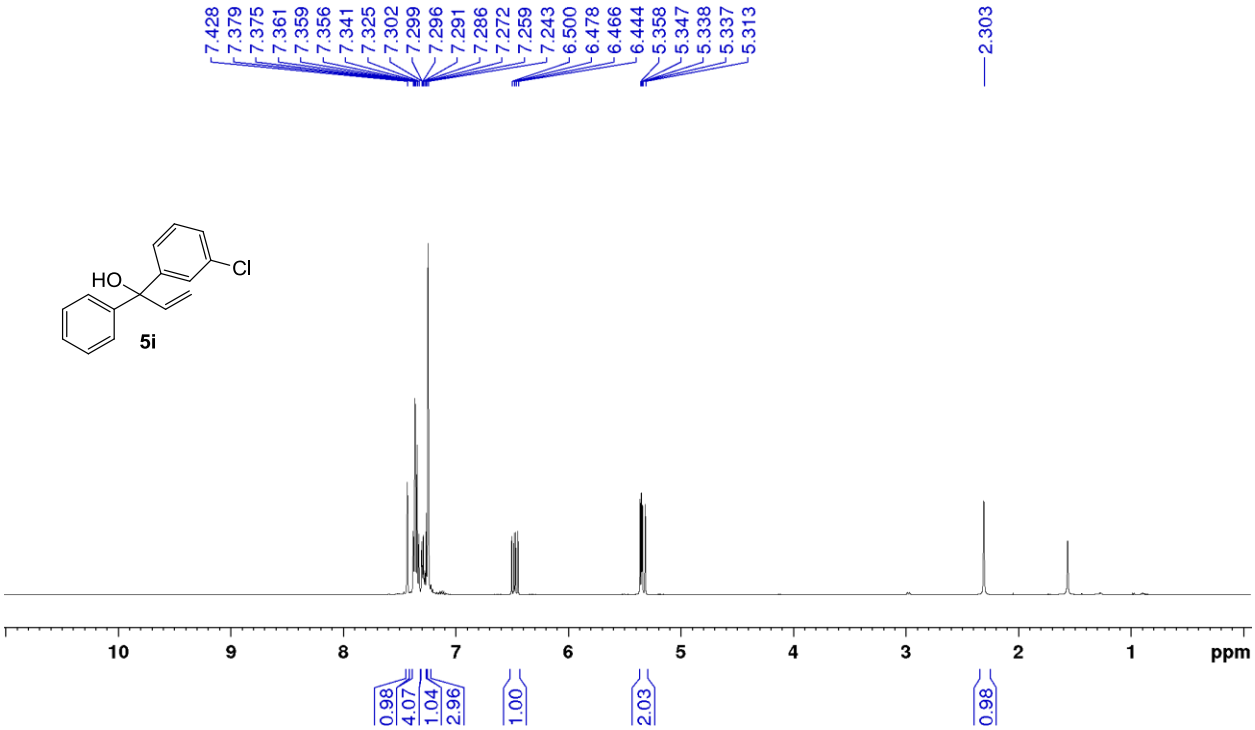
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5h)



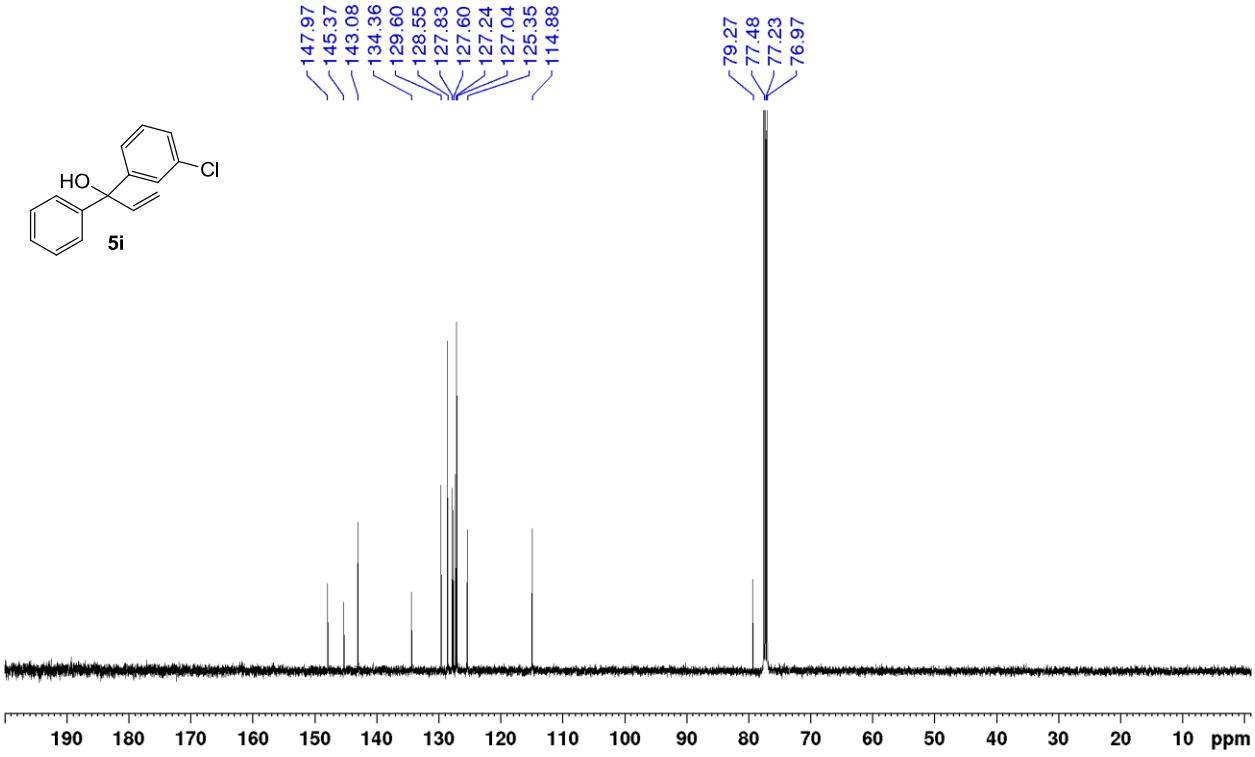
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5h)



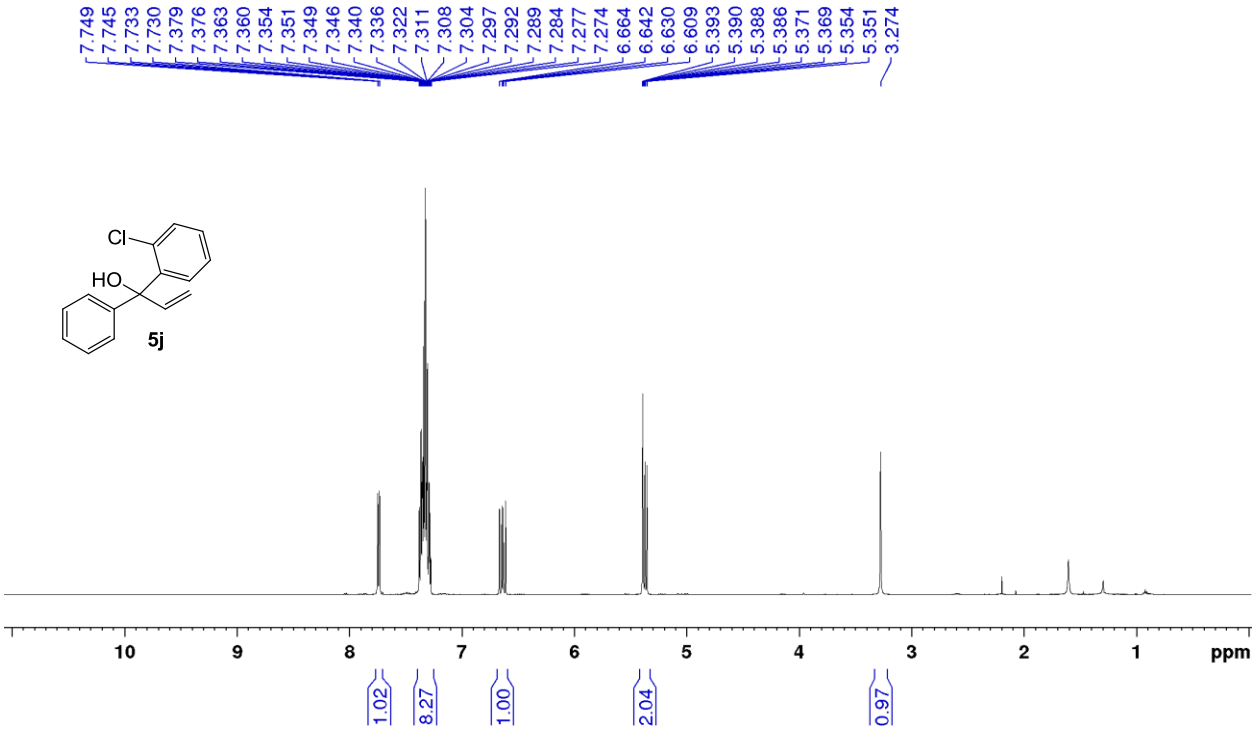
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5i)



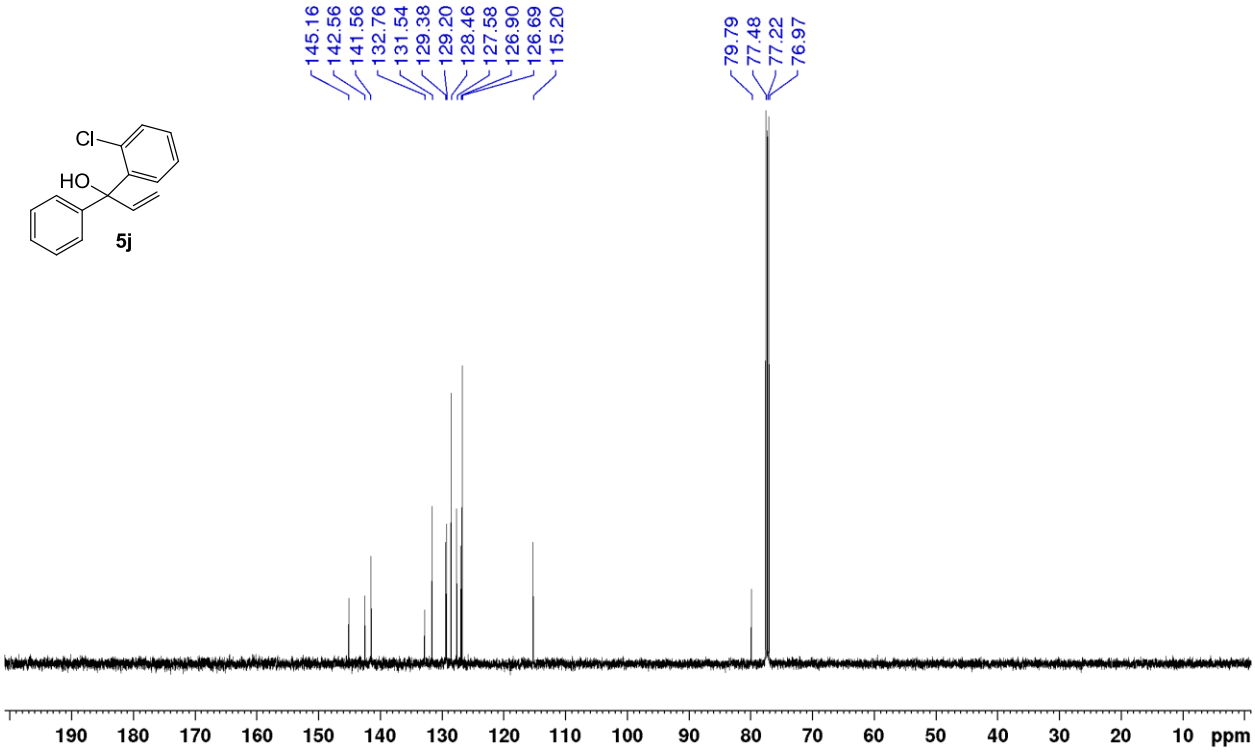
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5i)



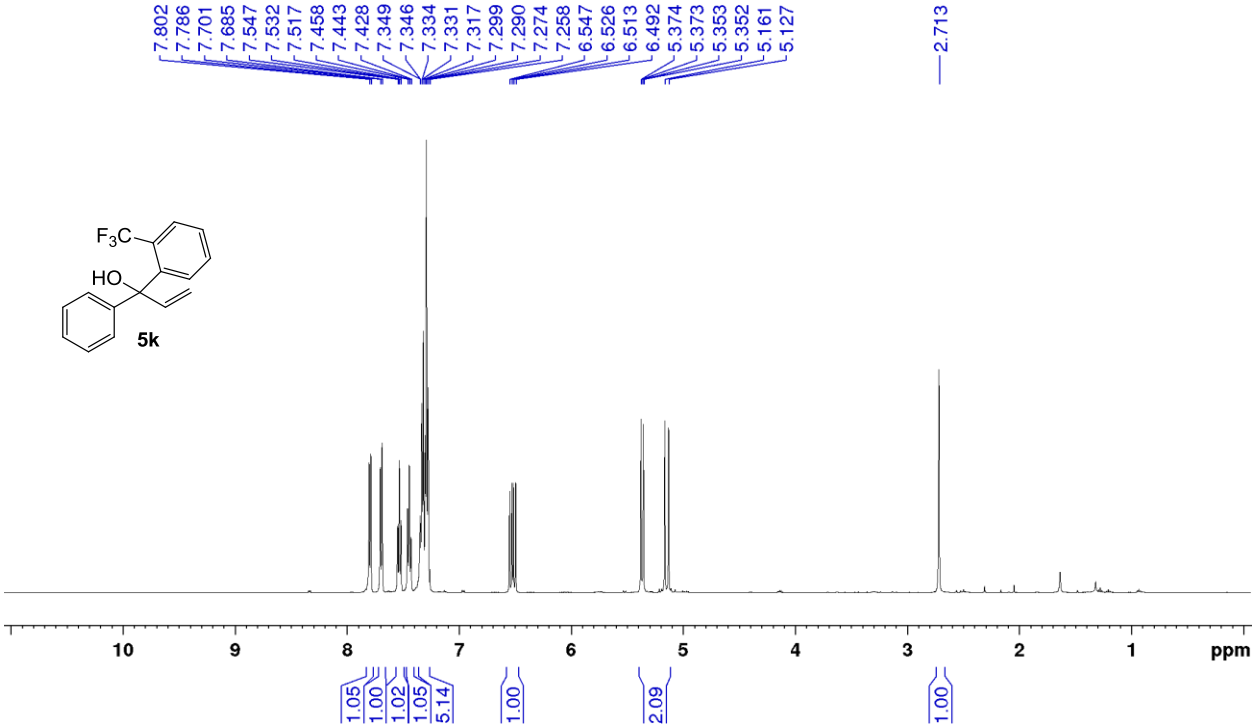
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (5j)



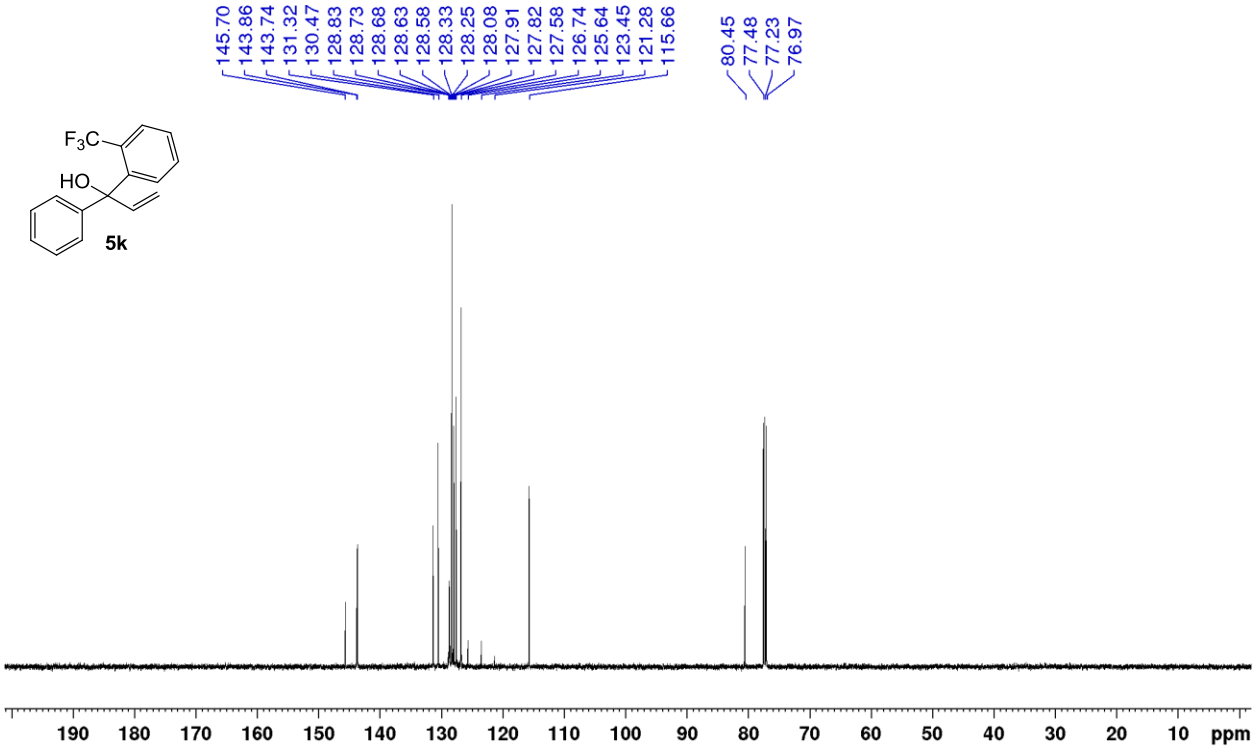
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (5j)



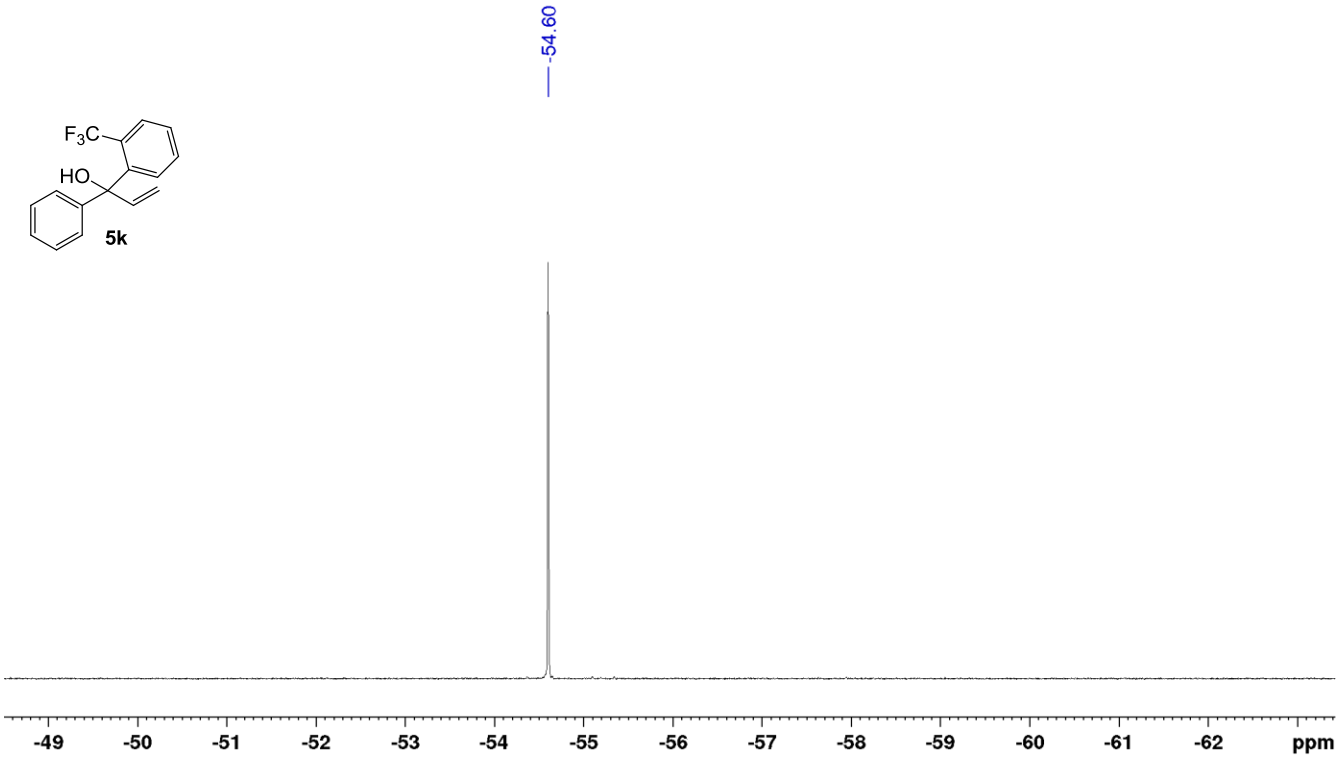
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (5k)



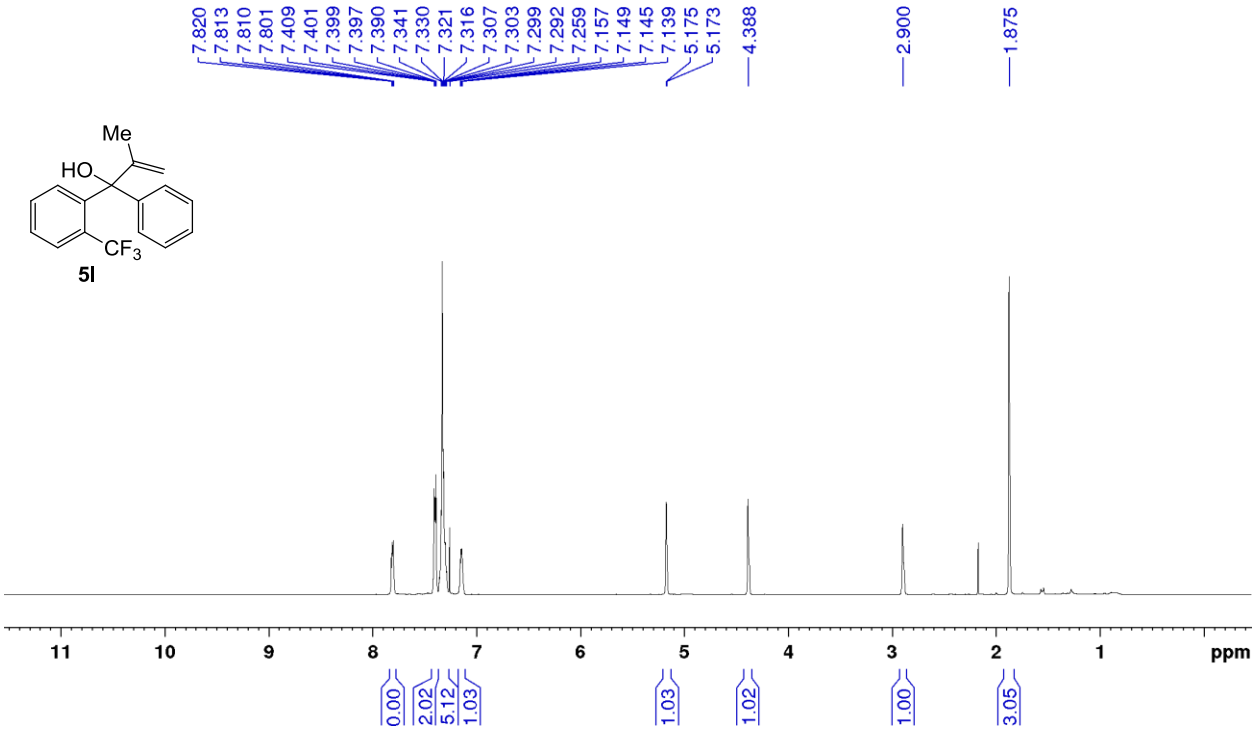
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (5k)



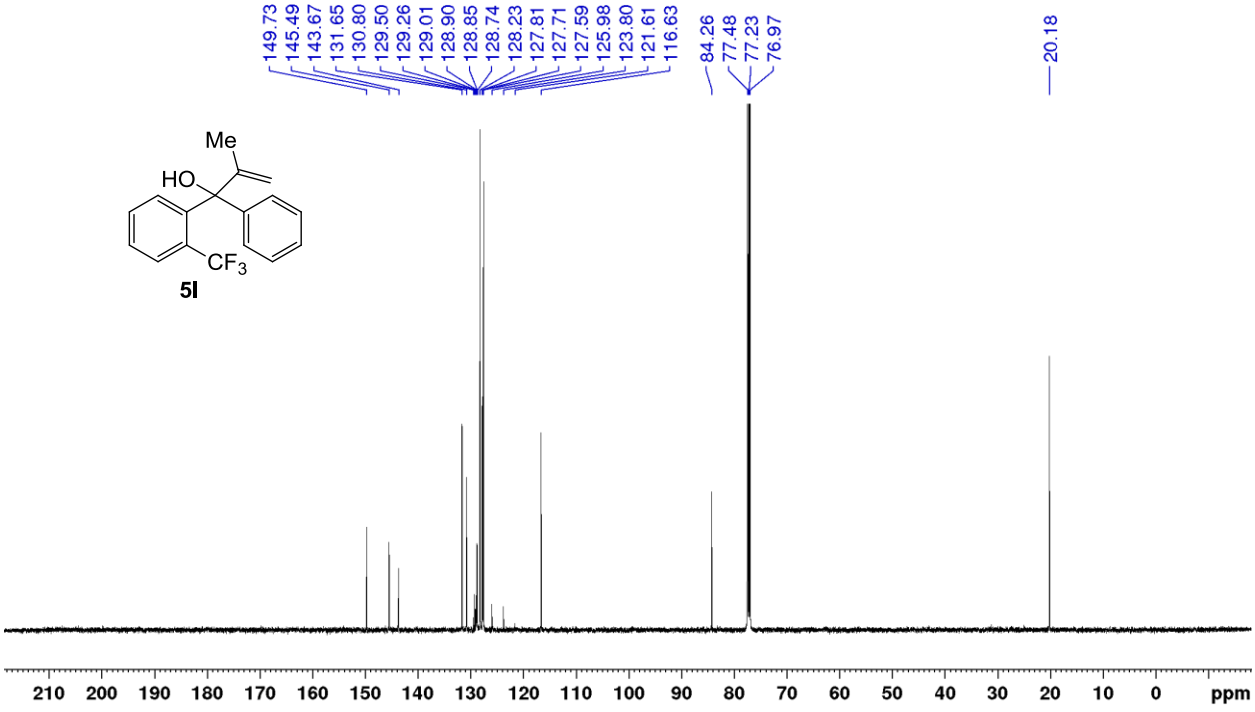
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (5k)



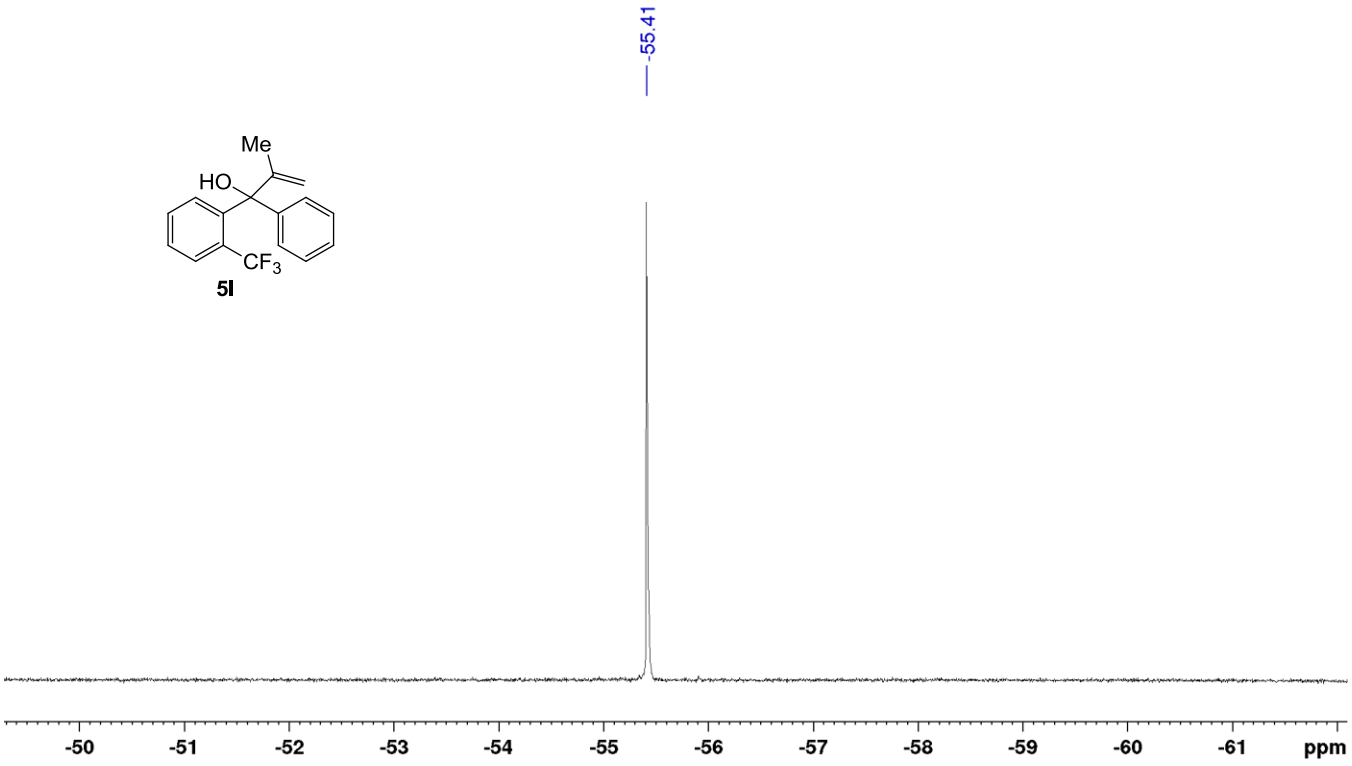
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5l)



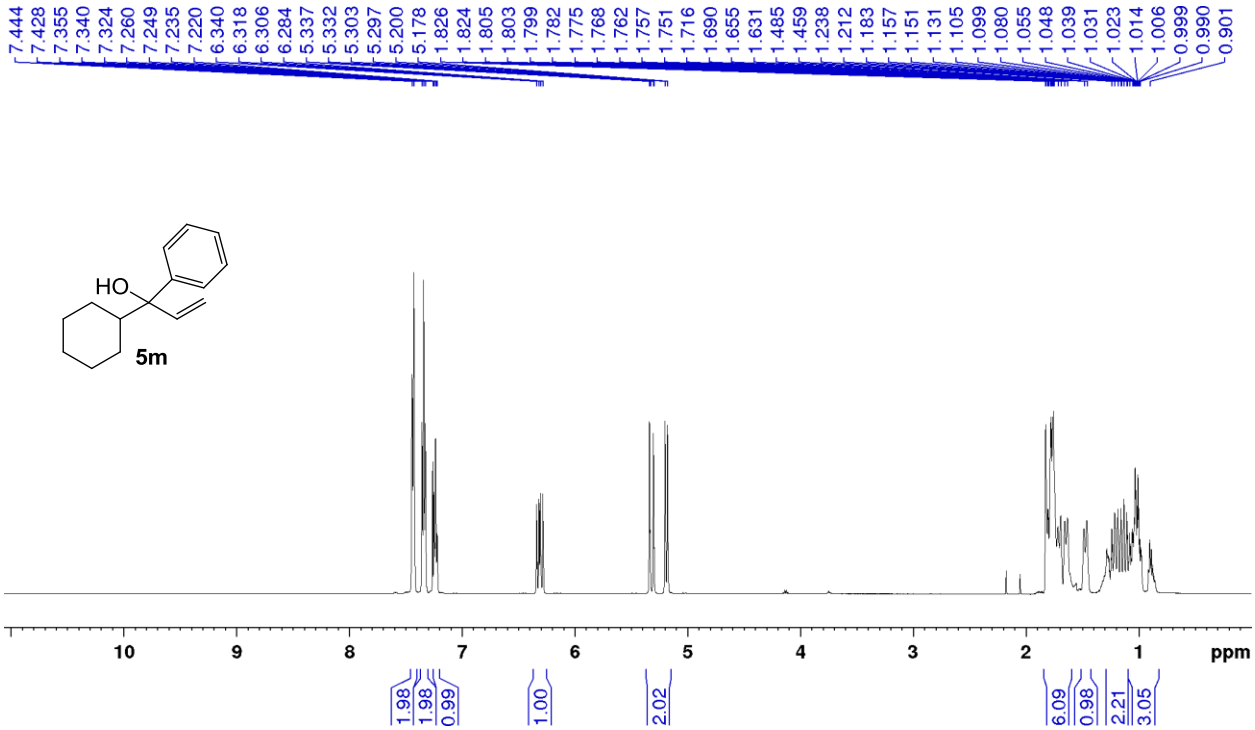
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5l)



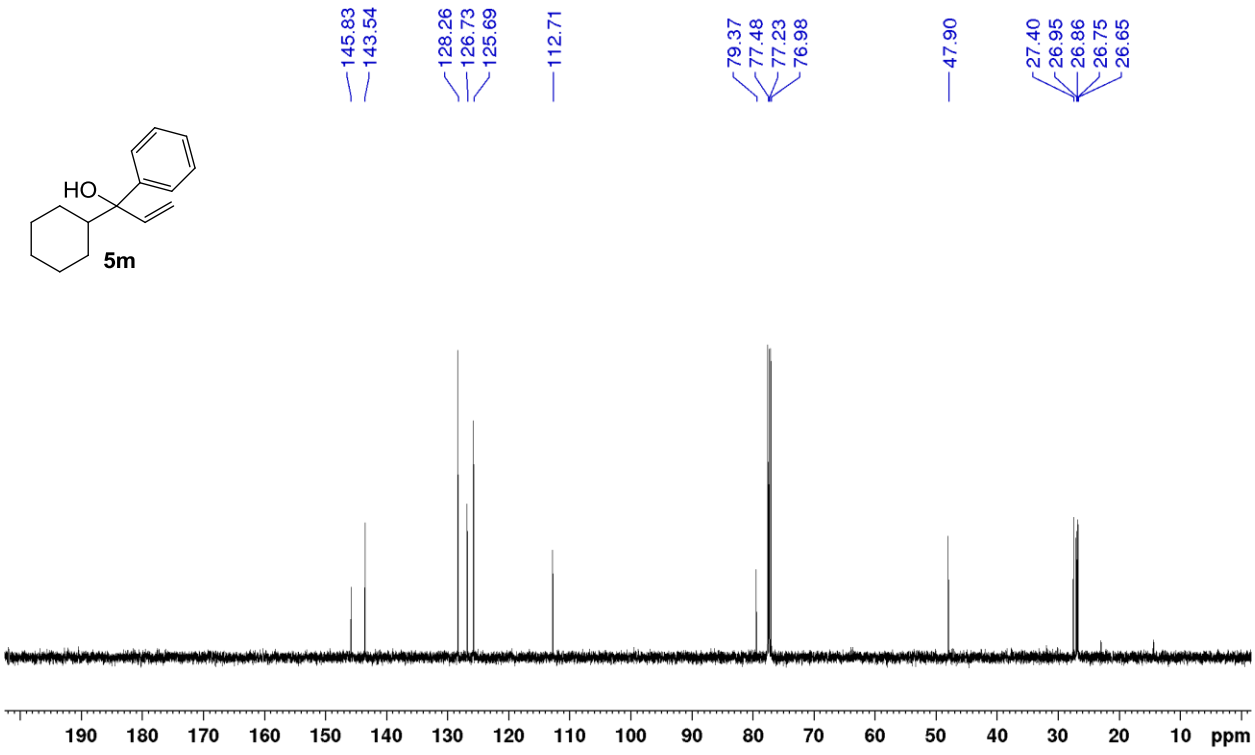
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (5l)



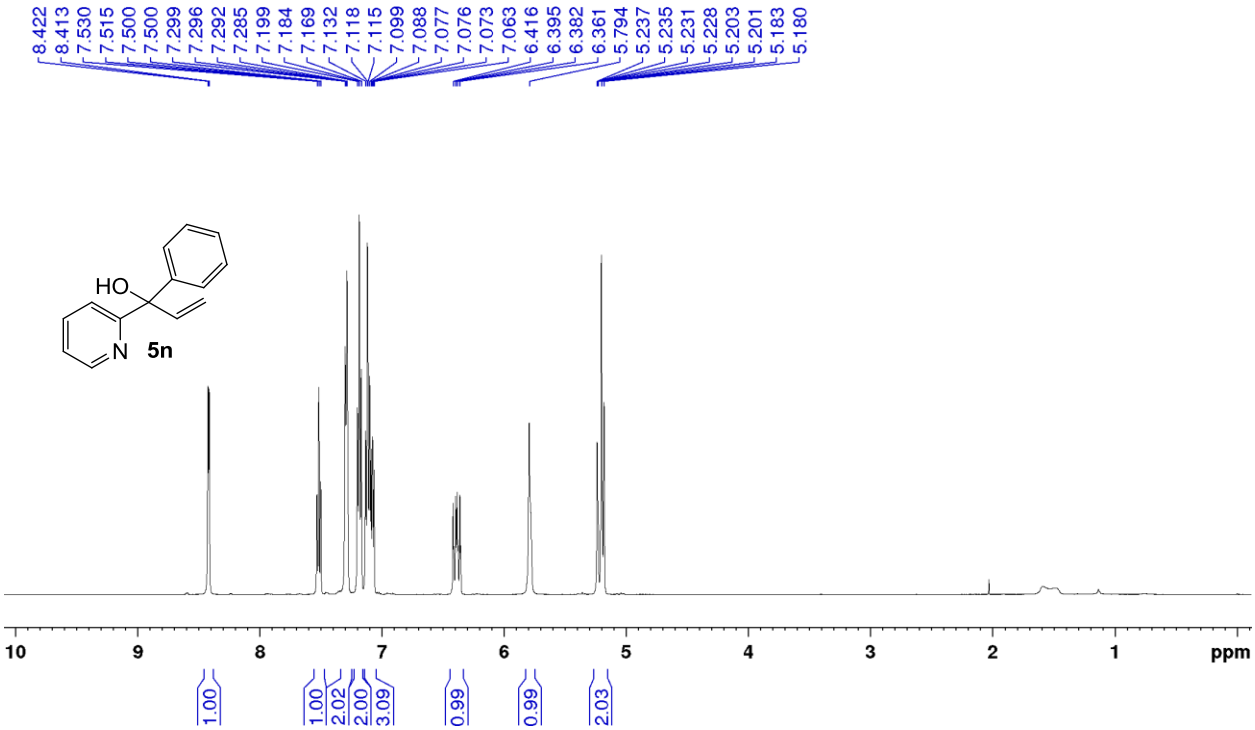
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5m)



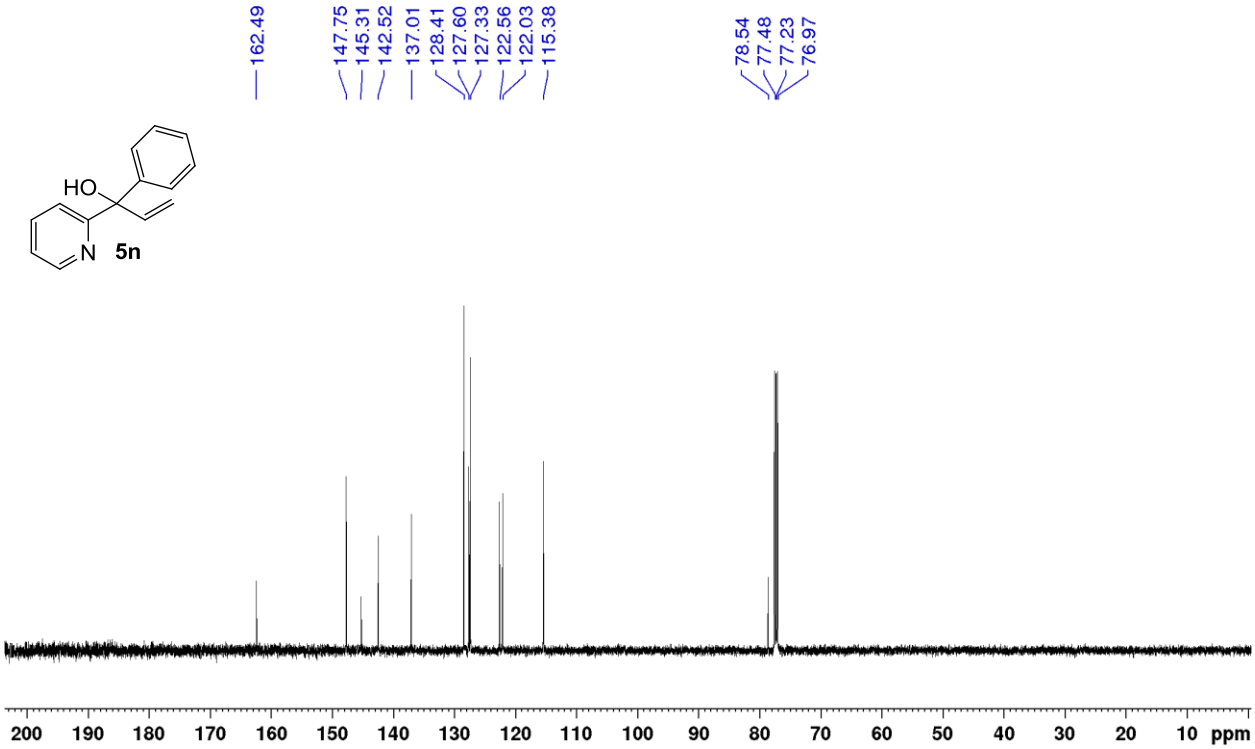
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5m)



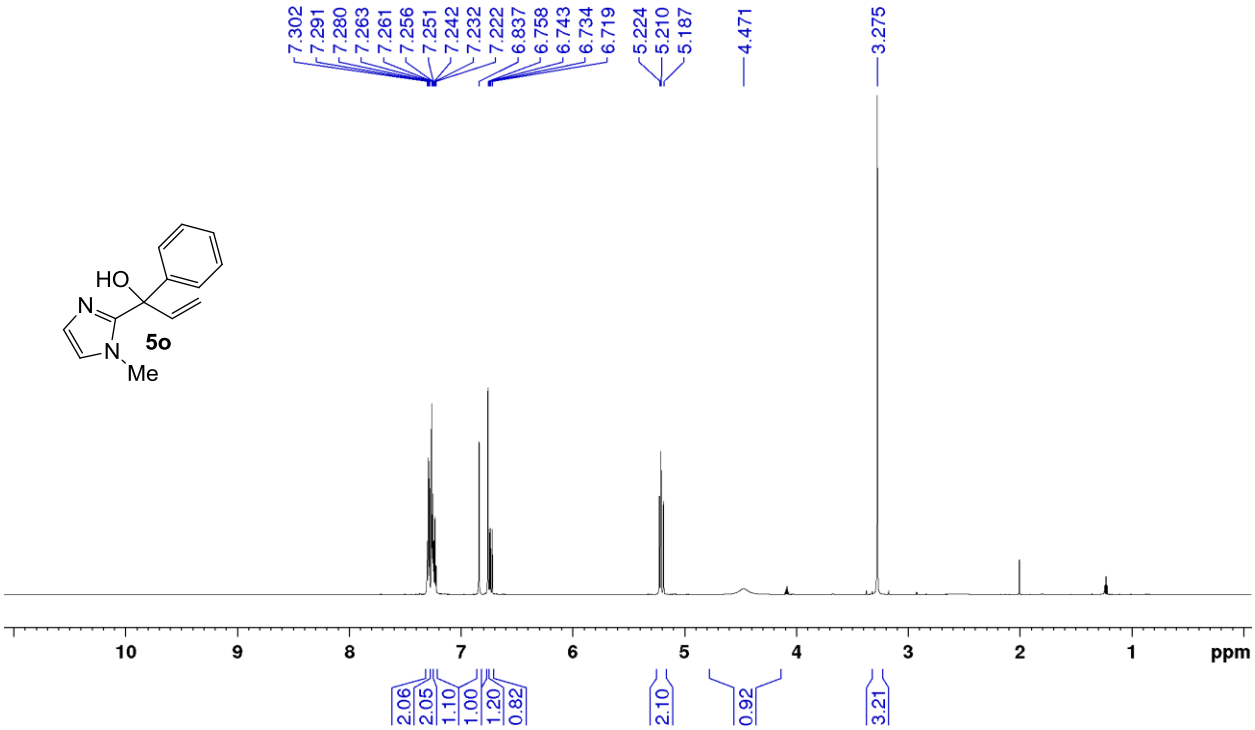
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (5n)



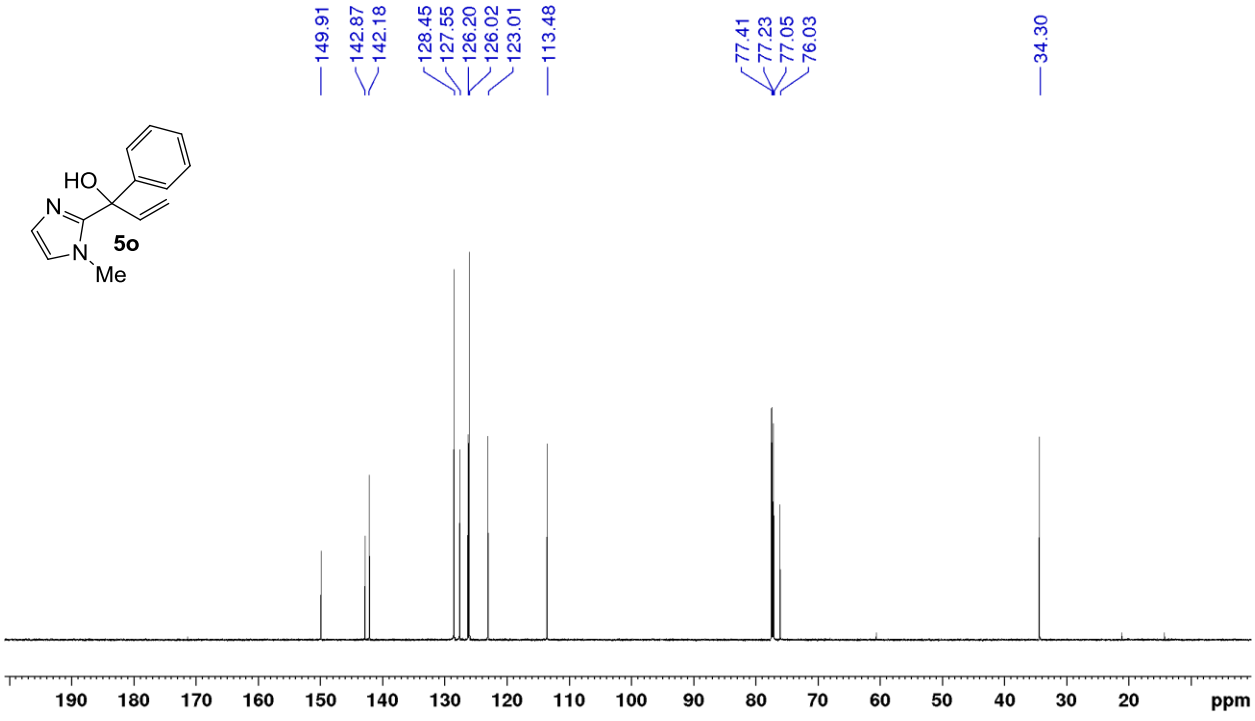
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (5n)



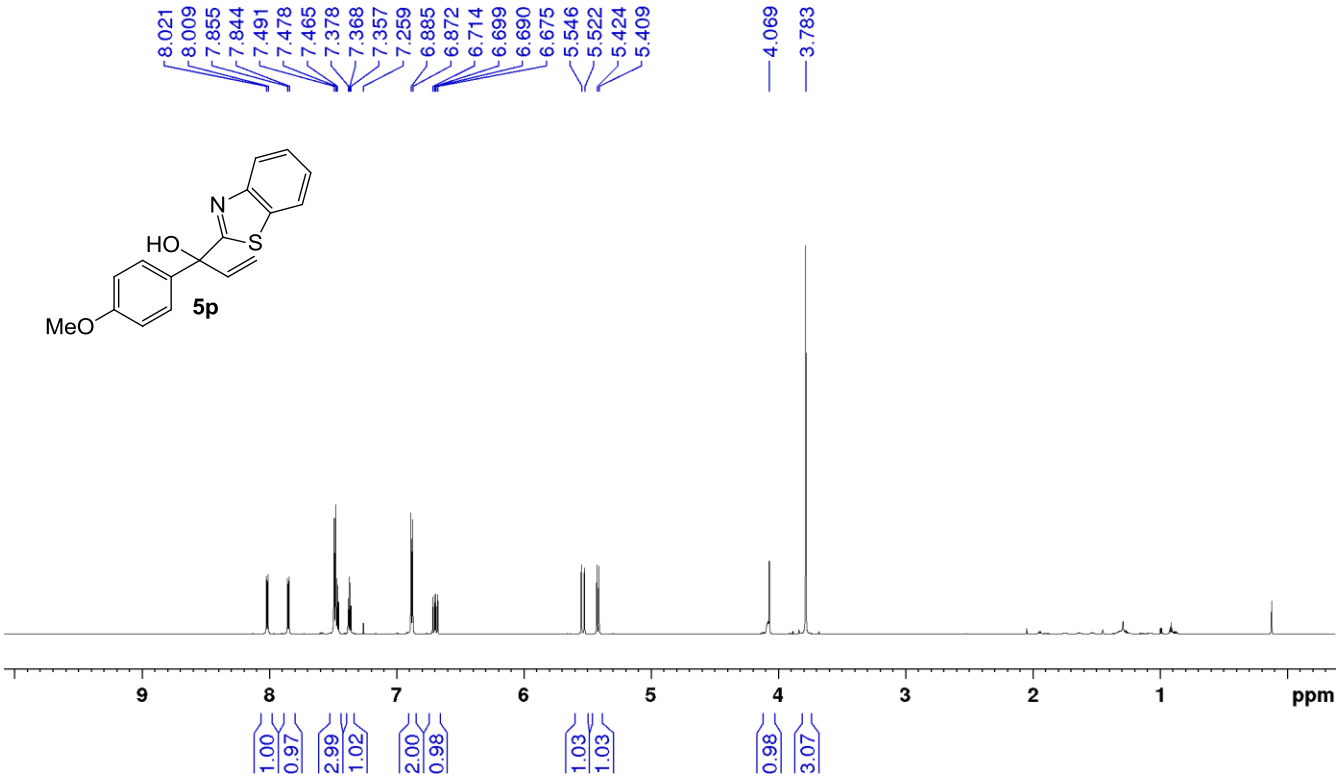
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (5o)



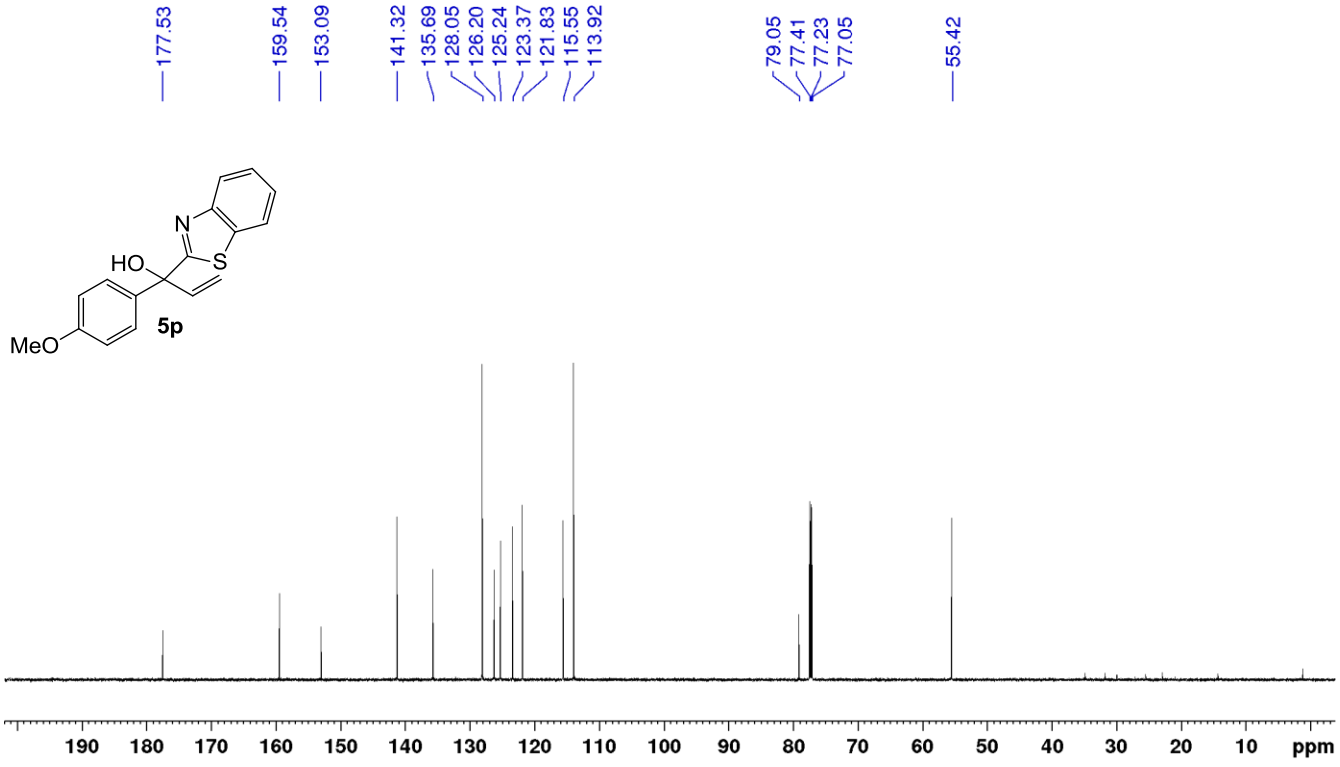
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (5o)



^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (5p)

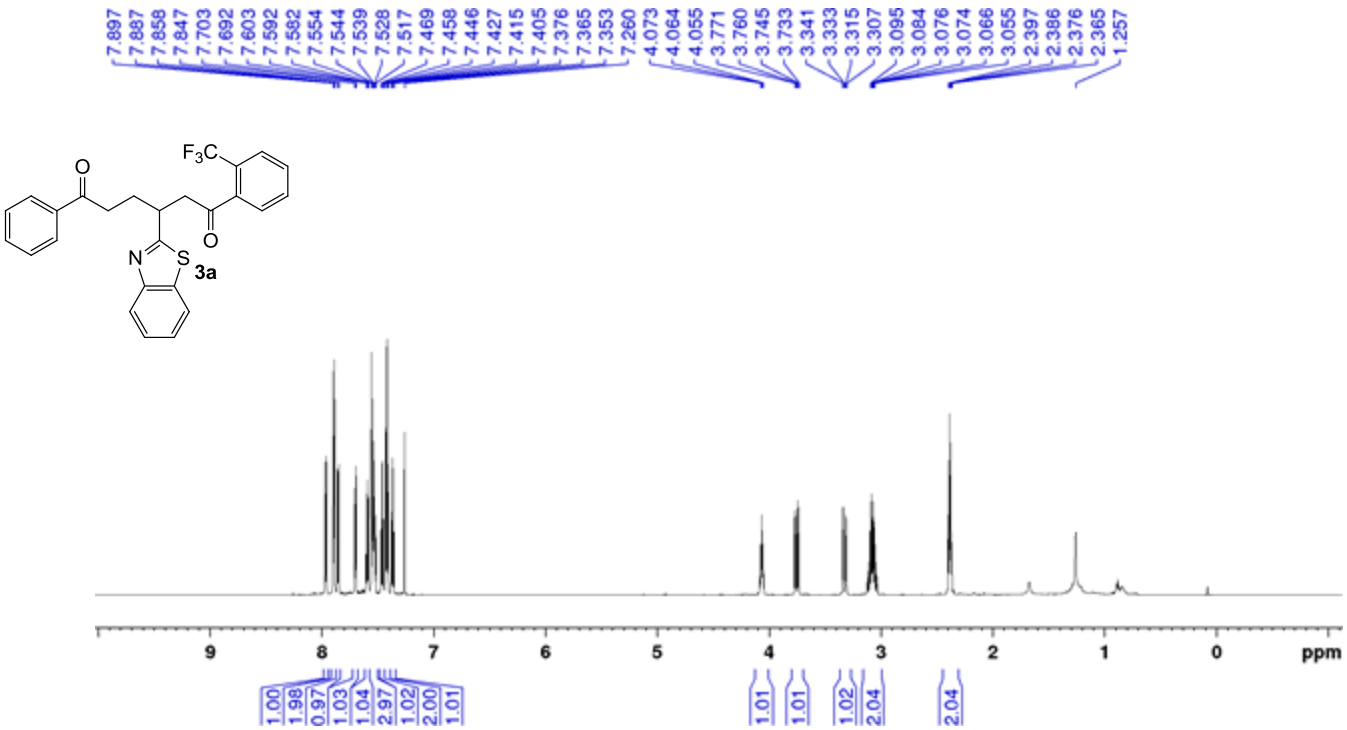


^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (5p)

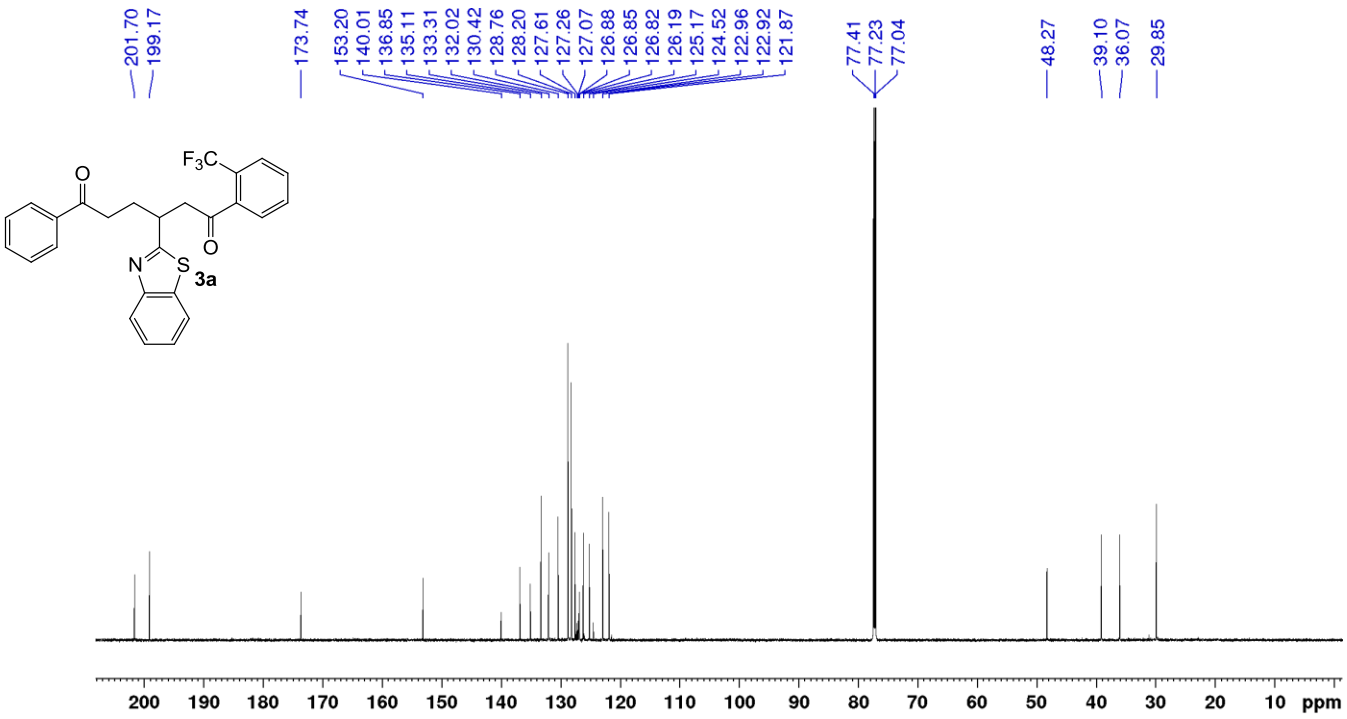


Spectra of Diketone products

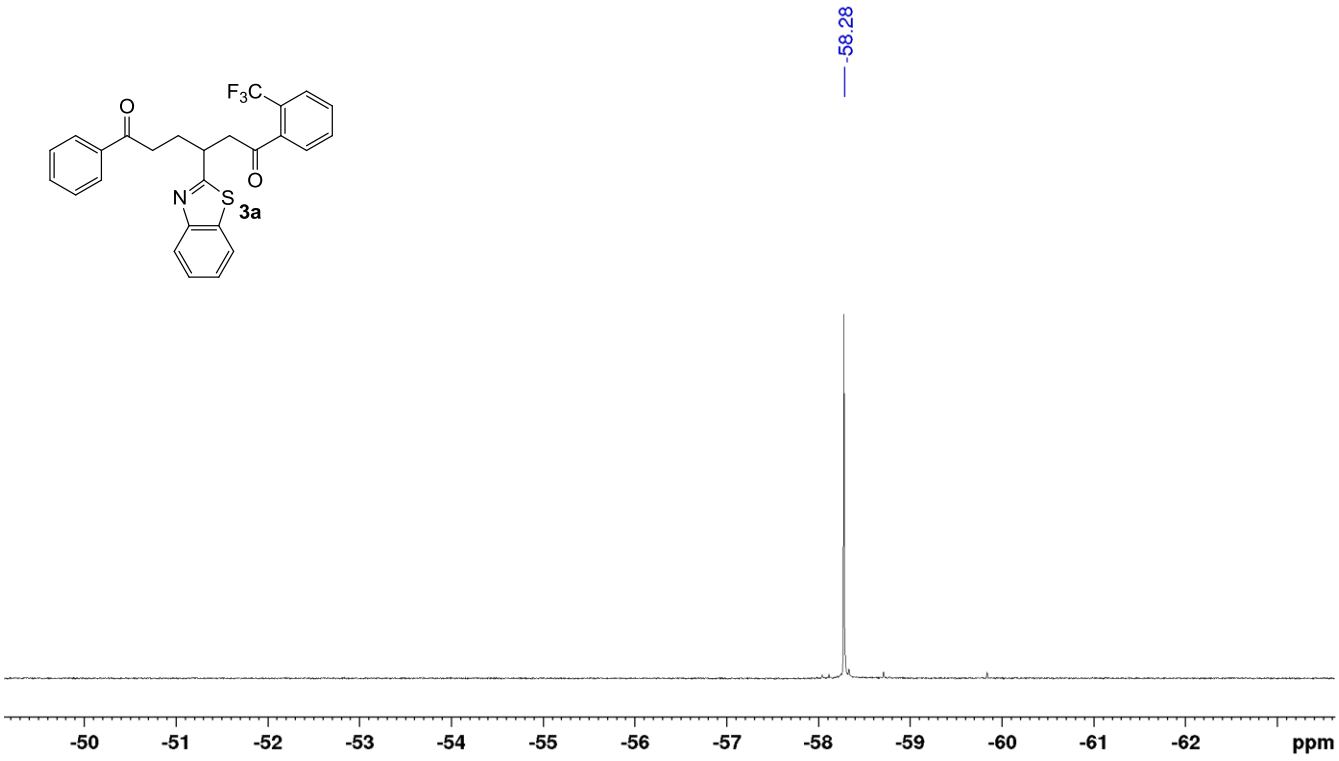
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3a)



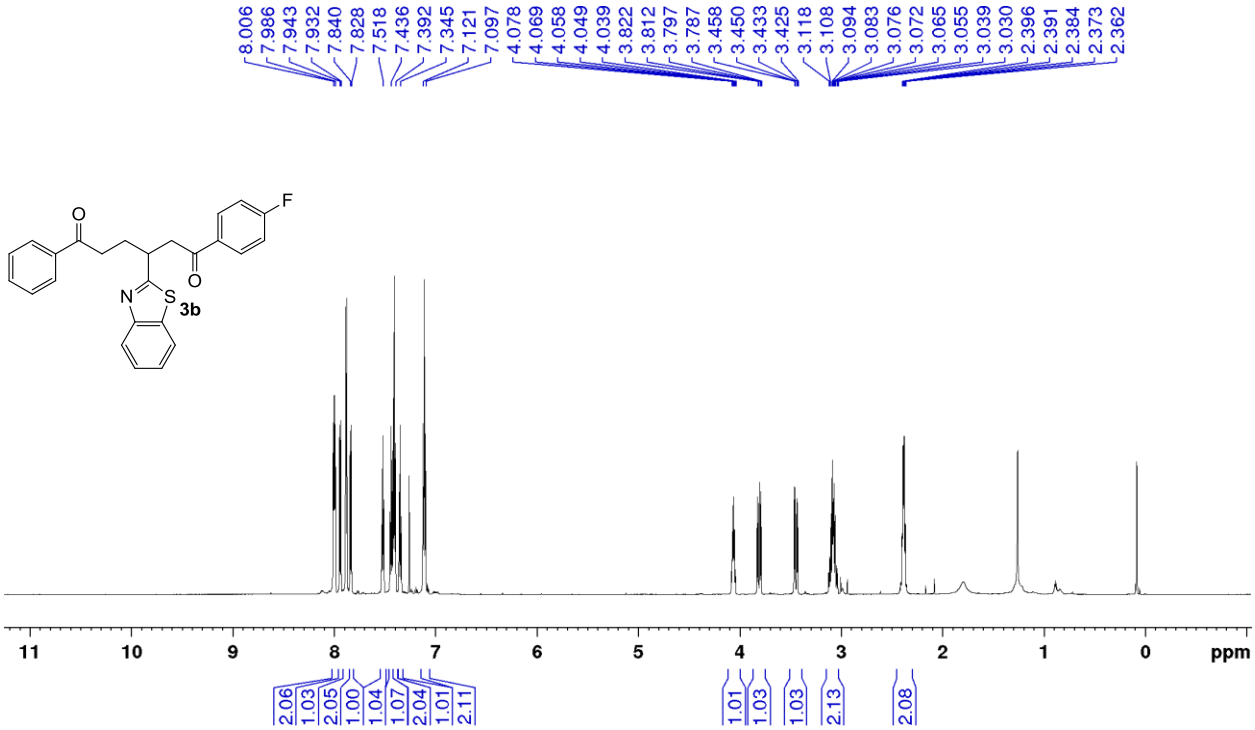
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3a)



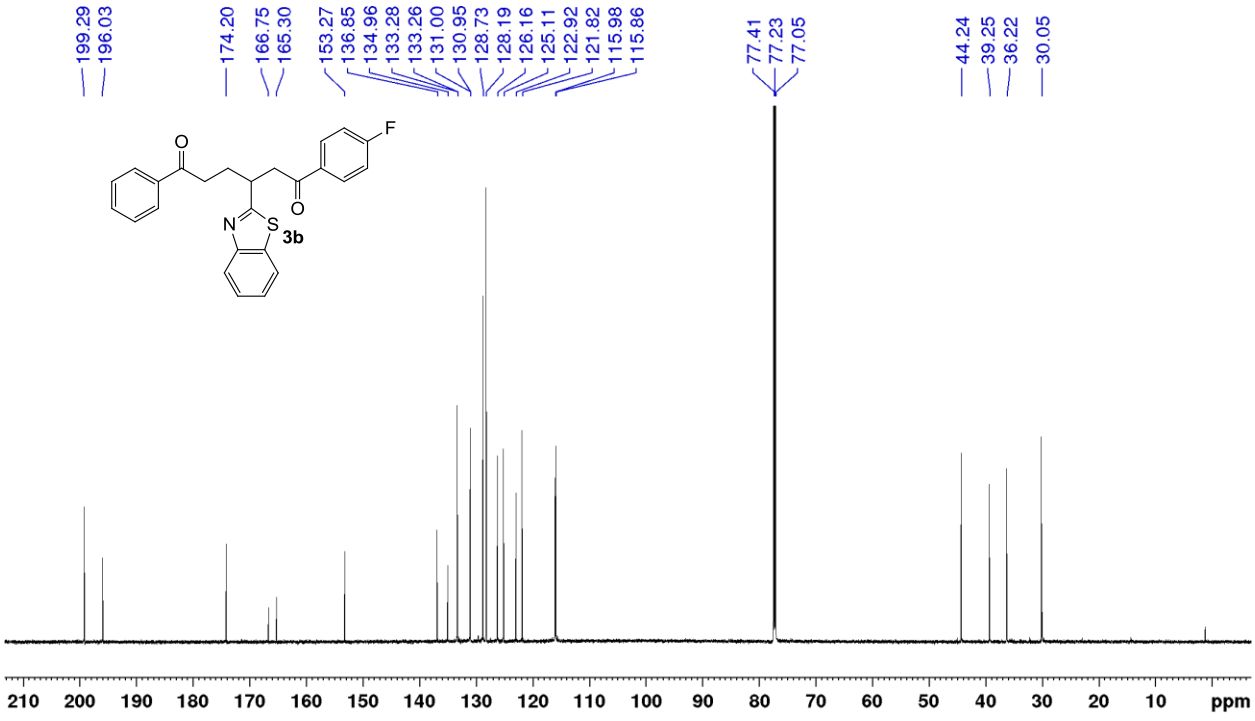
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (3a)



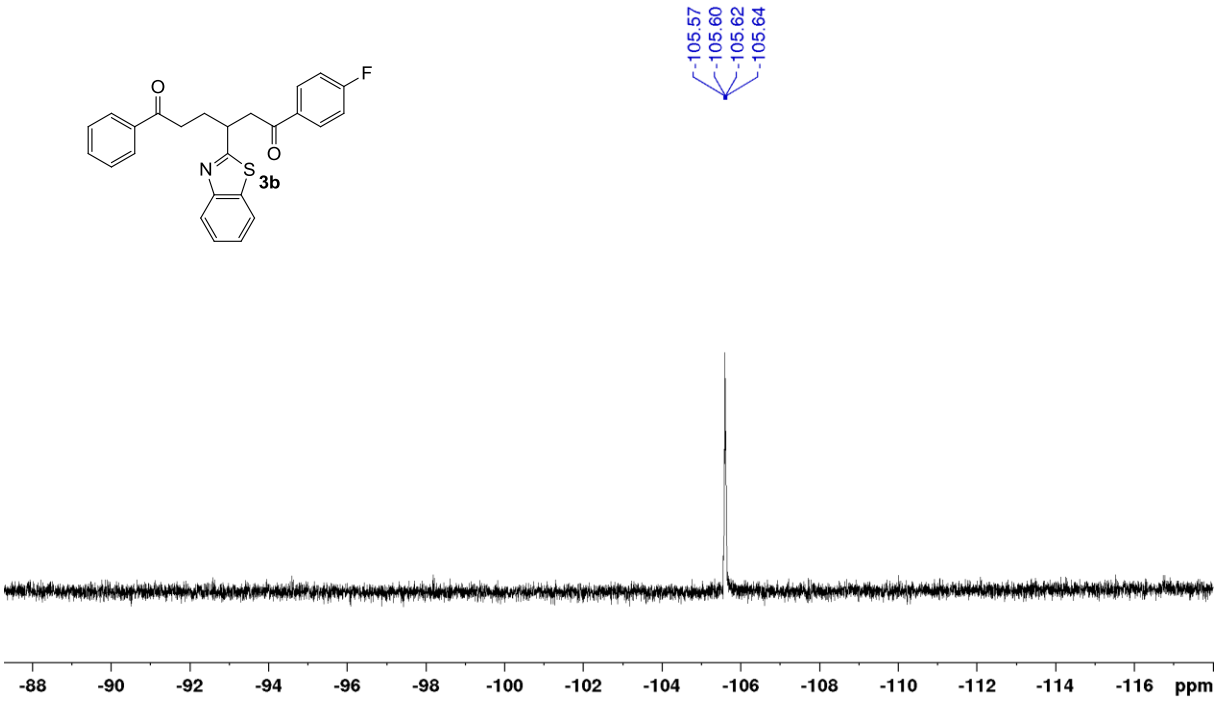
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (3b)



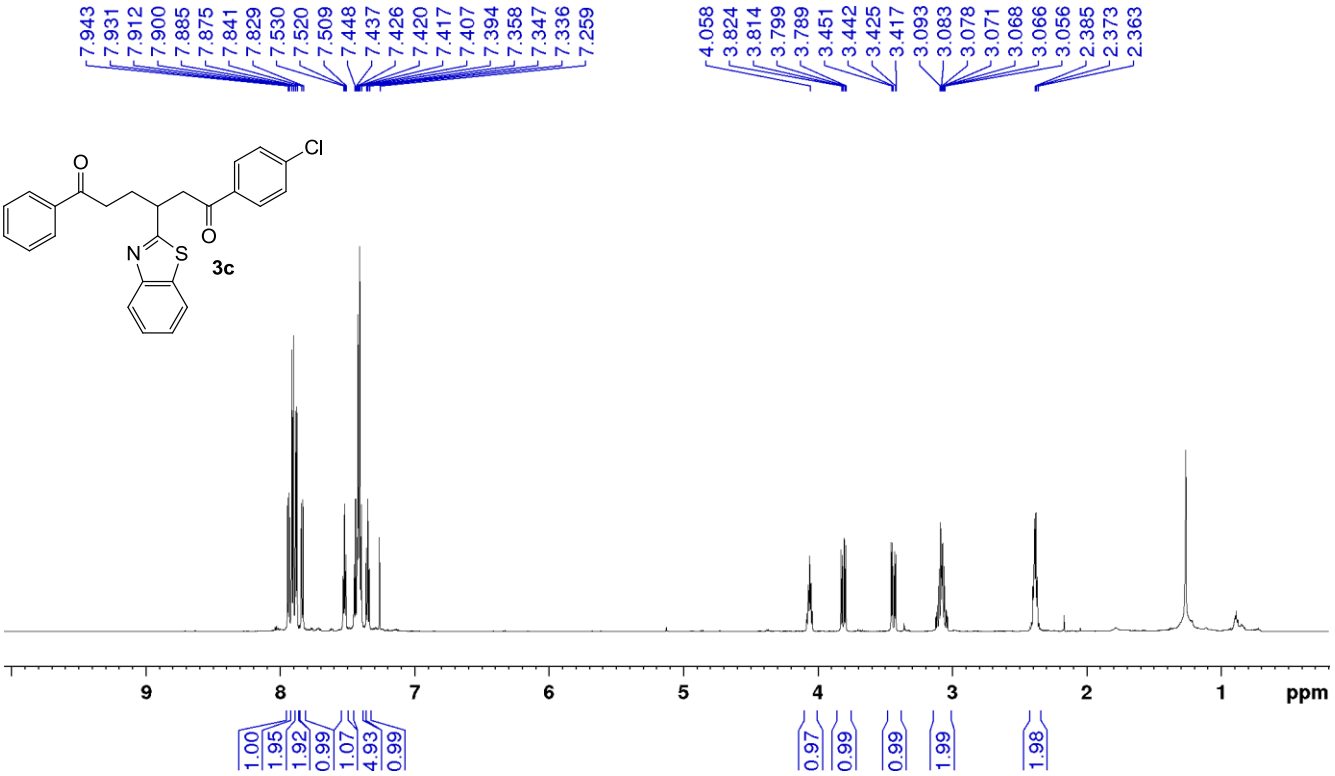
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (3b)



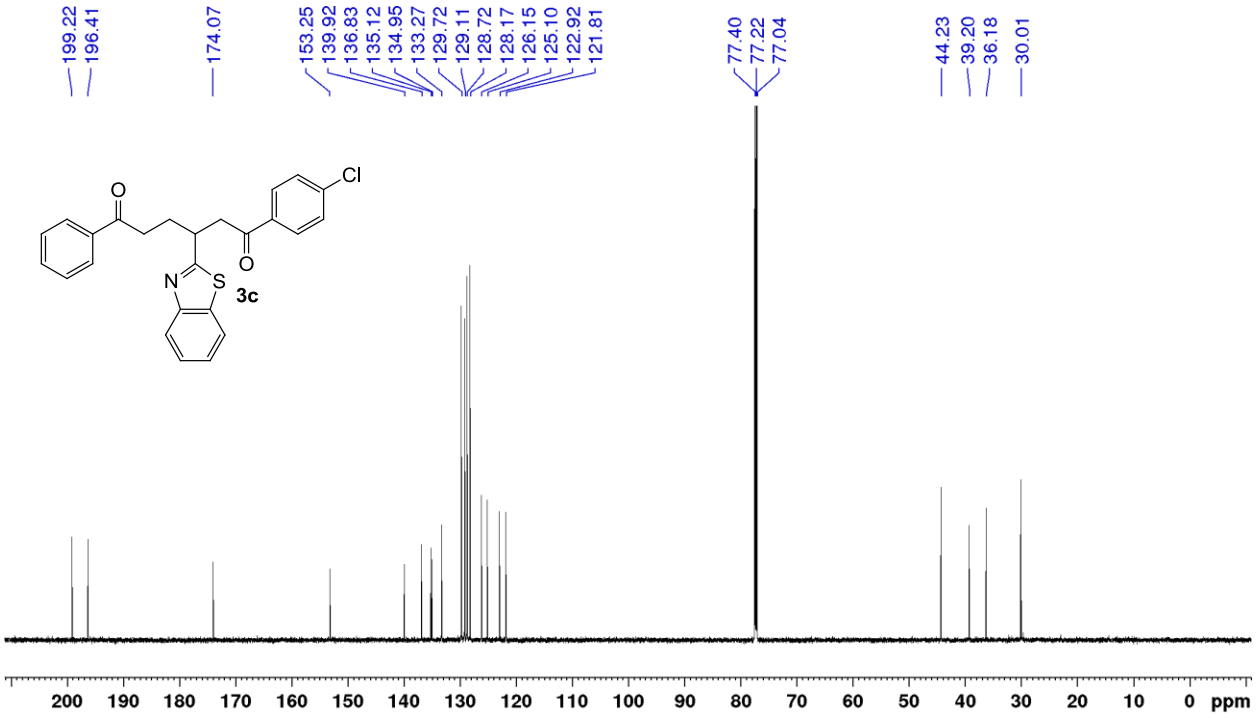
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (3b)



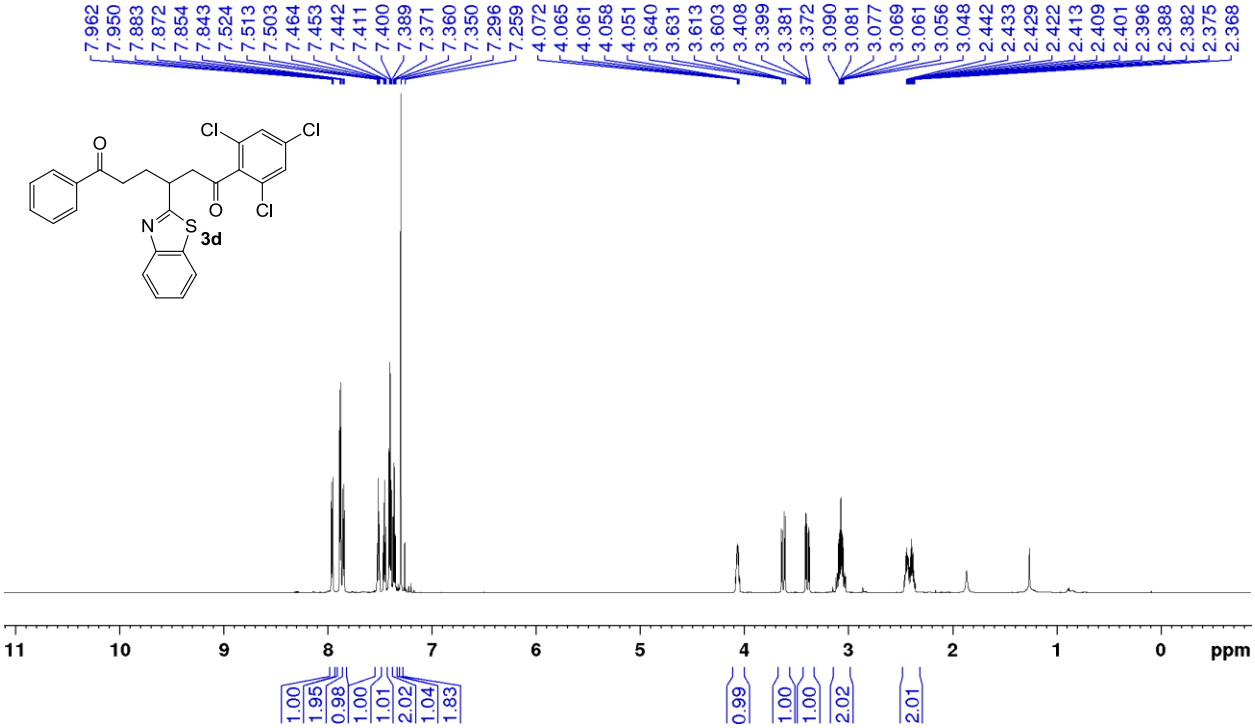
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (3c)



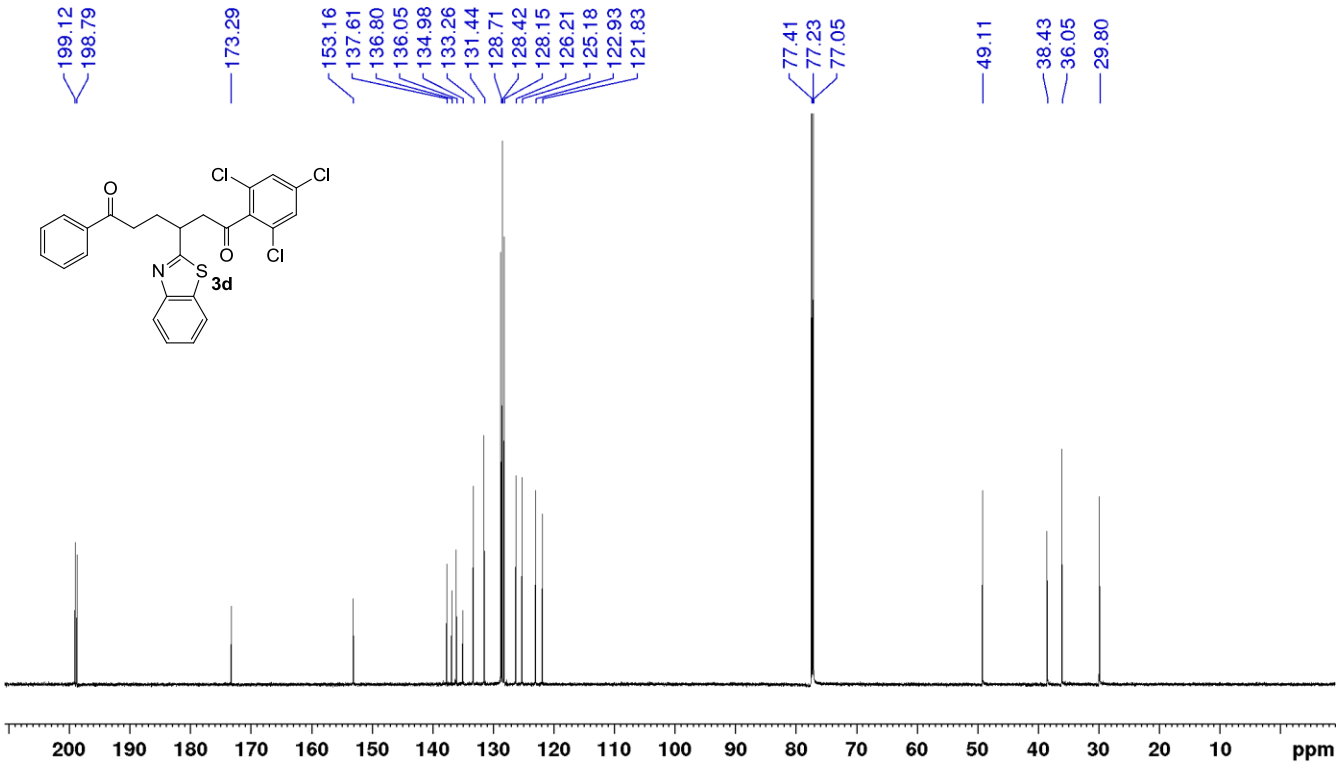
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (3c)



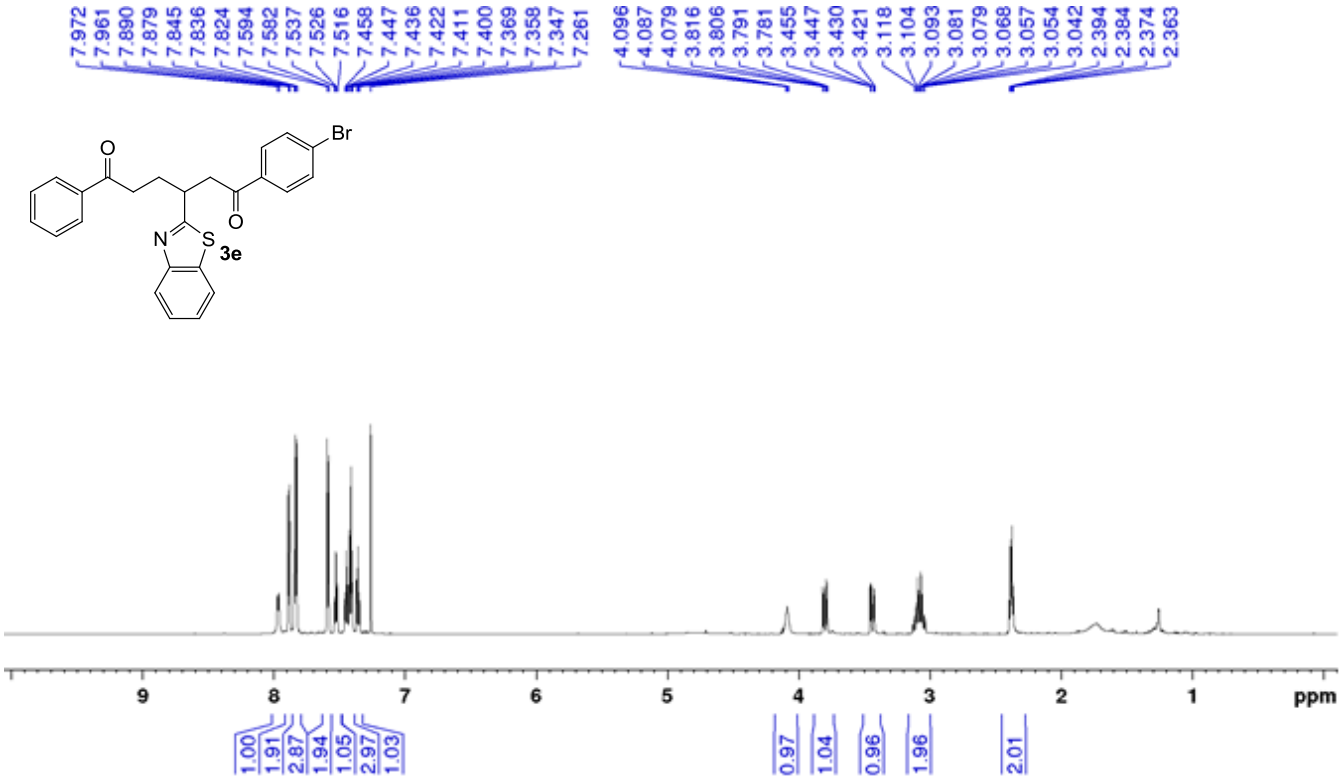
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3d)



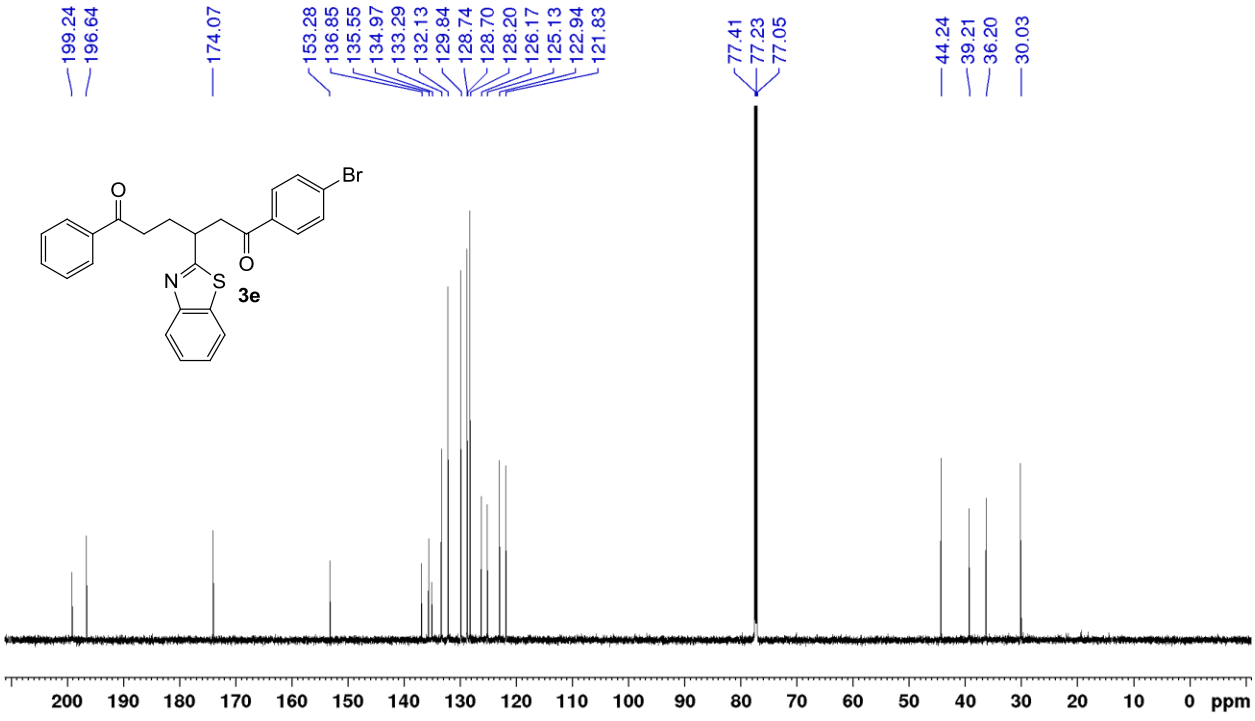
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3d)



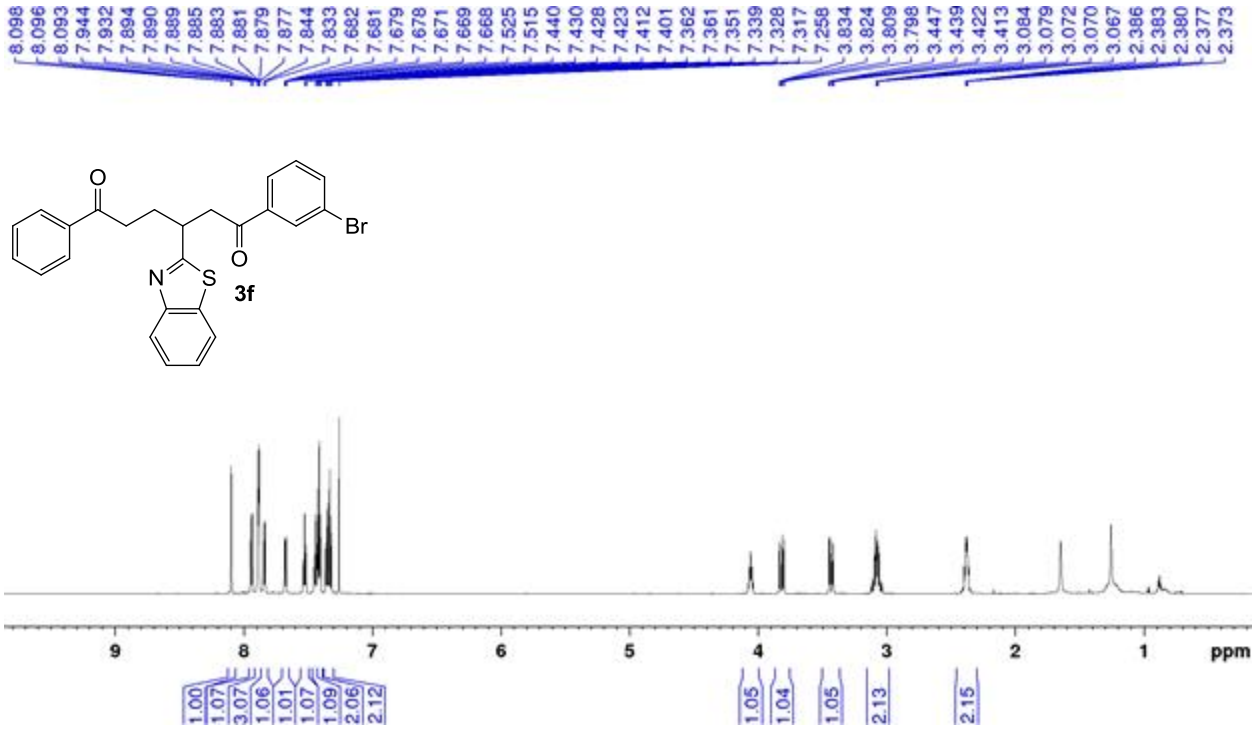
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3e)



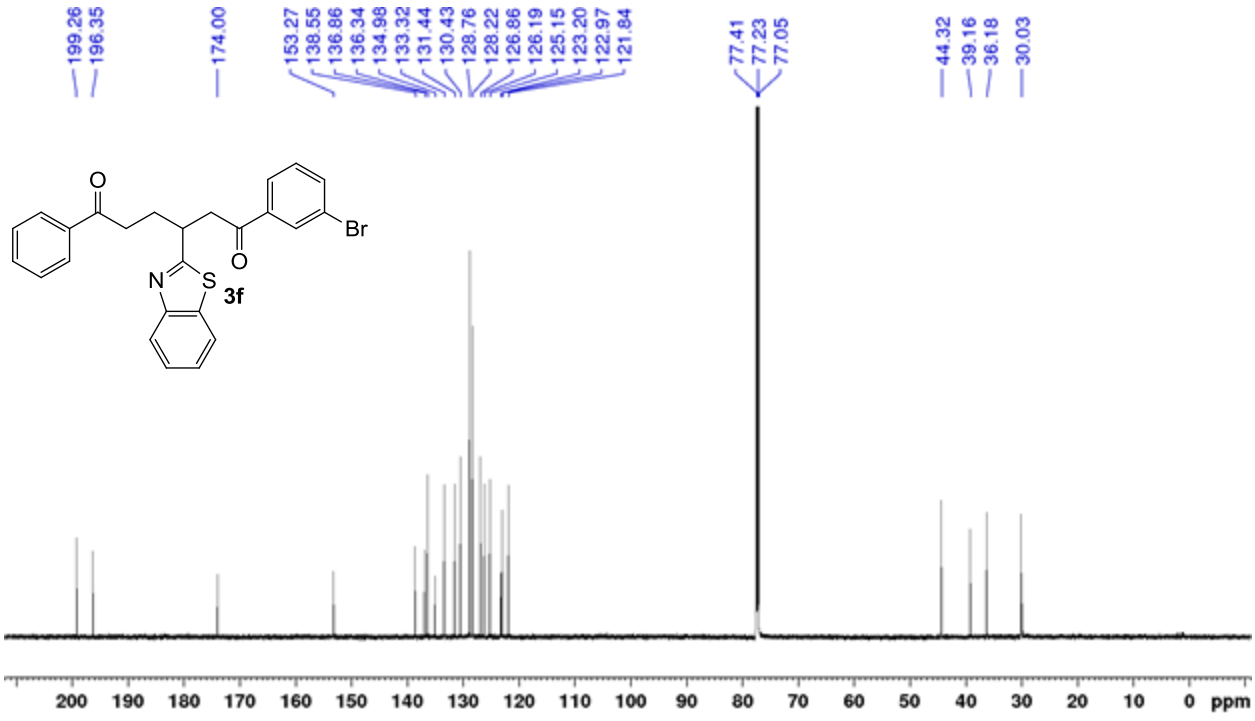
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3e)



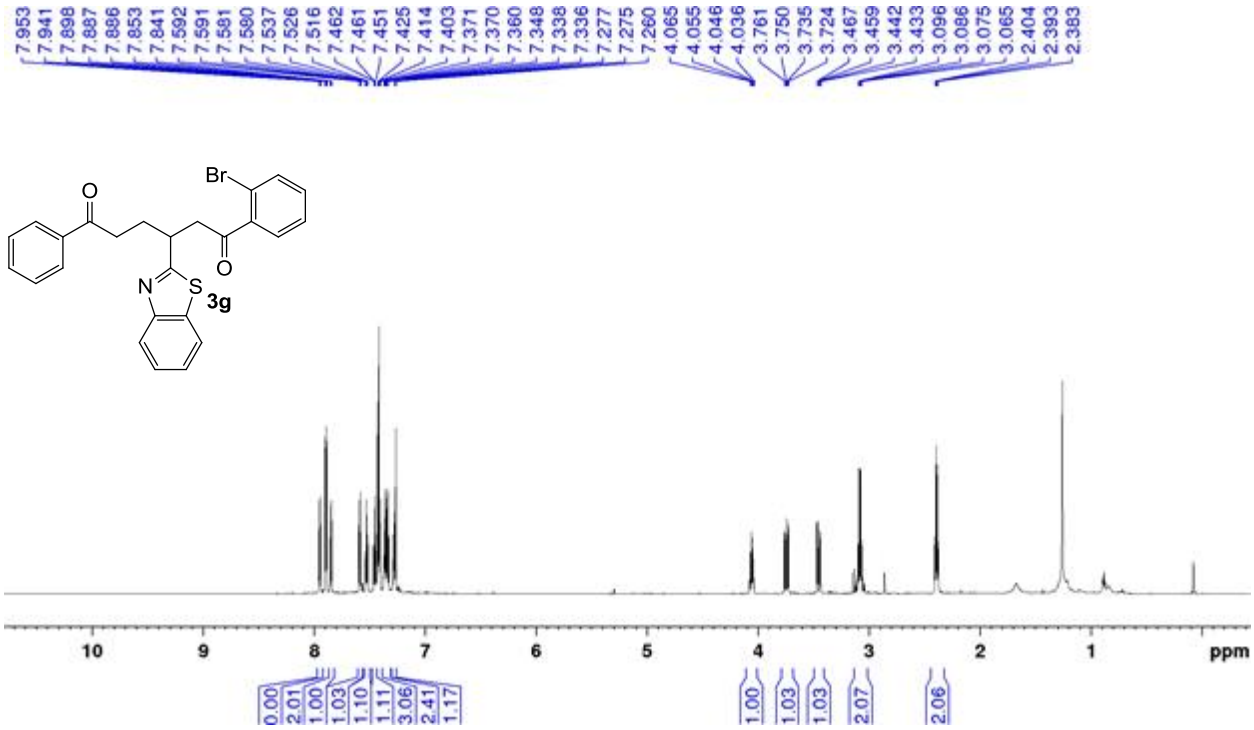
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3f)



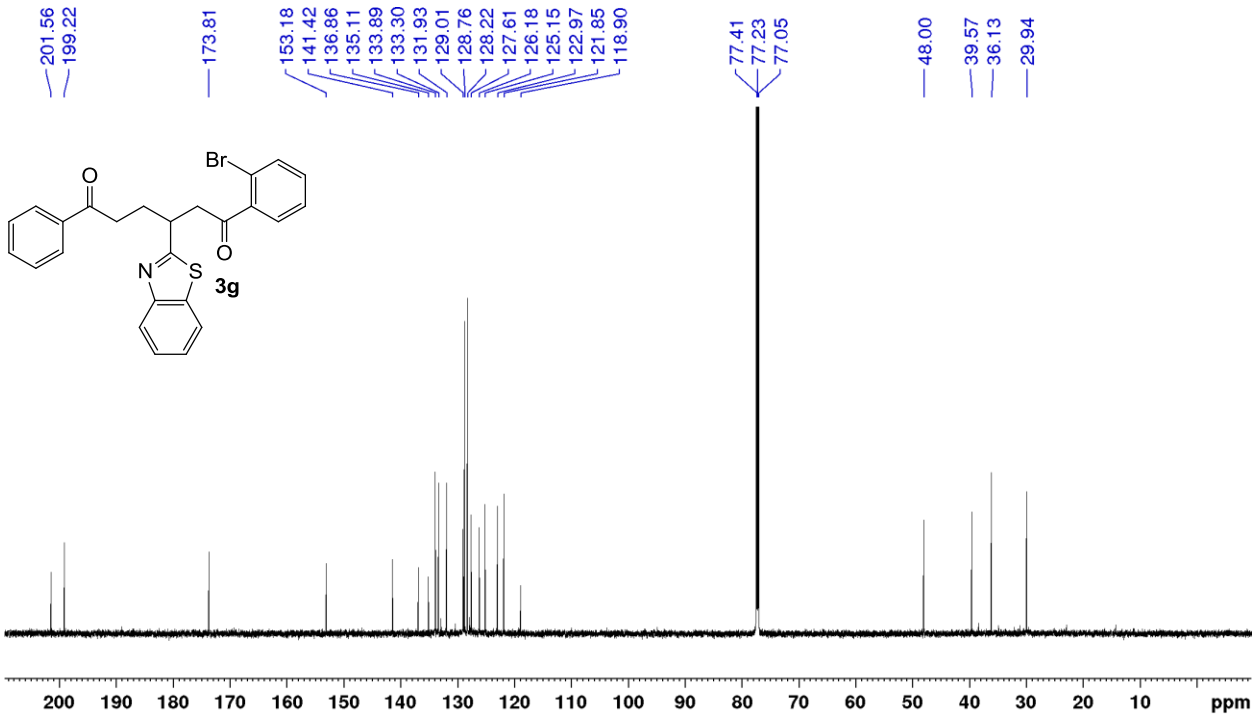
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3f)



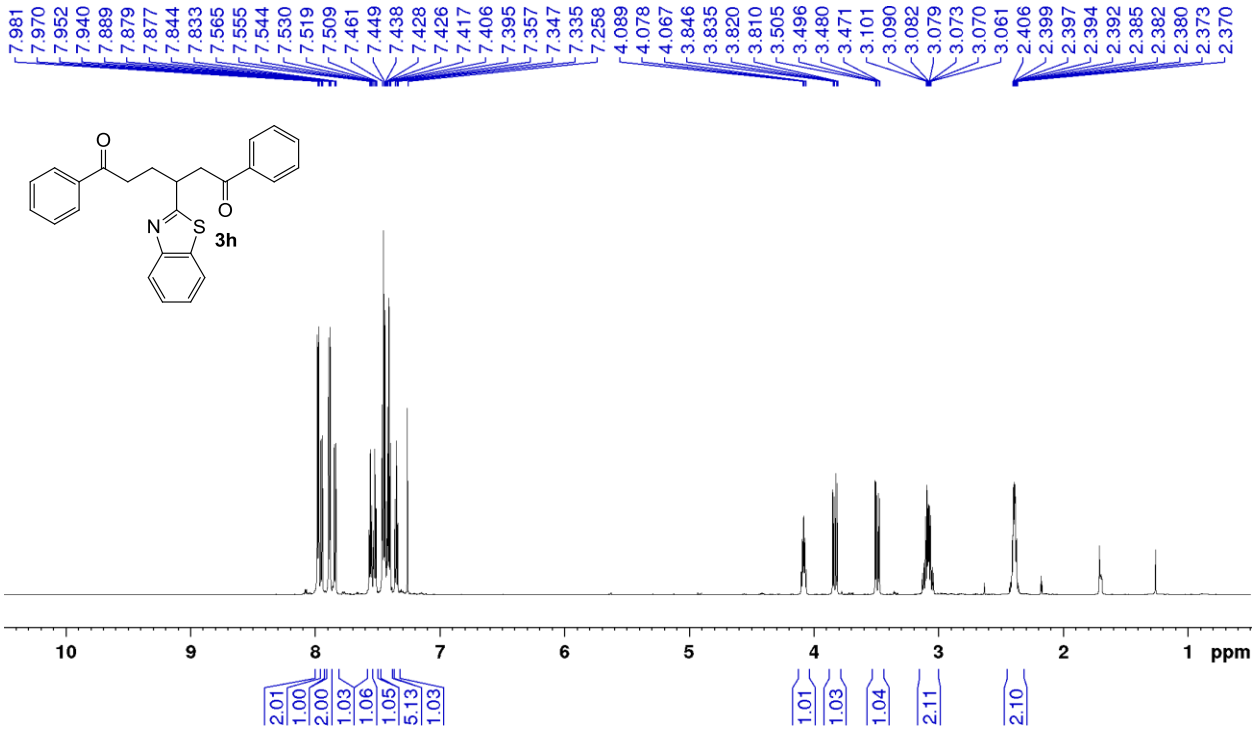
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3g)



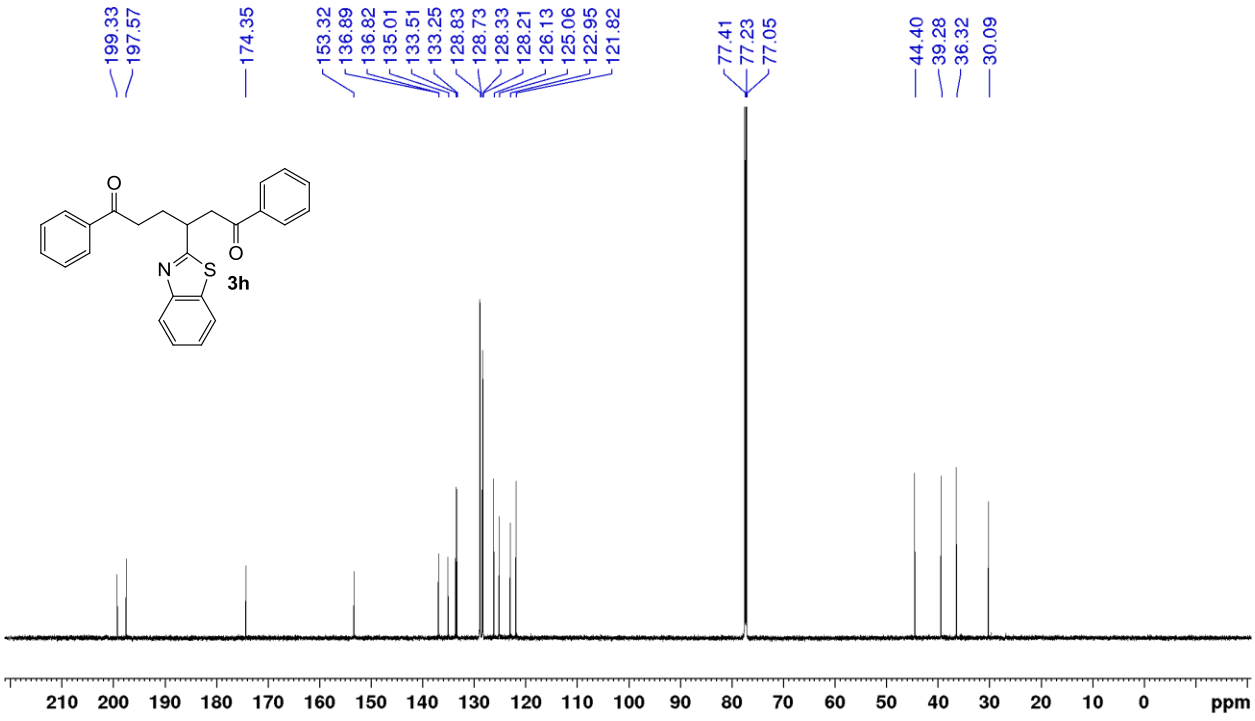
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3g)



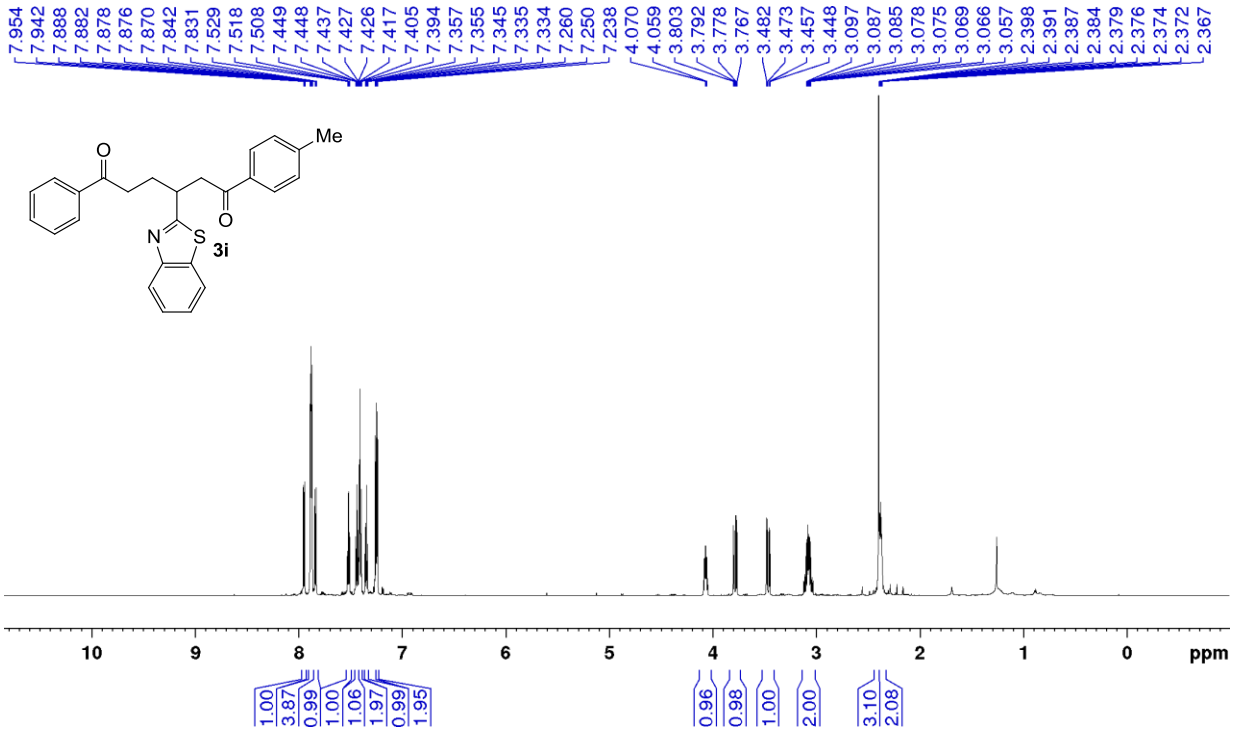
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3h)



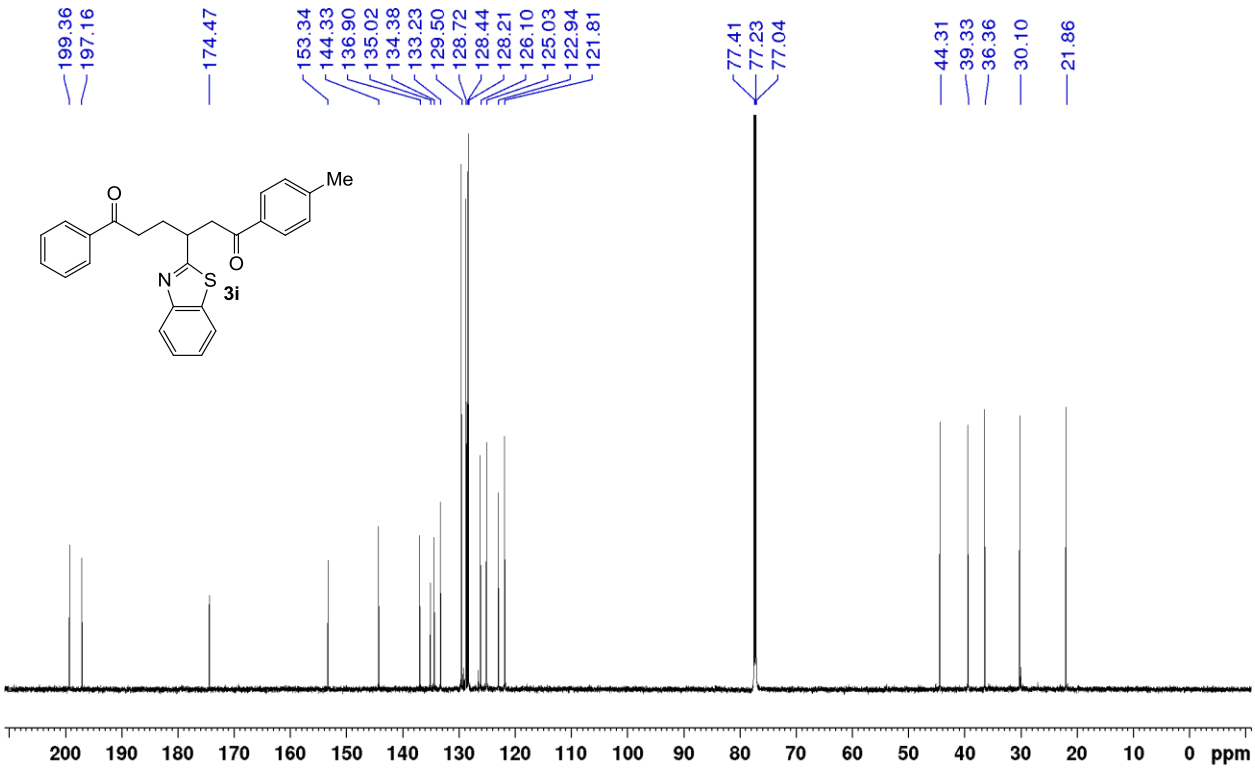
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3h)



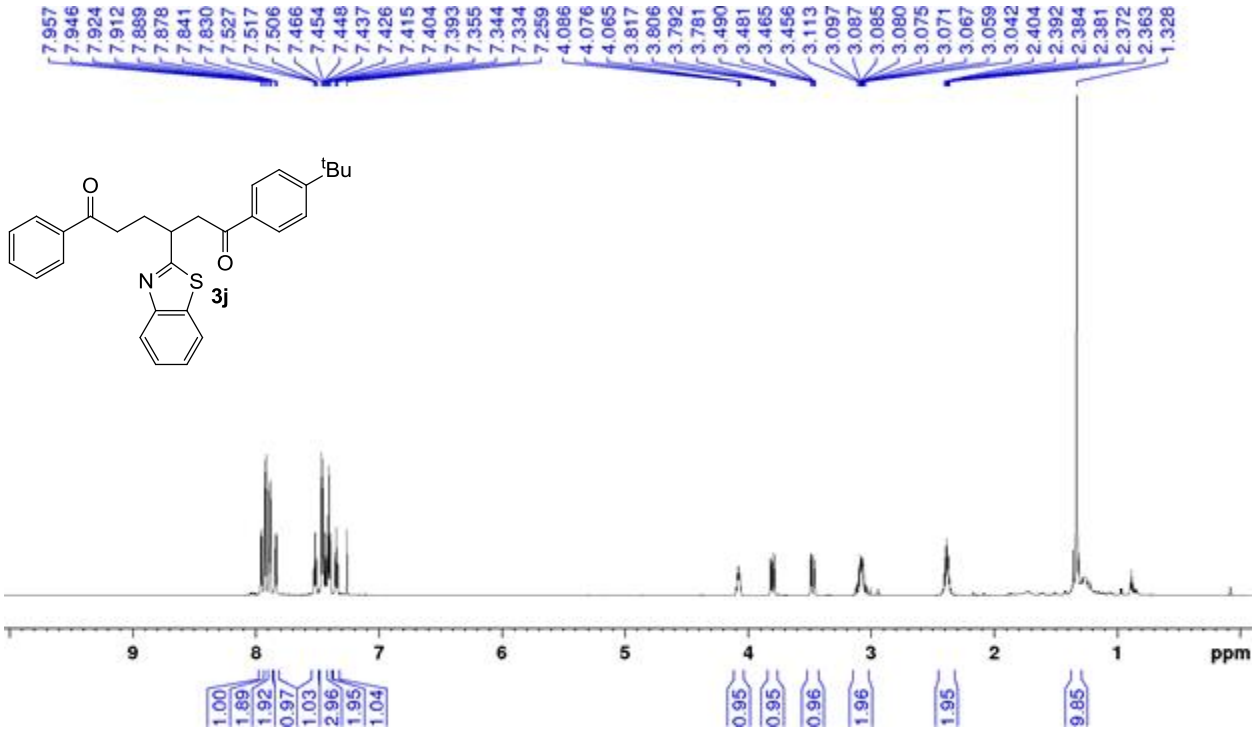
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3i)



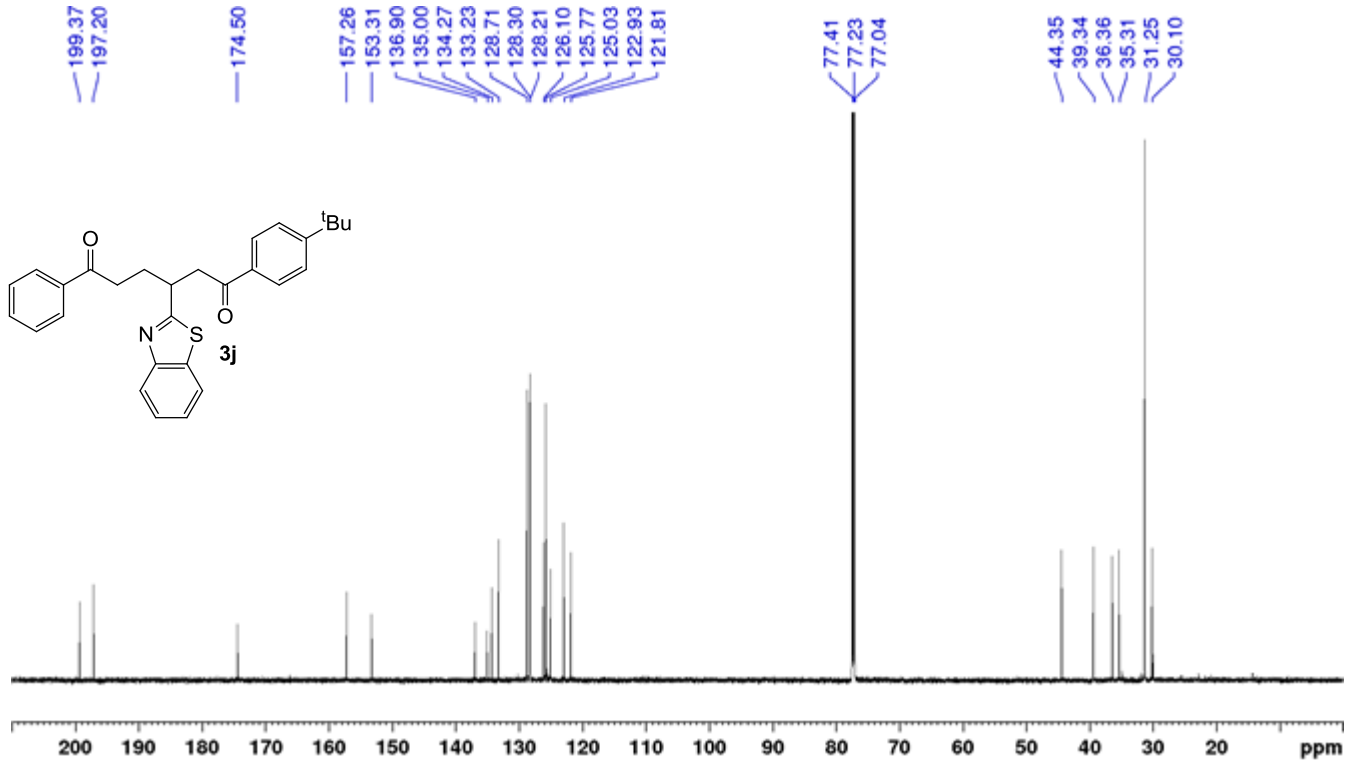
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3i)



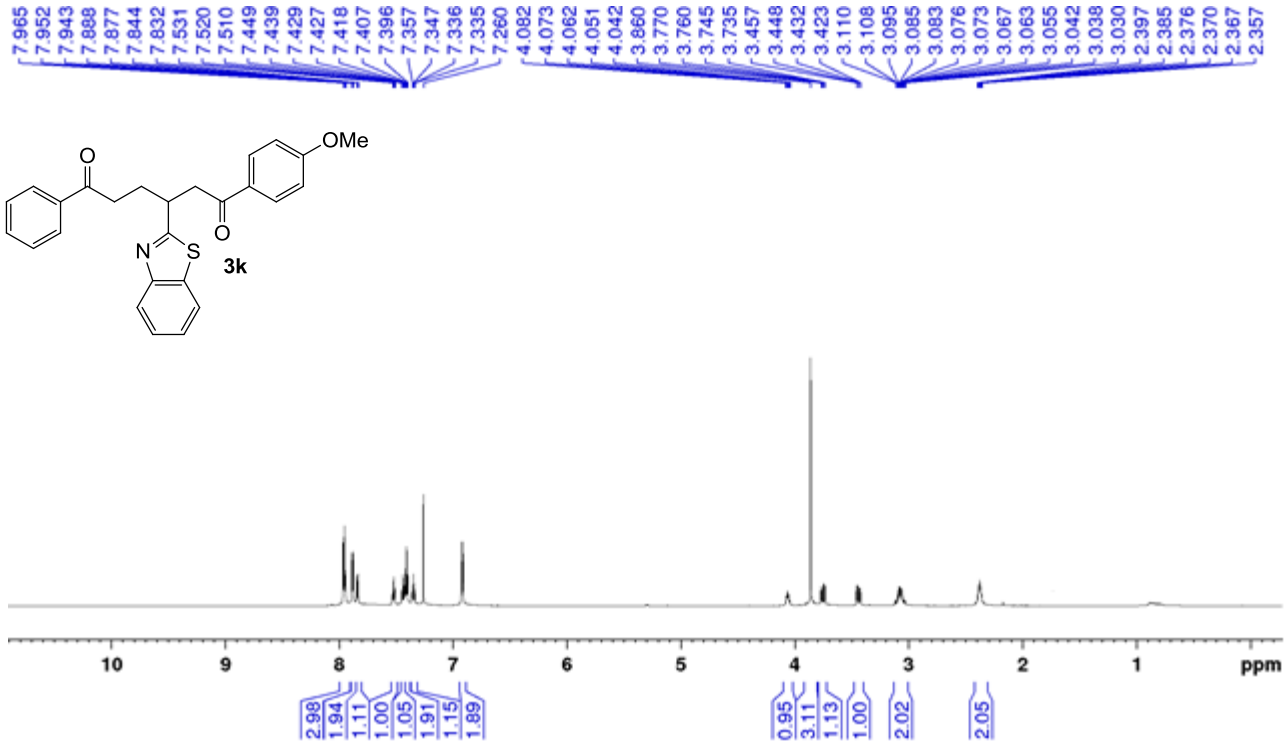
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3j)



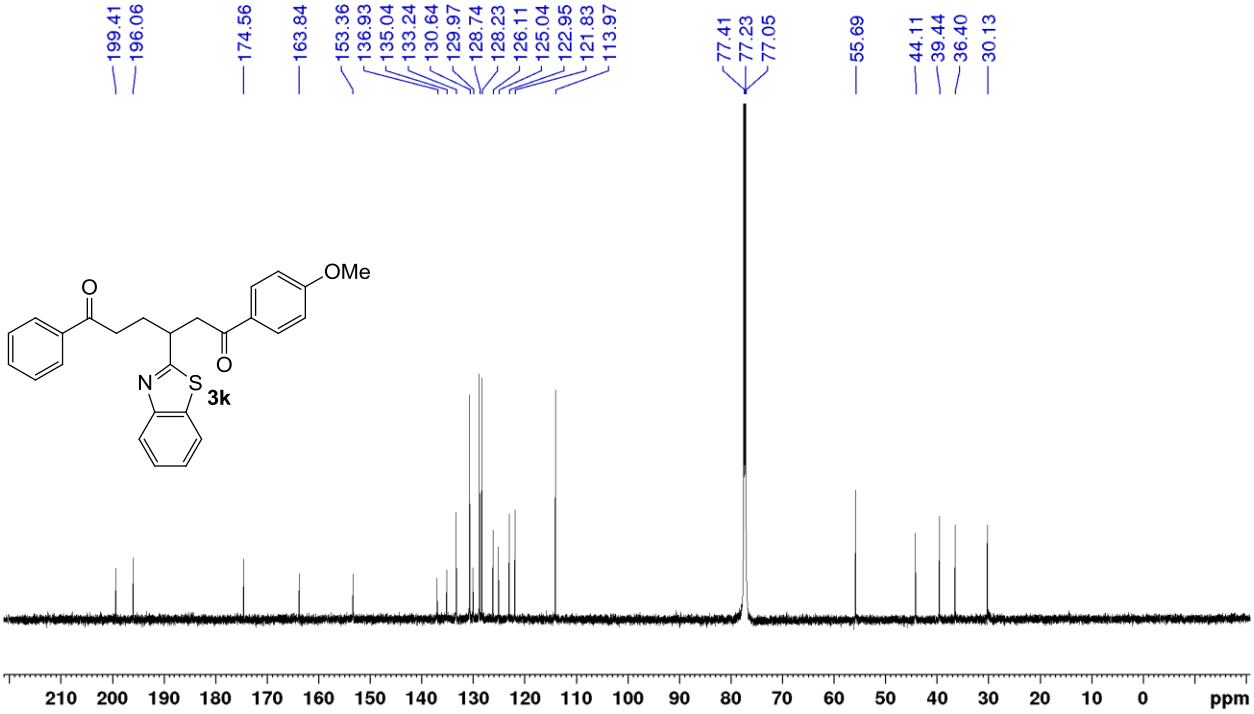
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3j)



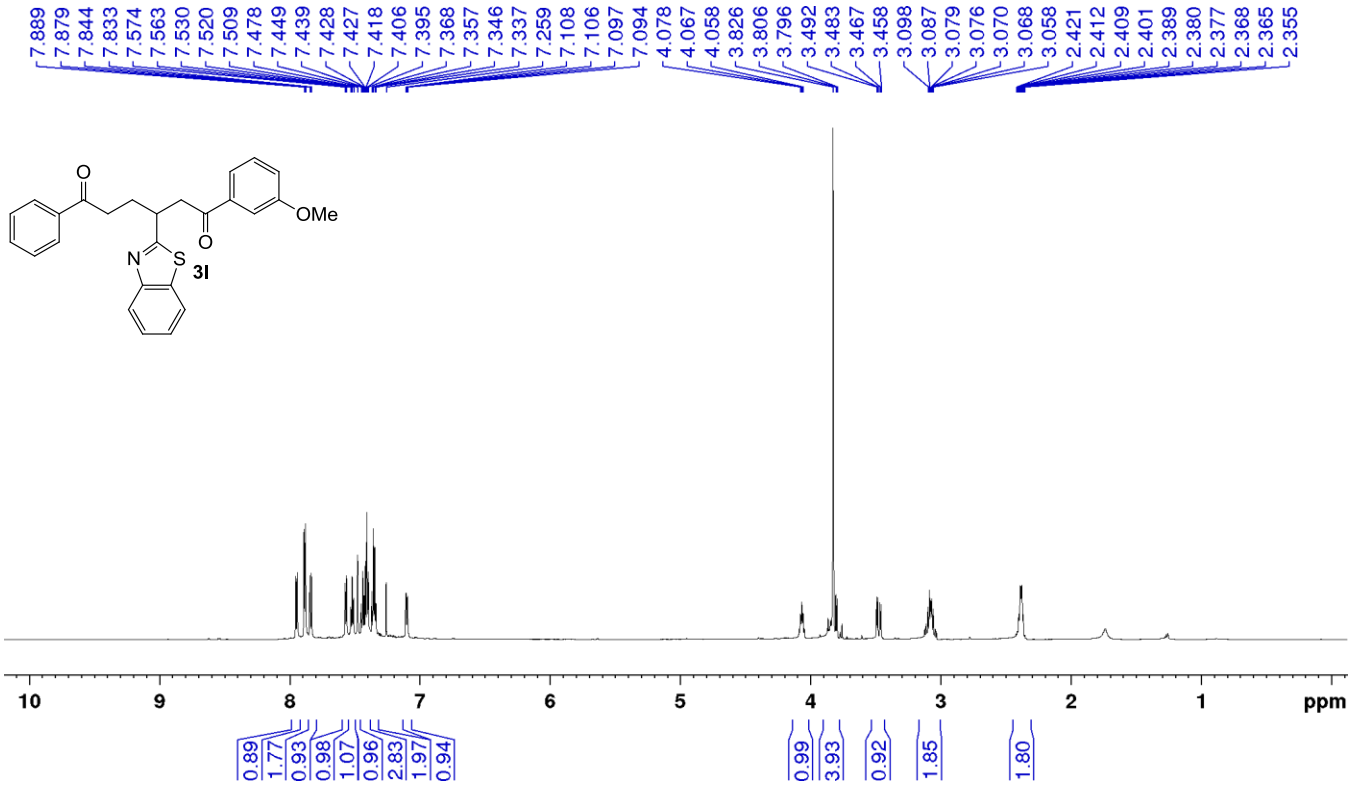
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (3k)



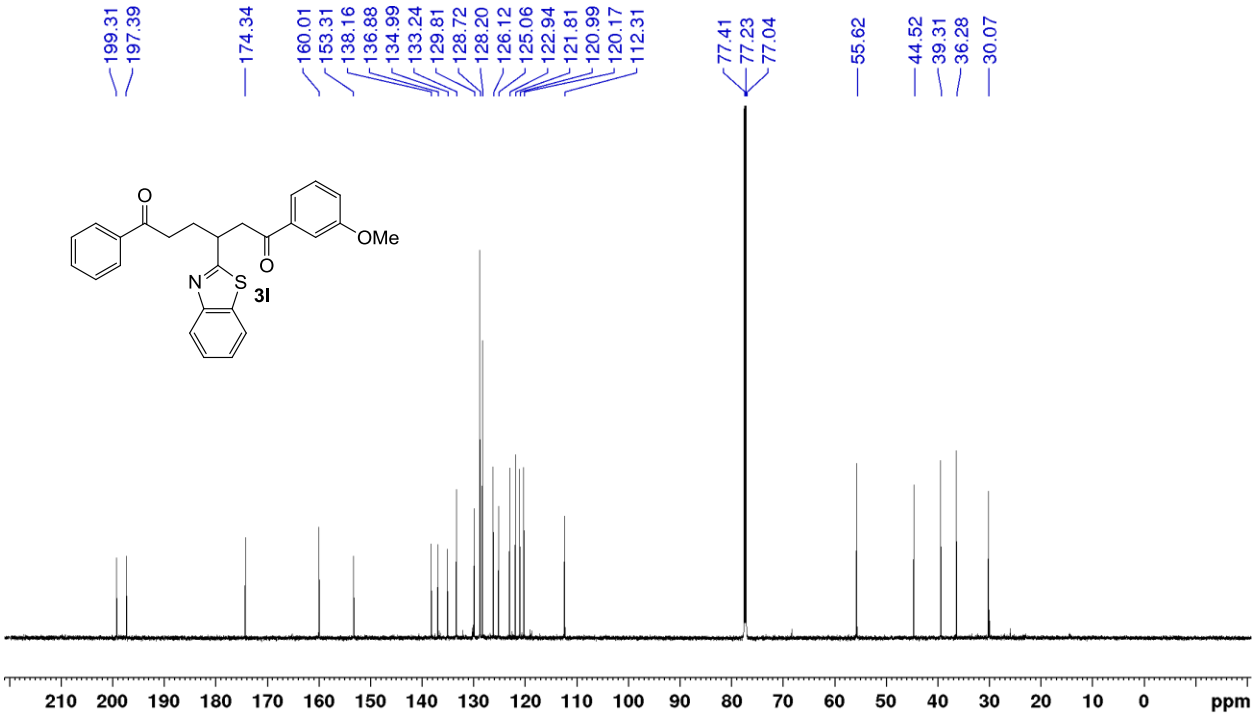
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (3k)



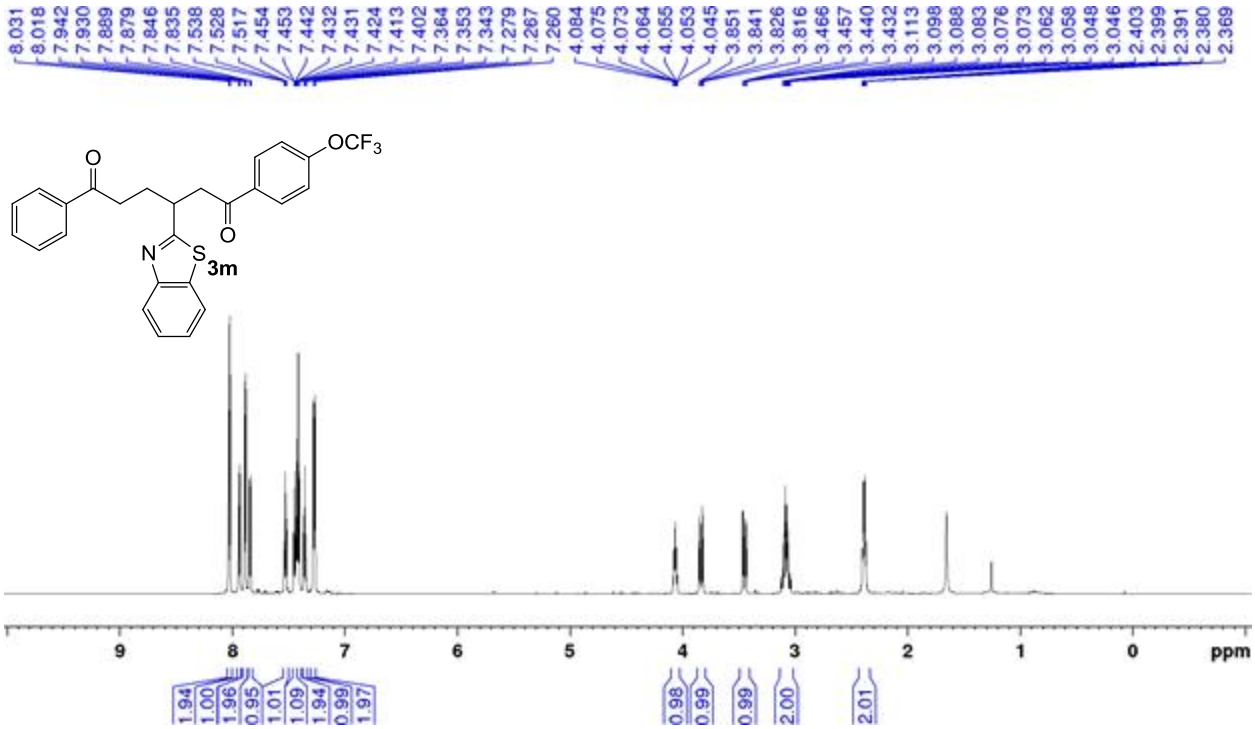
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (3l)



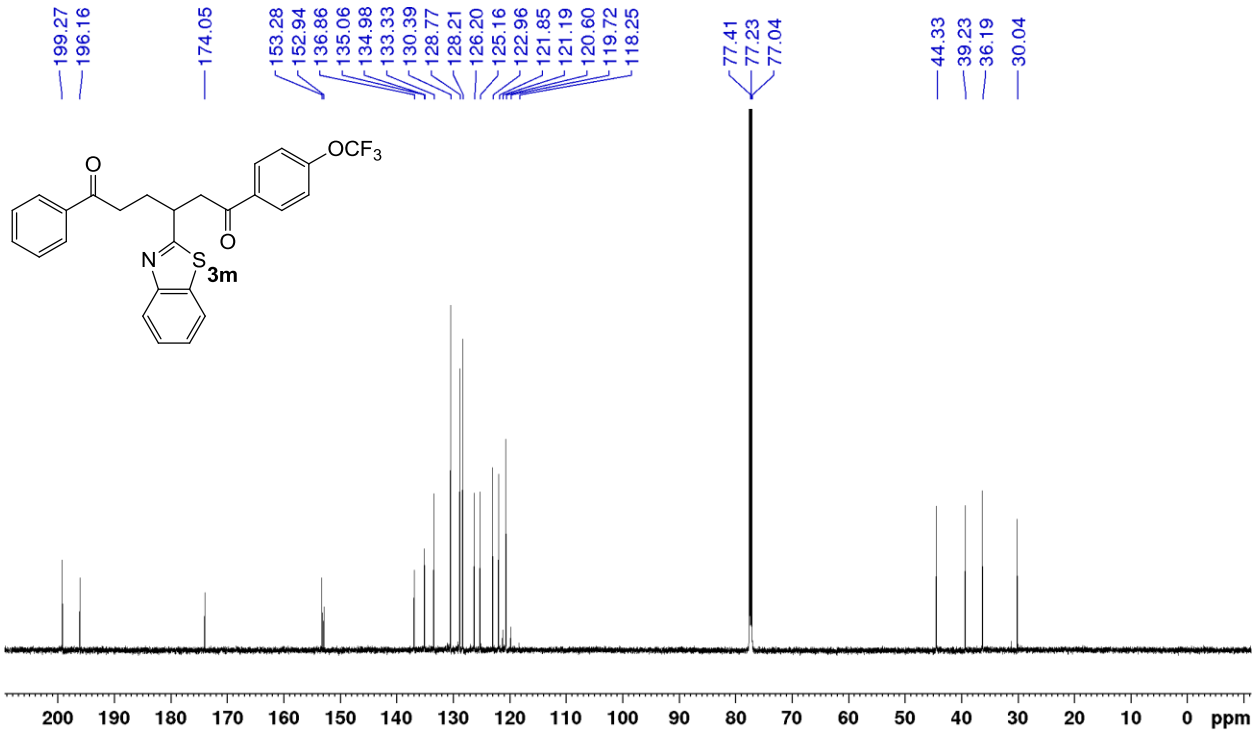
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (3l)



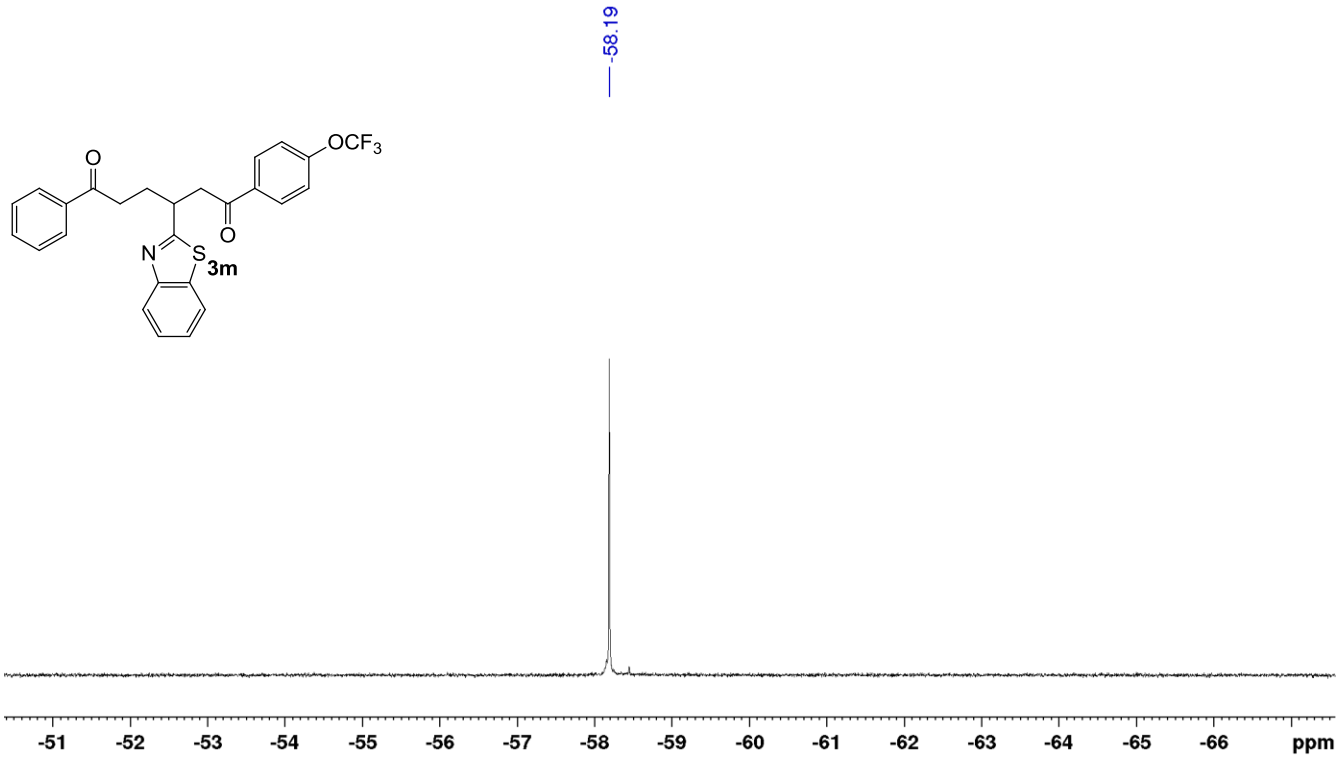
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3m)



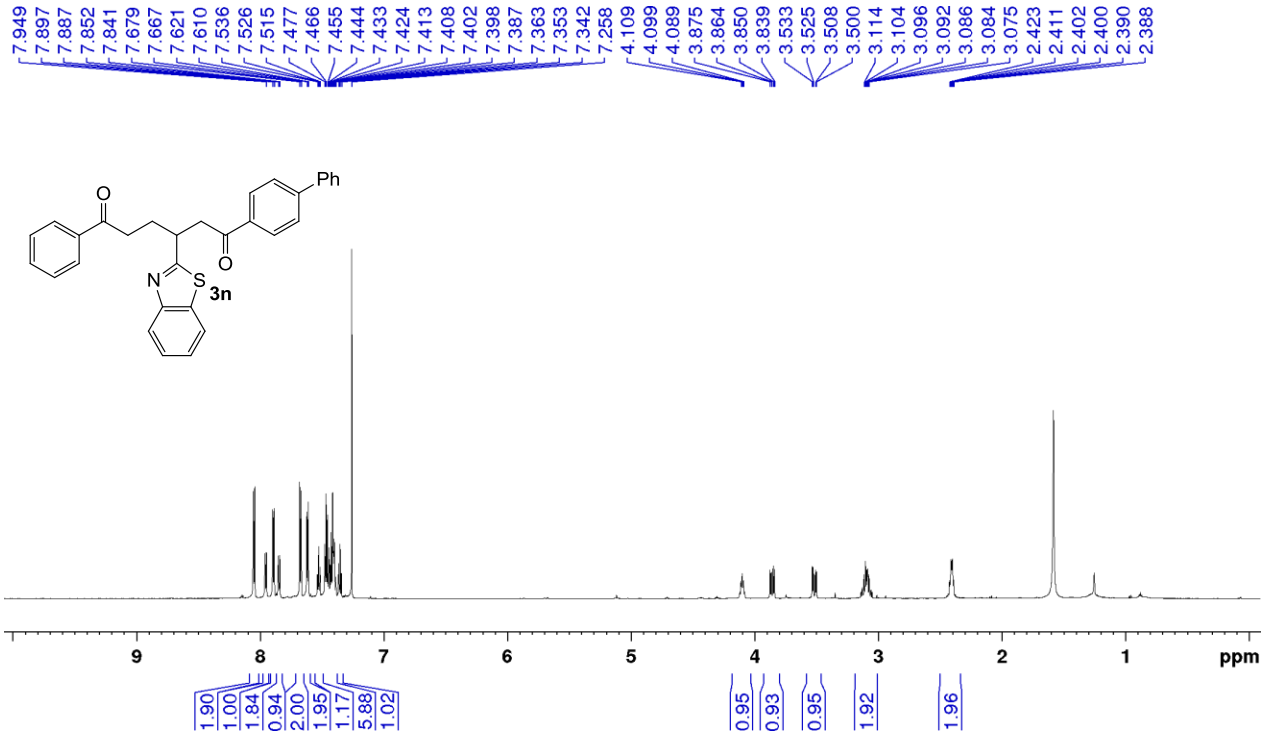
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3m)



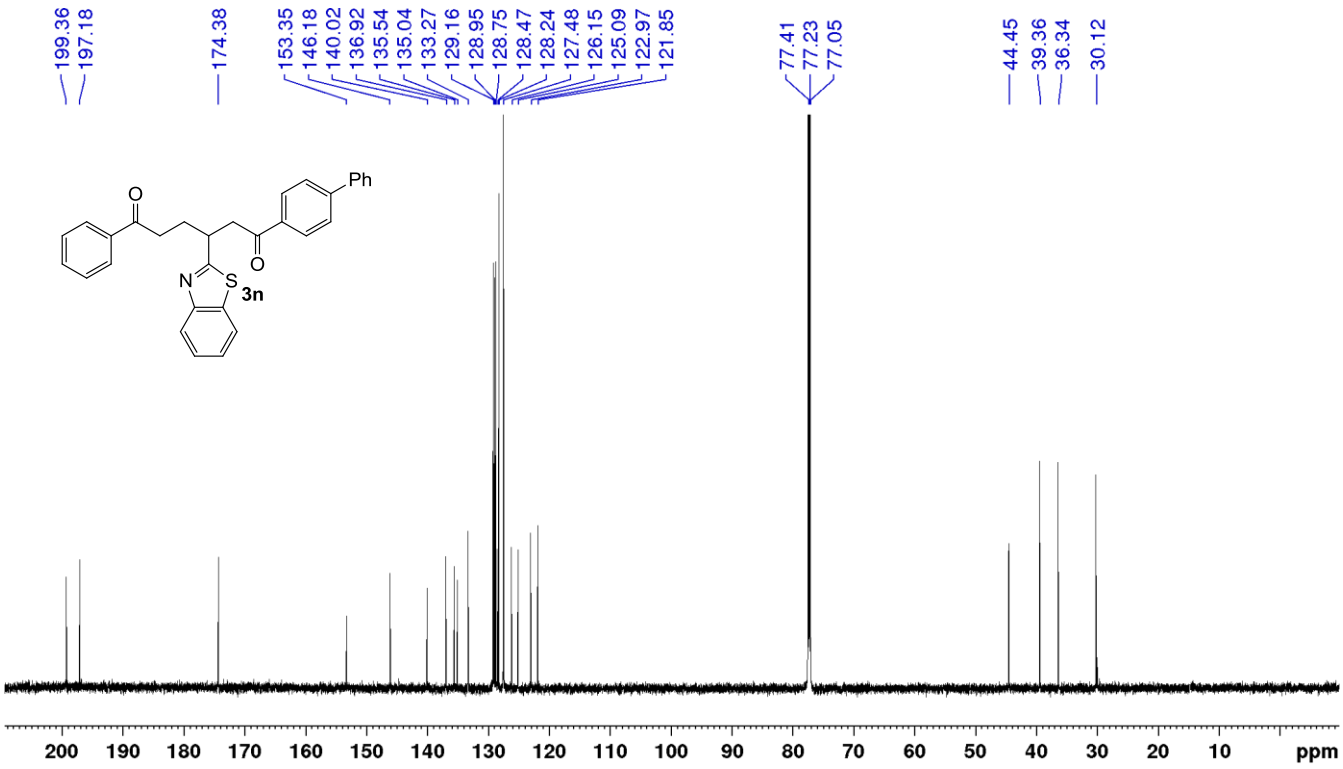
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (3m)



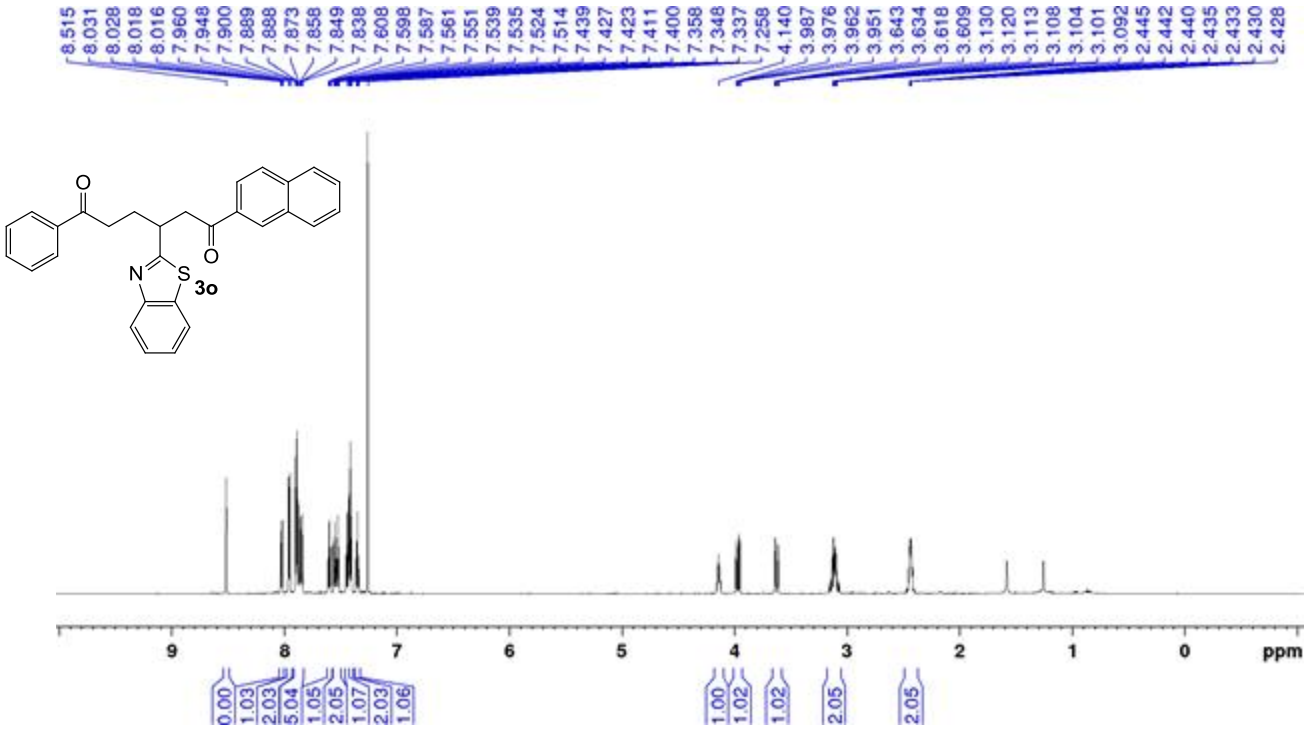
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3n)



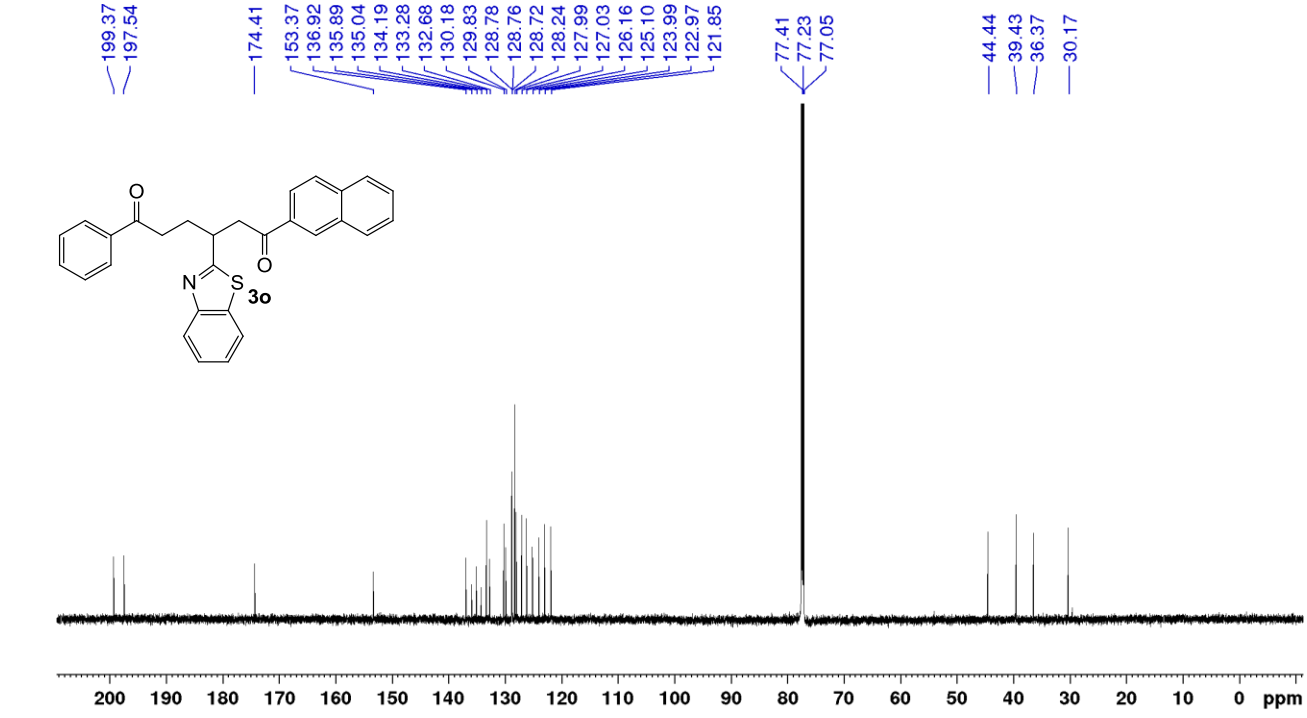
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3n)



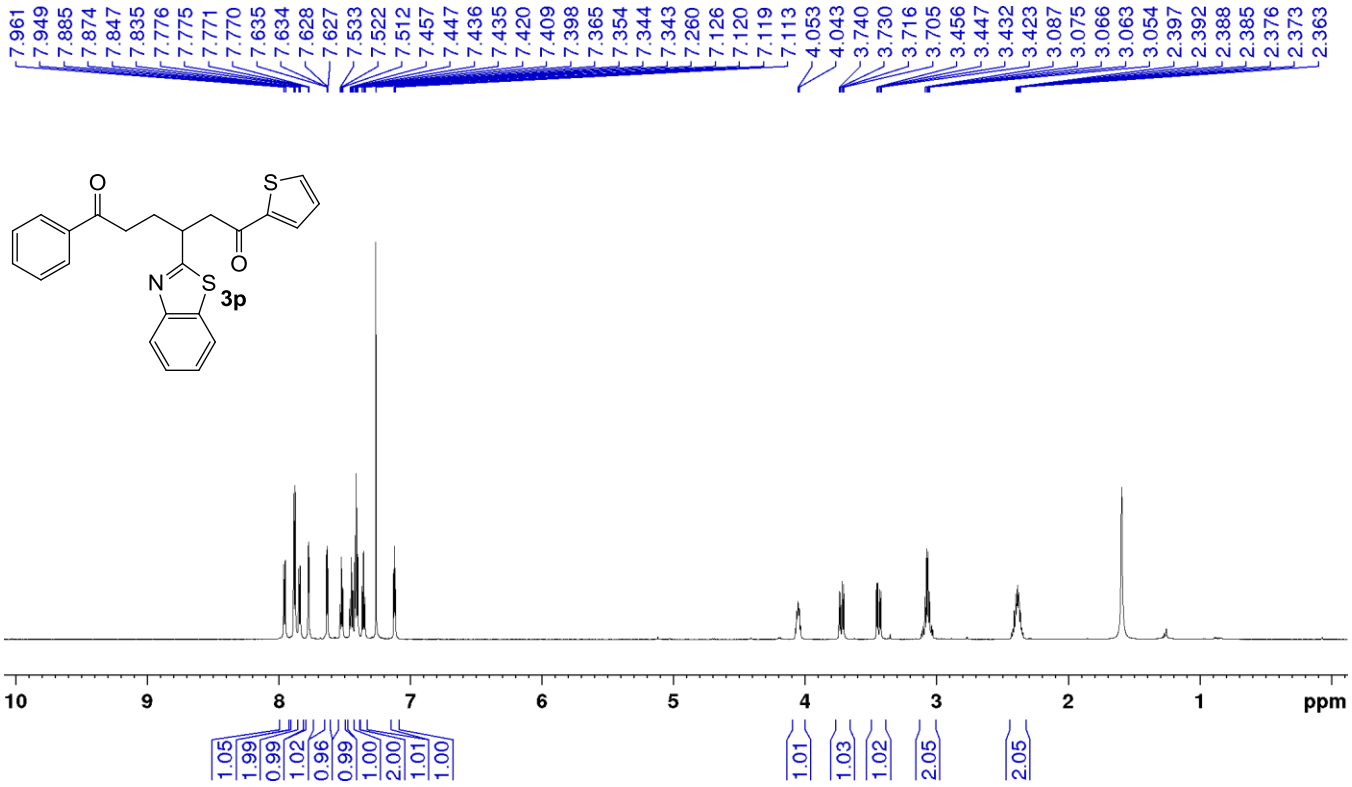
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3o)



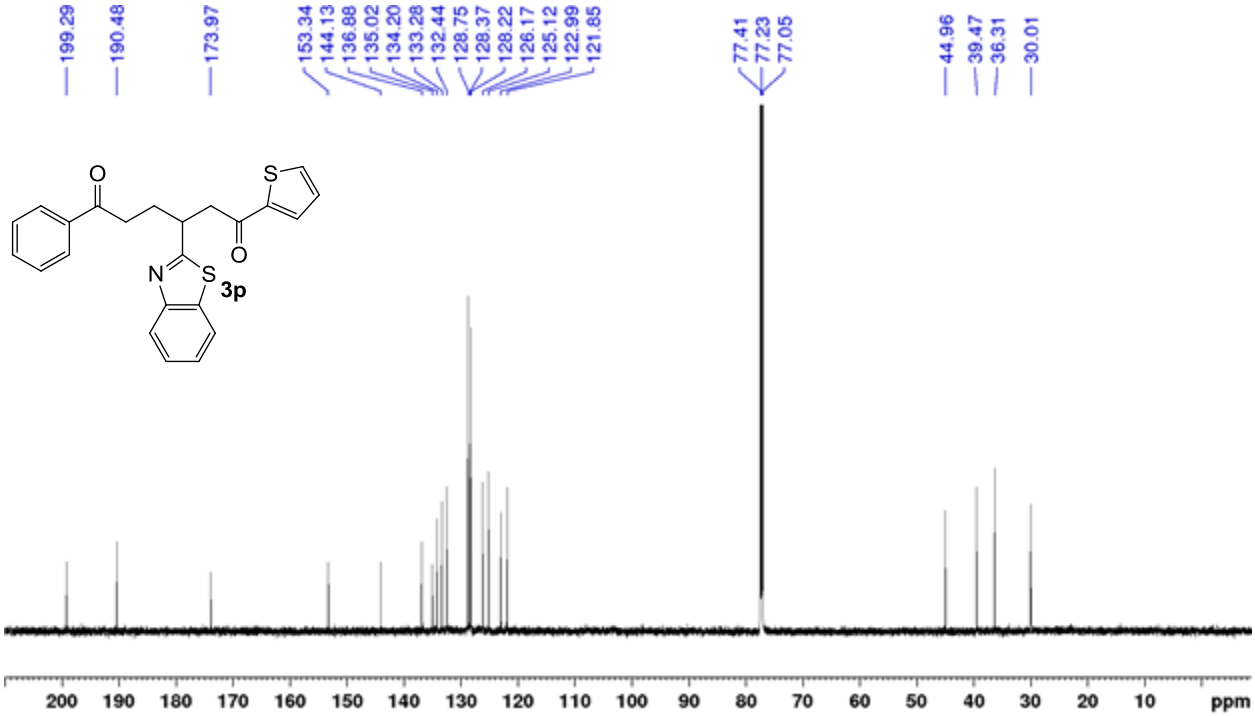
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3o)



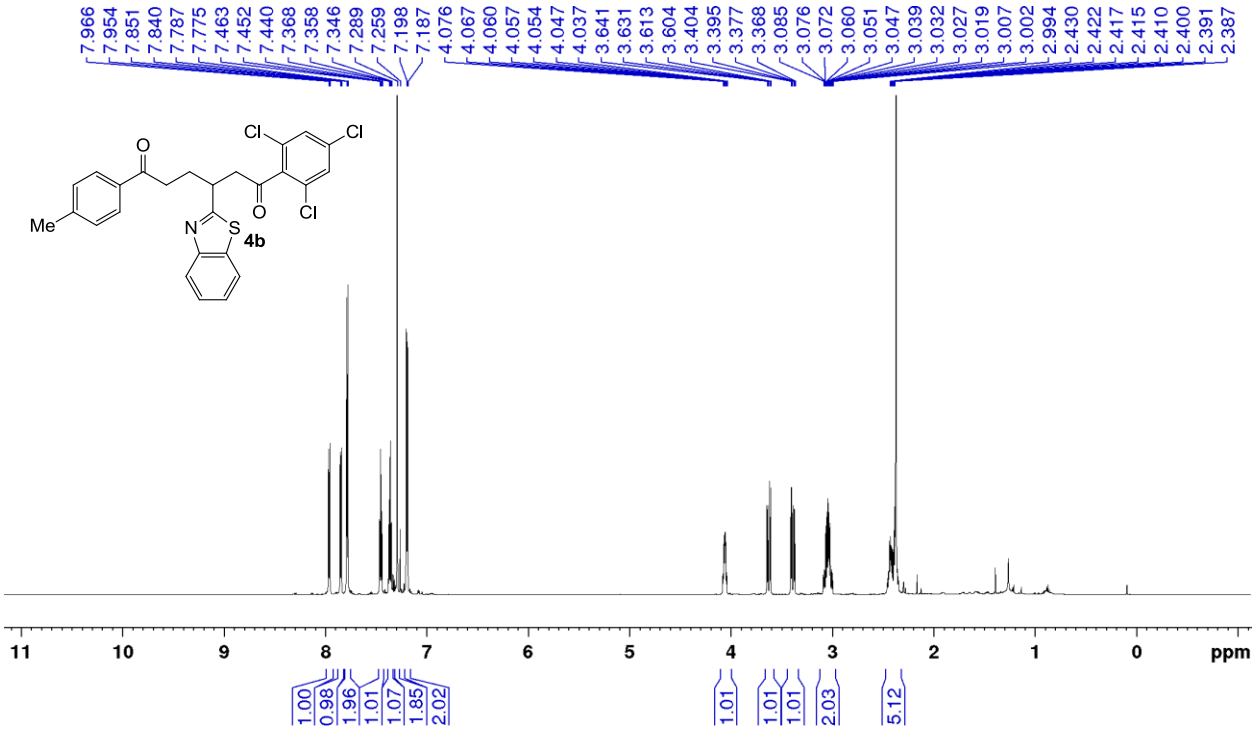
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (3p)



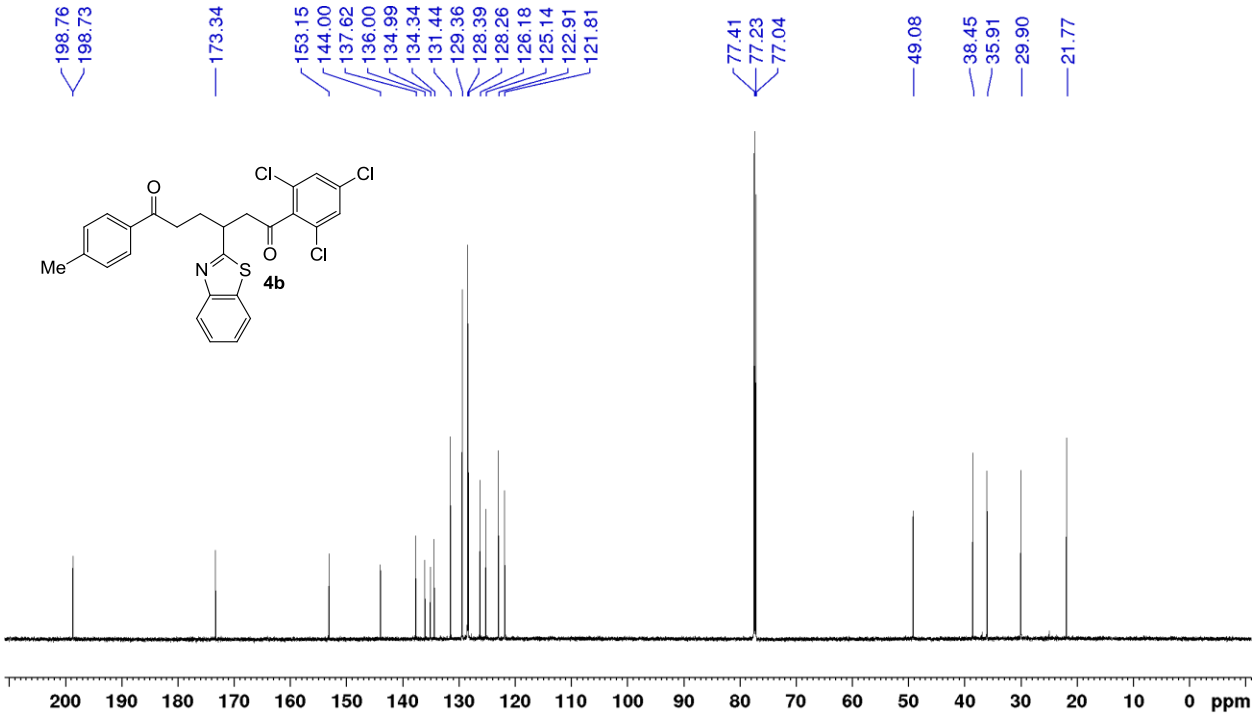
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (3p)



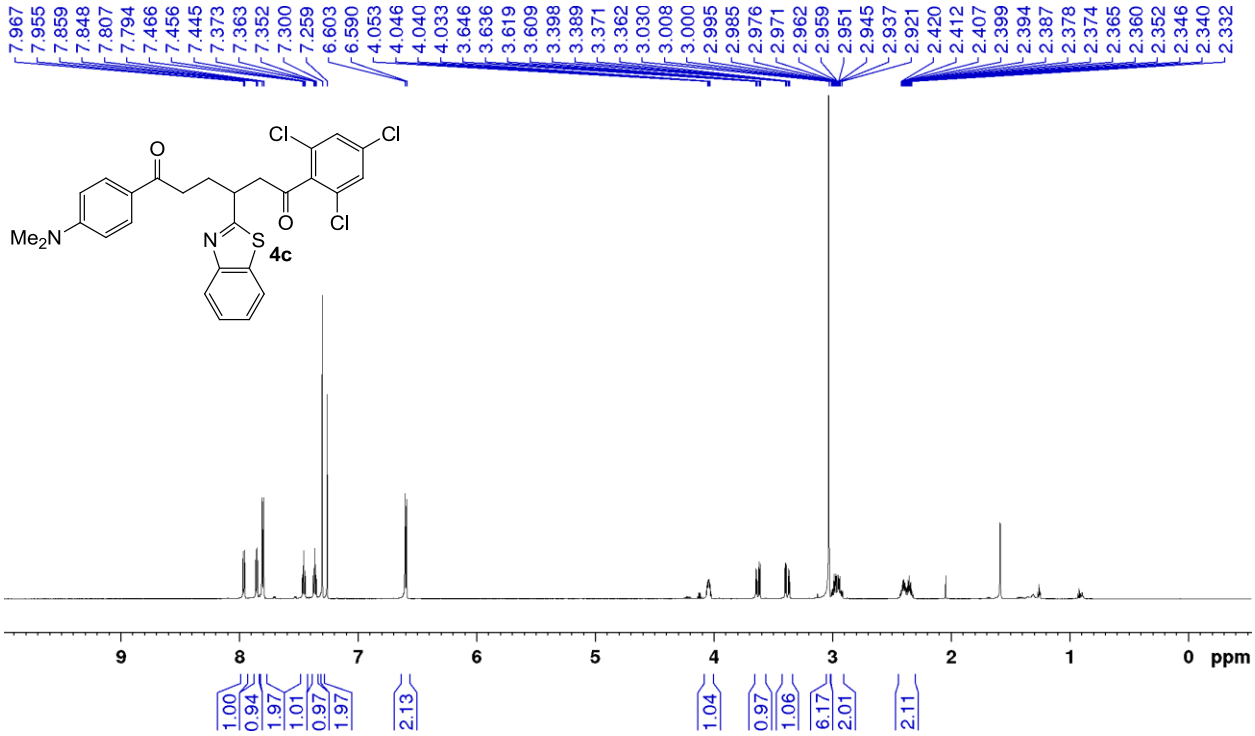
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4b)



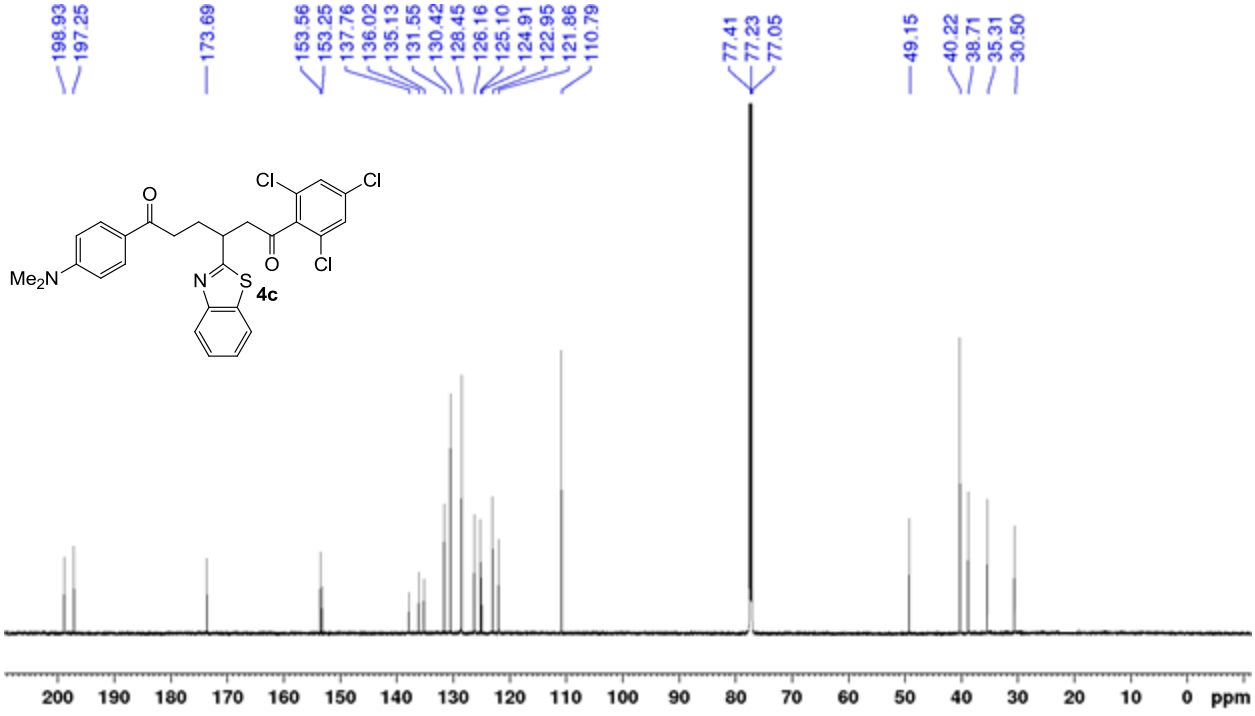
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4b)



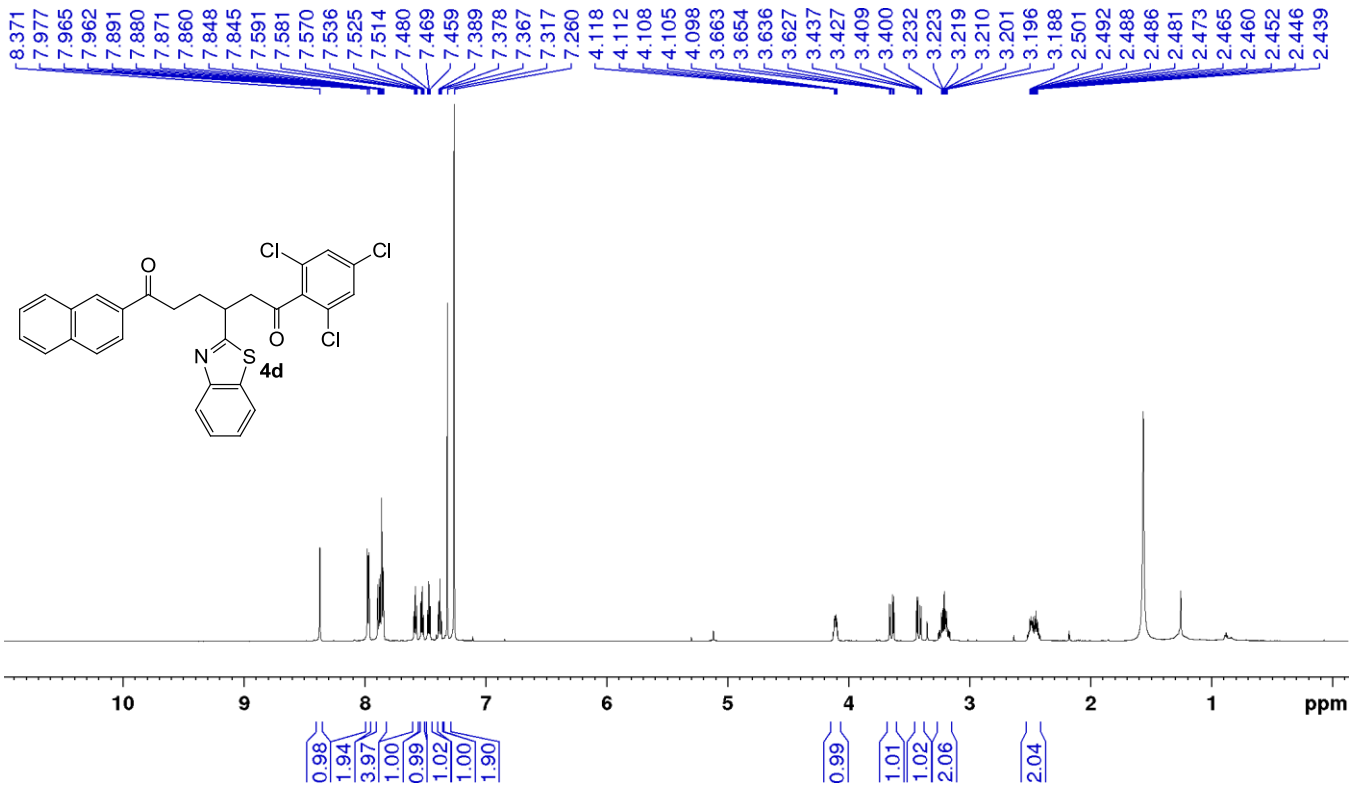
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4c)



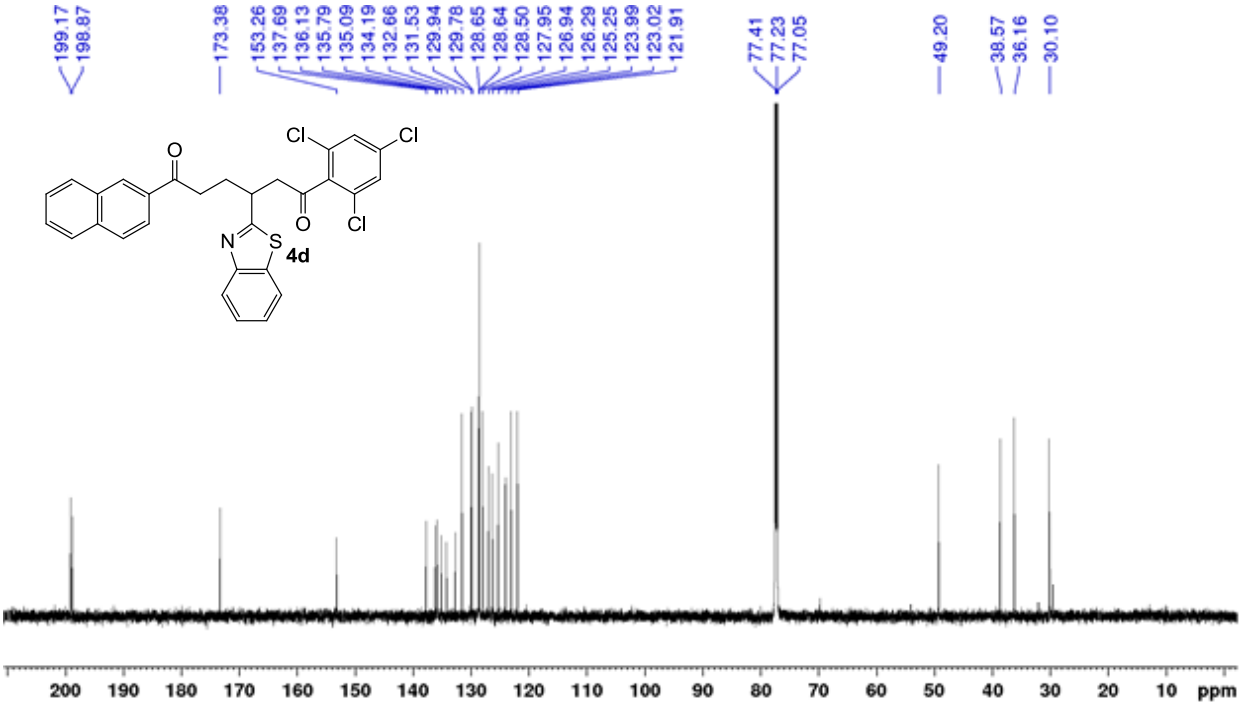
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4c)



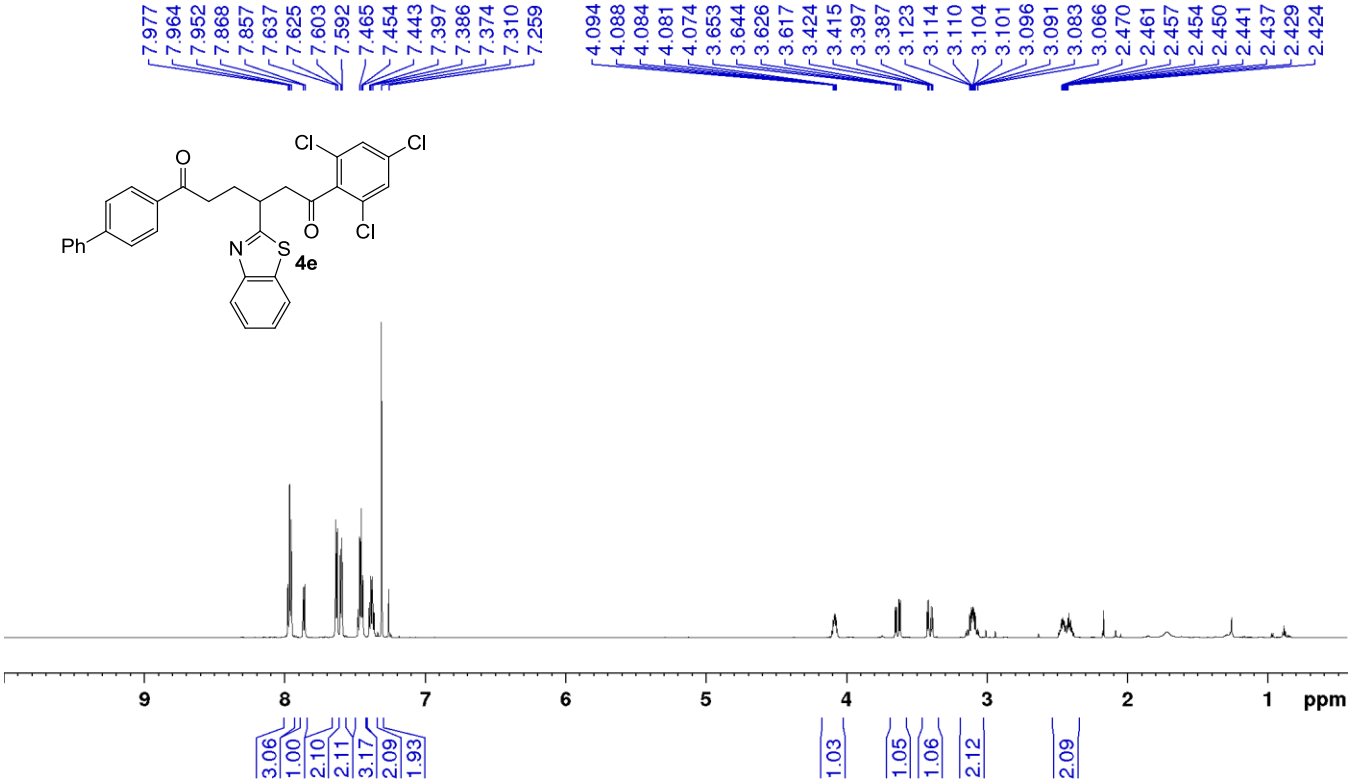
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4d)



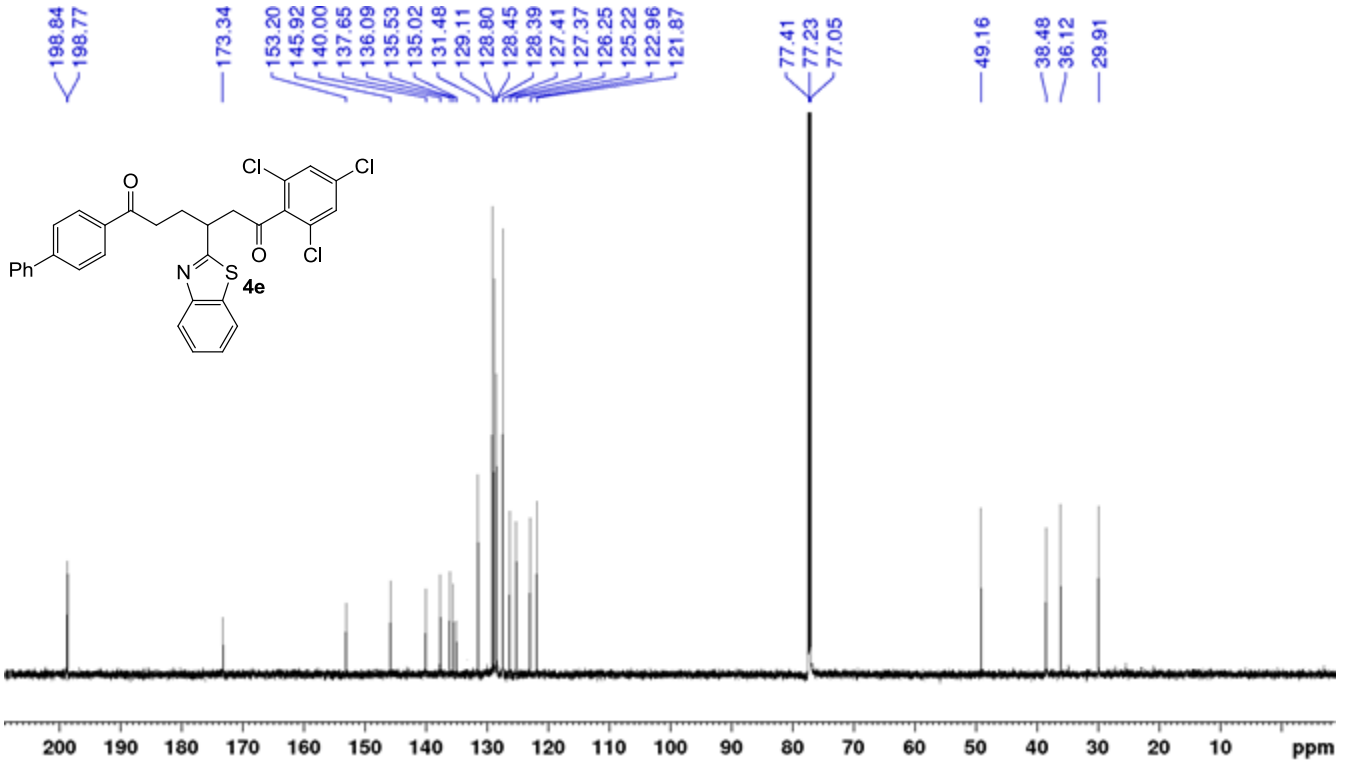
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4d)



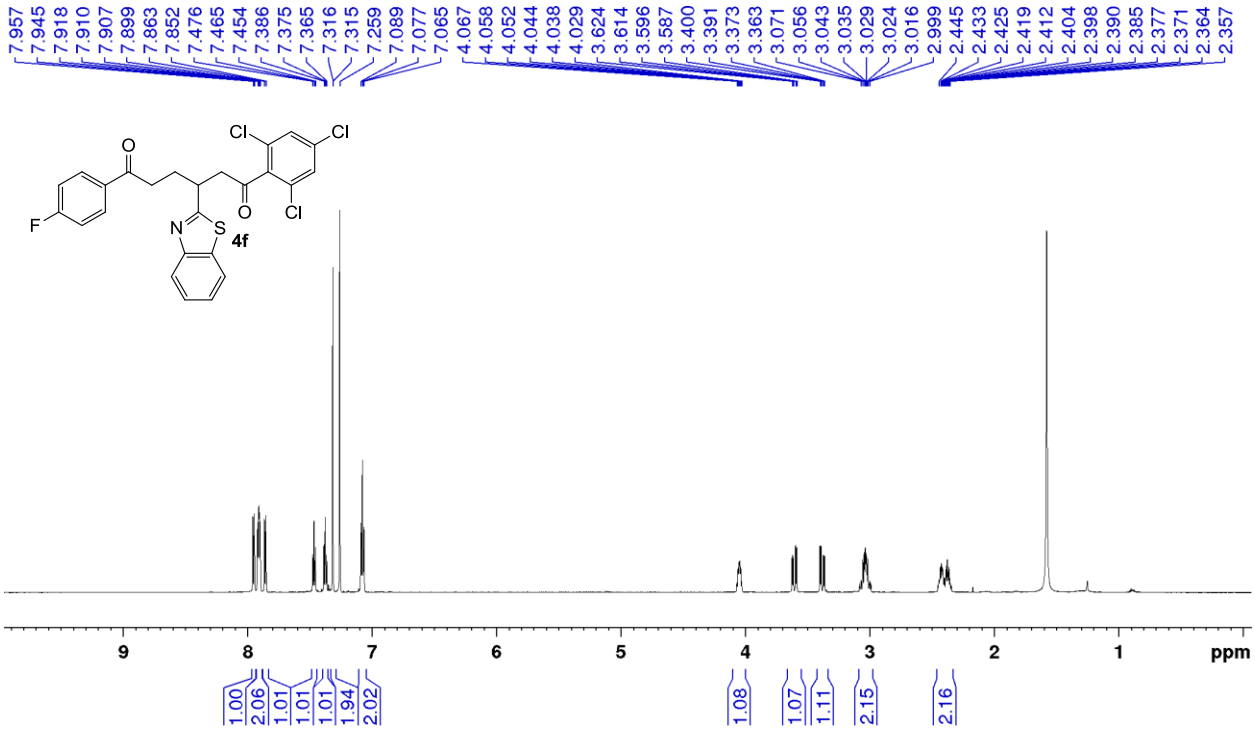
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4e)



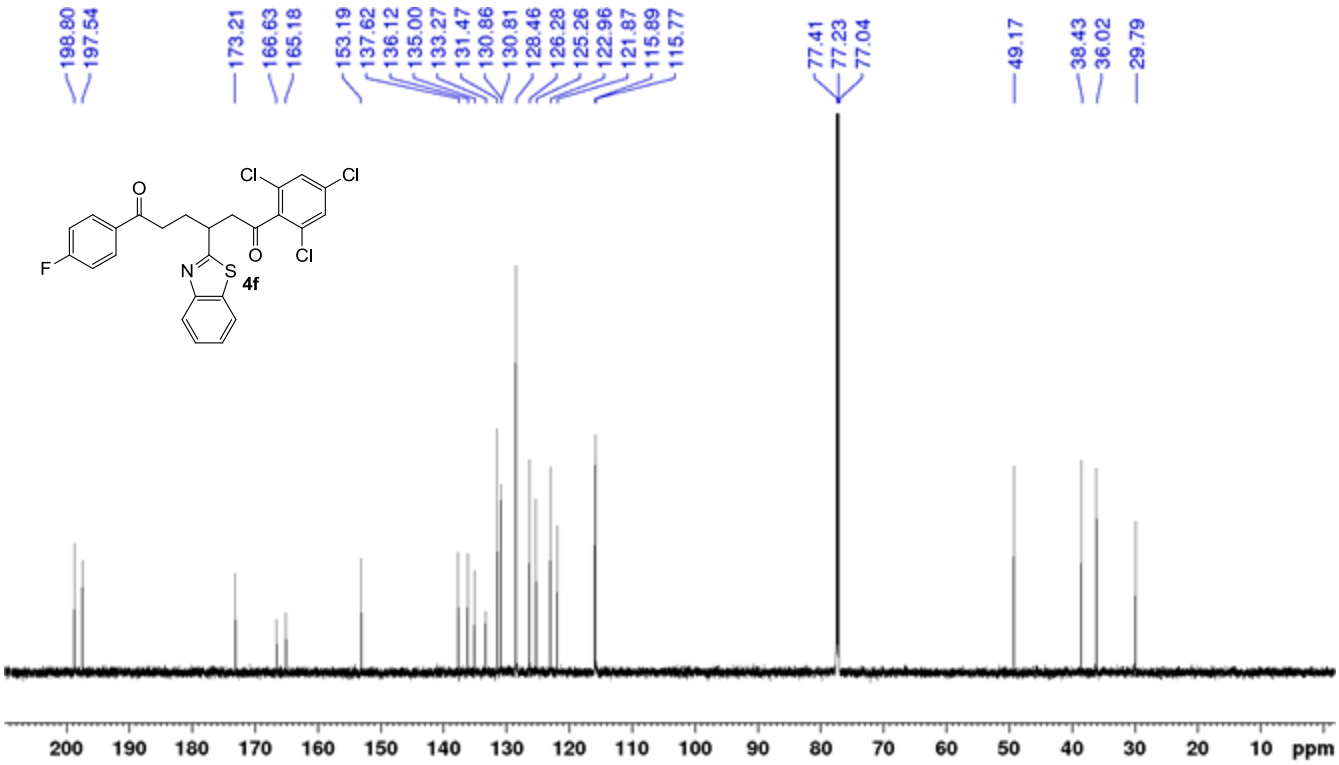
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4e)



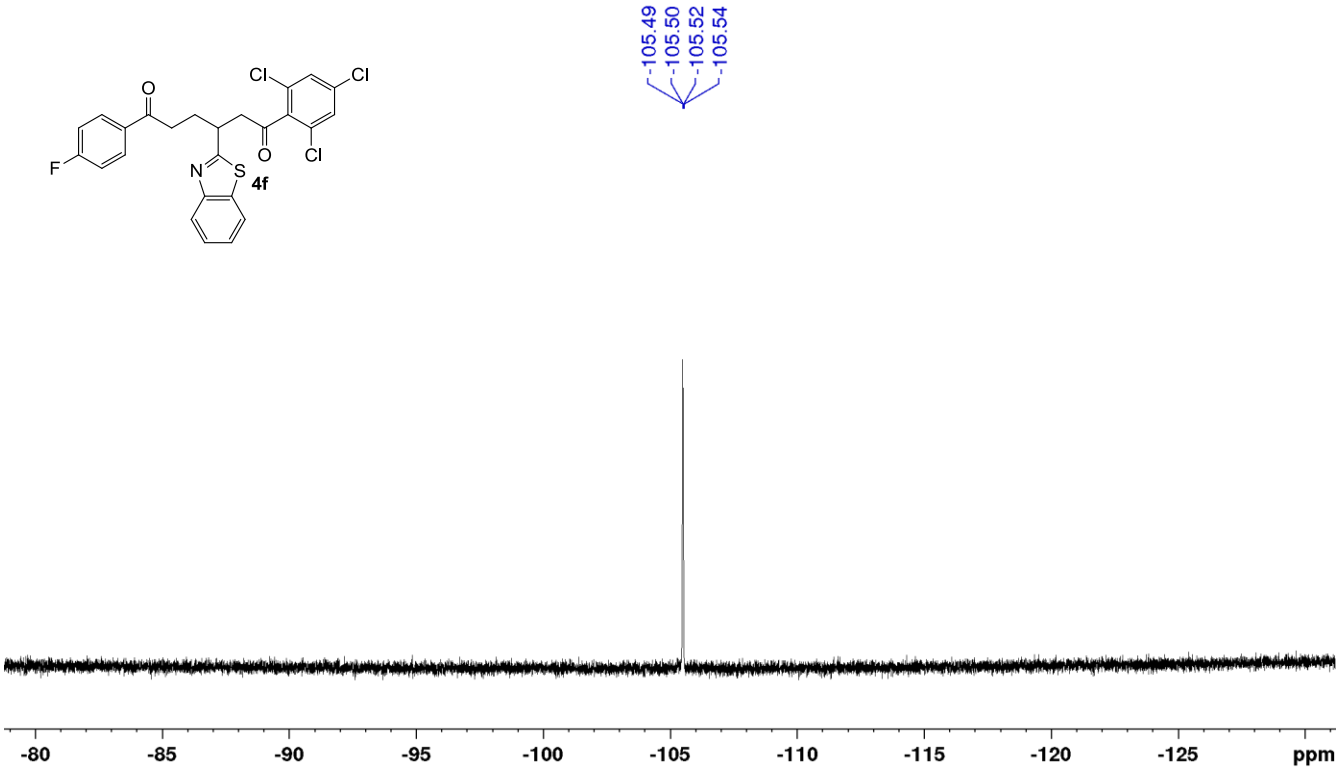
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4f)



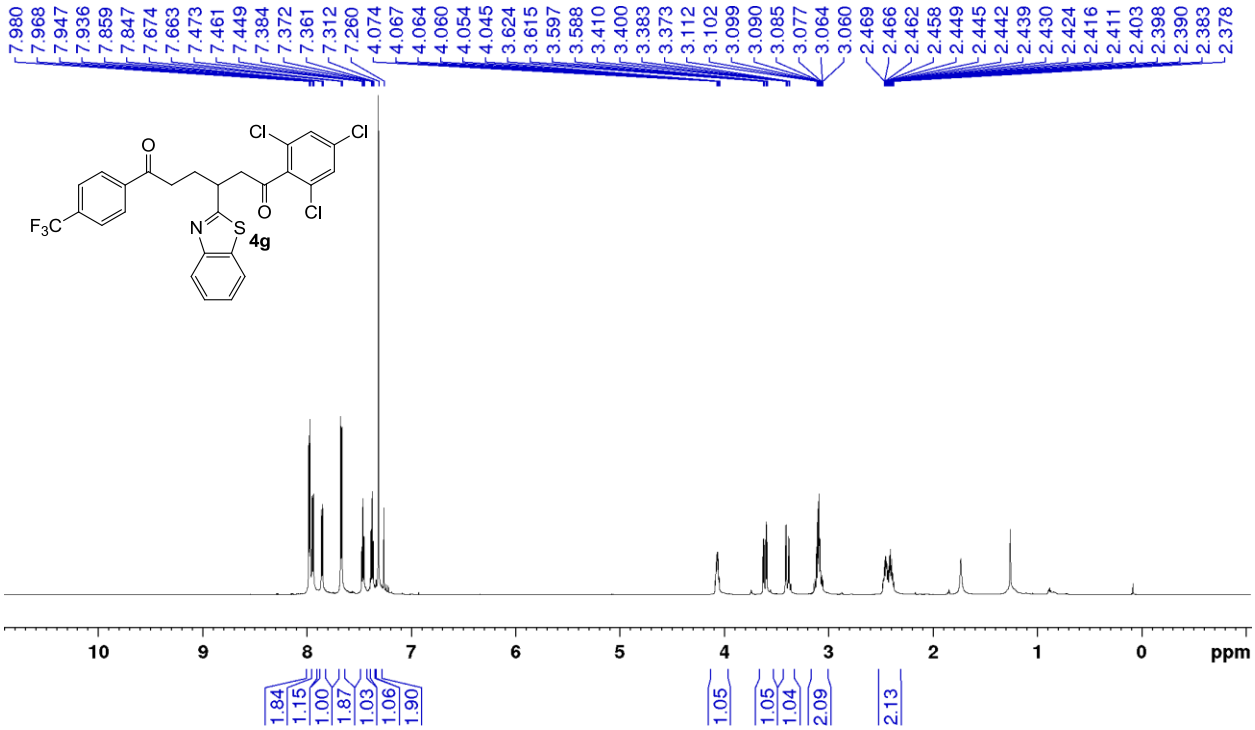
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4f)



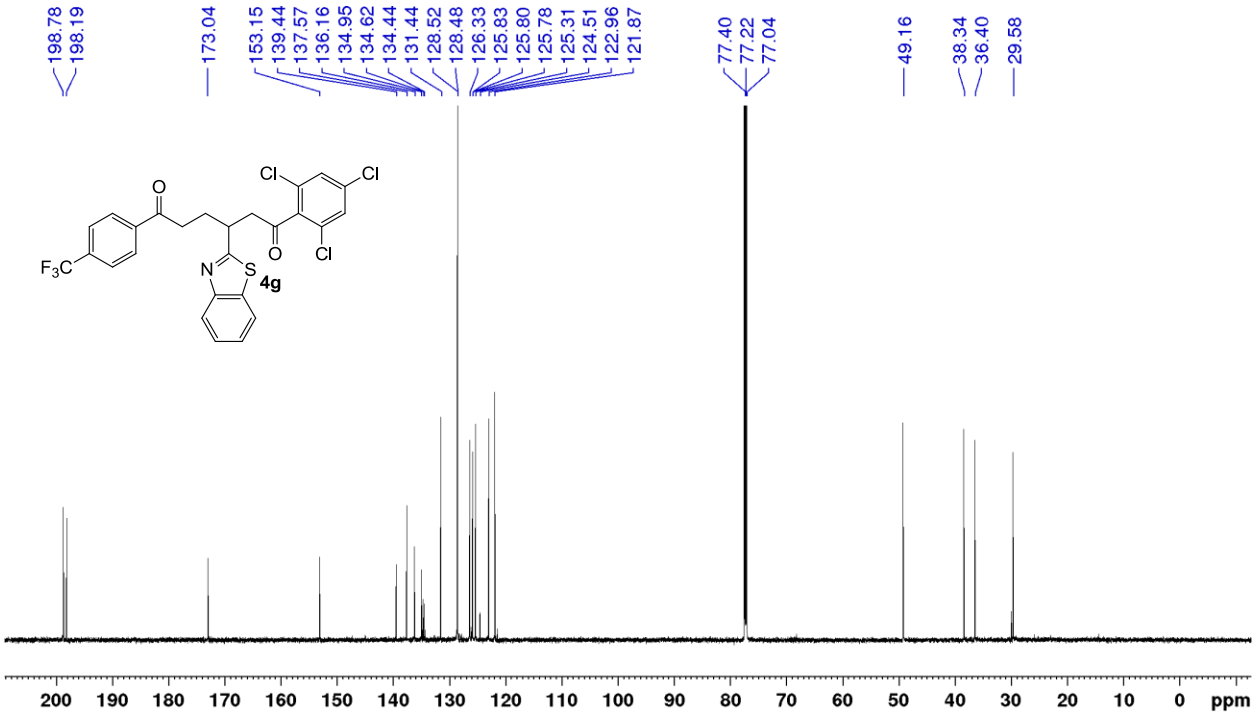
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4f)



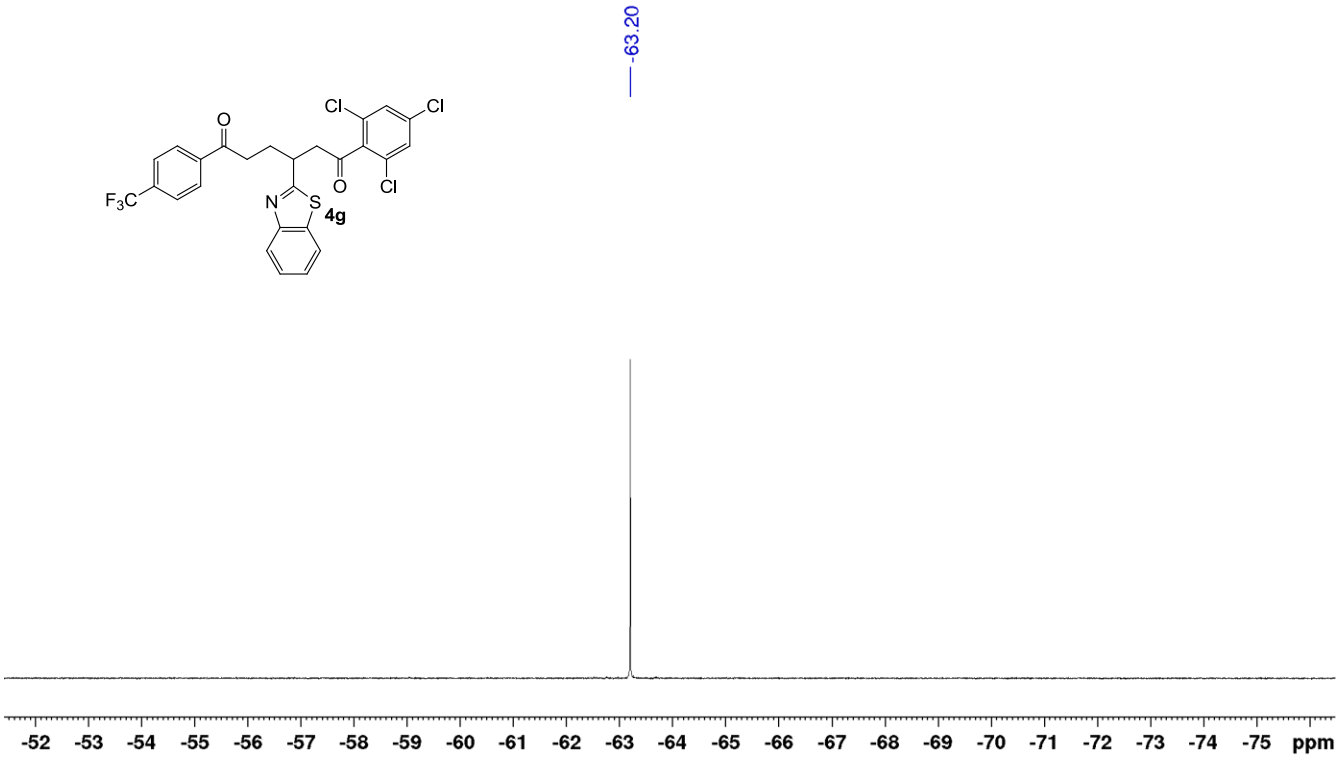
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4g)



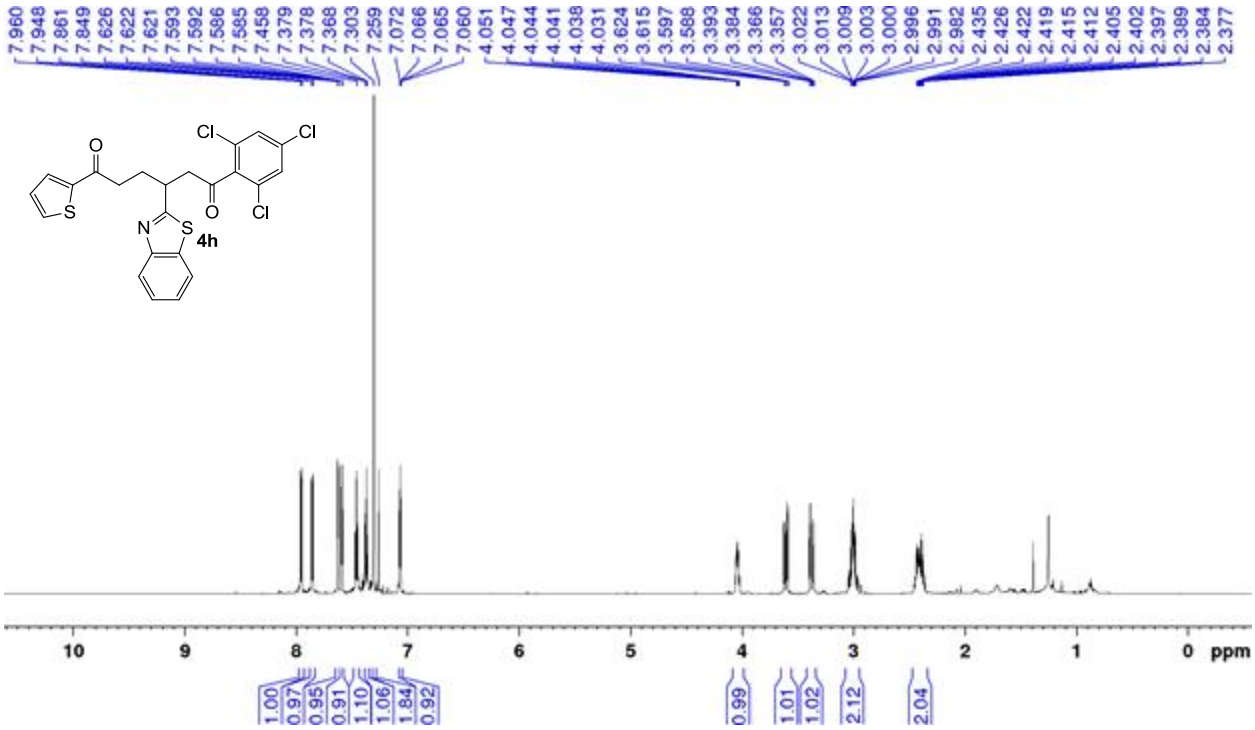
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4g)



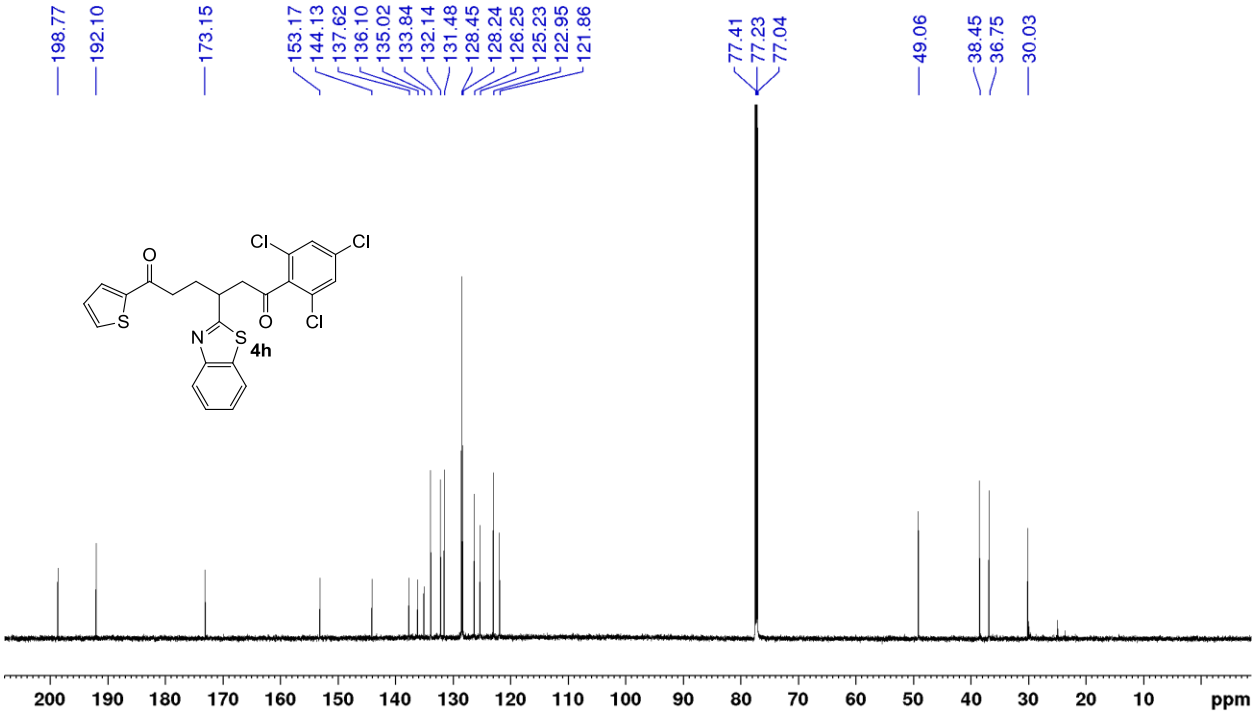
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4g)



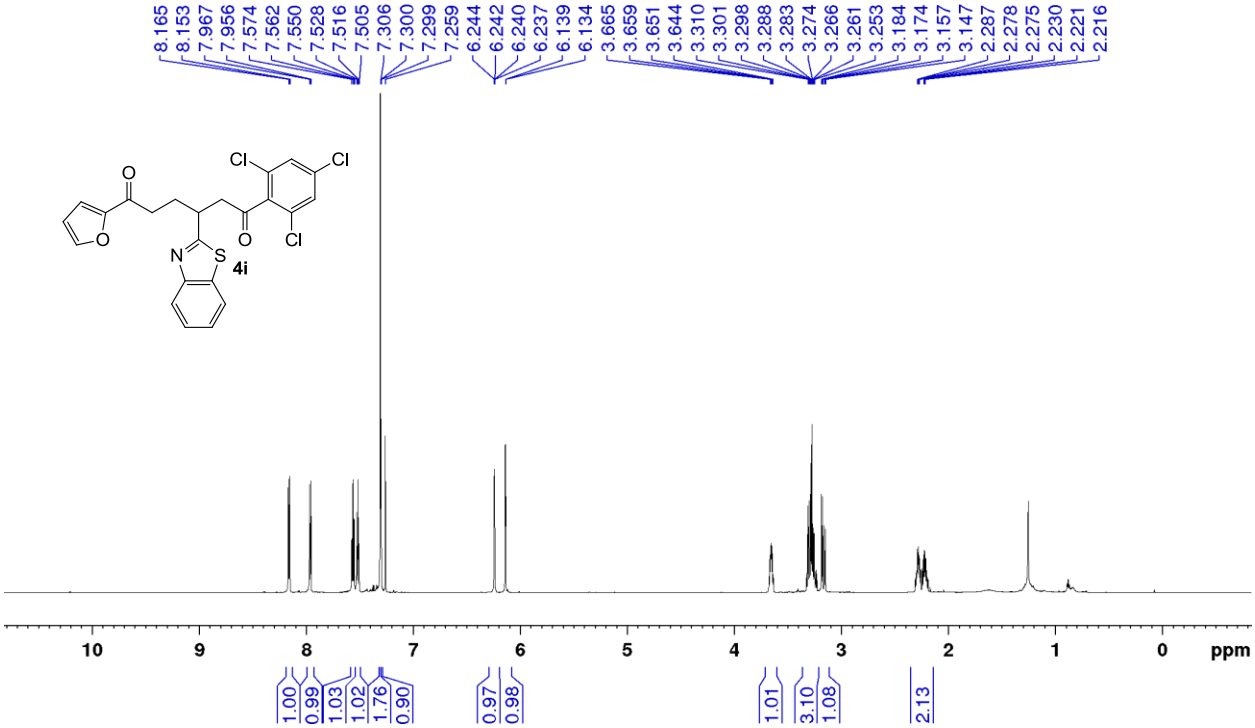
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4h)



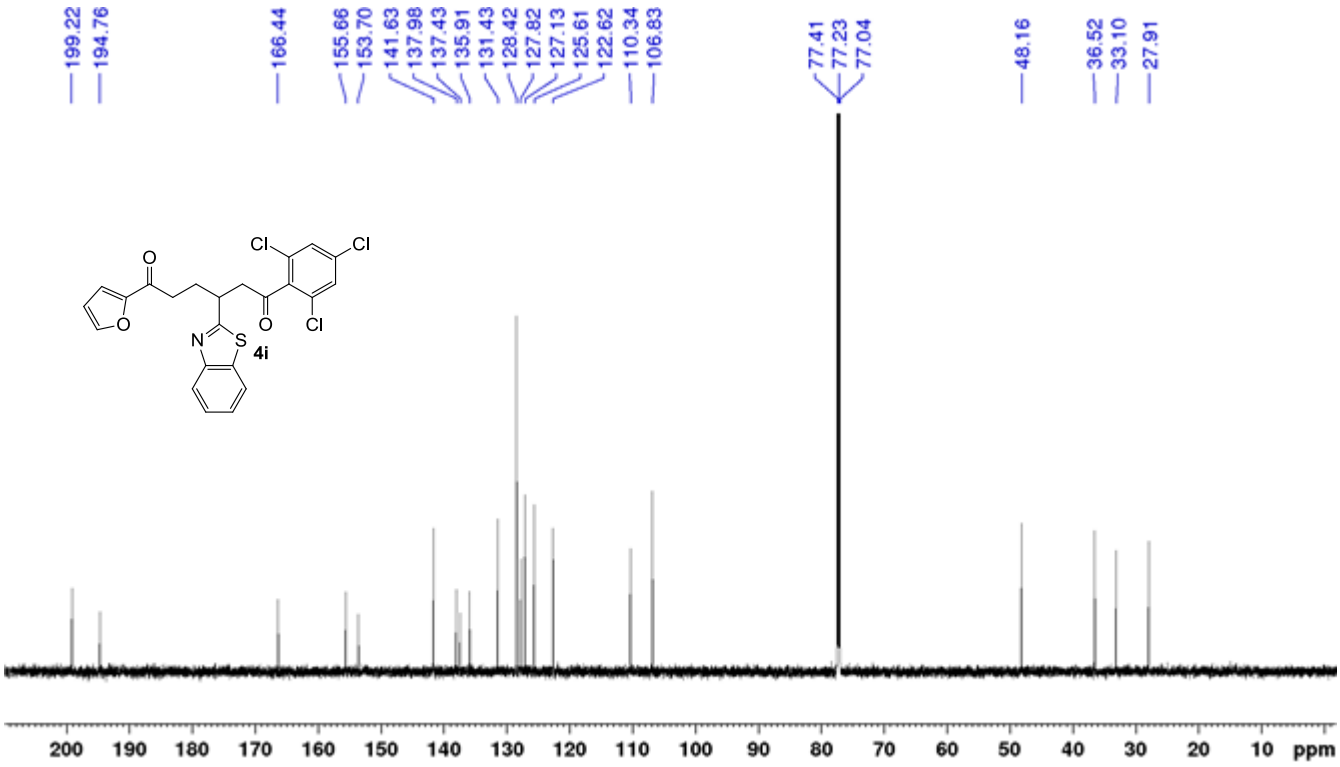
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4h)



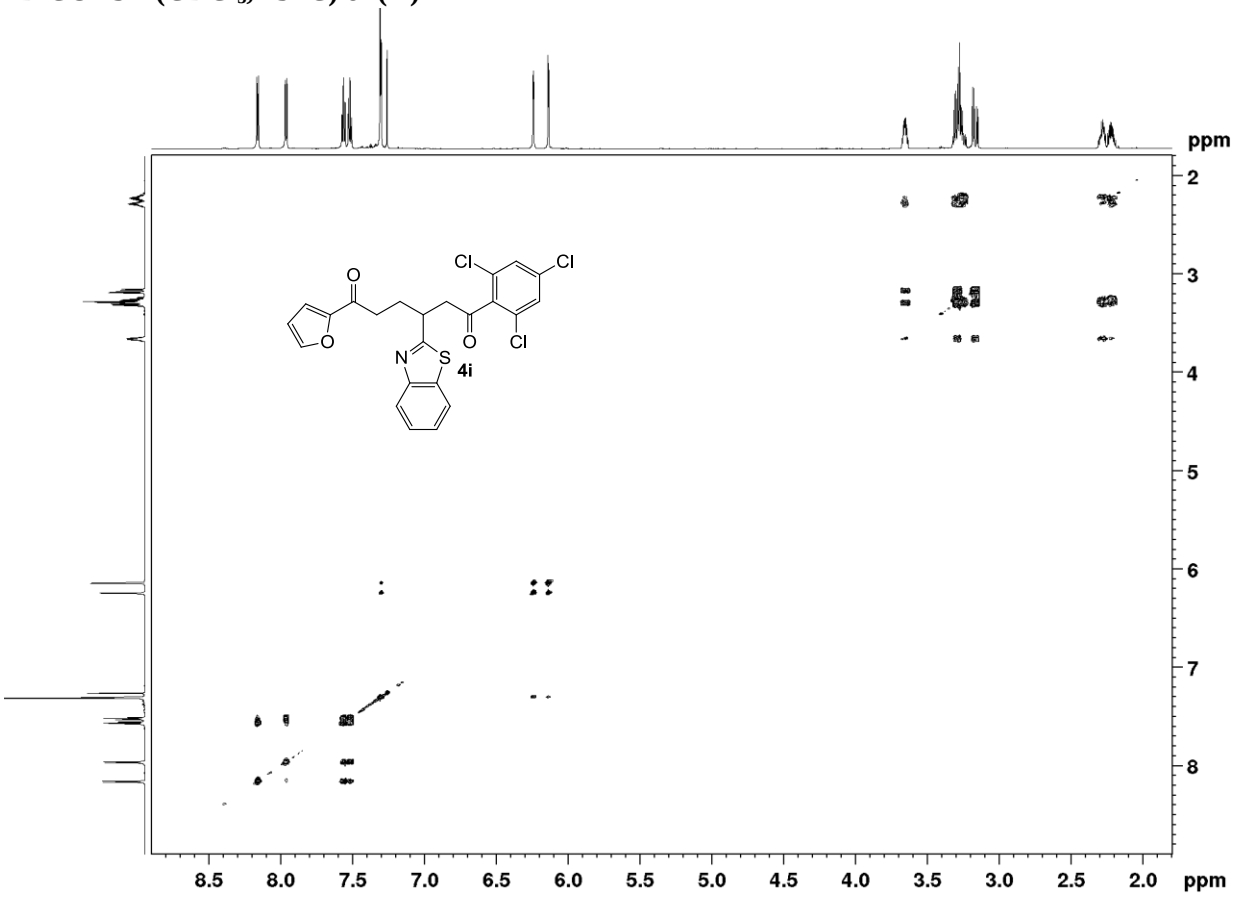
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4i)



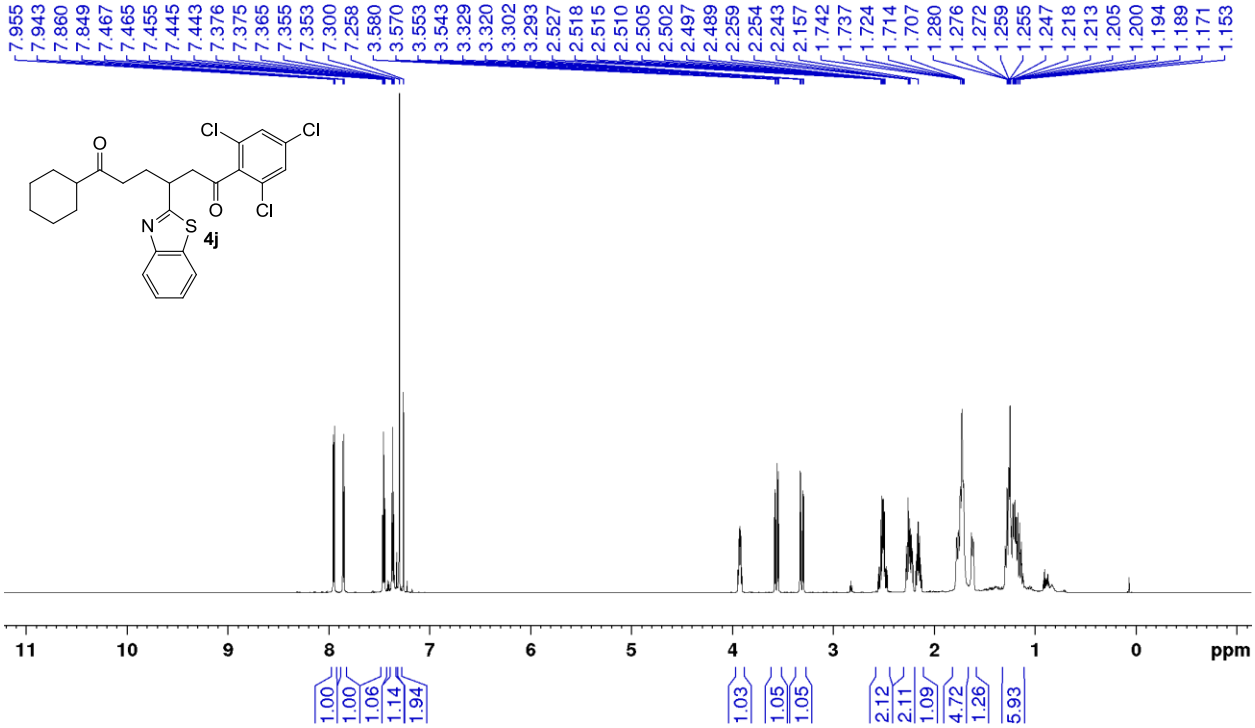
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4i)



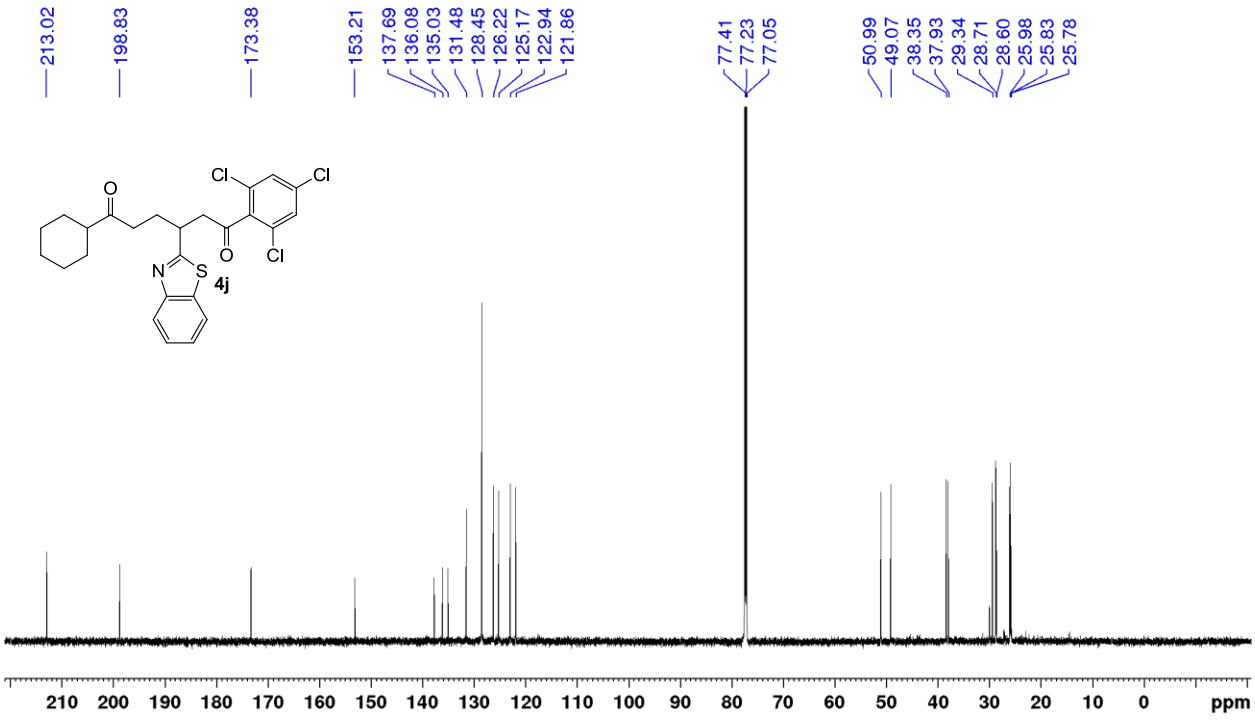
2D COESY ($CDCl_3$, 25 ºC) of (4i)



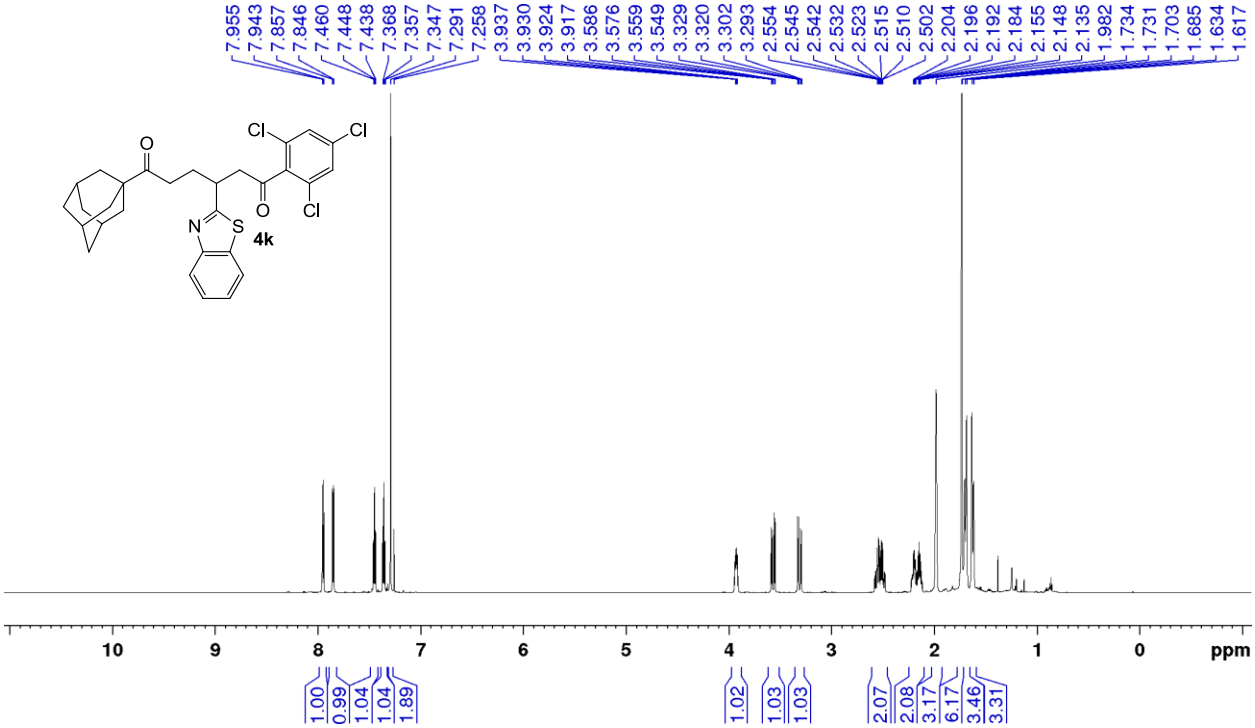
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4j)



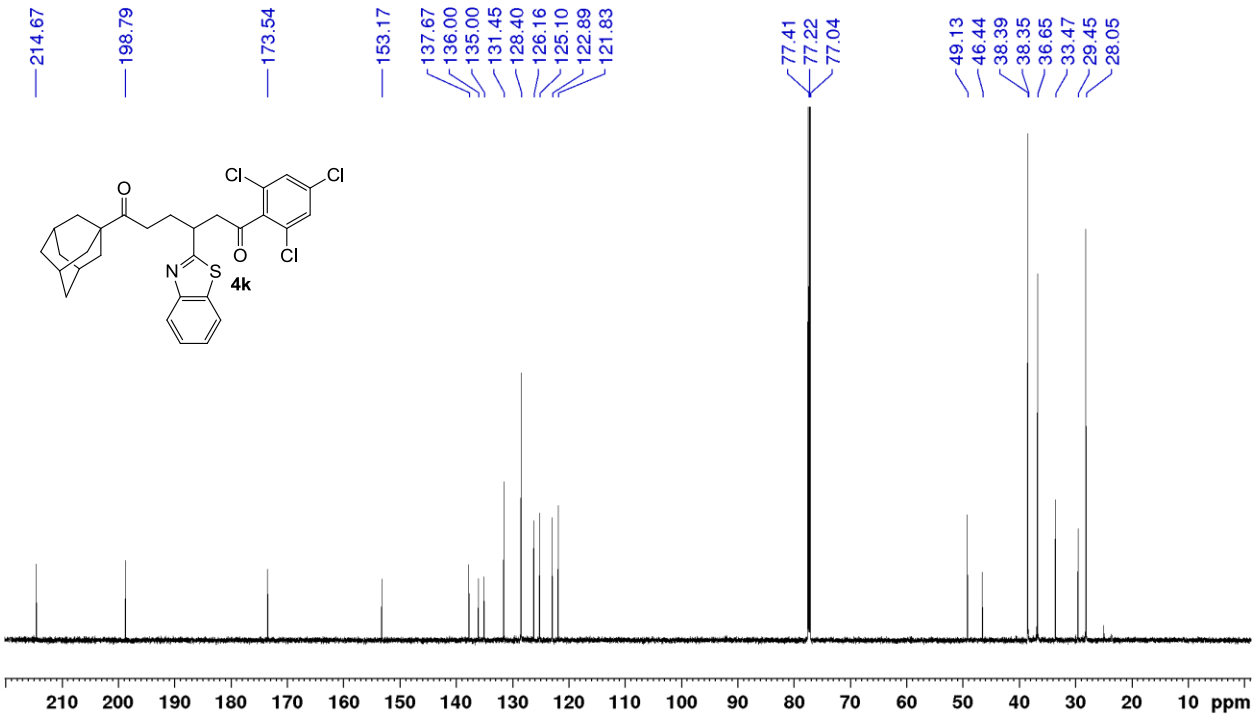
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4j)



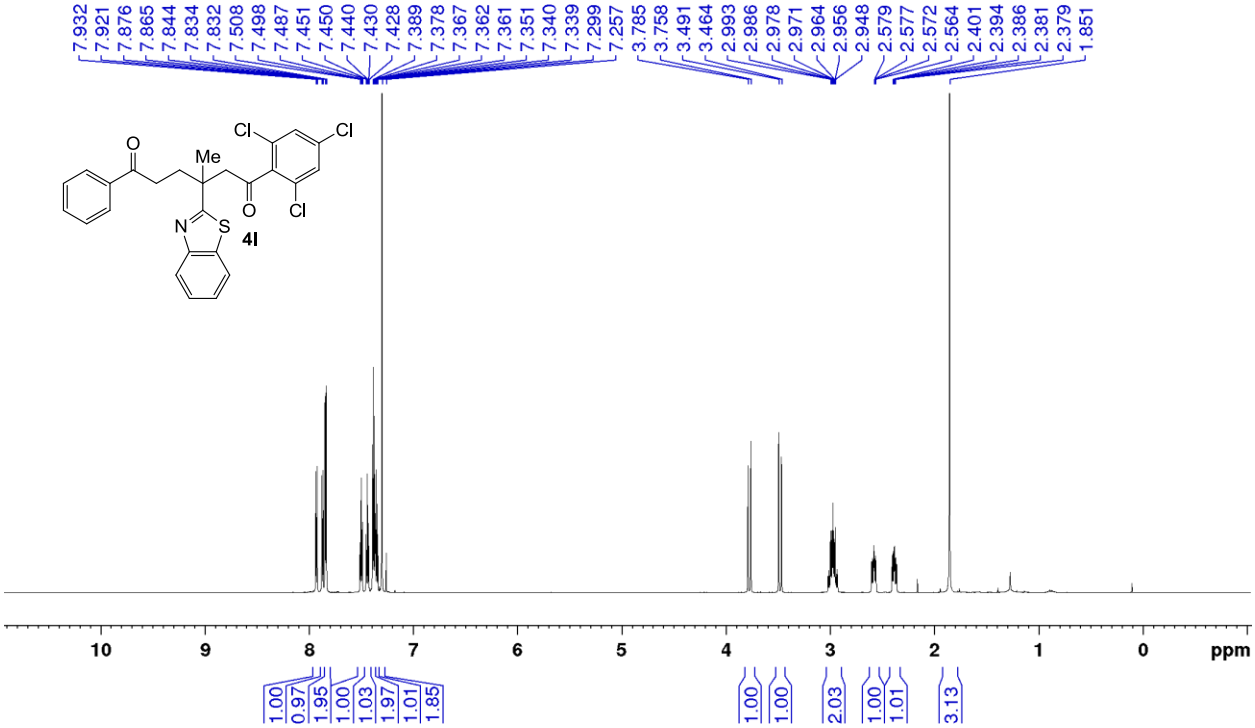
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4k)



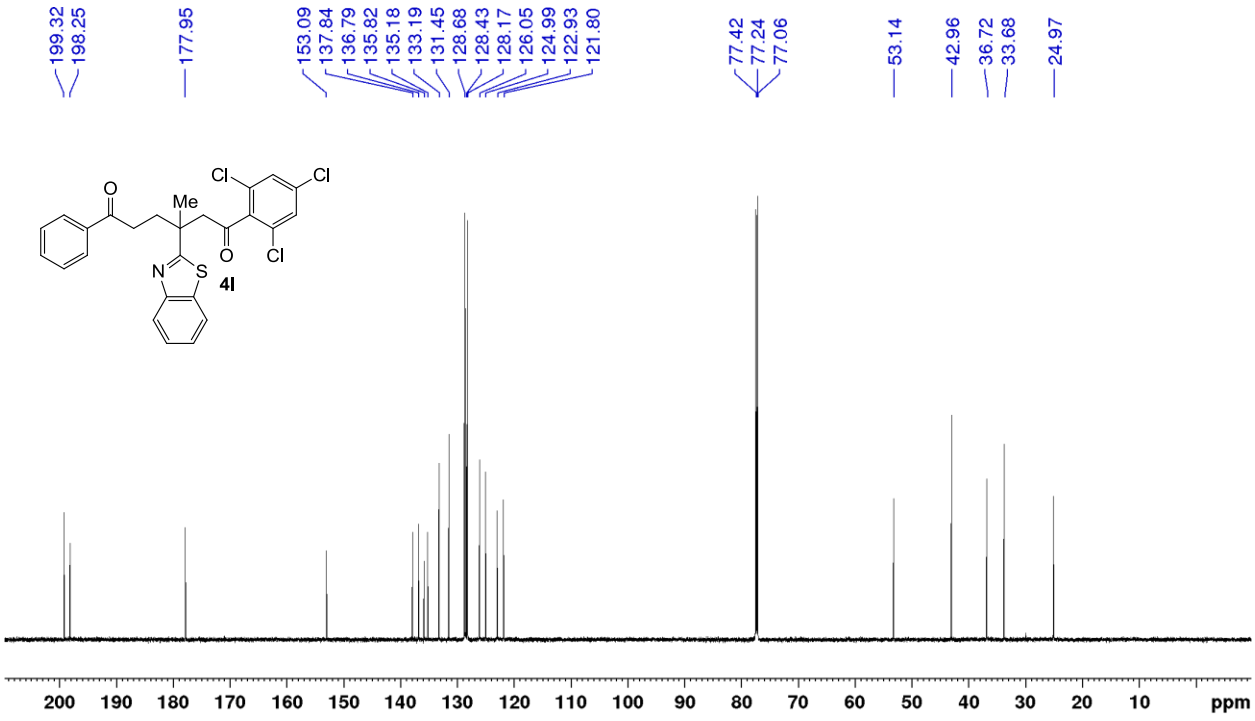
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4k)



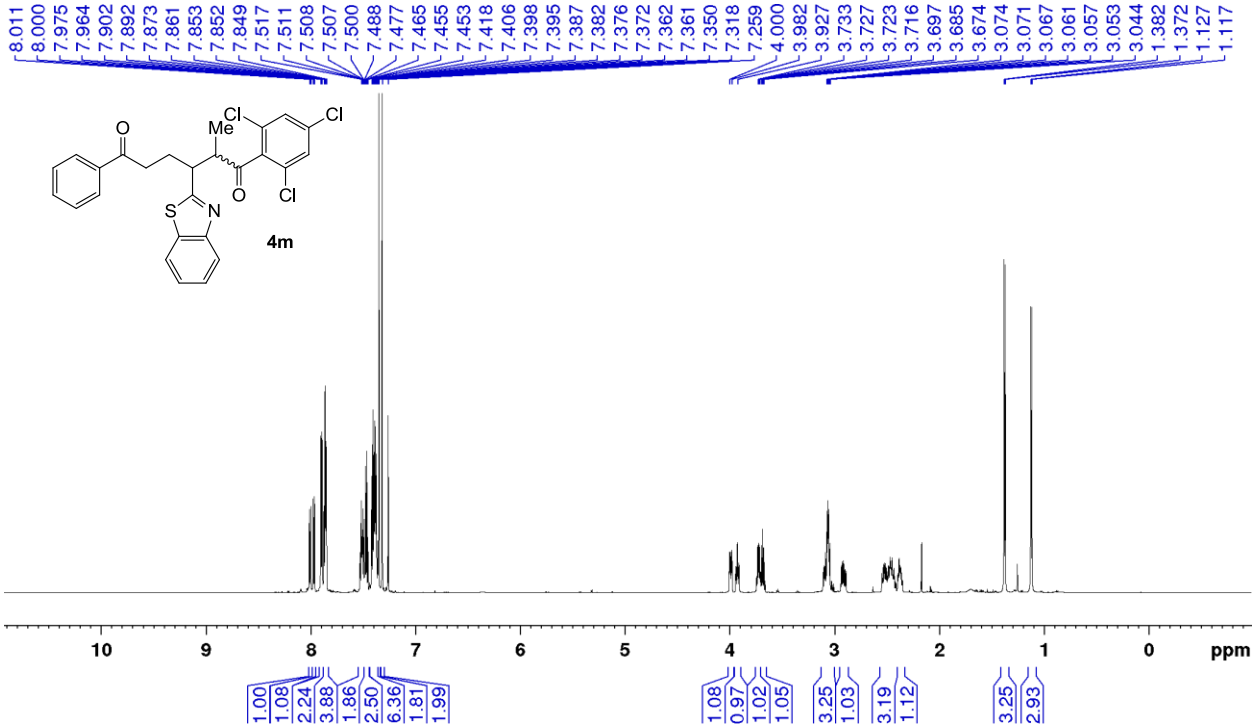
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4l)



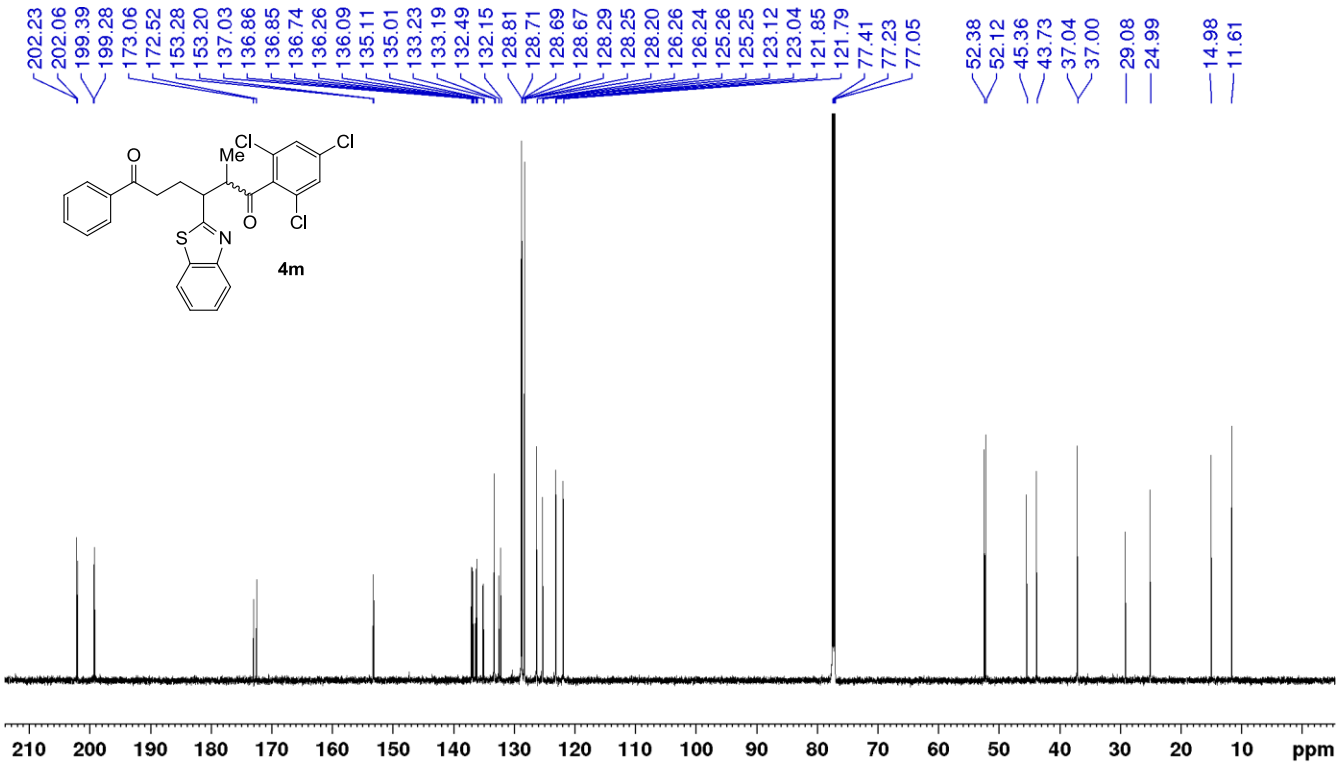
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4l)



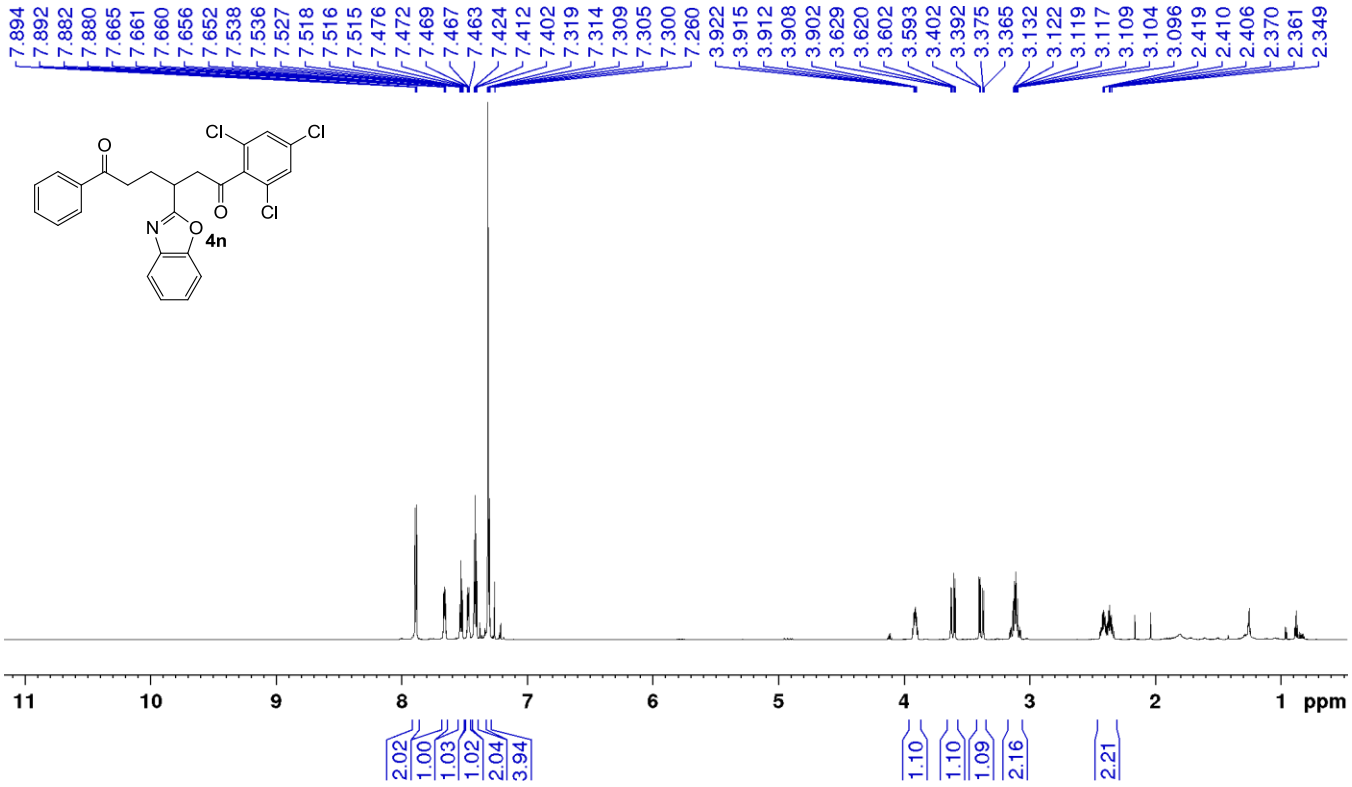
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4m)



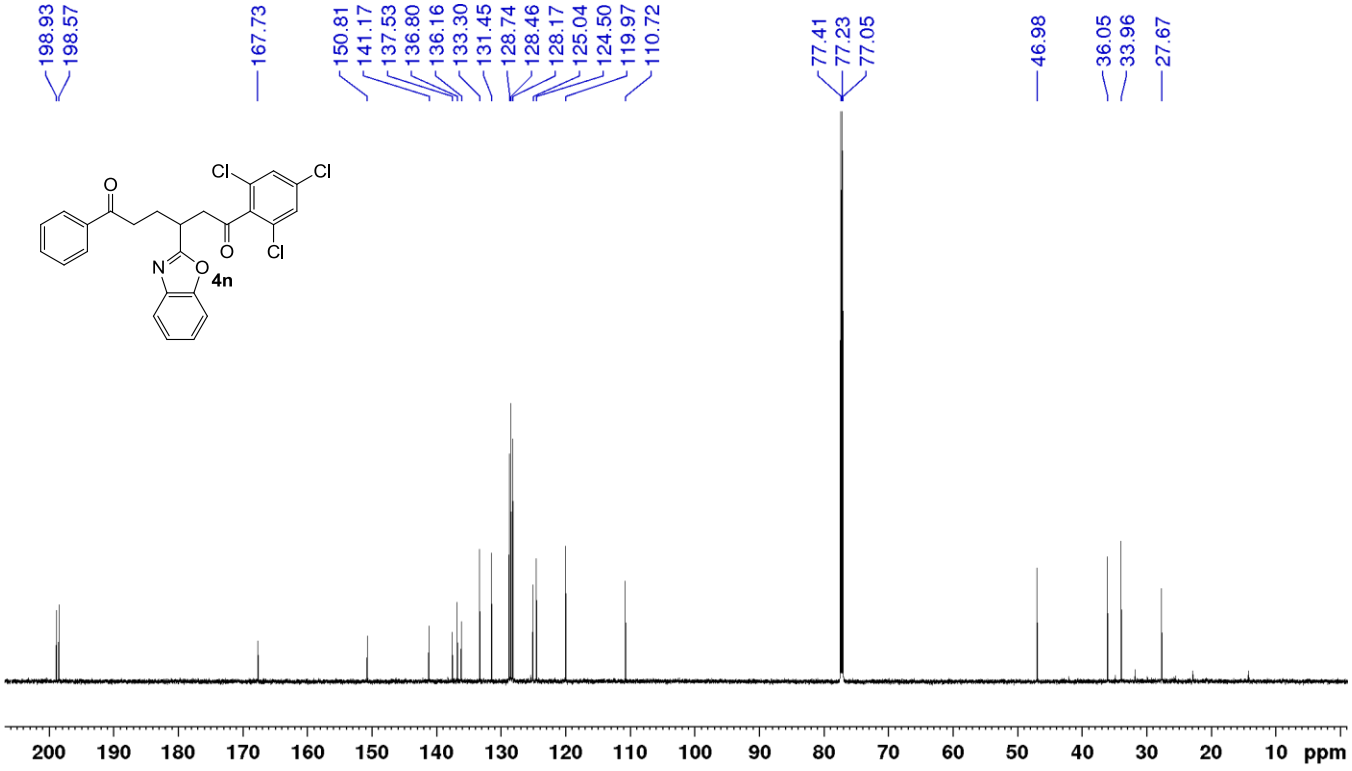
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4m)



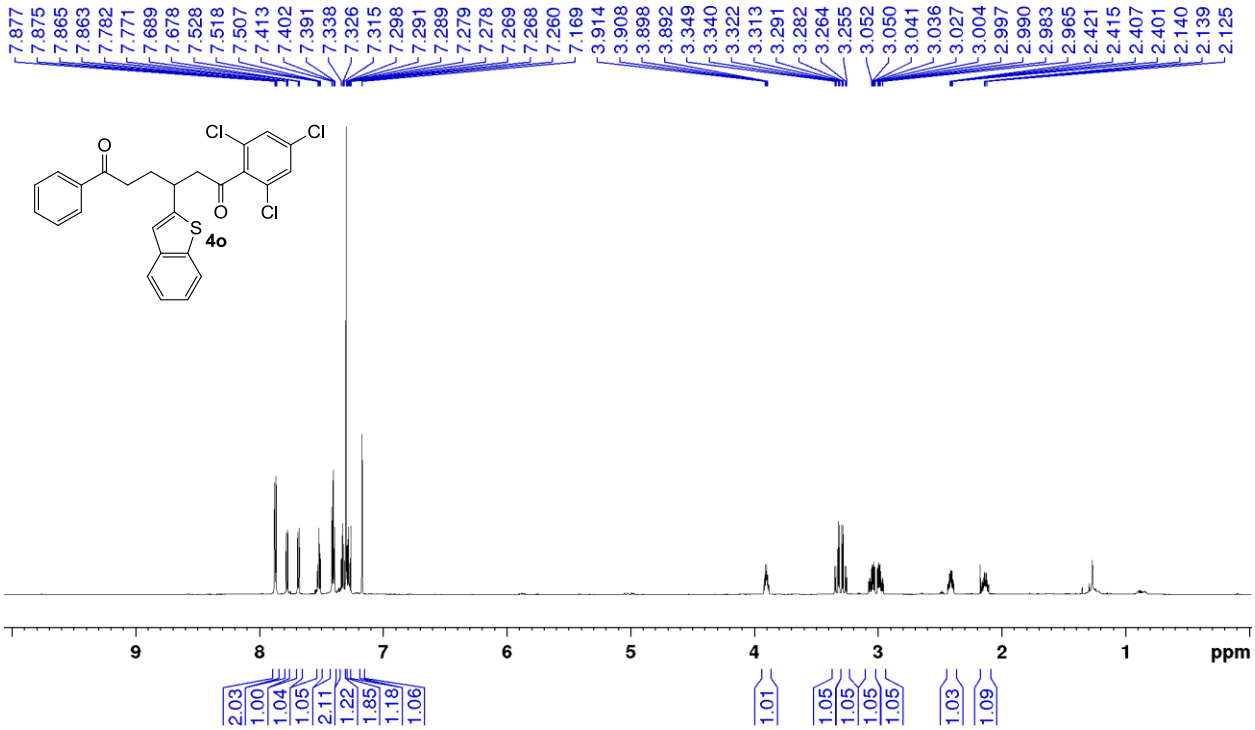
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4n)



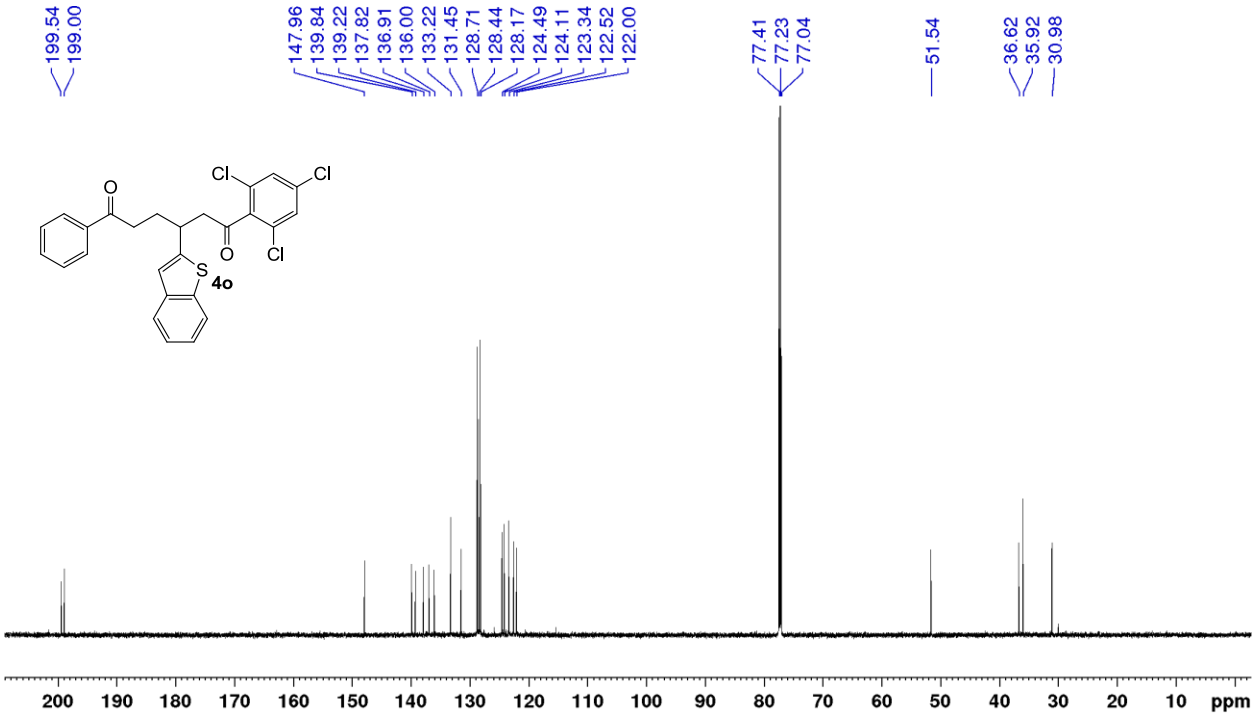
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4n)



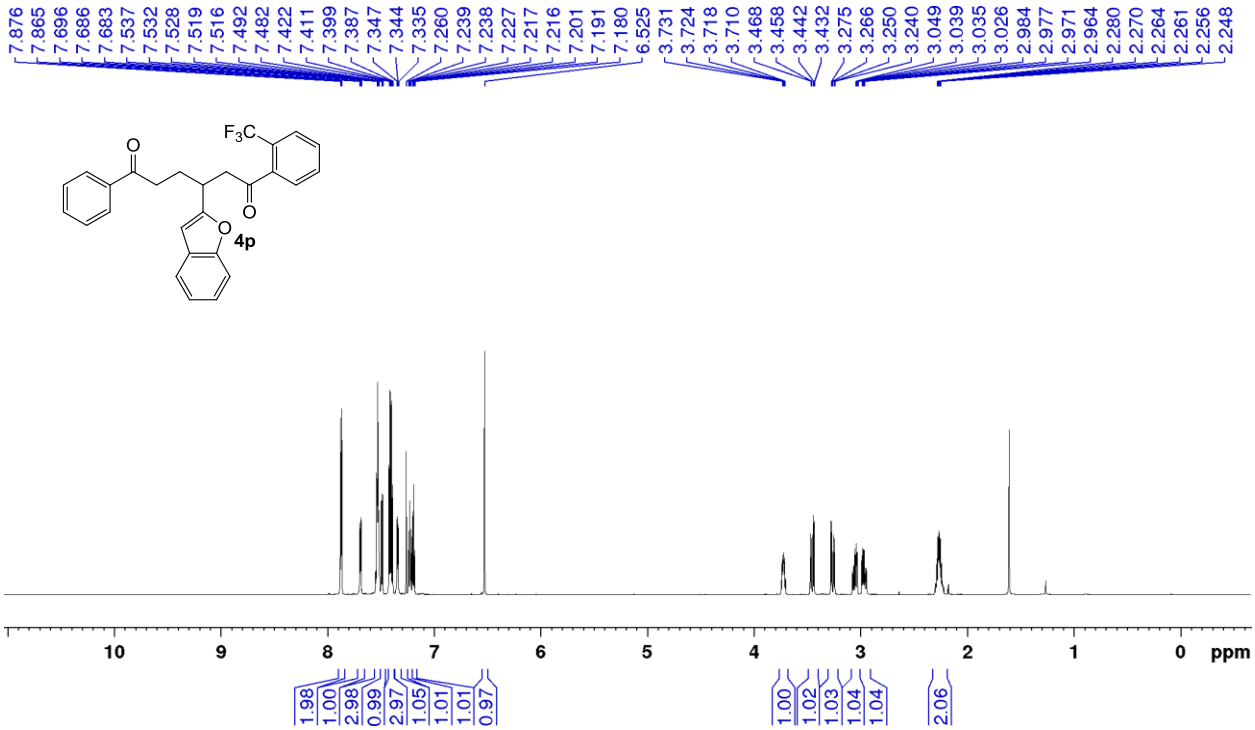
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4o)



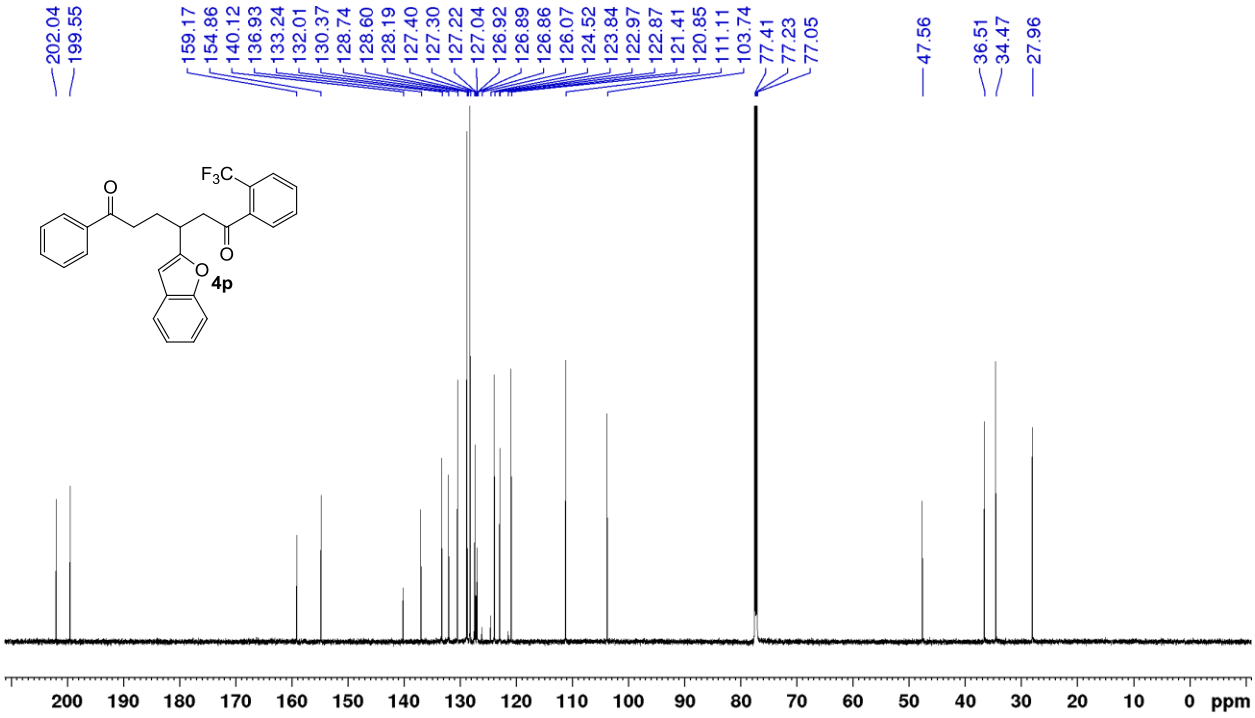
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4o)



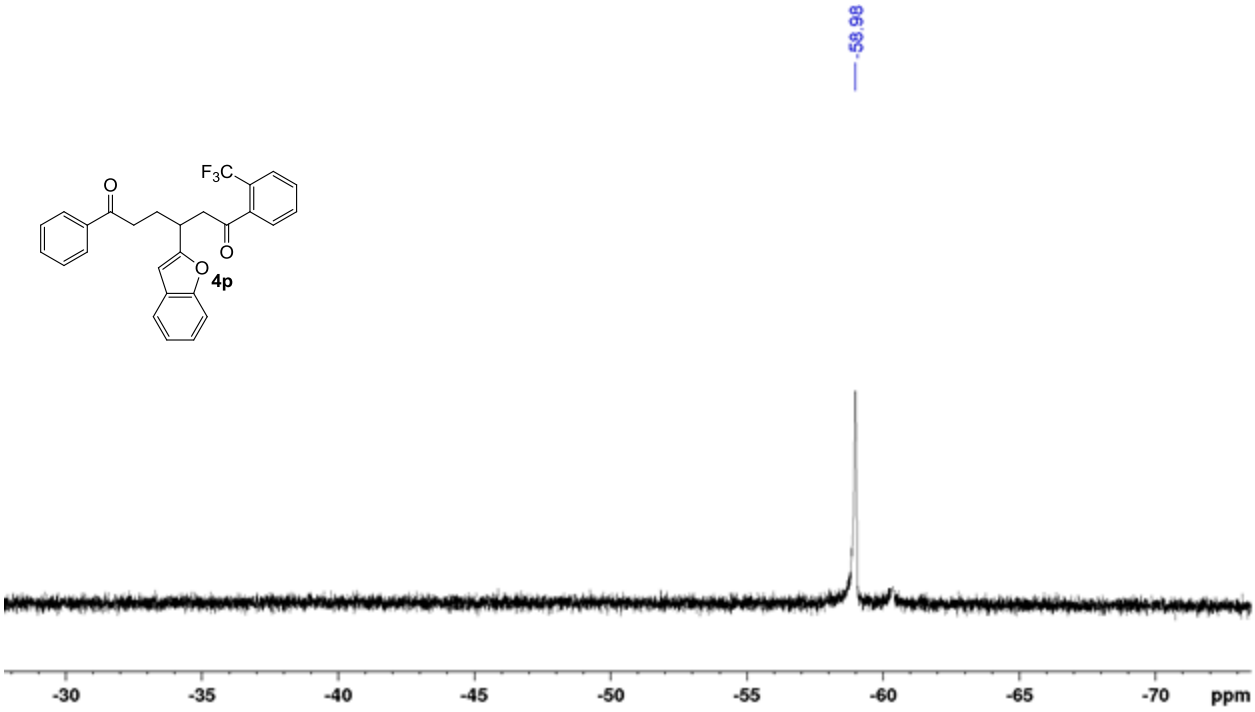
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4p)



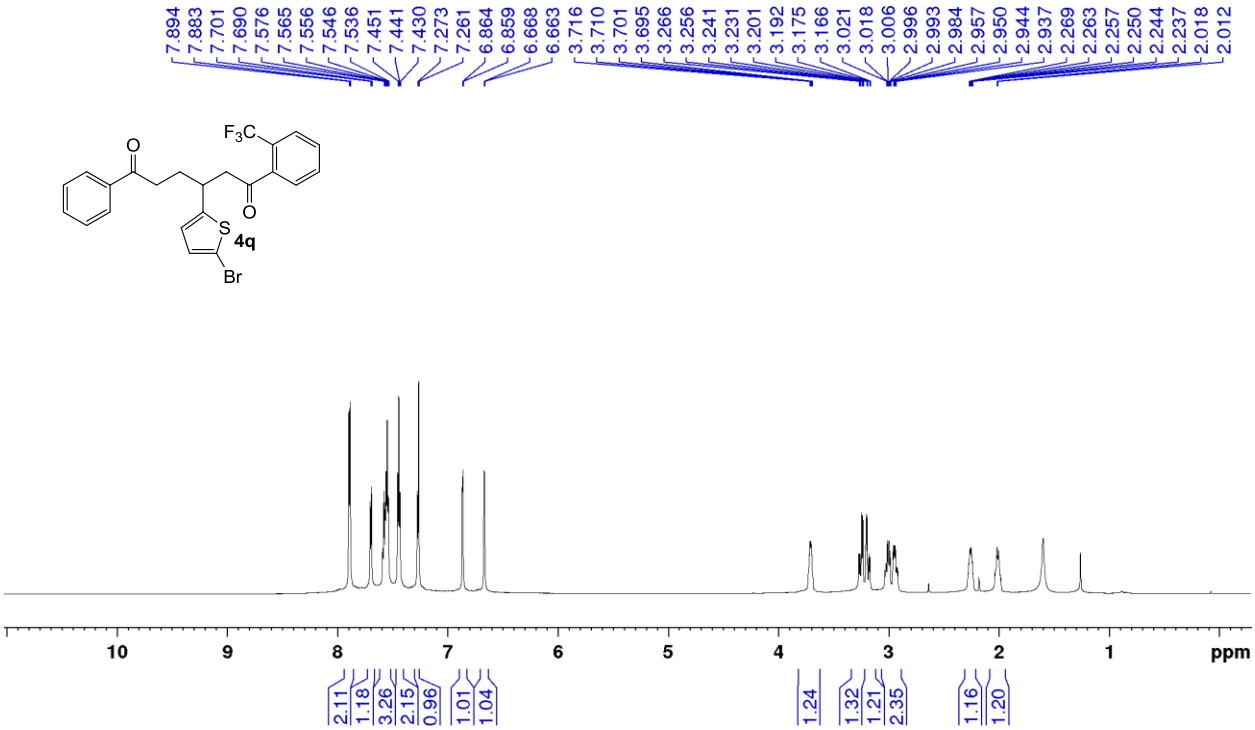
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4p)



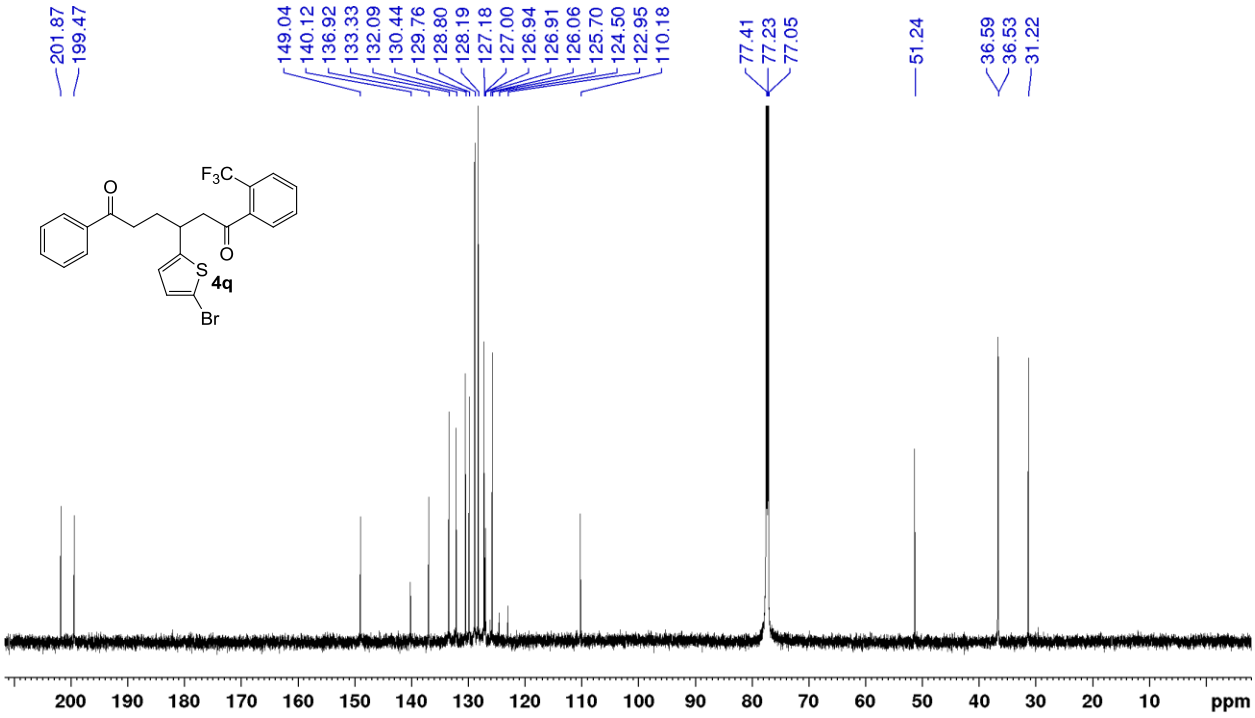
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4p)



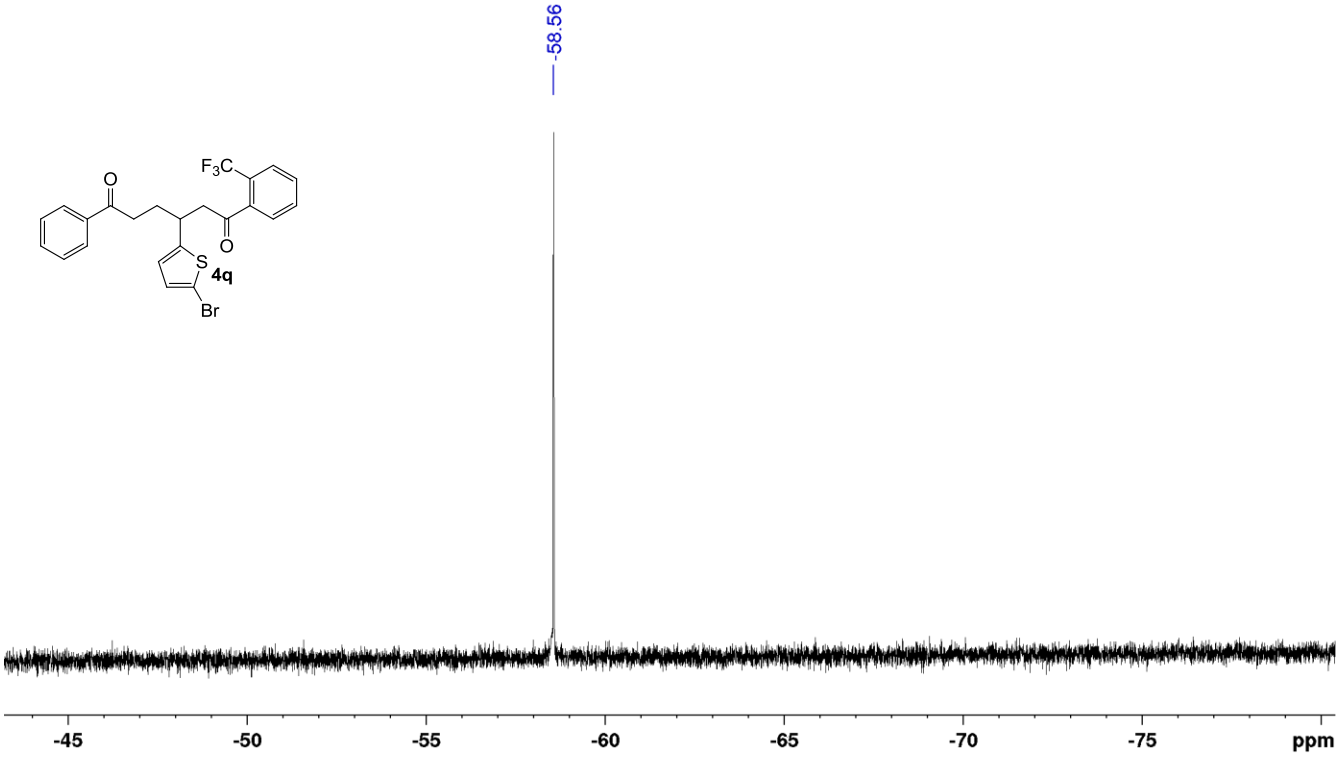
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4q)



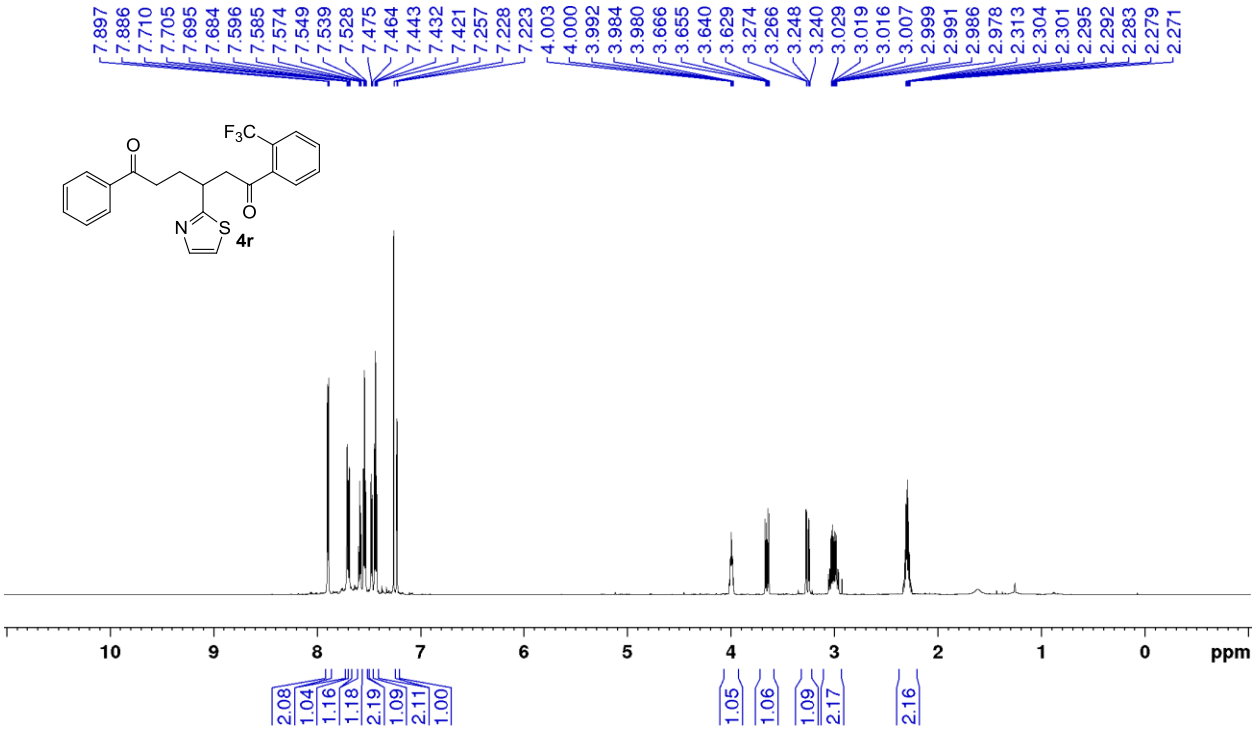
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4q)



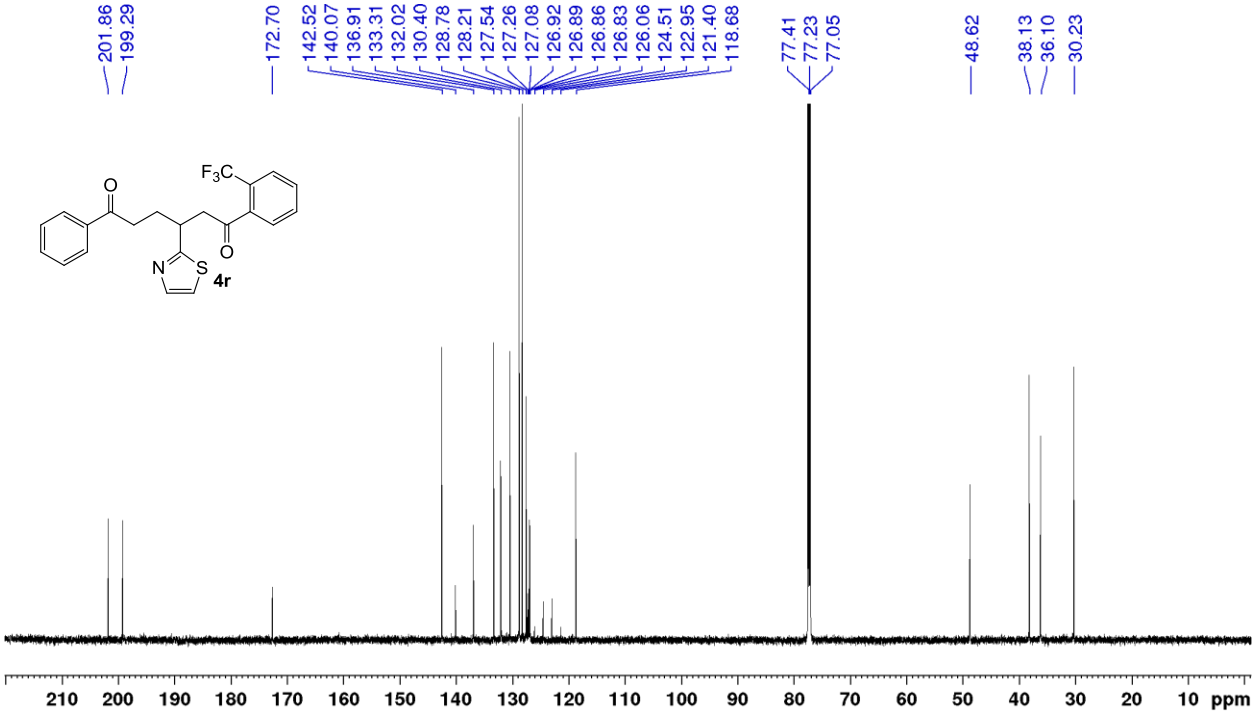
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4q)



^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4r)

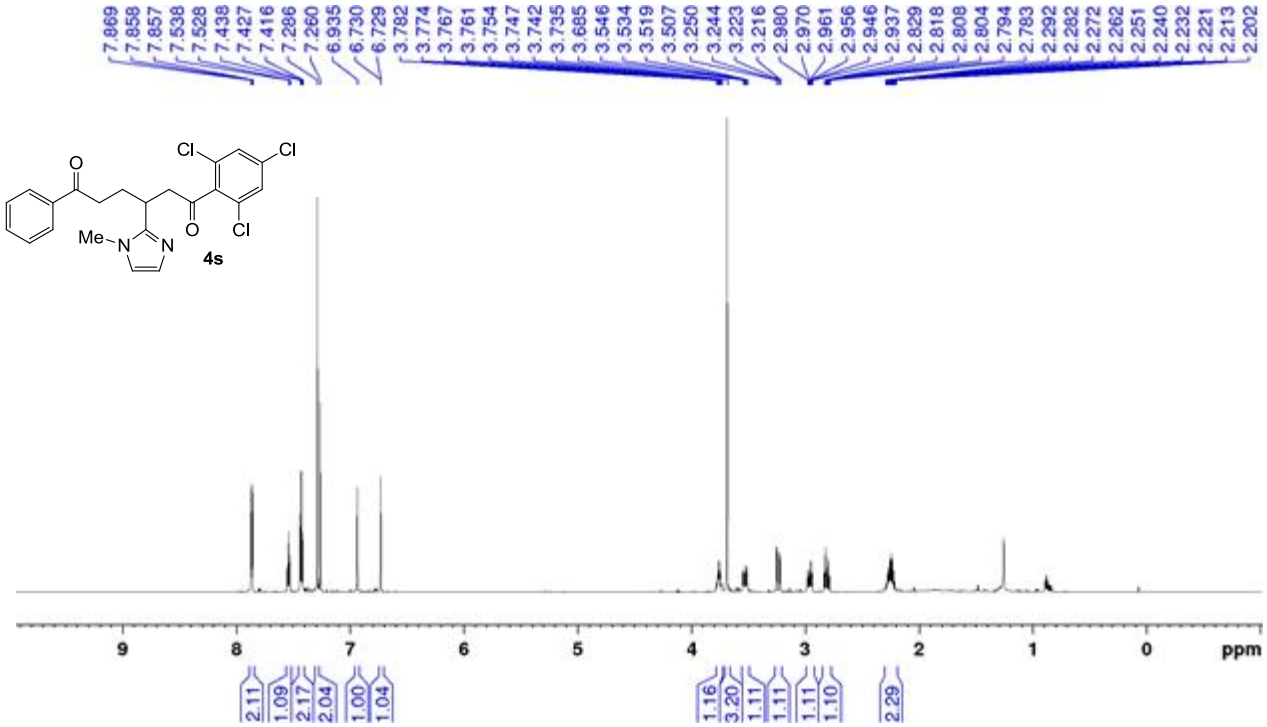


^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4r)

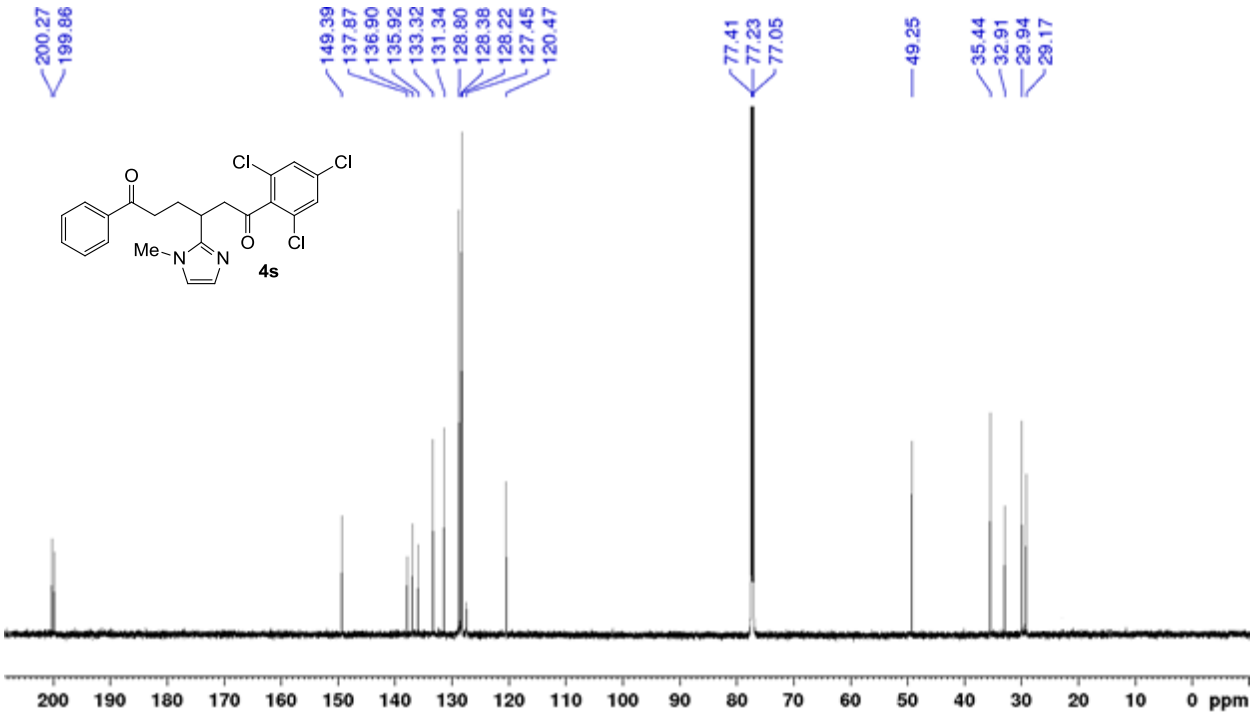


^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4r)

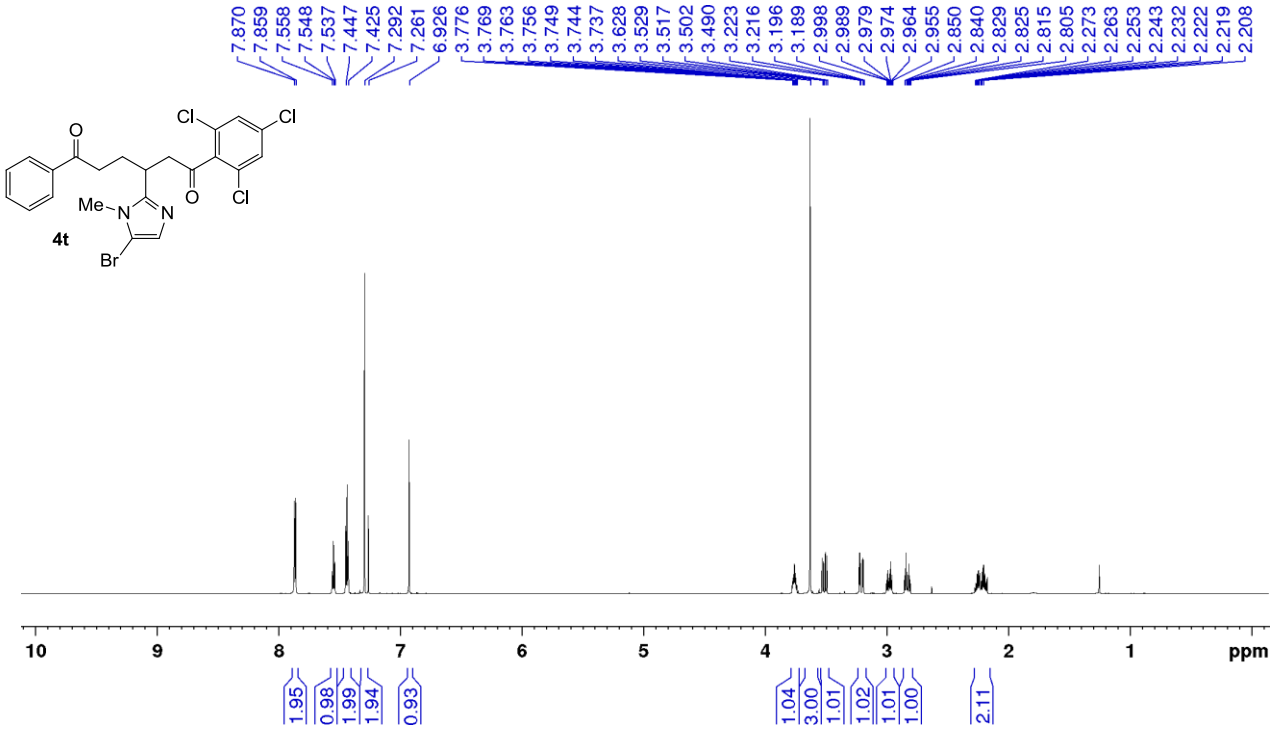
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4s)



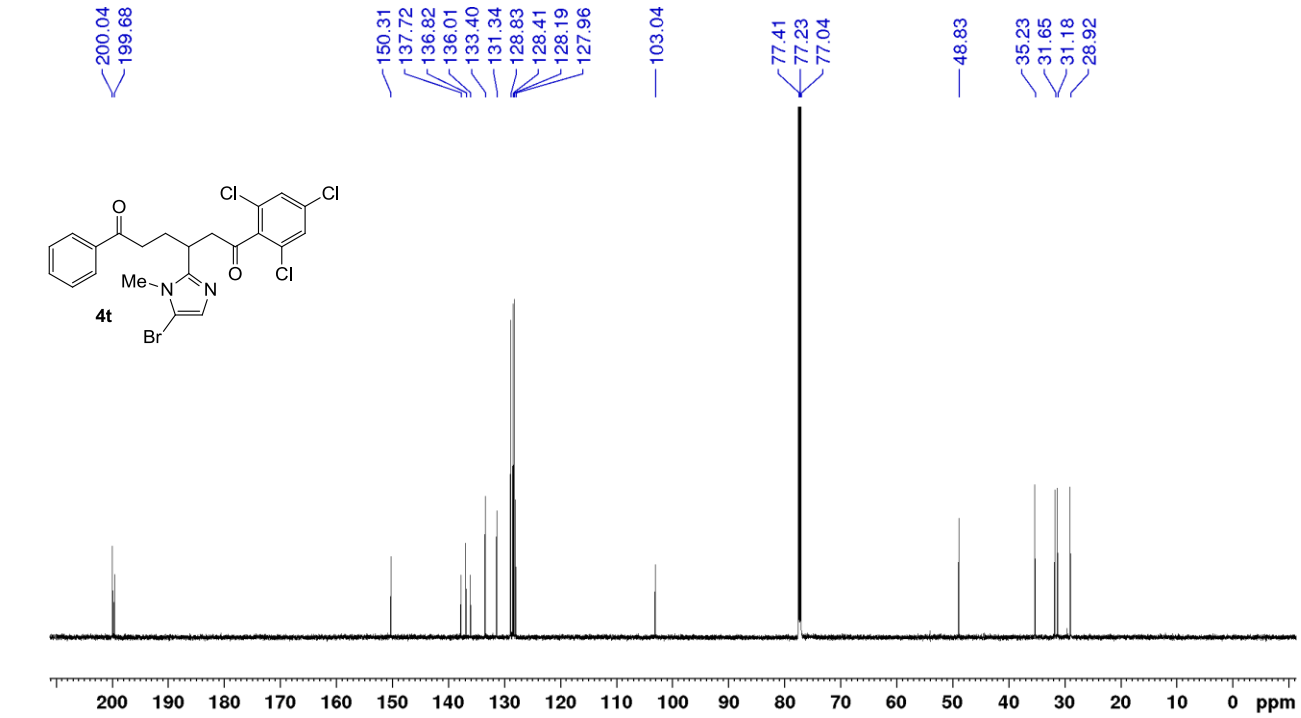
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4s)



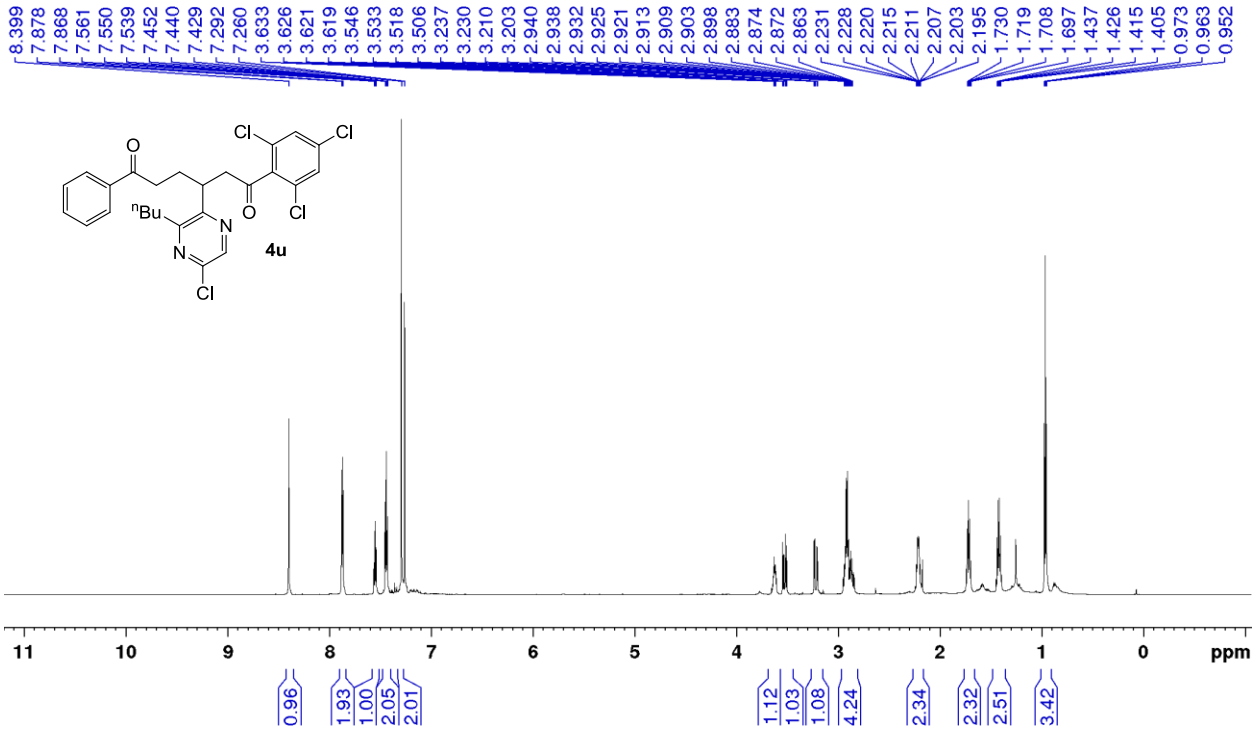
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4t)



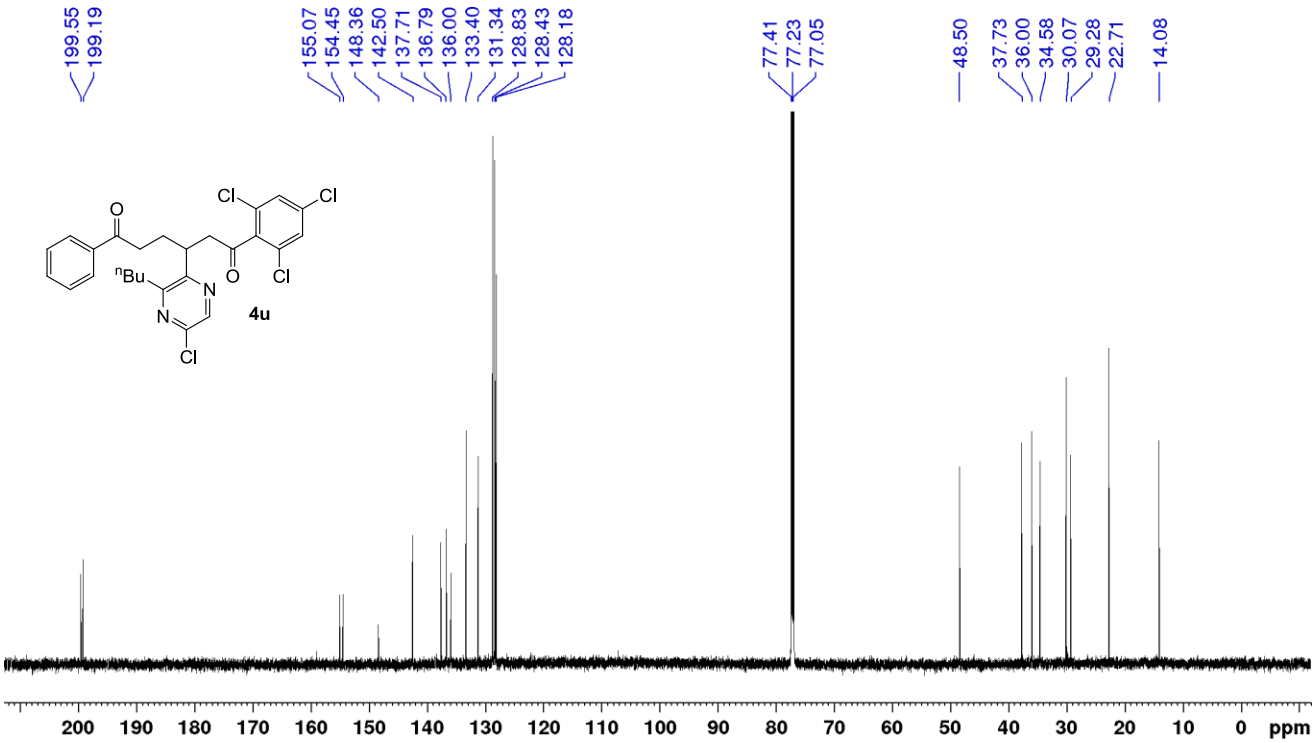
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4t)



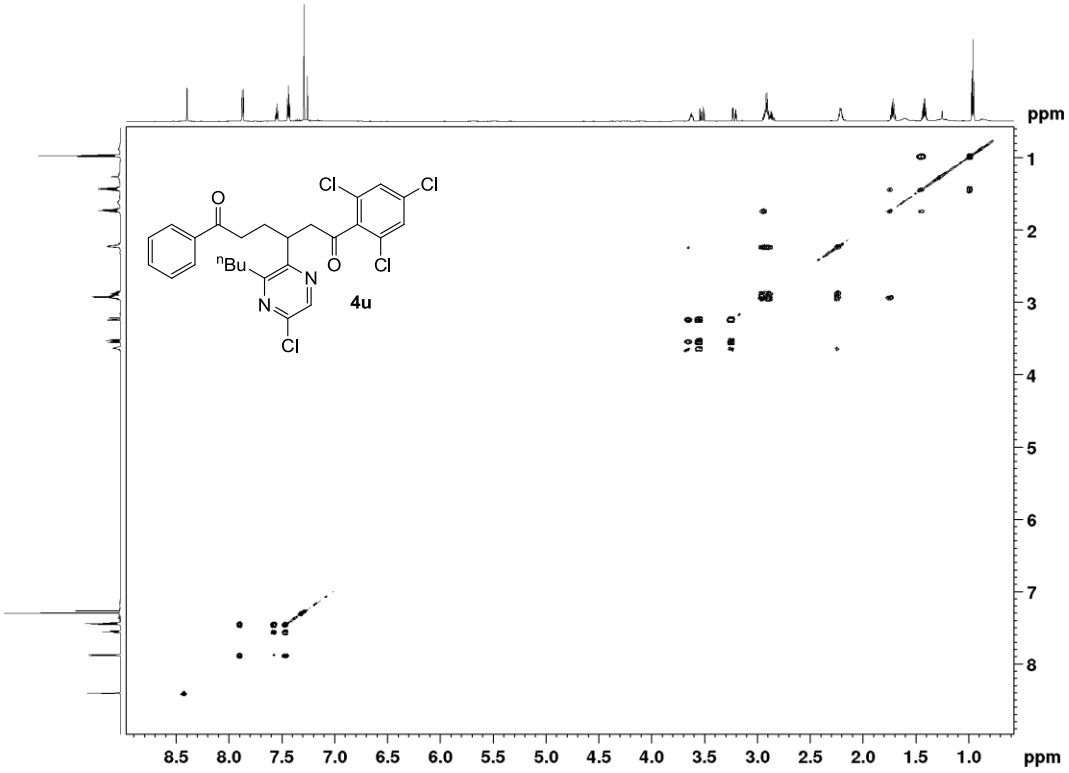
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4u)



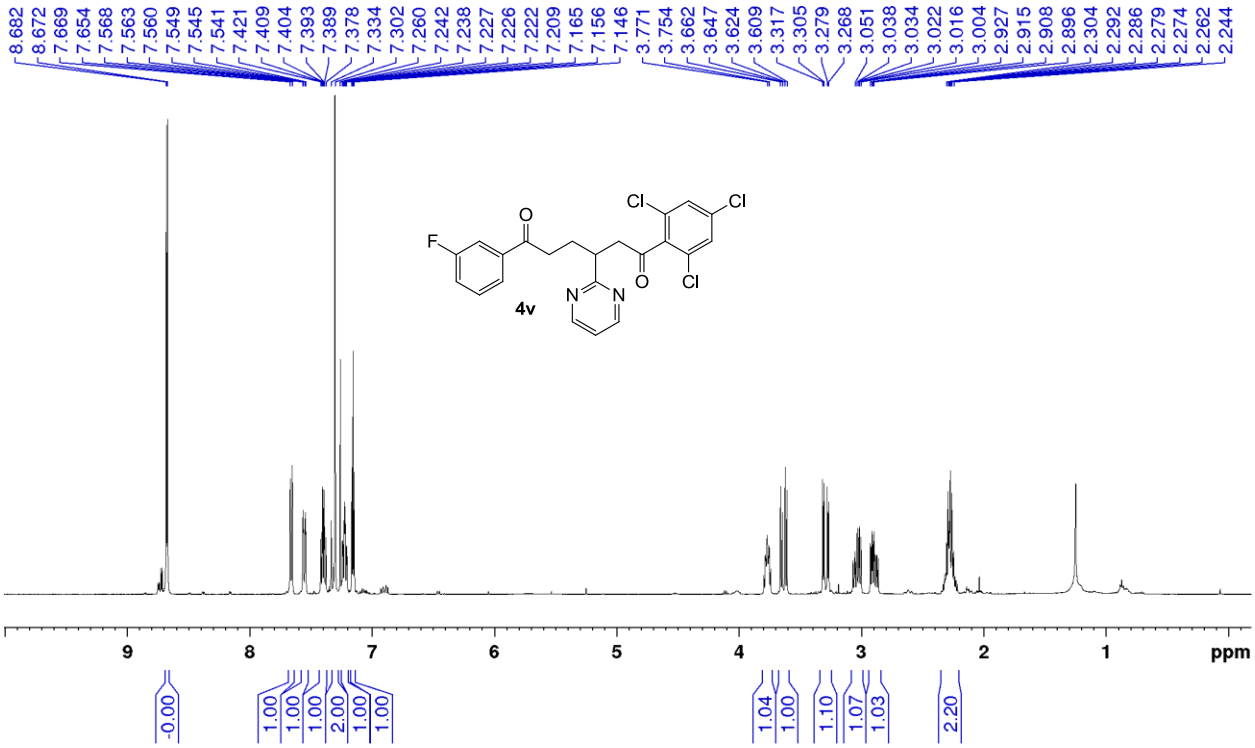
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4u)



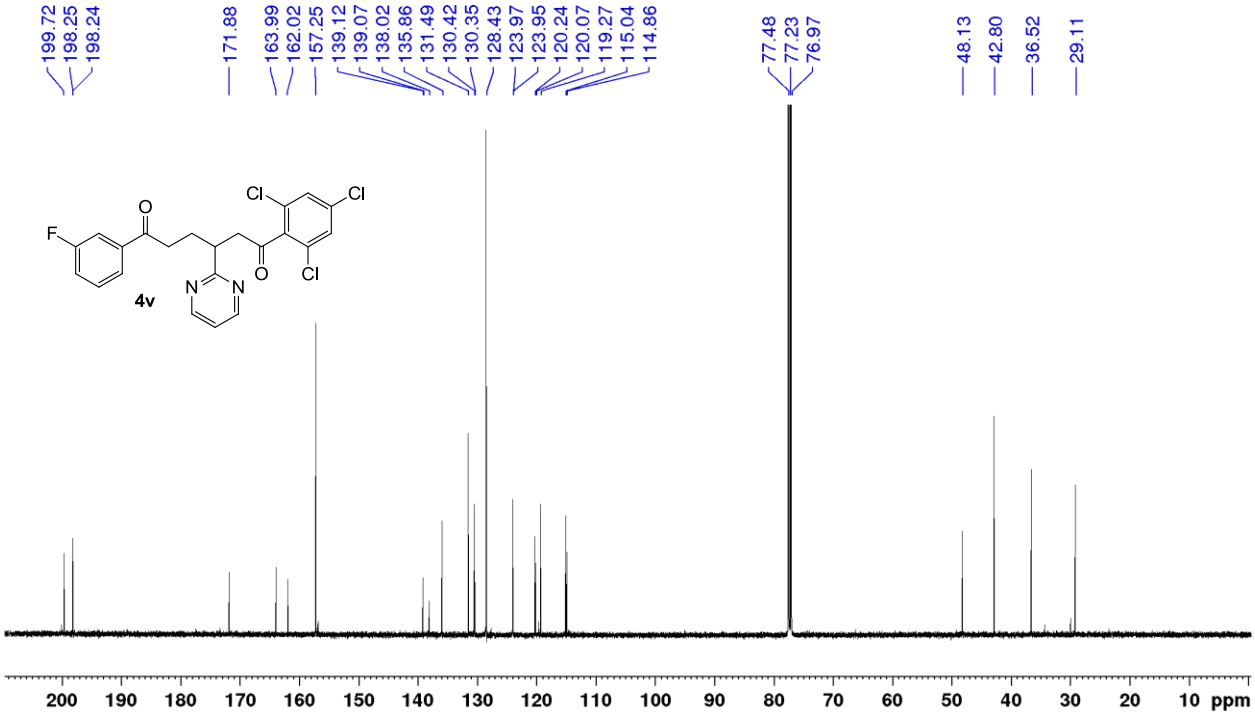
2D COESY ($CDCl_3$, 25 ºC) of (4u)



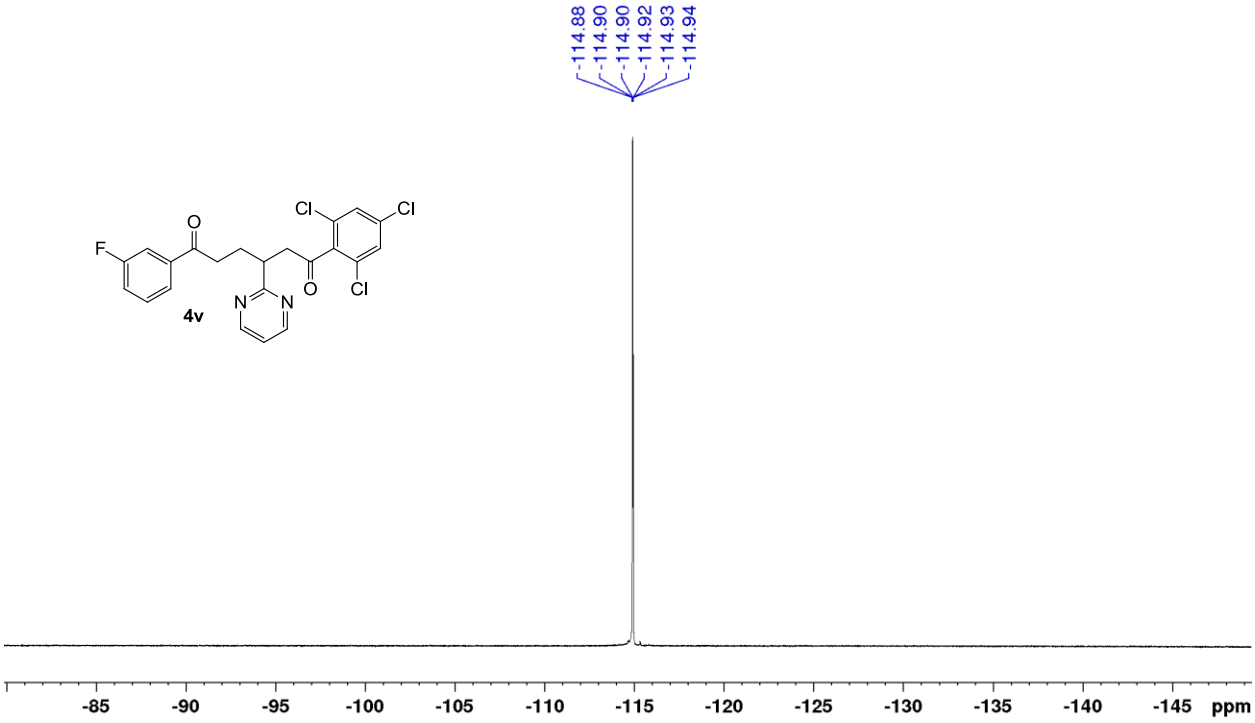
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (4v)



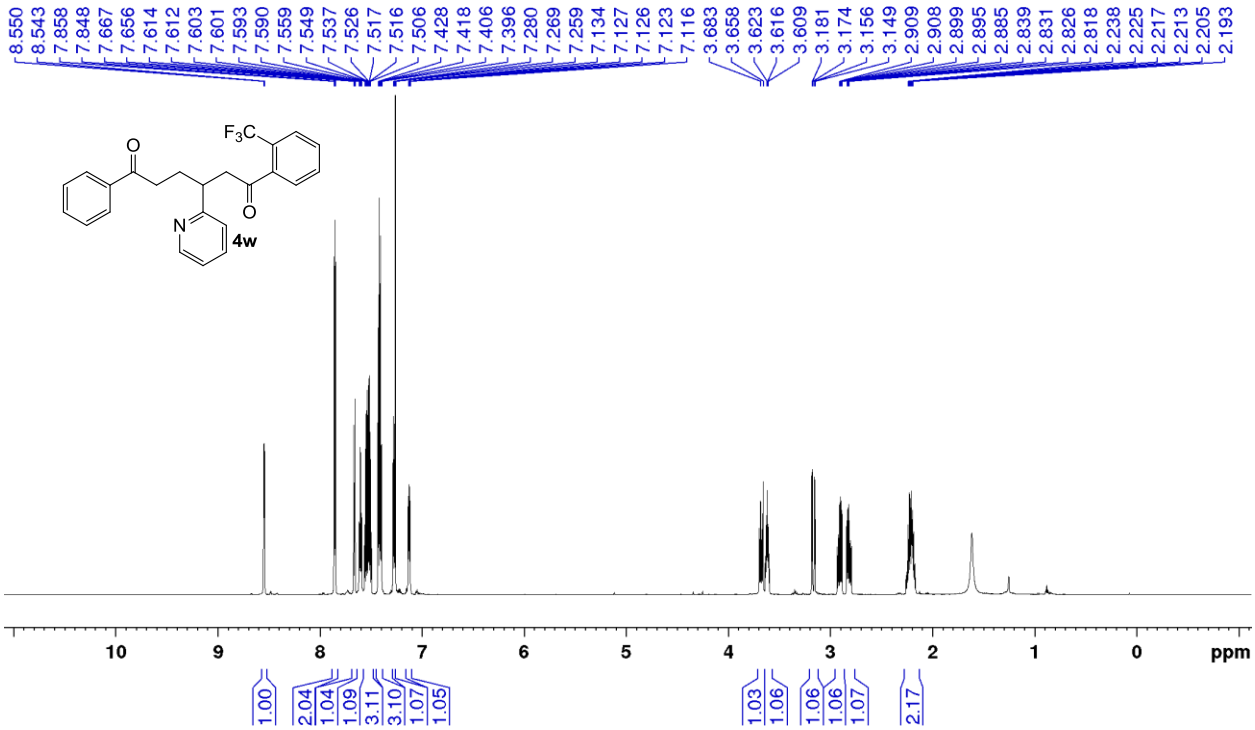
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (4v)



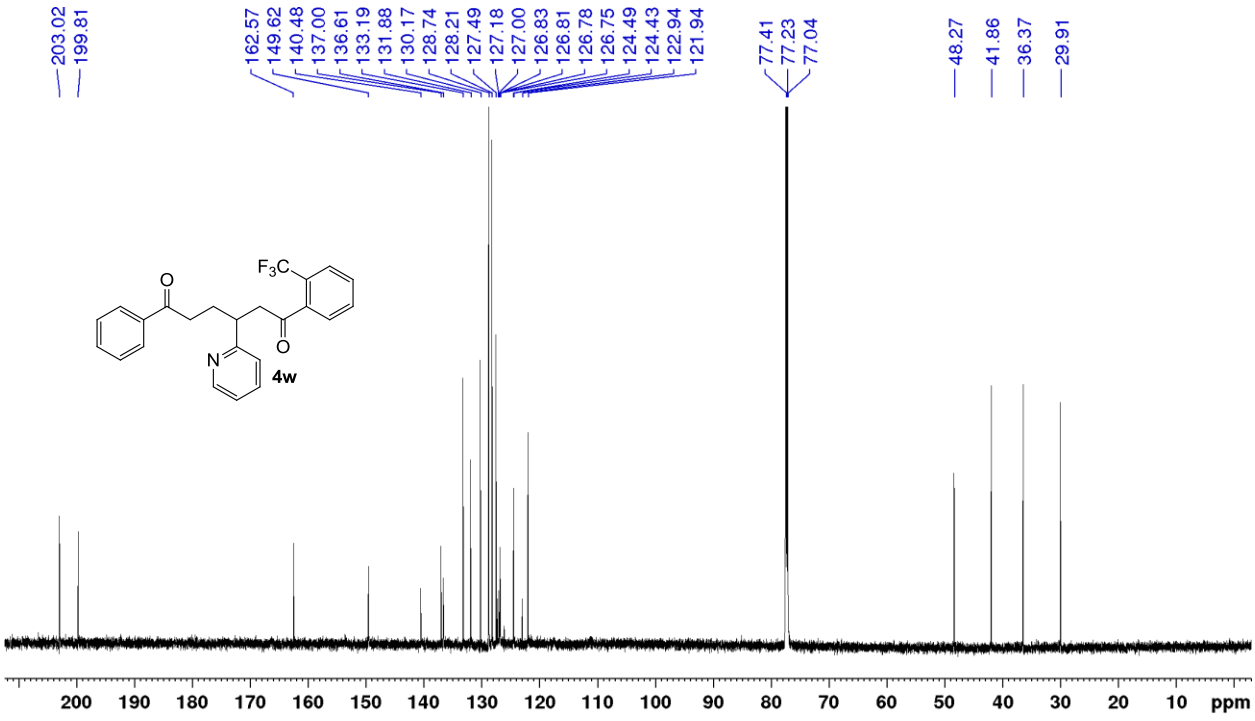
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4v)



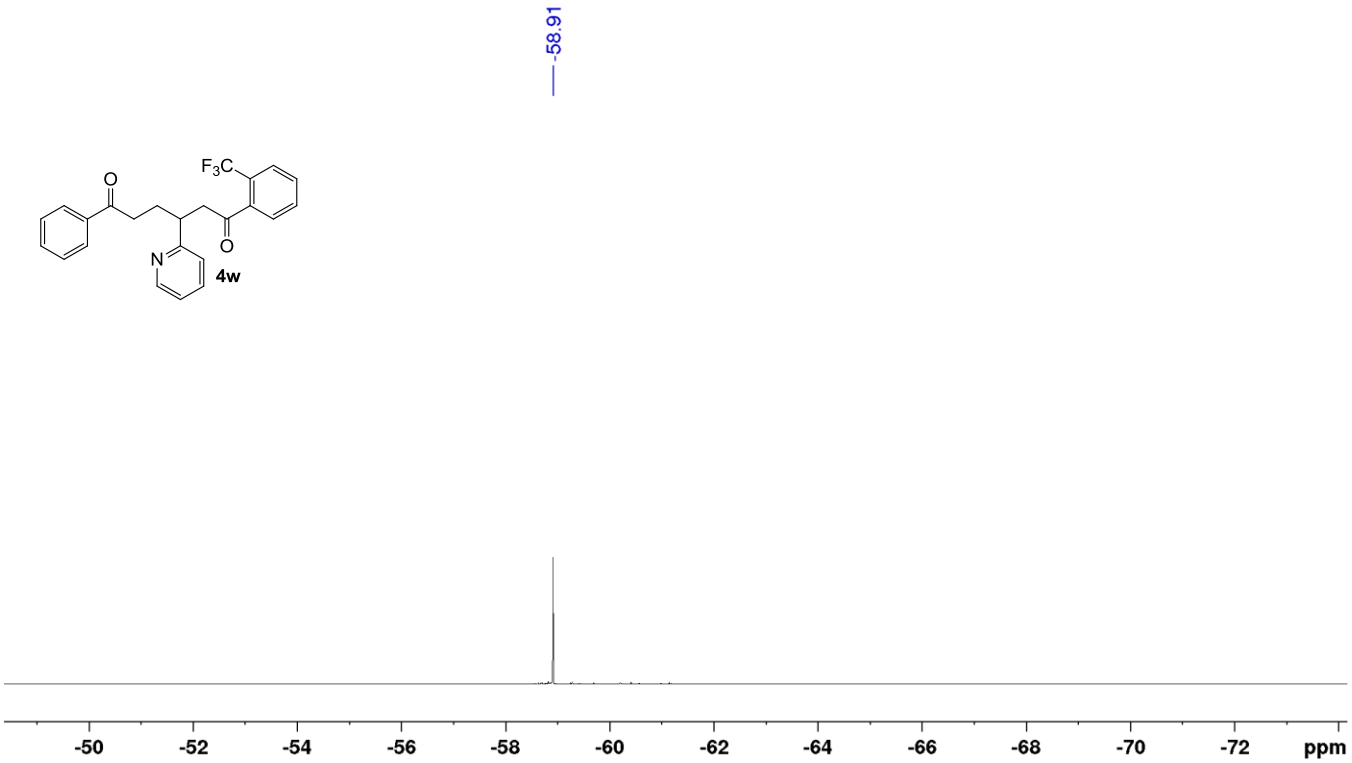
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4w)



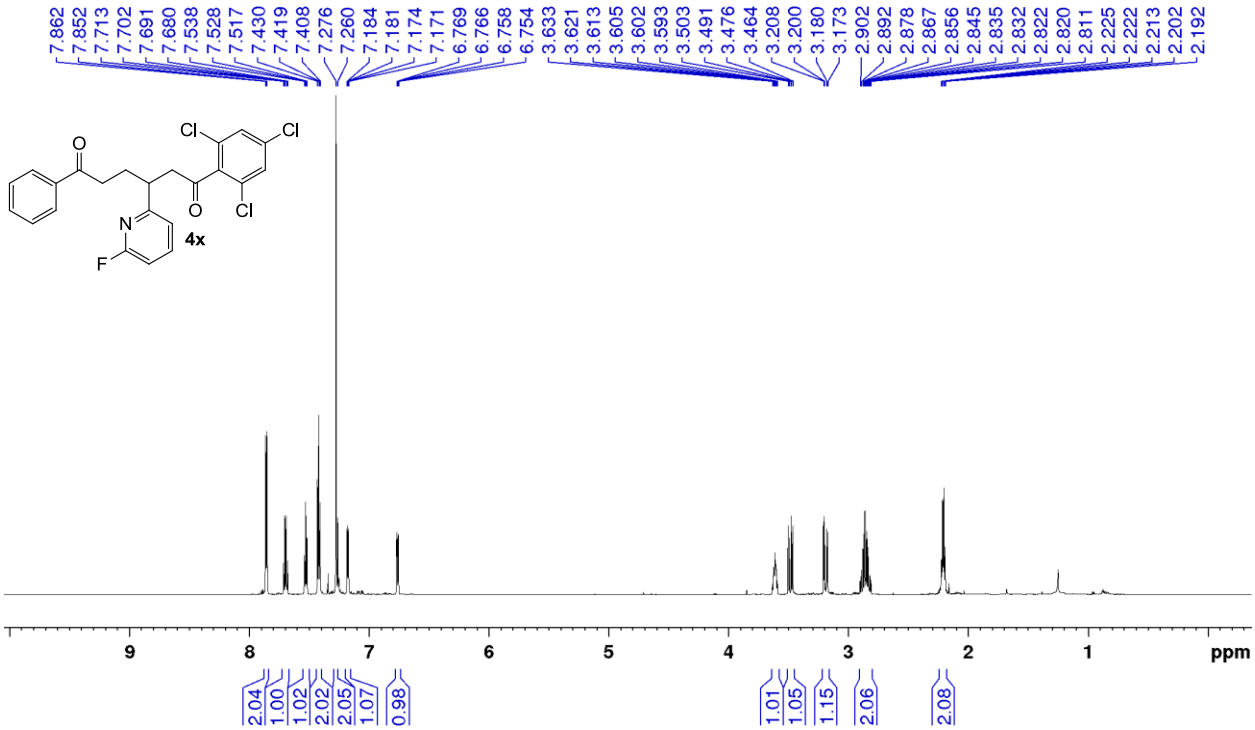
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4w)



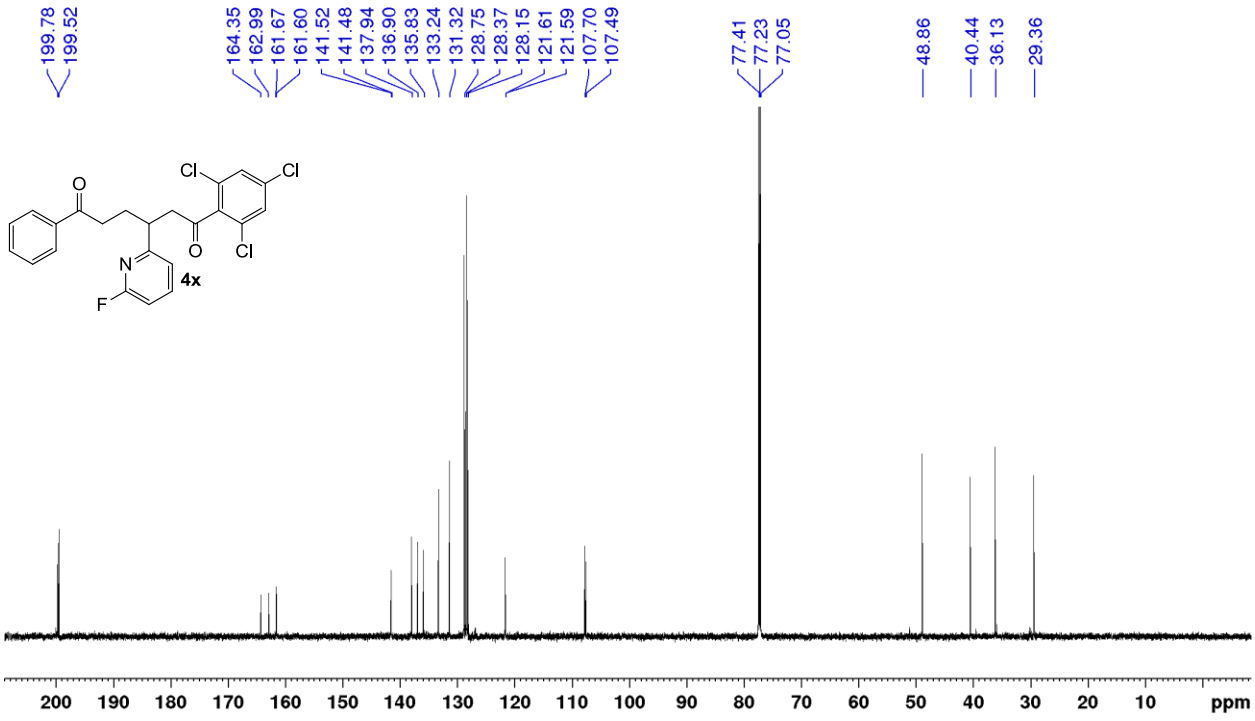
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4w)



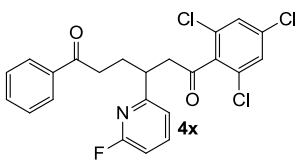
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4x)



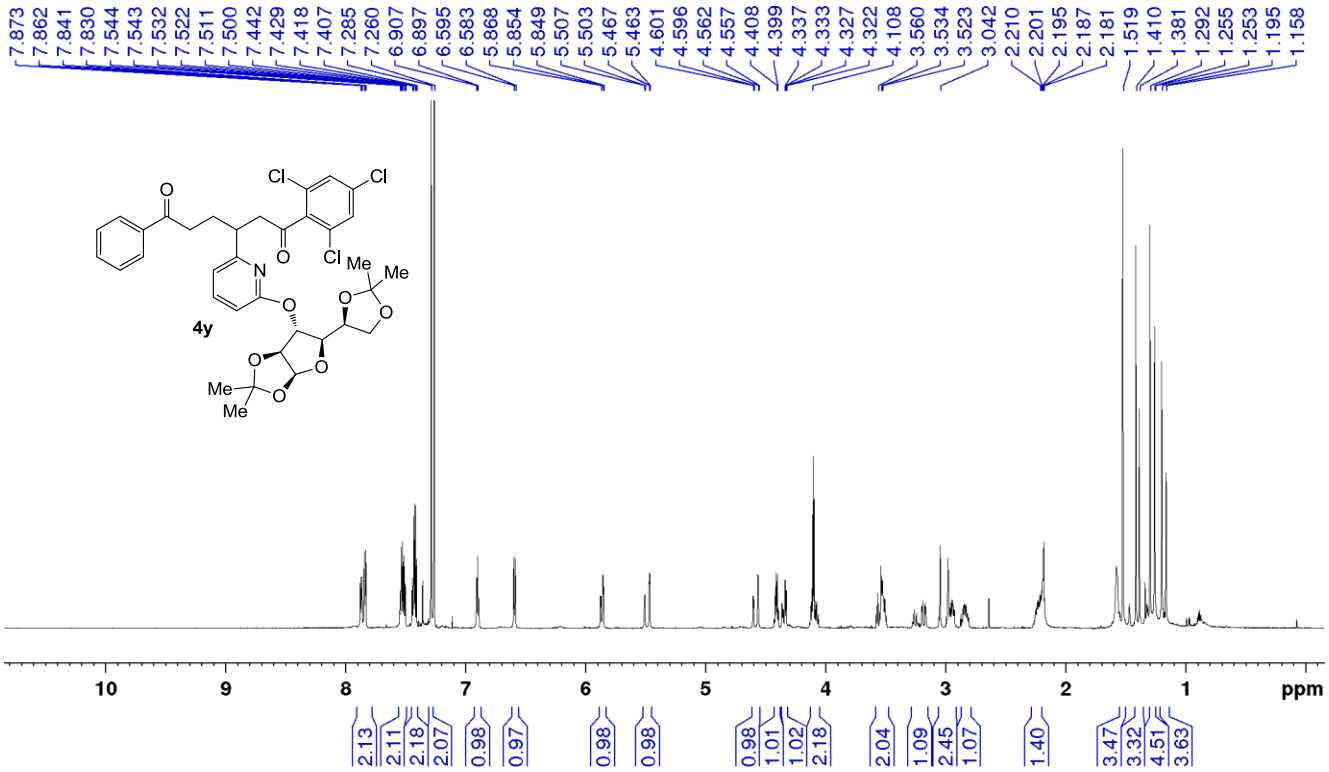
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4x)



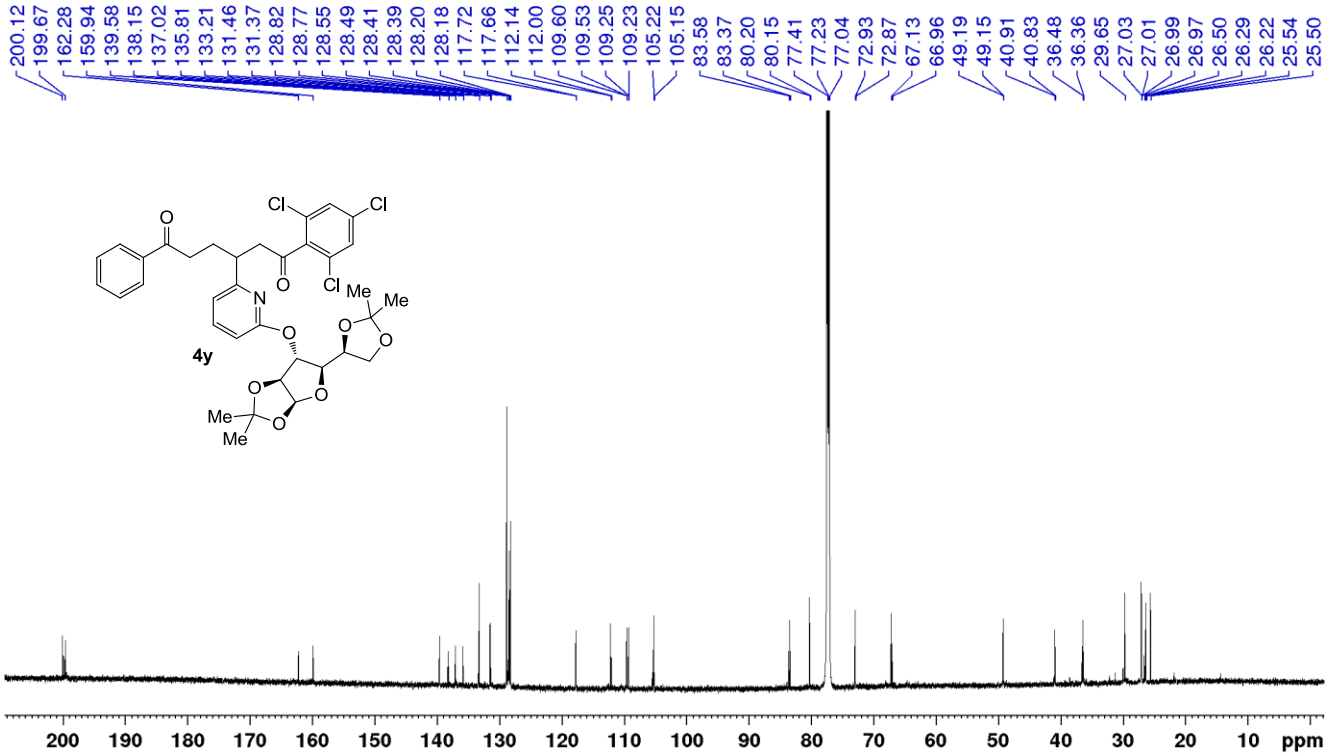
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4x)



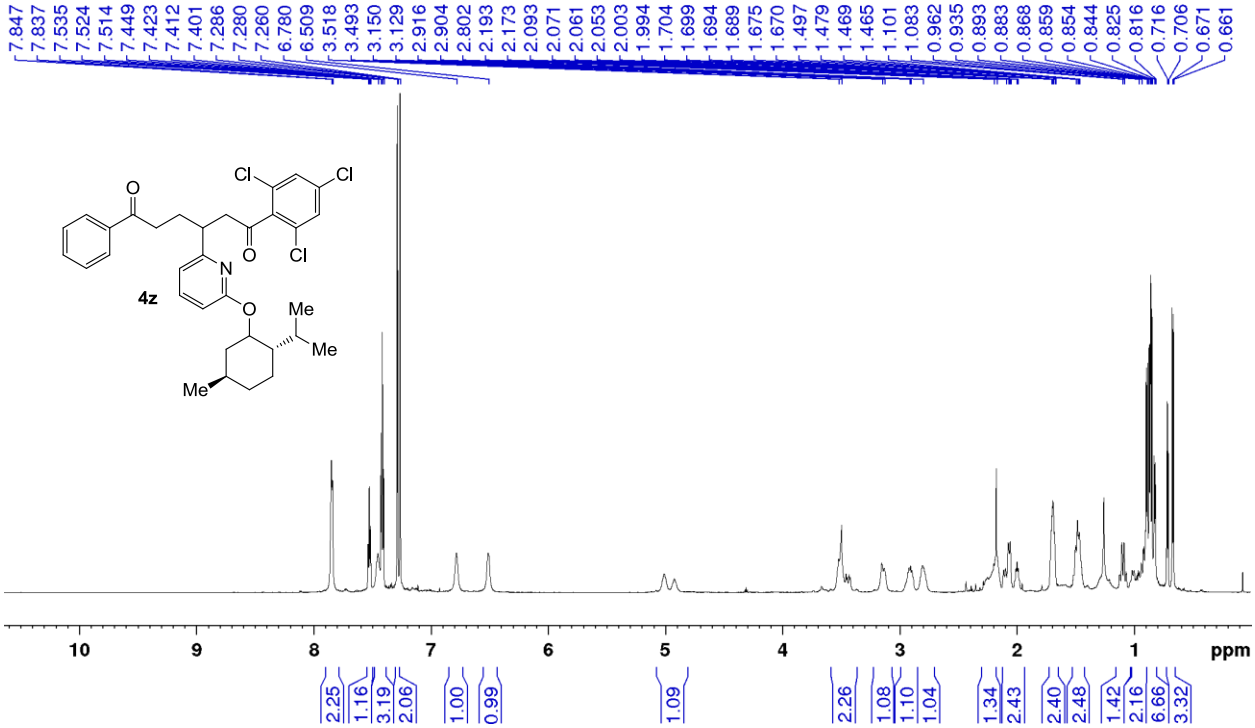
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4y)



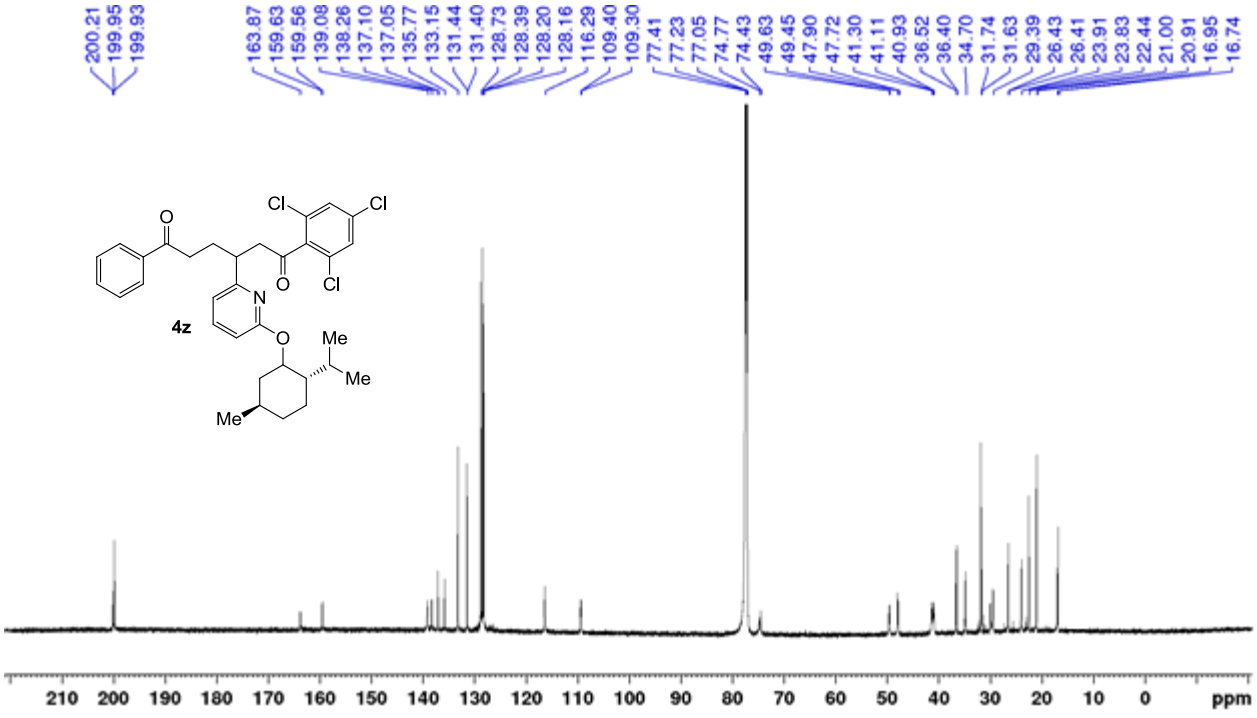
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4y)



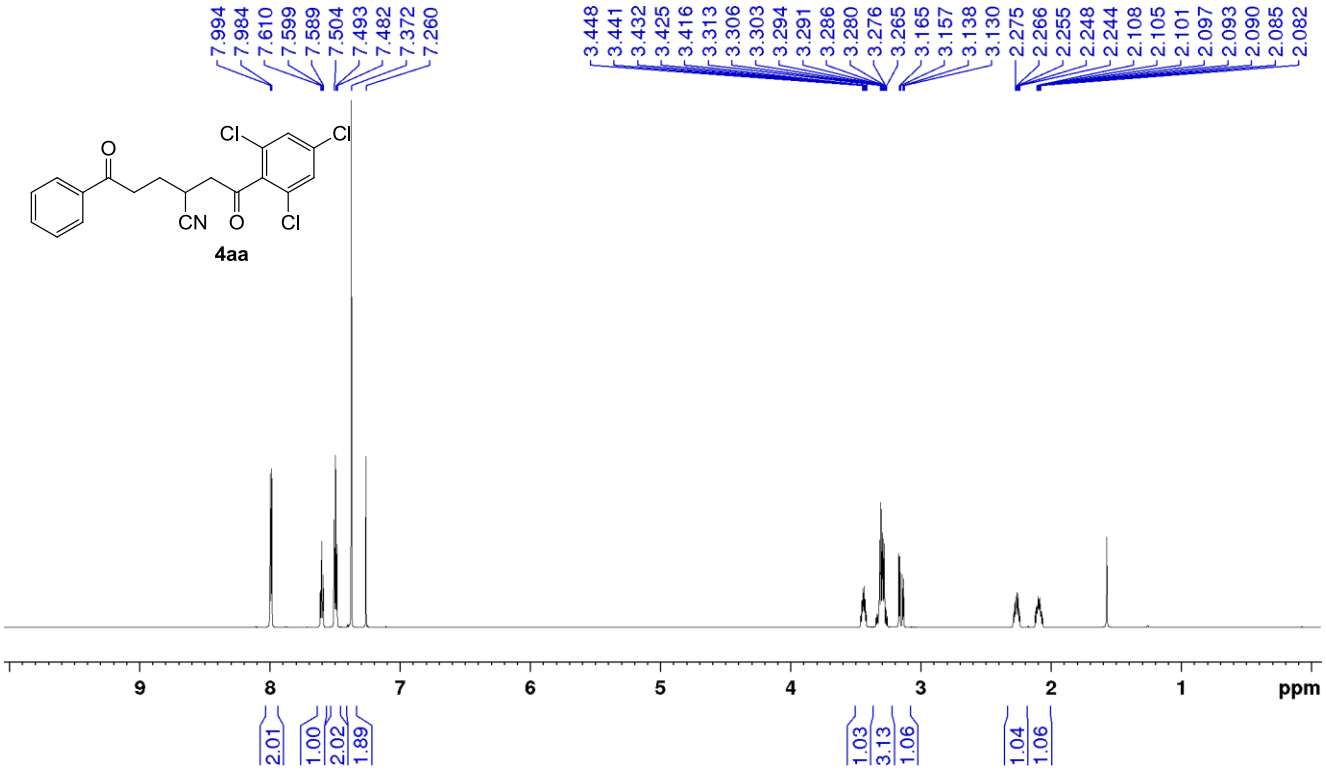
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (4z)



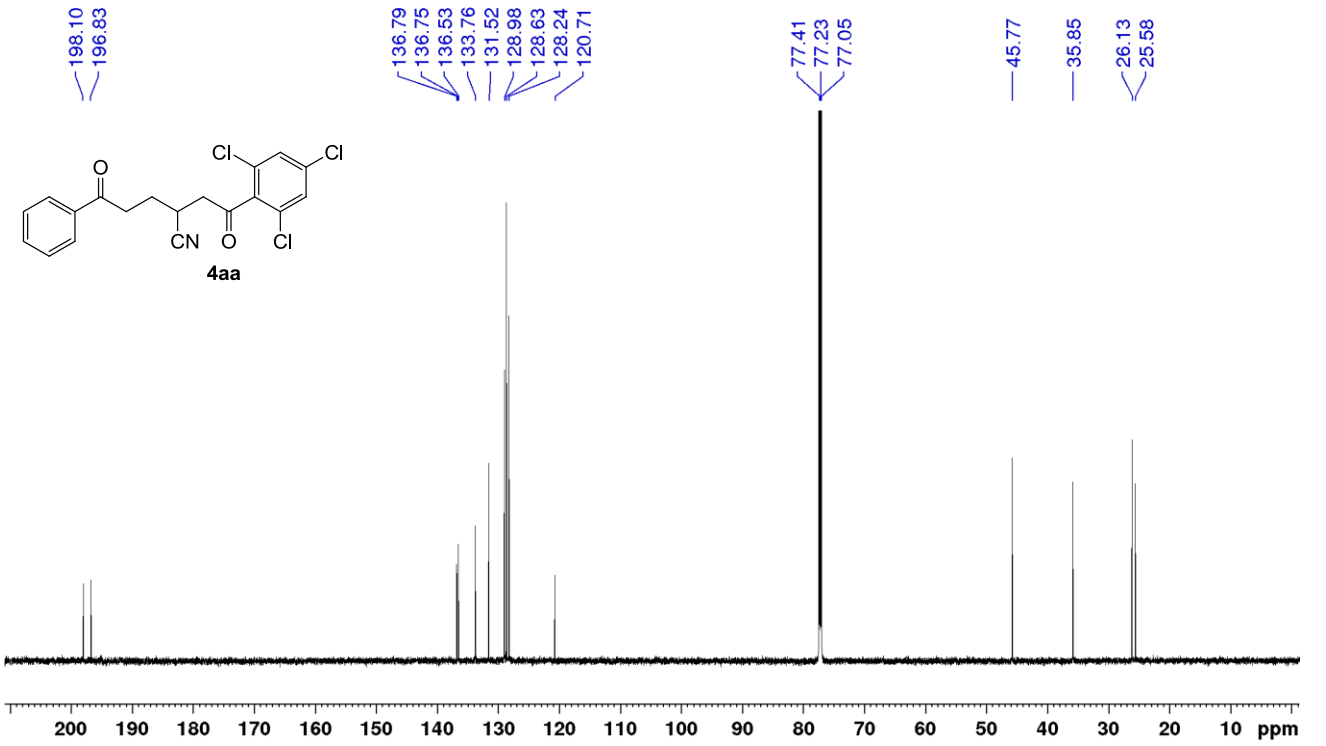
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (4z)



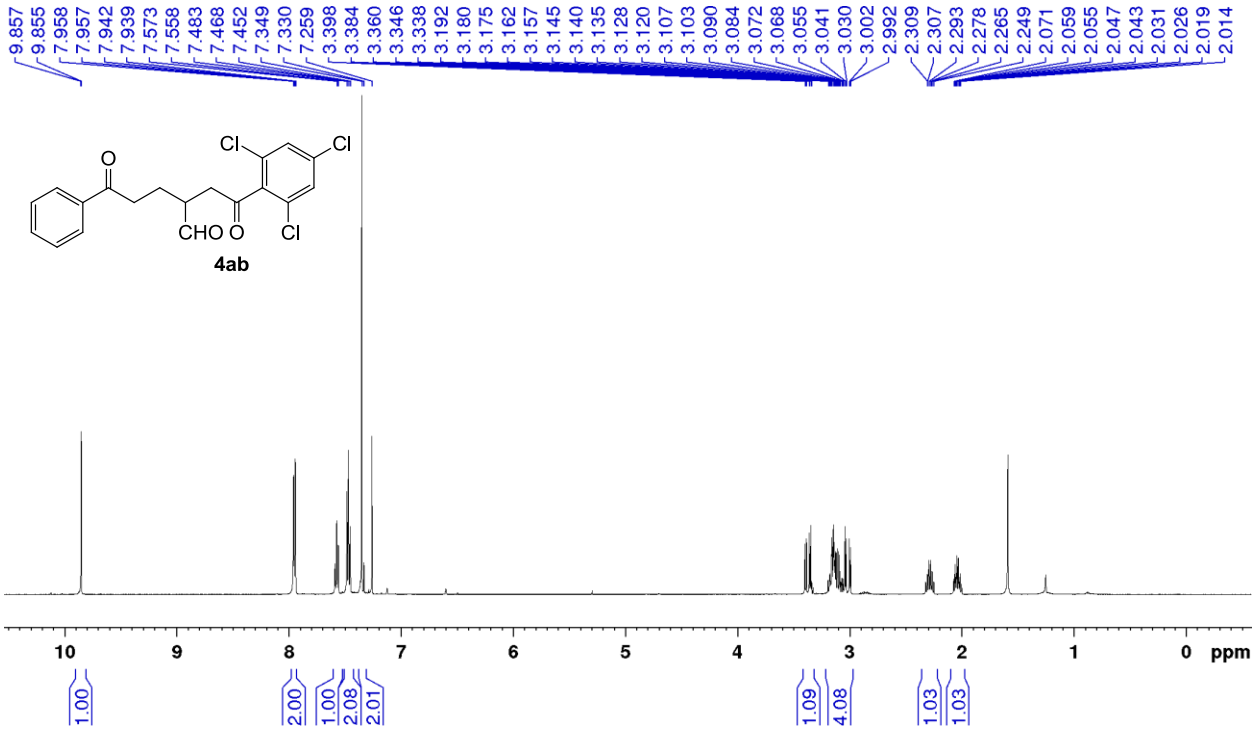
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4aa)



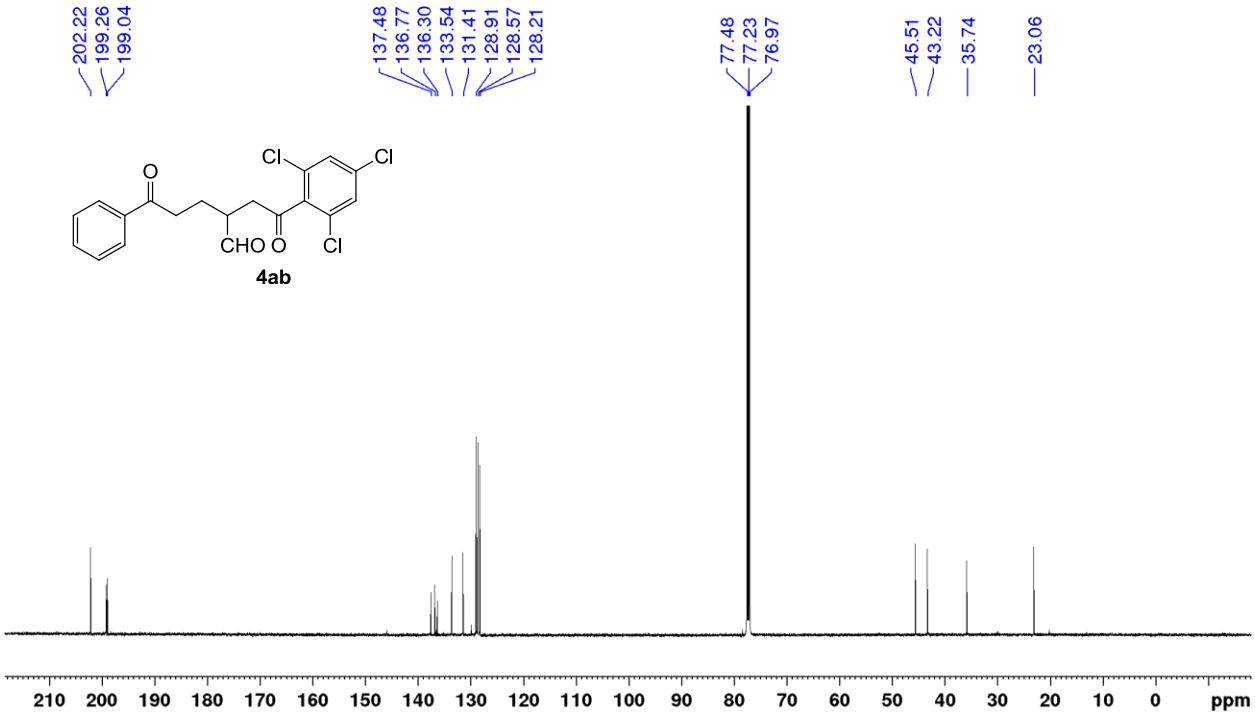
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4aa)



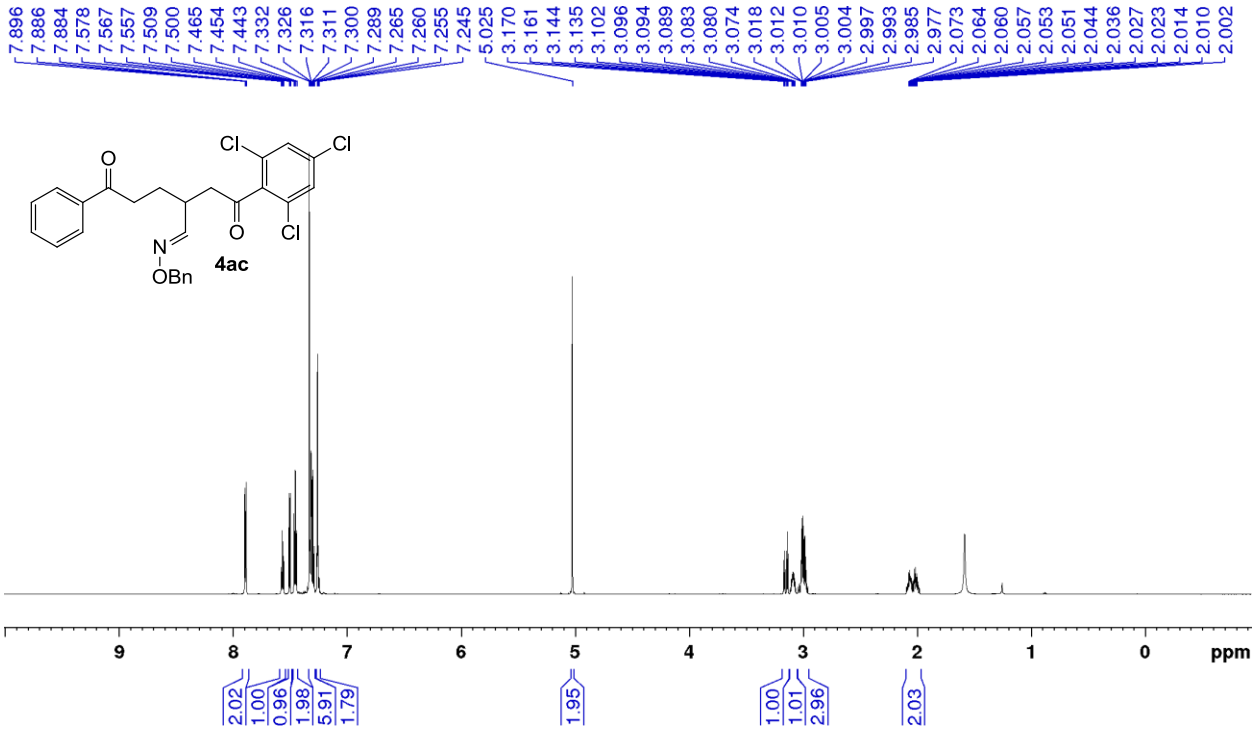
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4ab)



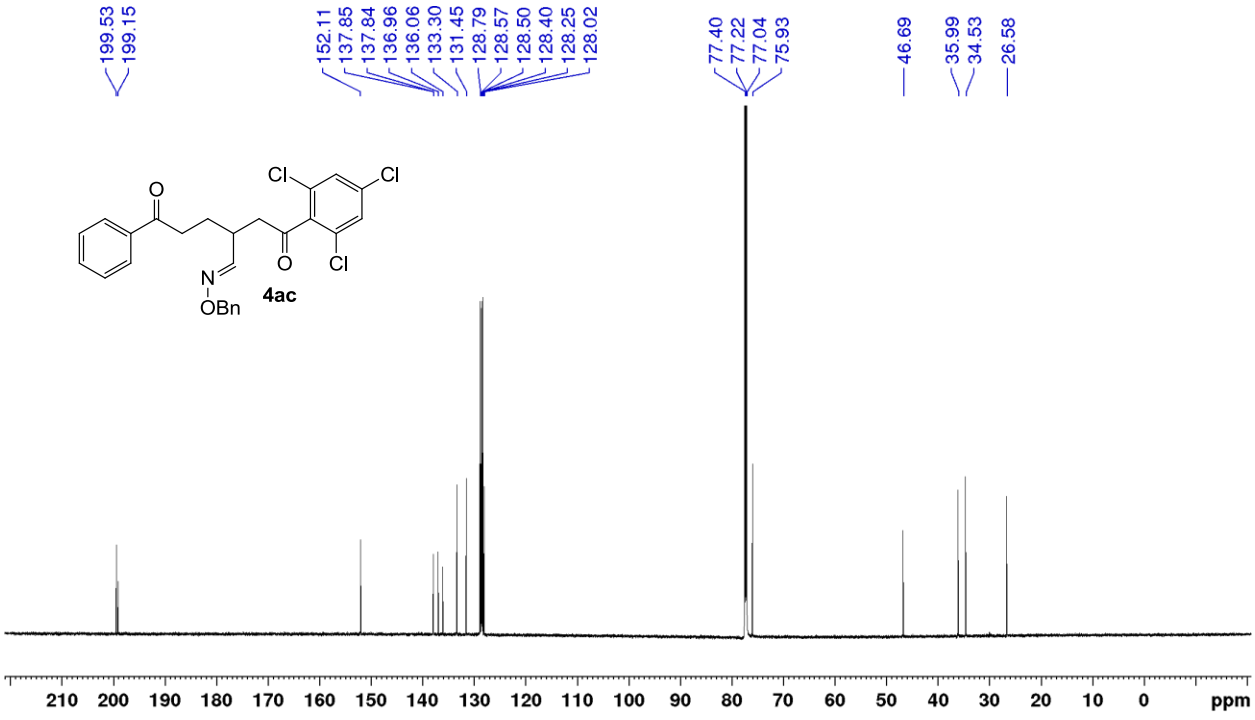
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4ab)



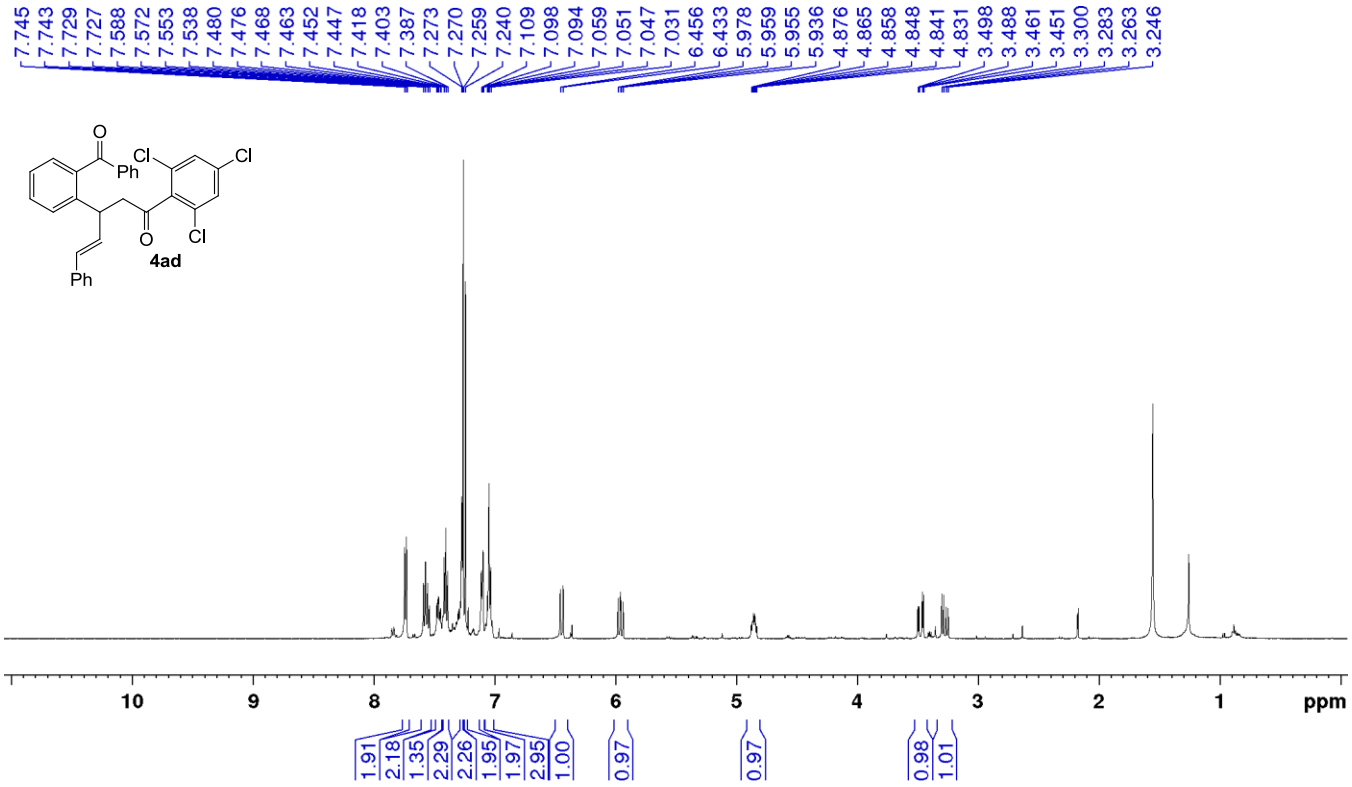
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4ac)



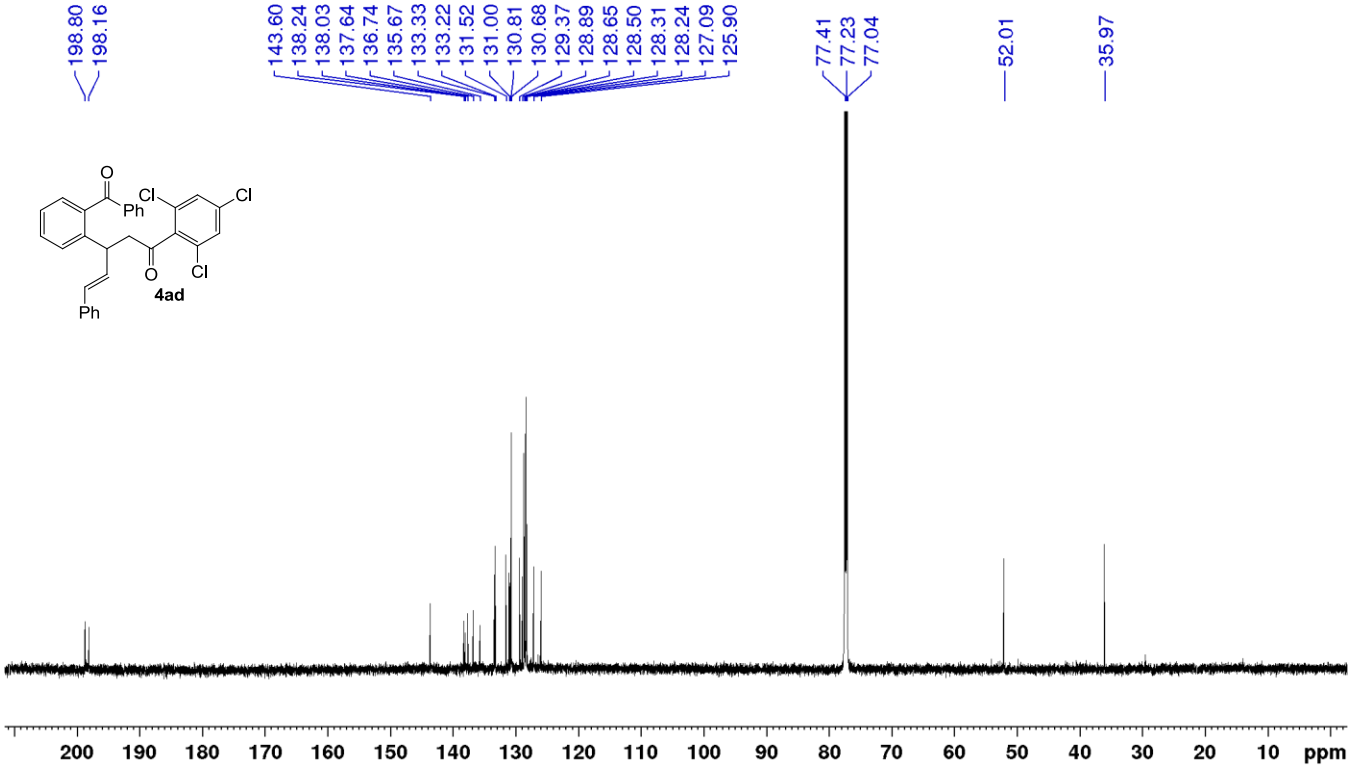
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4ac)



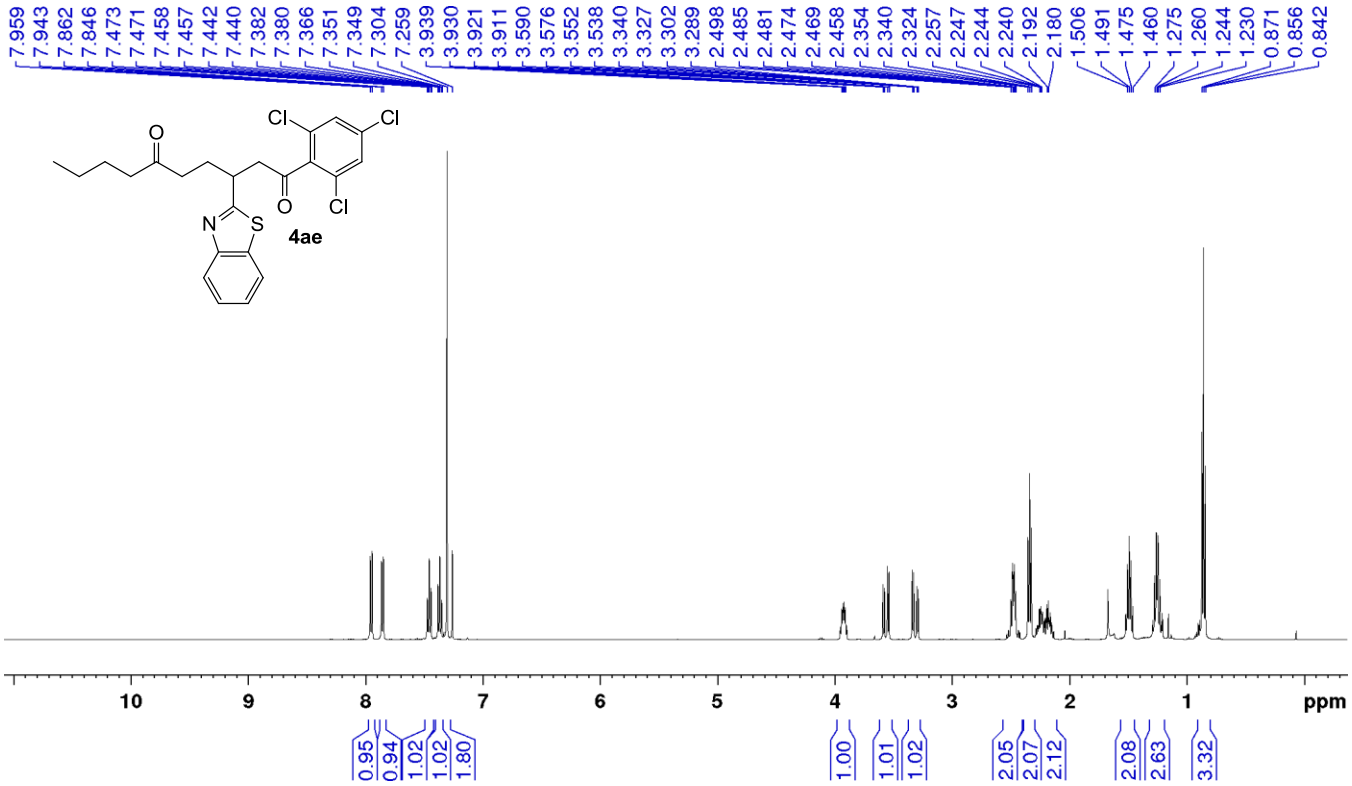
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (4ad)



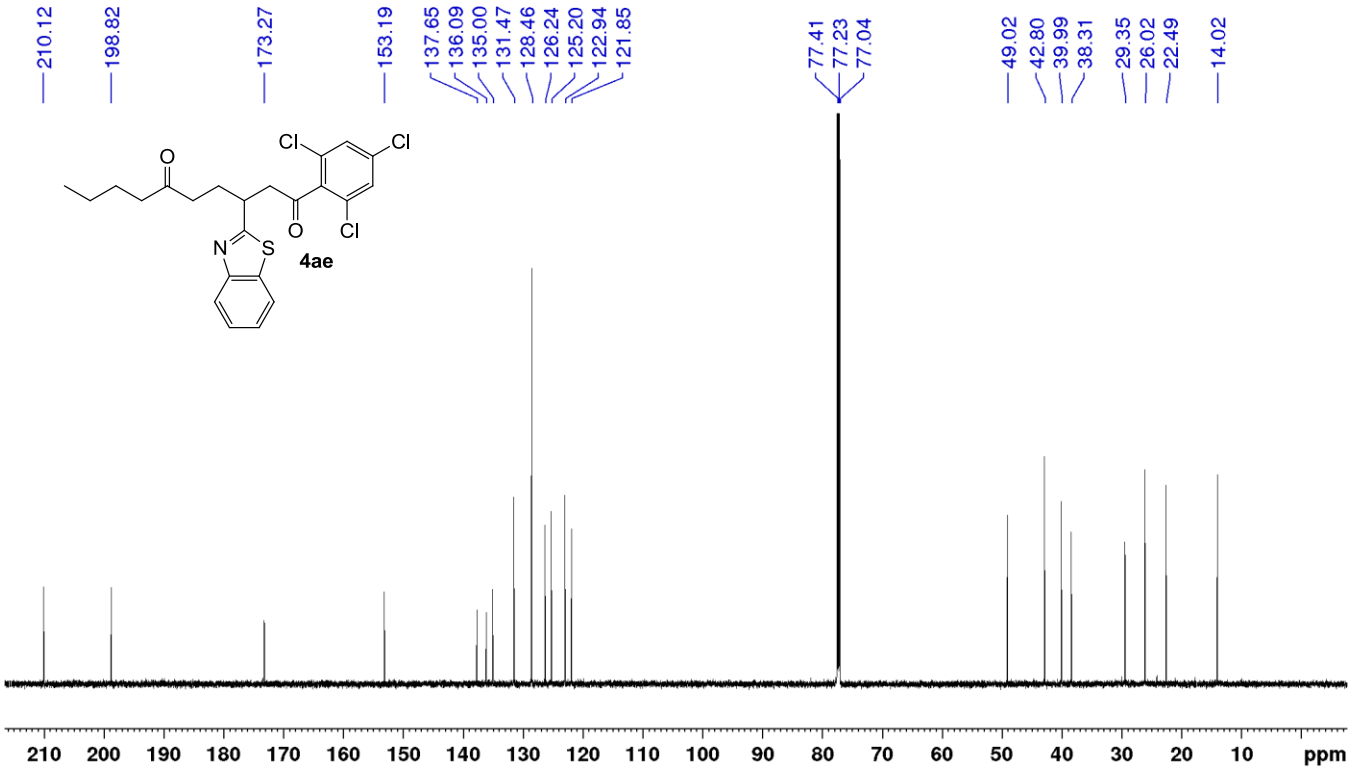
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4ad)



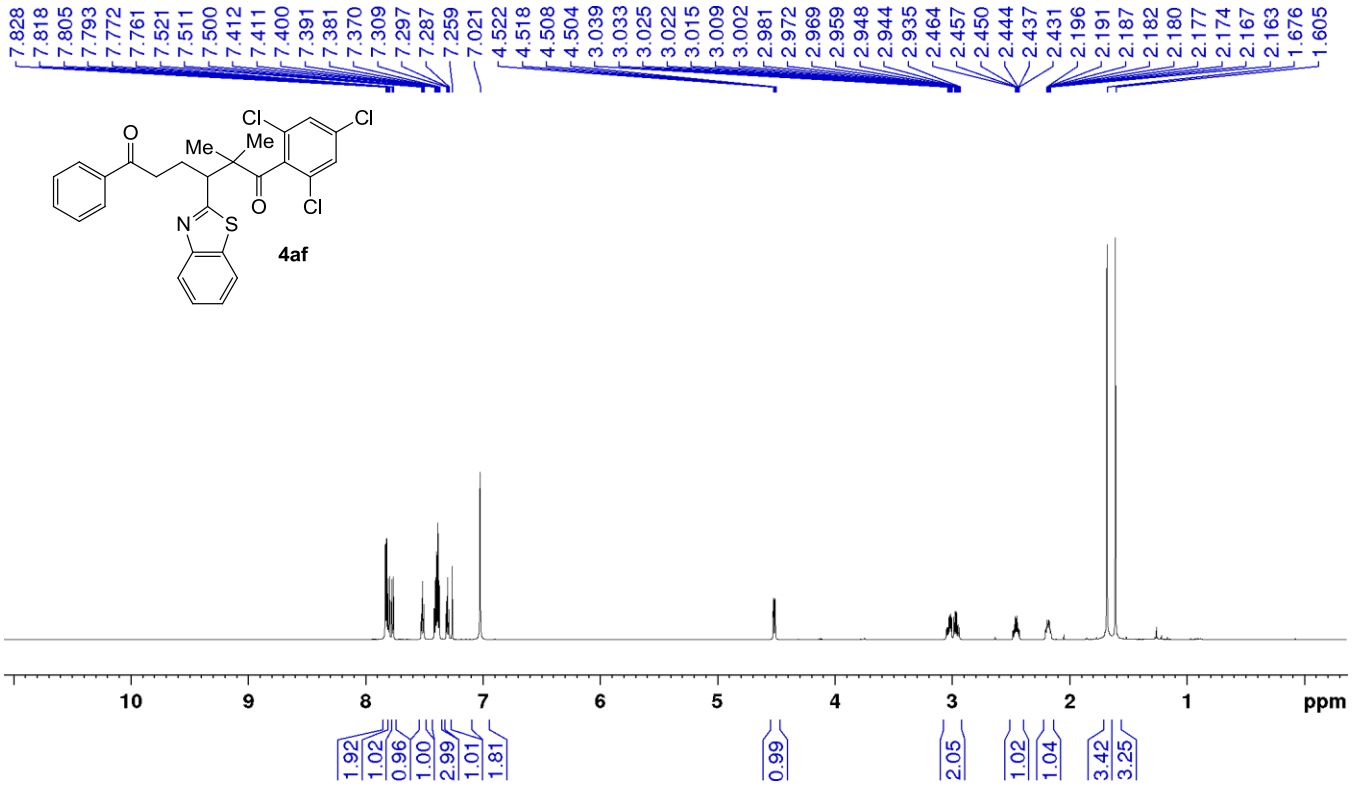
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (4ae)



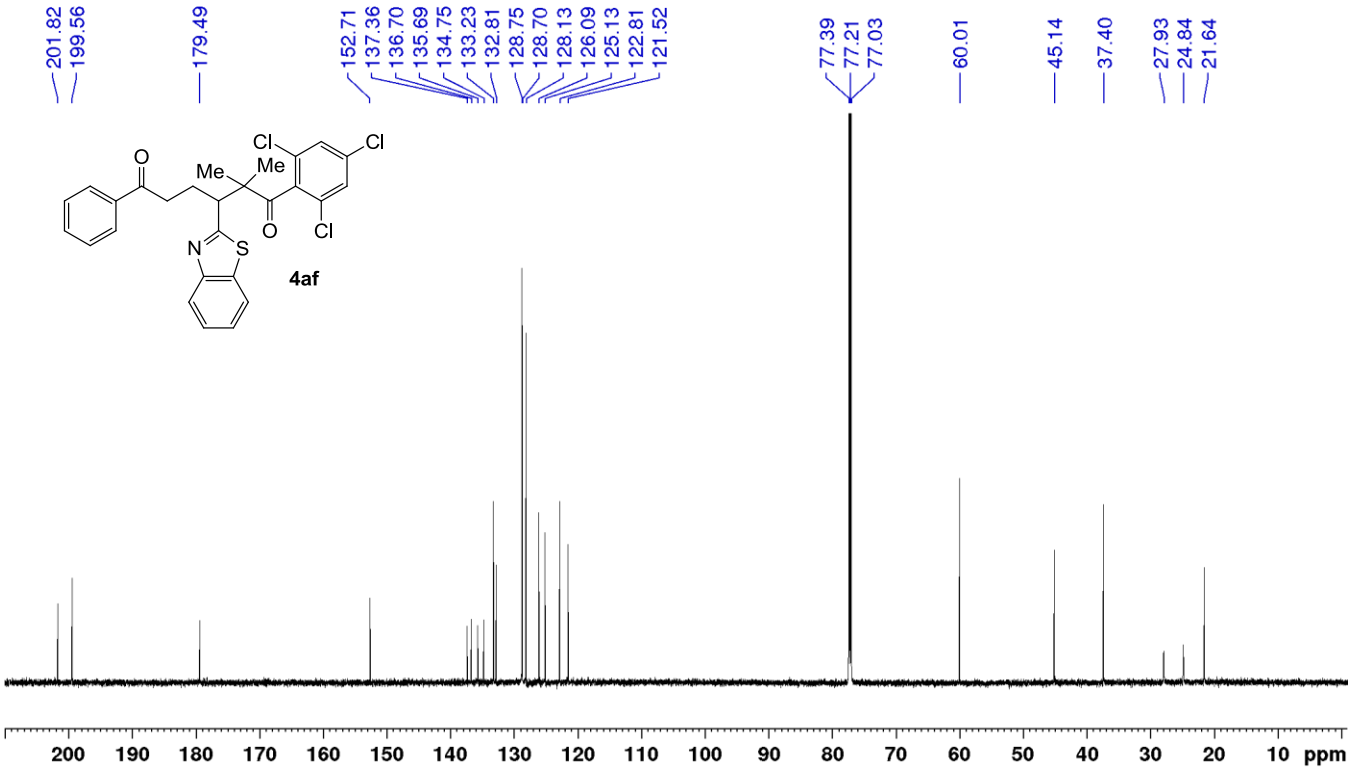
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4ae)



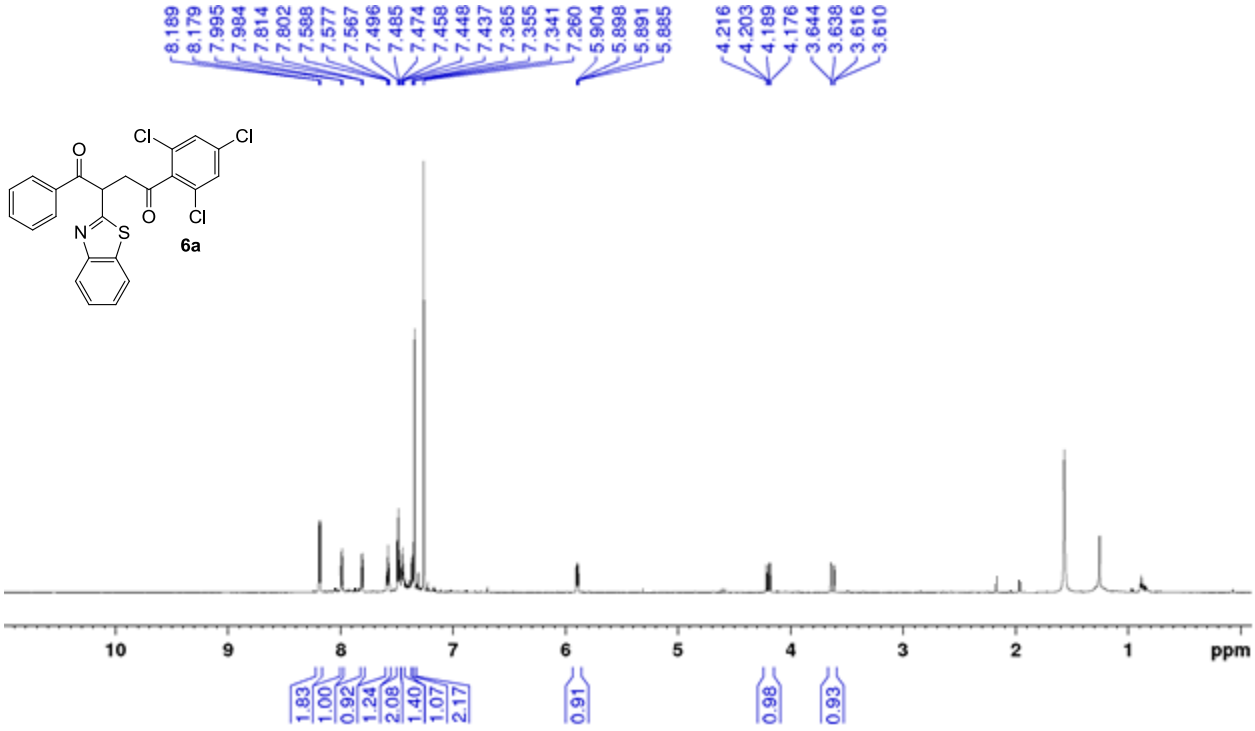
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (4af)



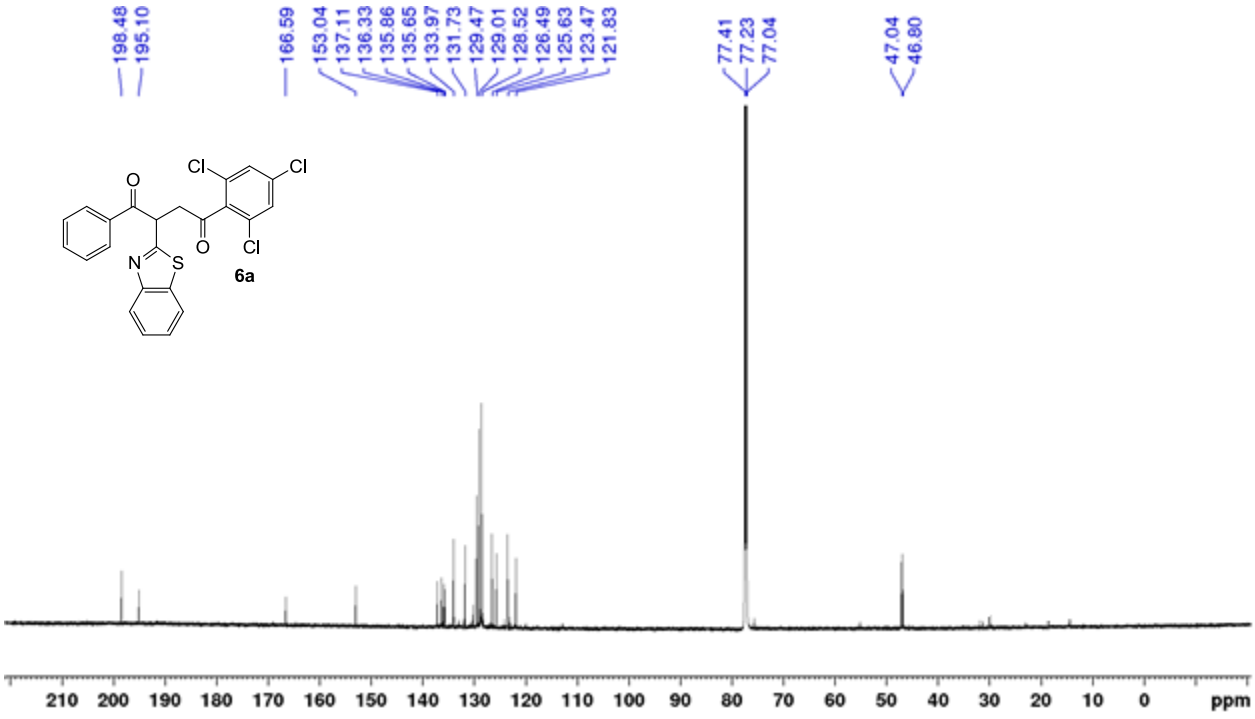
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (4af)



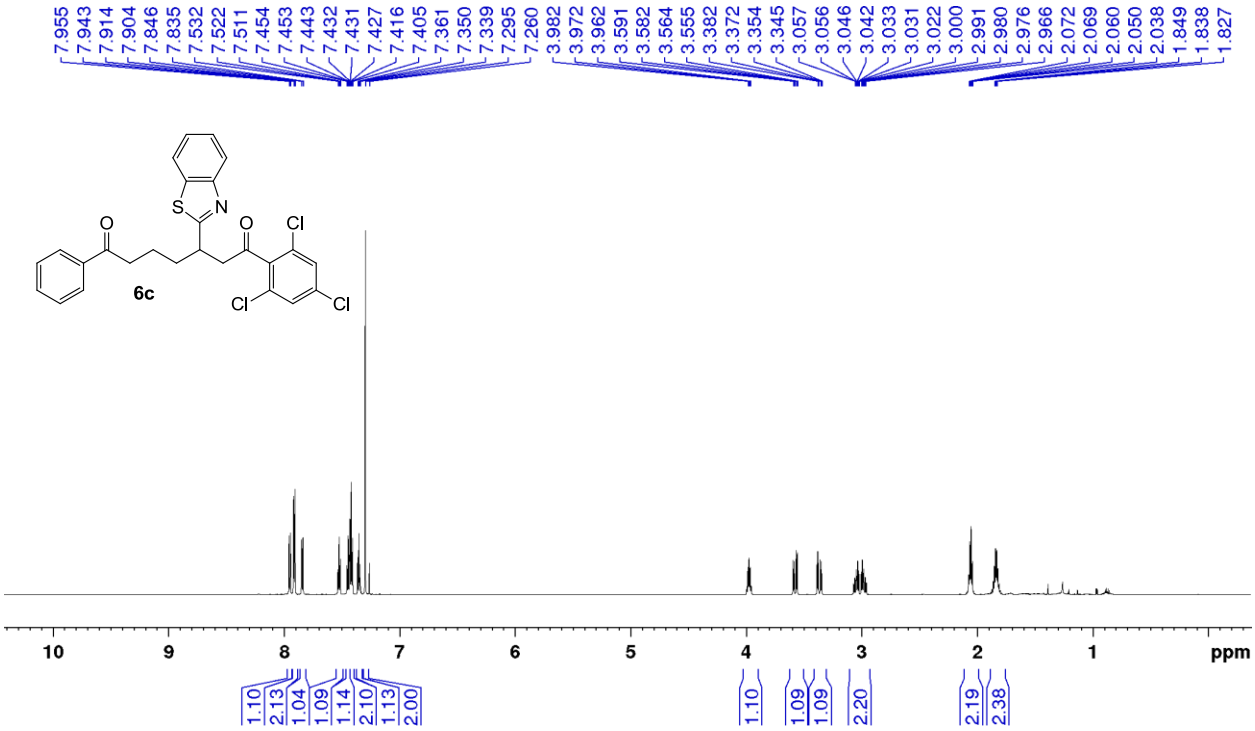
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6a)



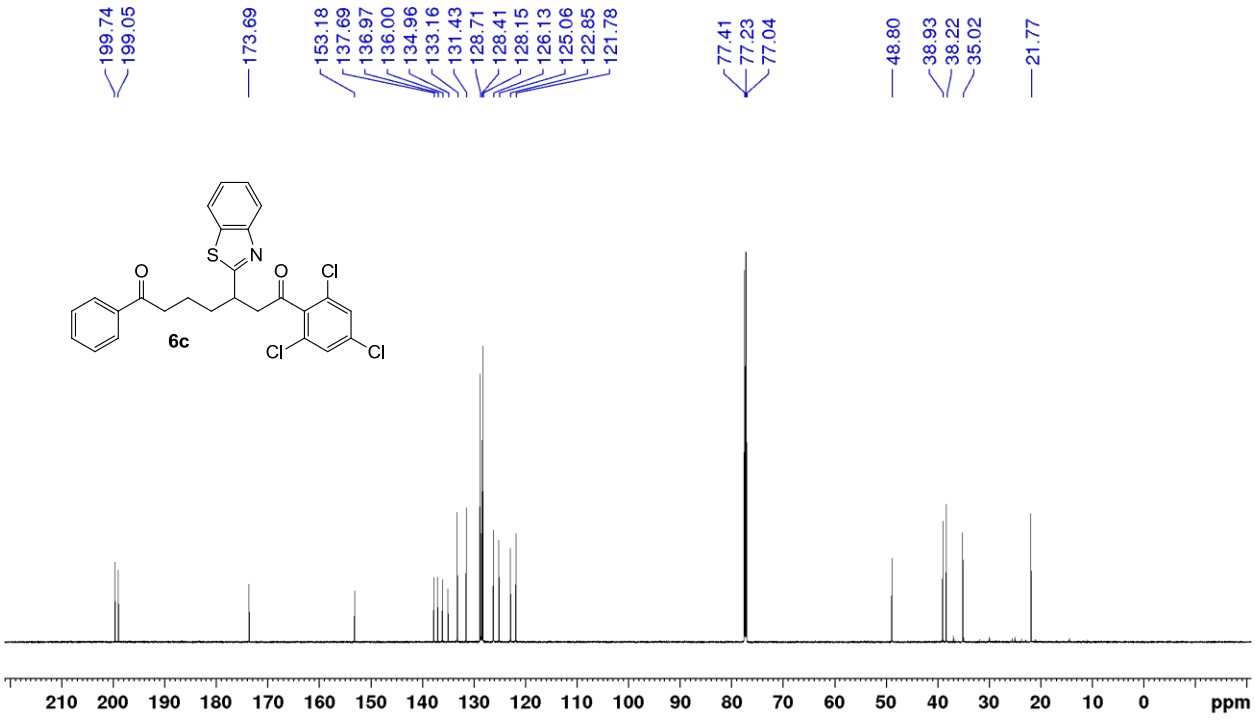
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6a)



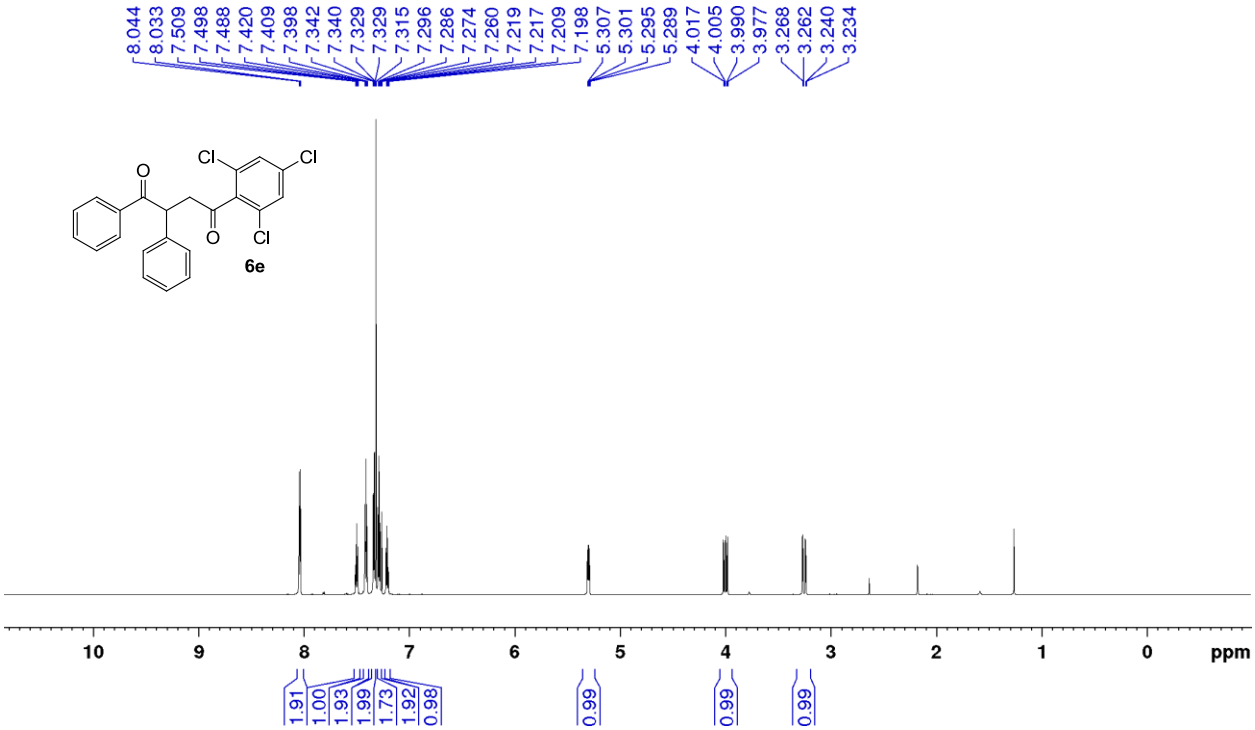
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6c)



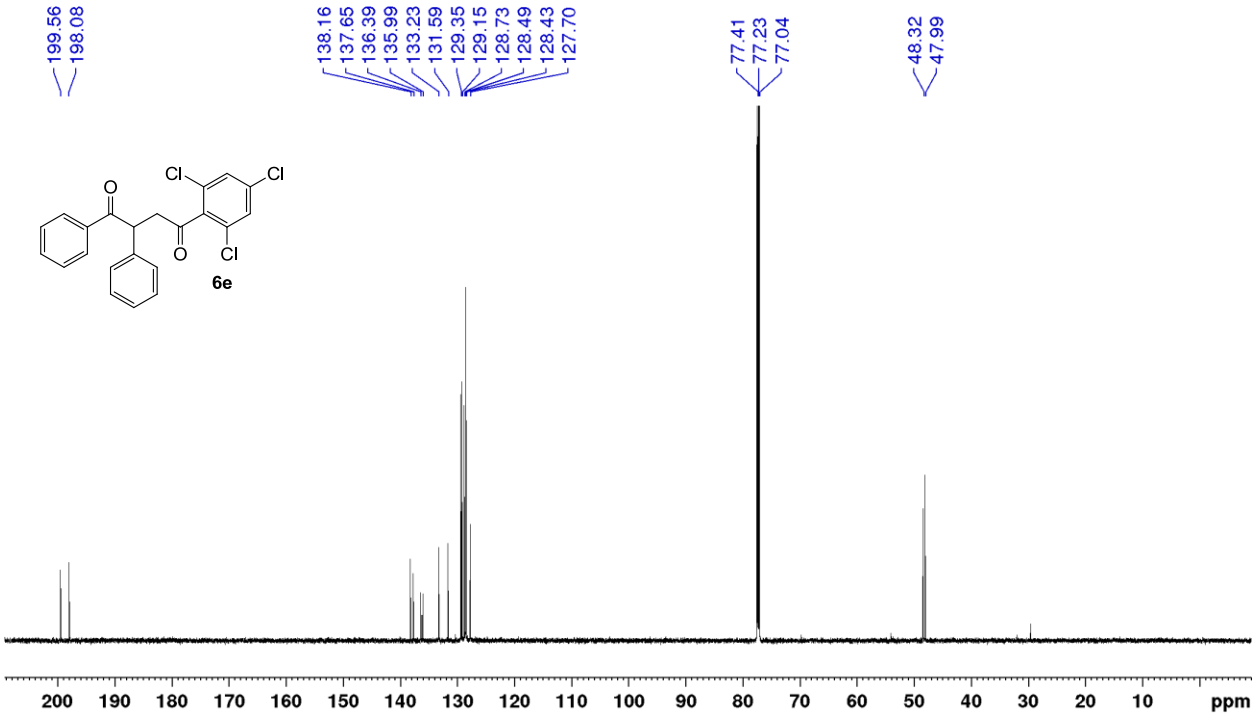
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6c)



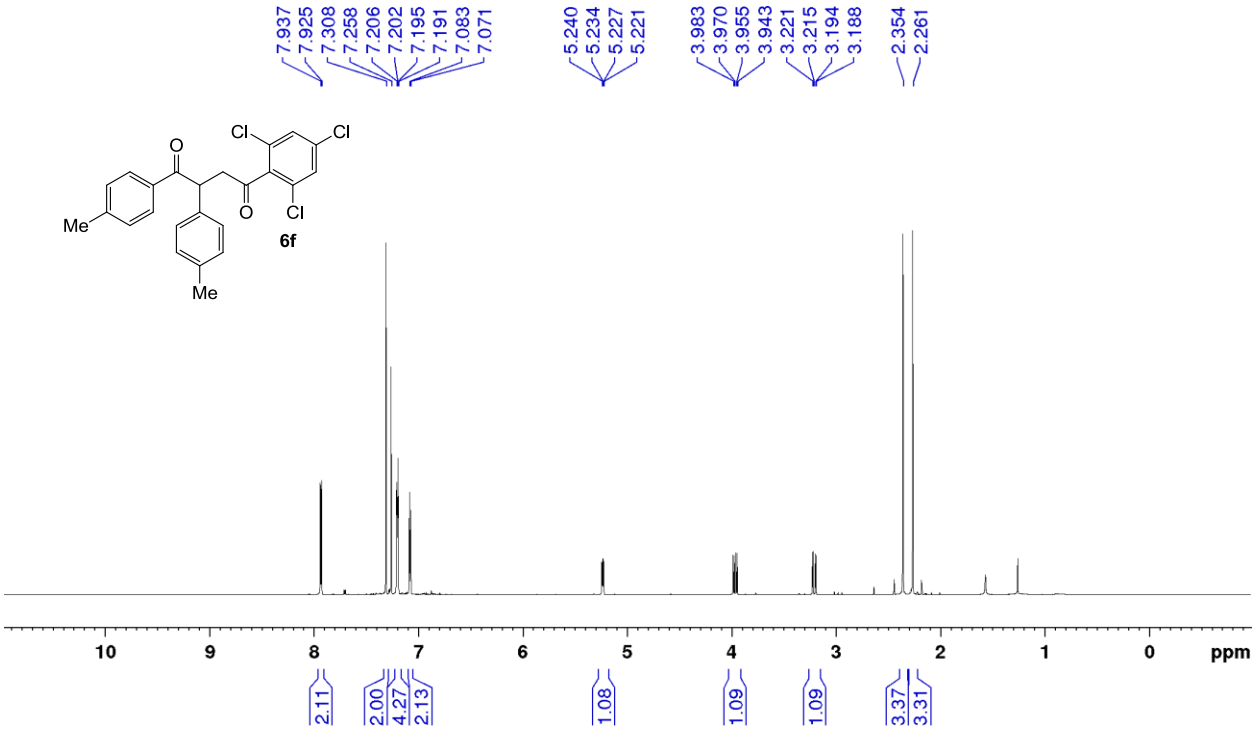
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (6e)



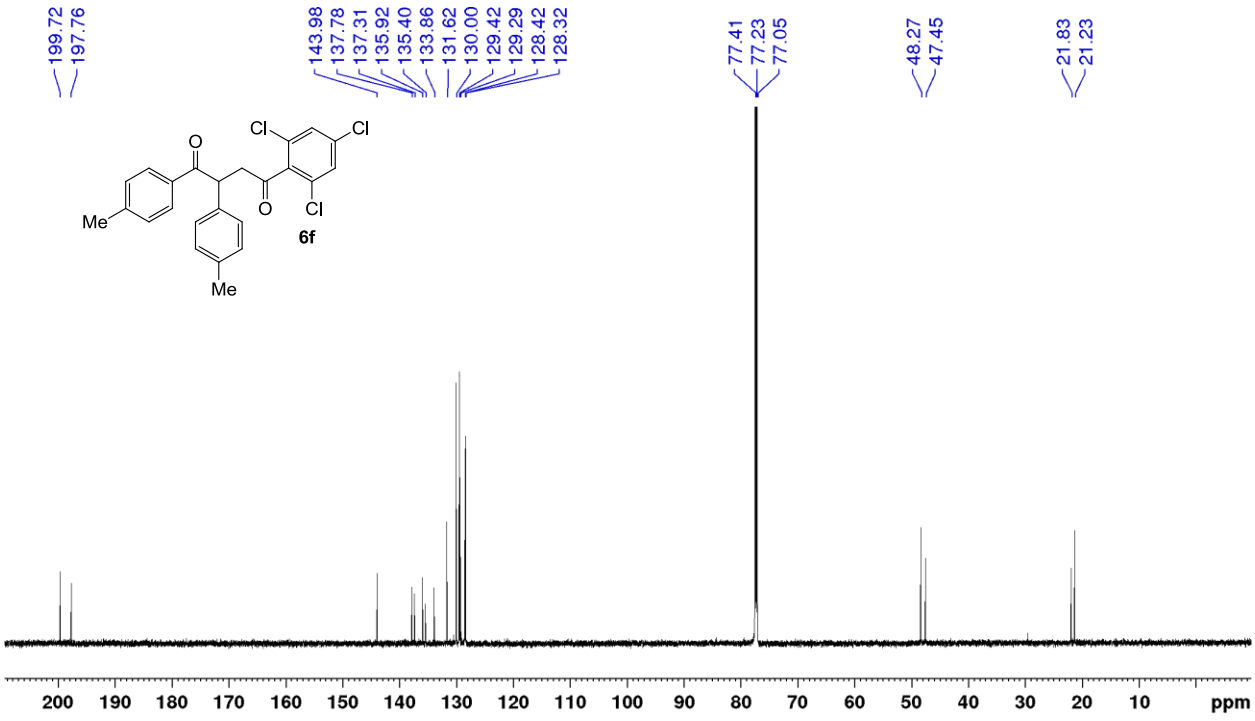
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (6e)



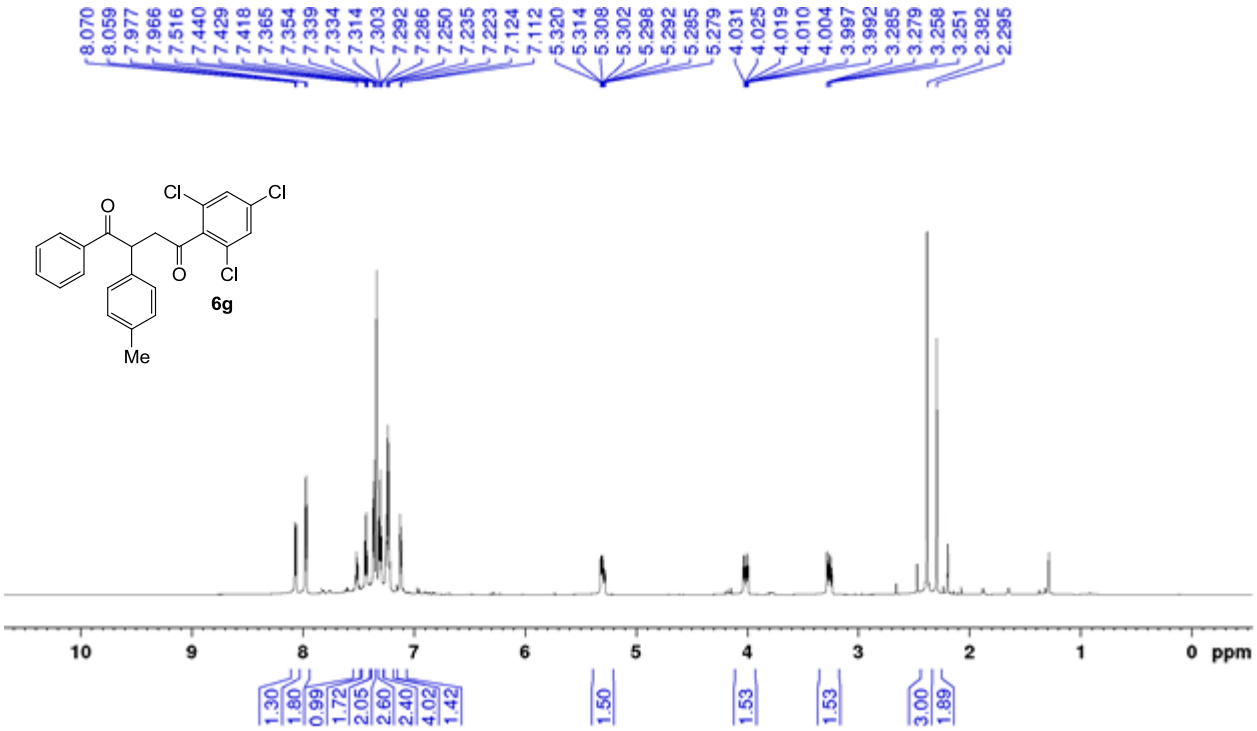
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6f)



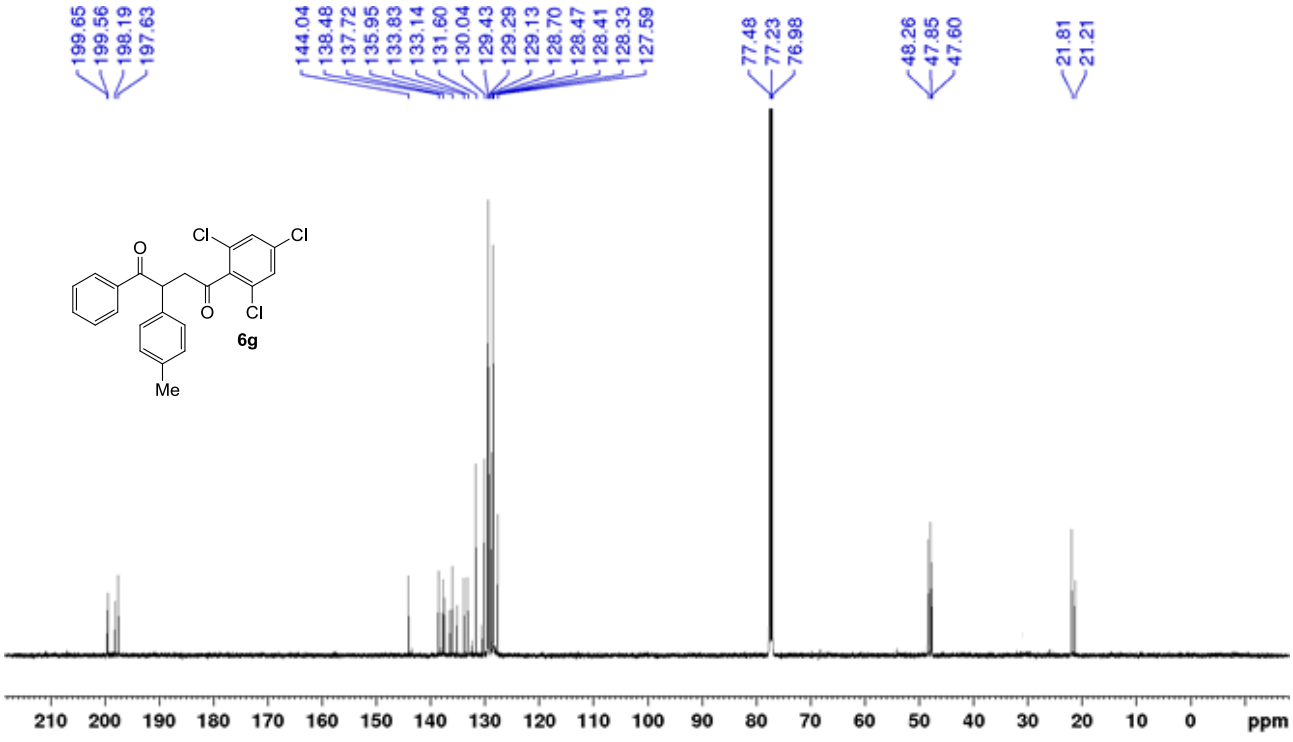
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6f)



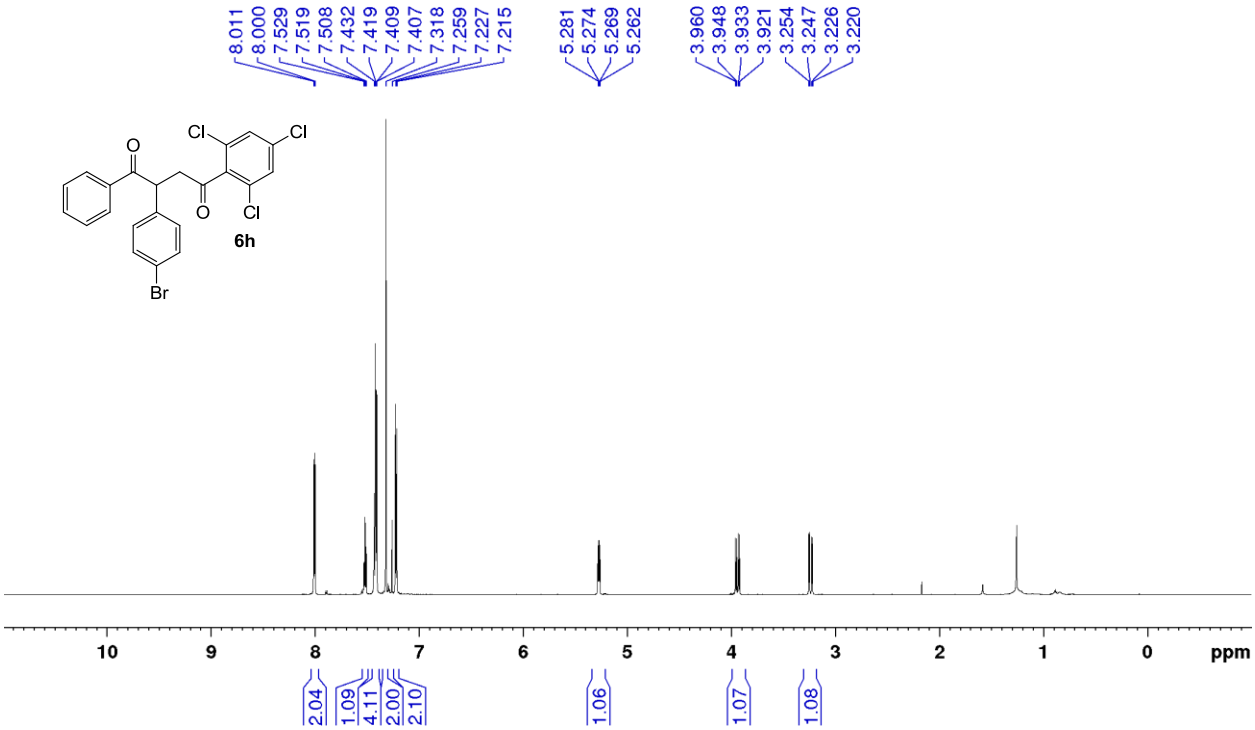
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6g)



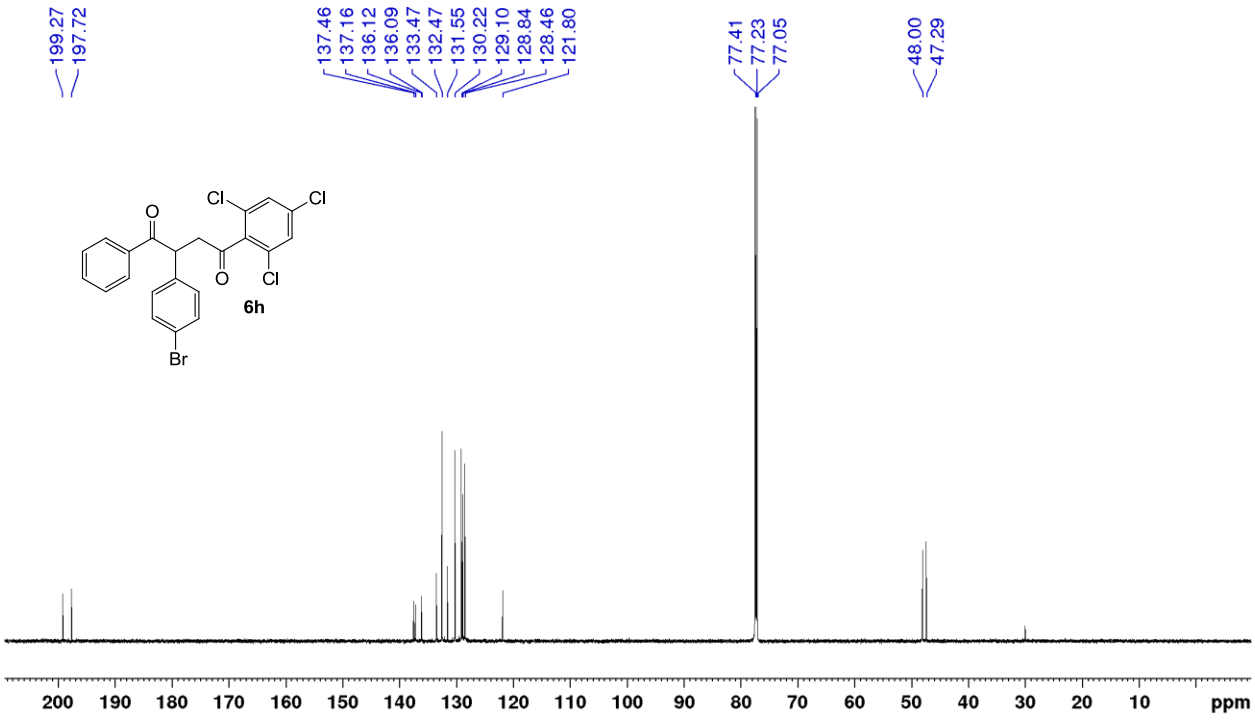
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6g)



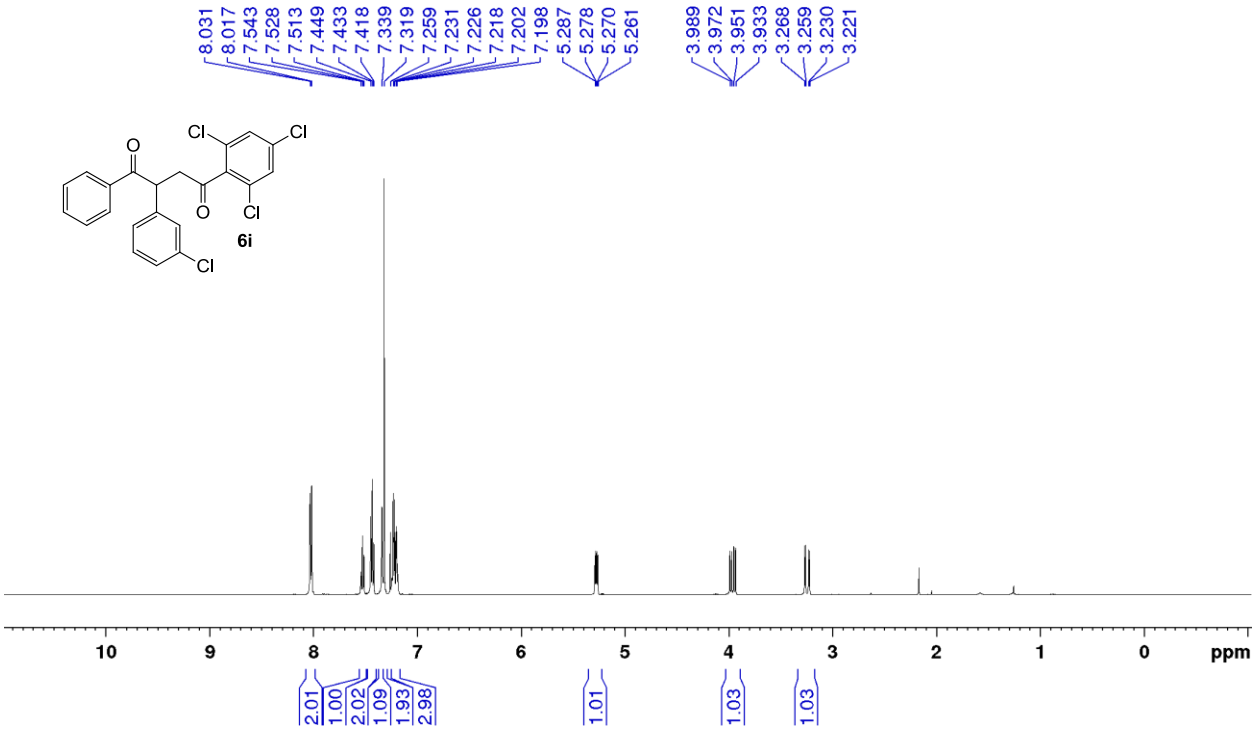
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6h)



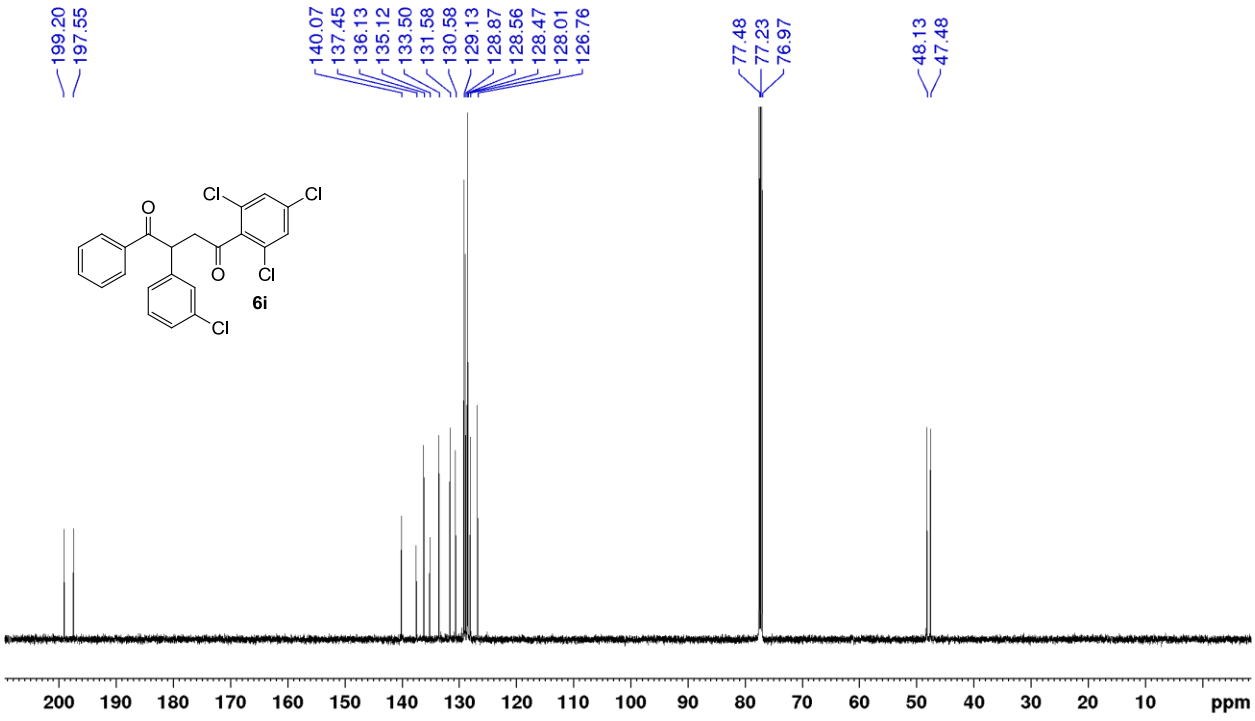
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6h)



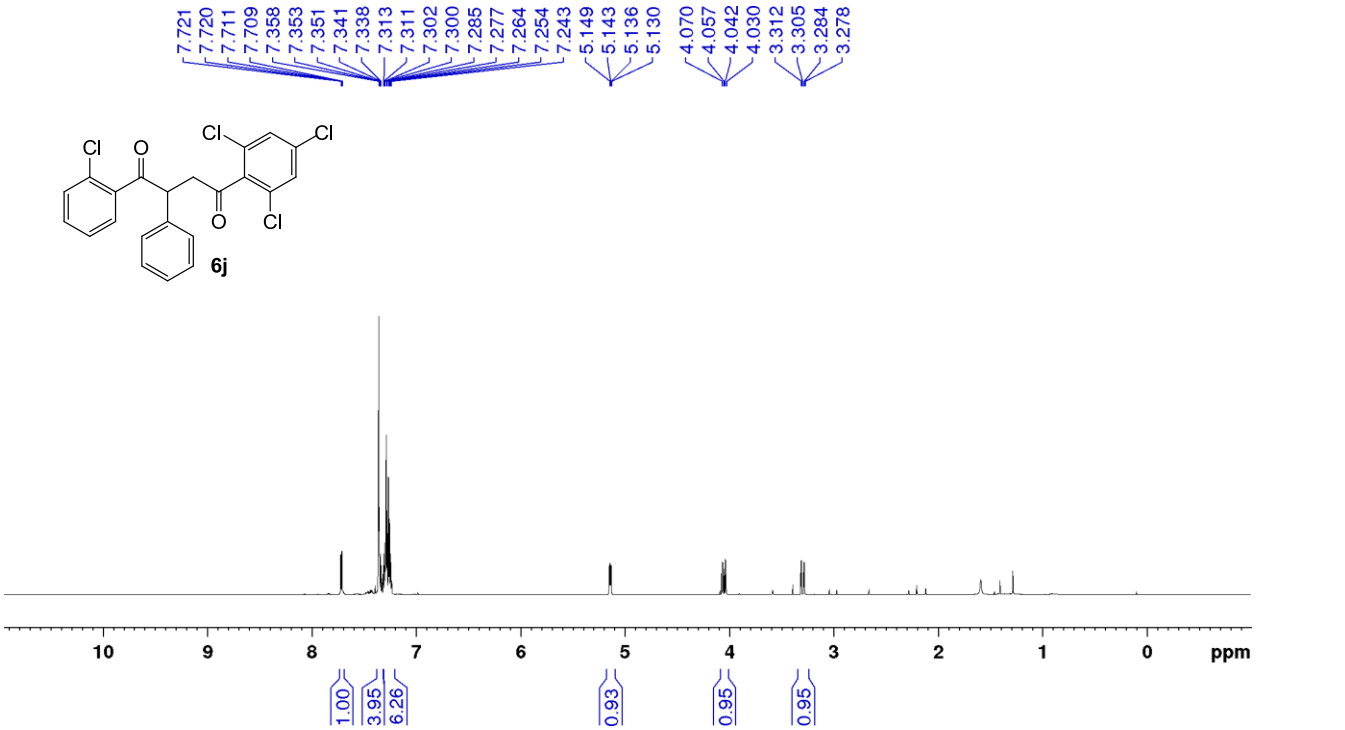
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (6i)



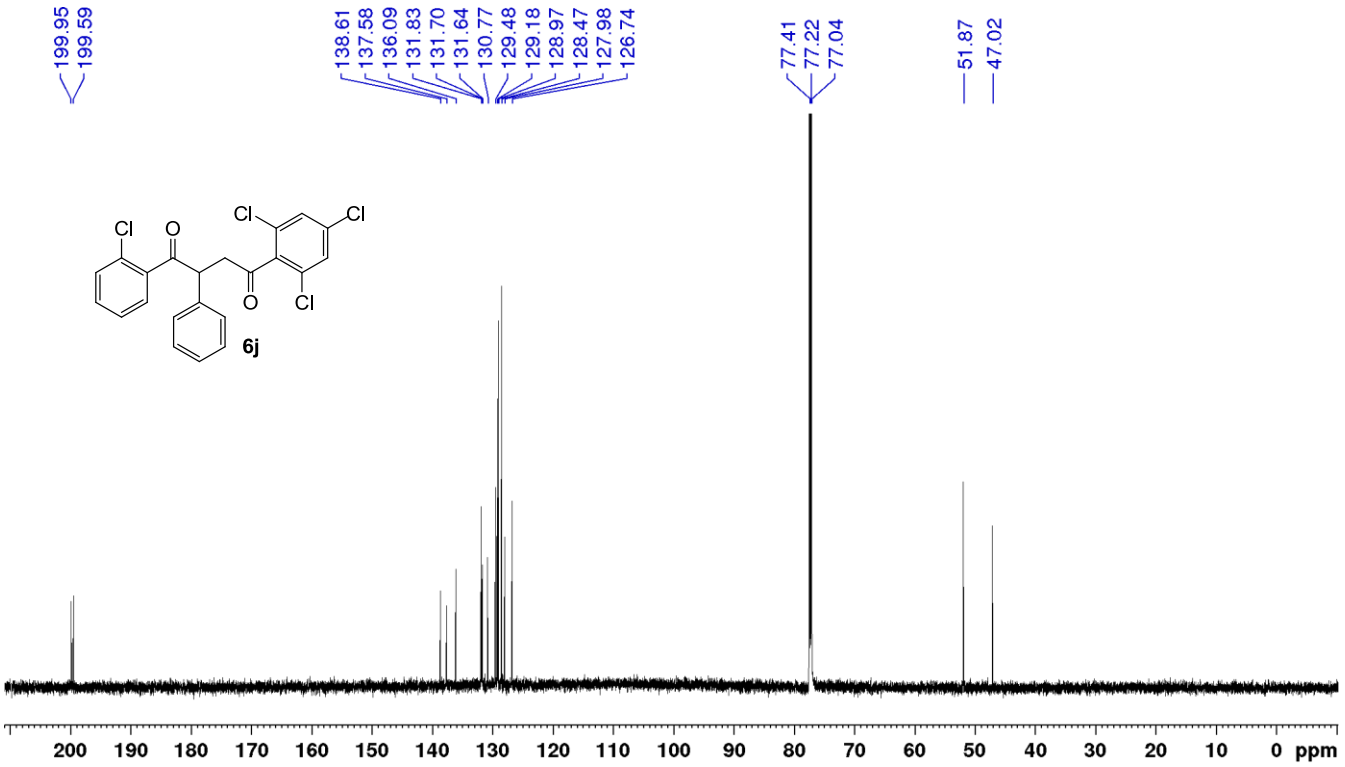
^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (6i)



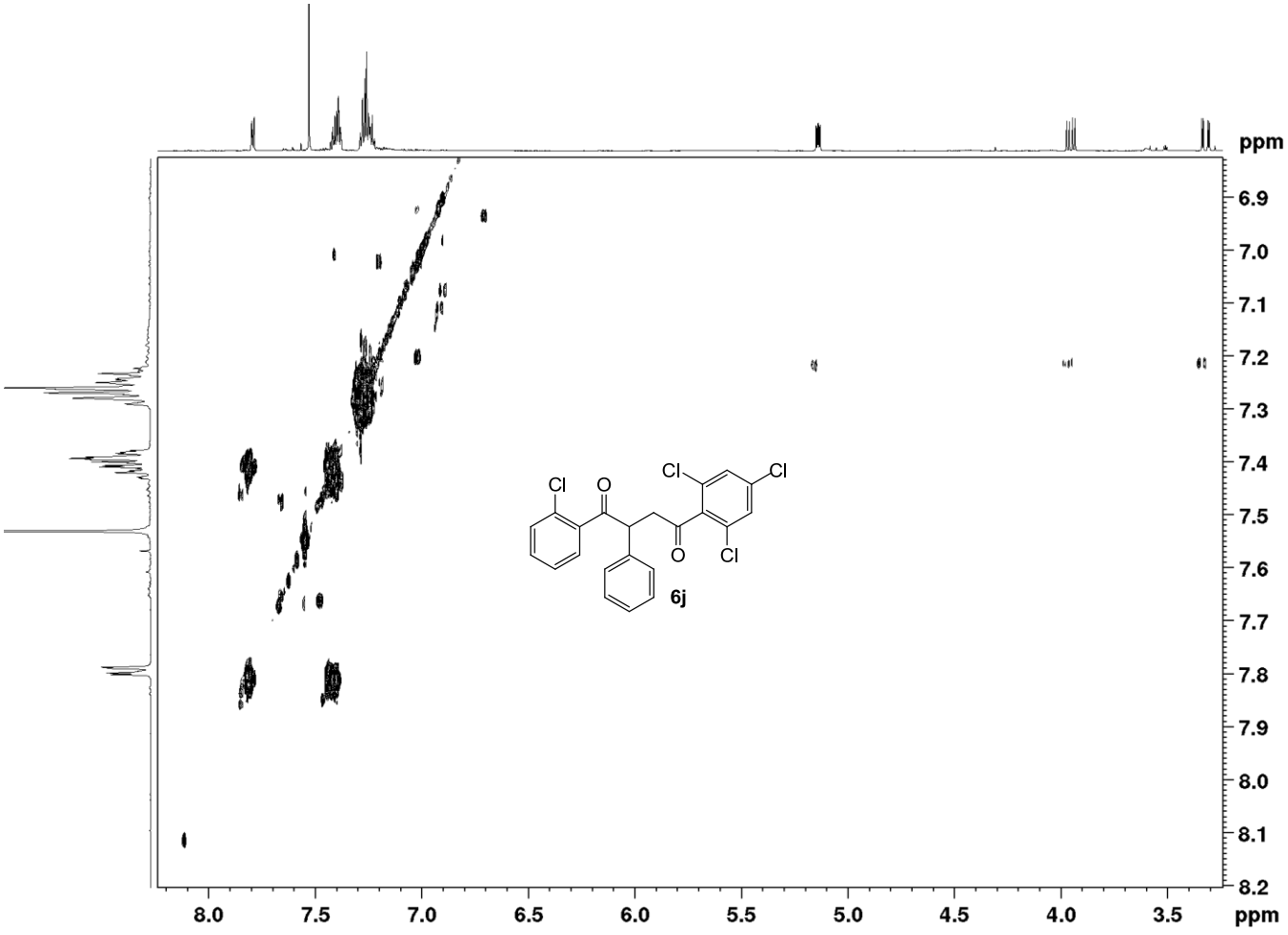
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6j)



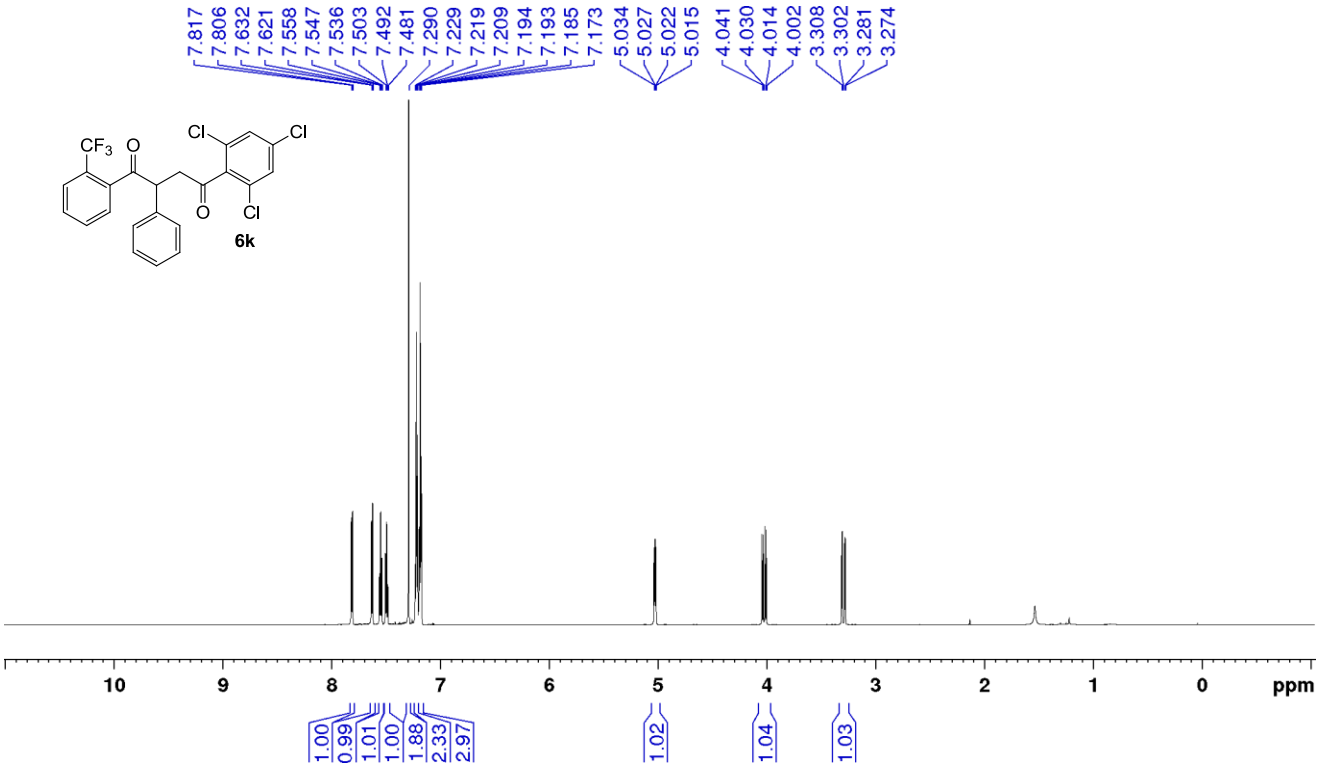
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6j)



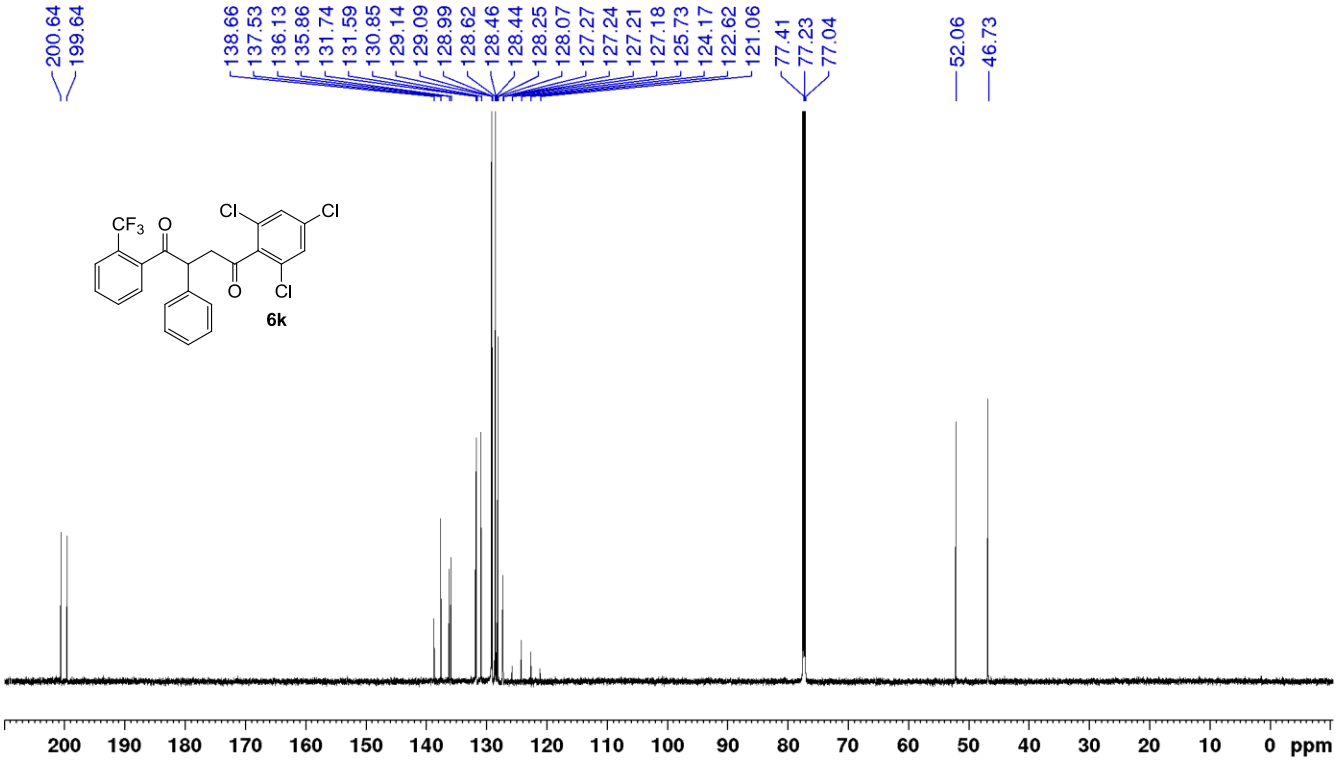
2D COESY (CD_3CN, 25 ºC) of (6j)



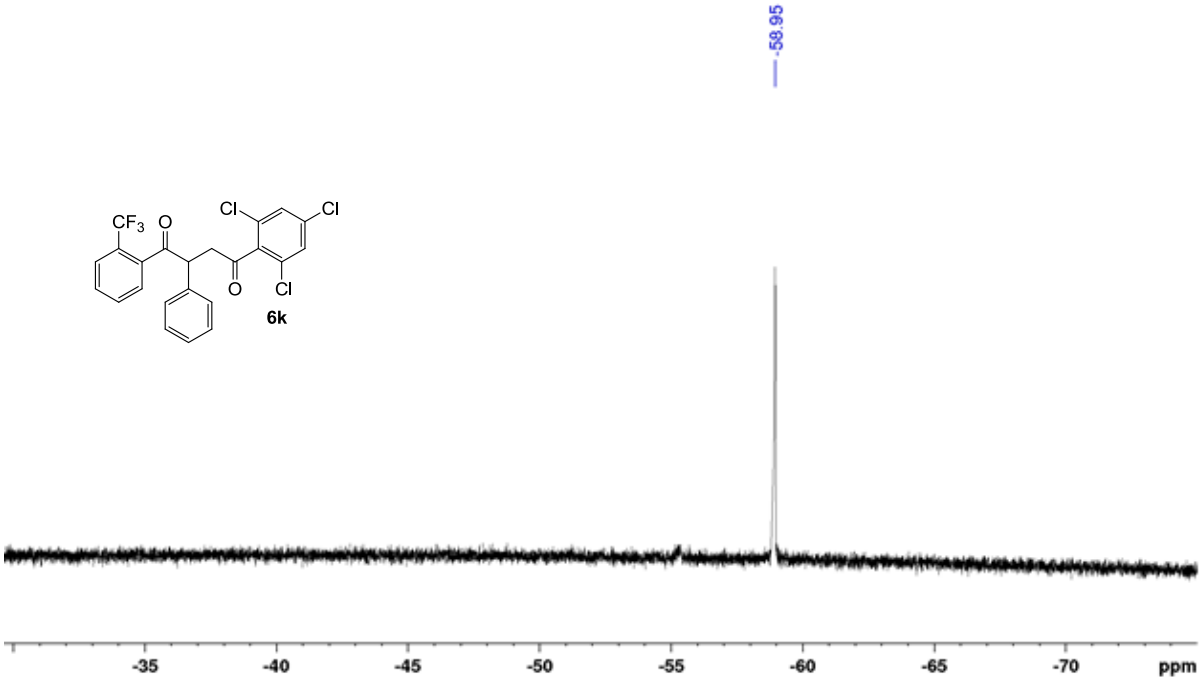
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (6k)



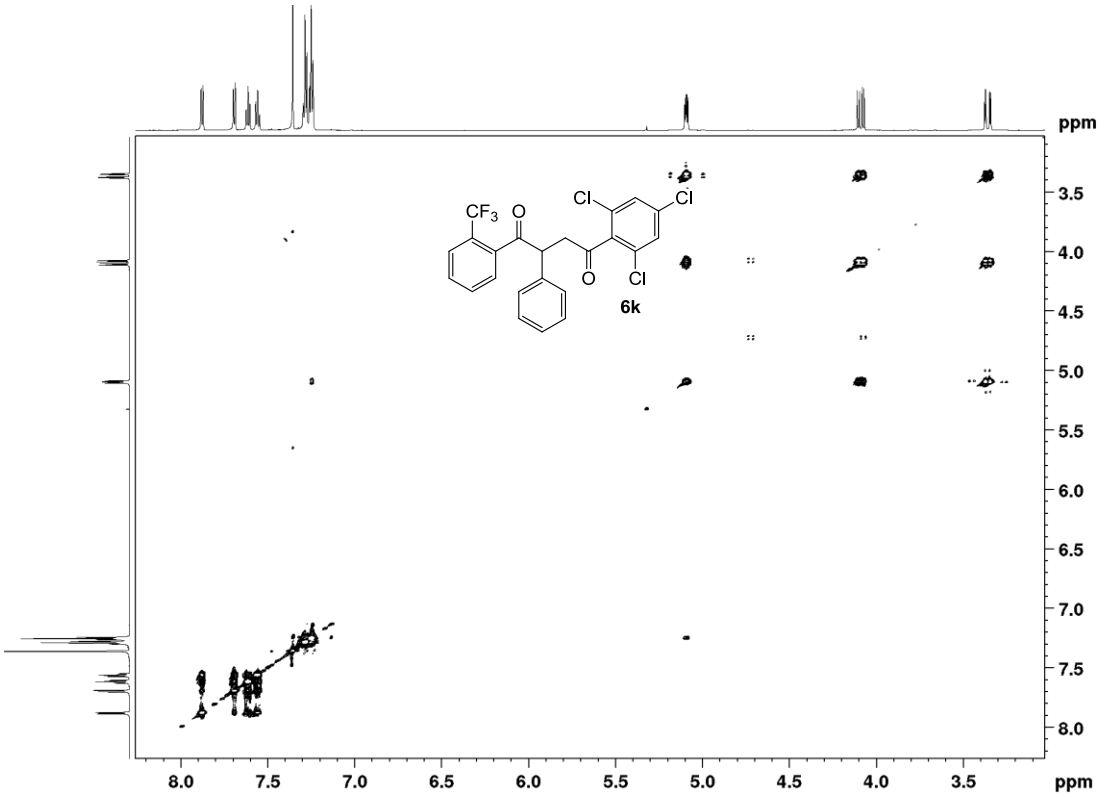
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (6k)



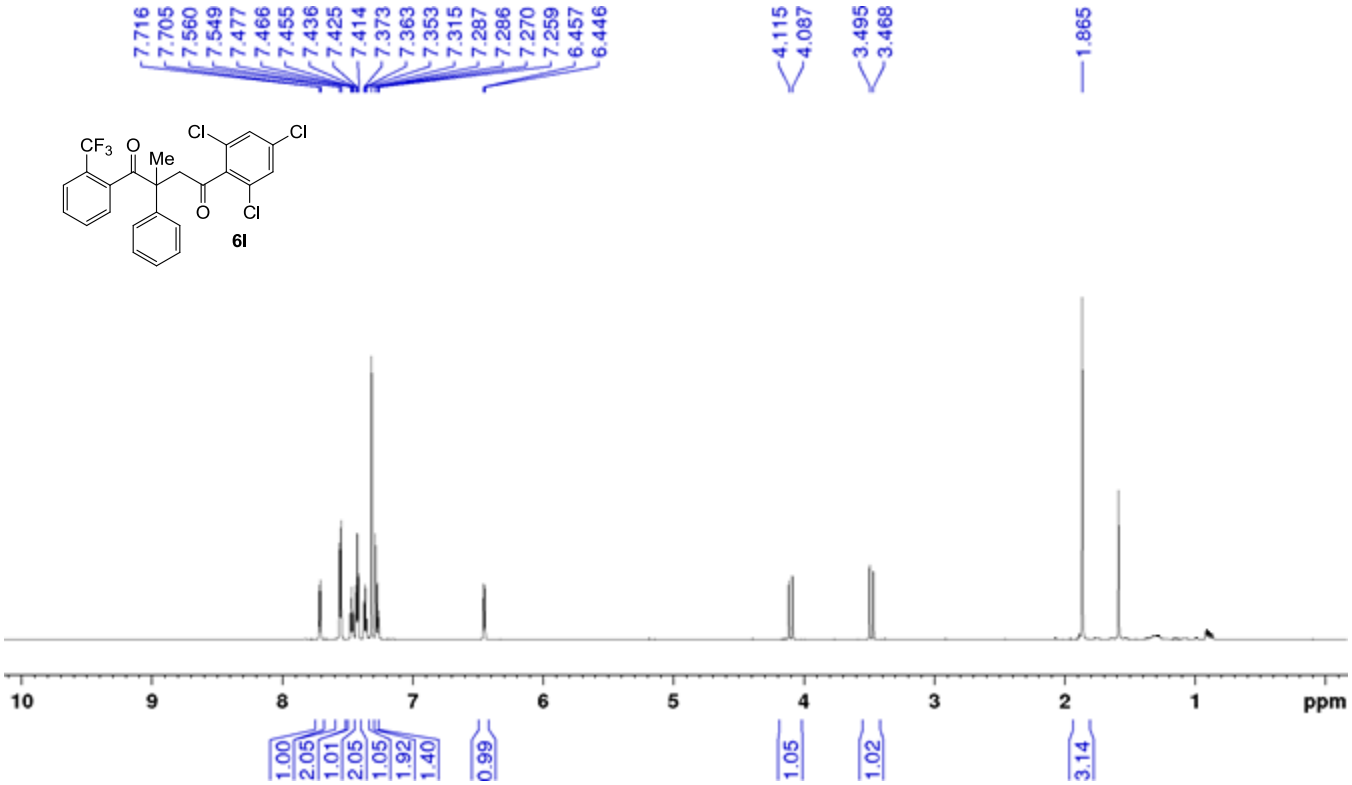
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (6k)



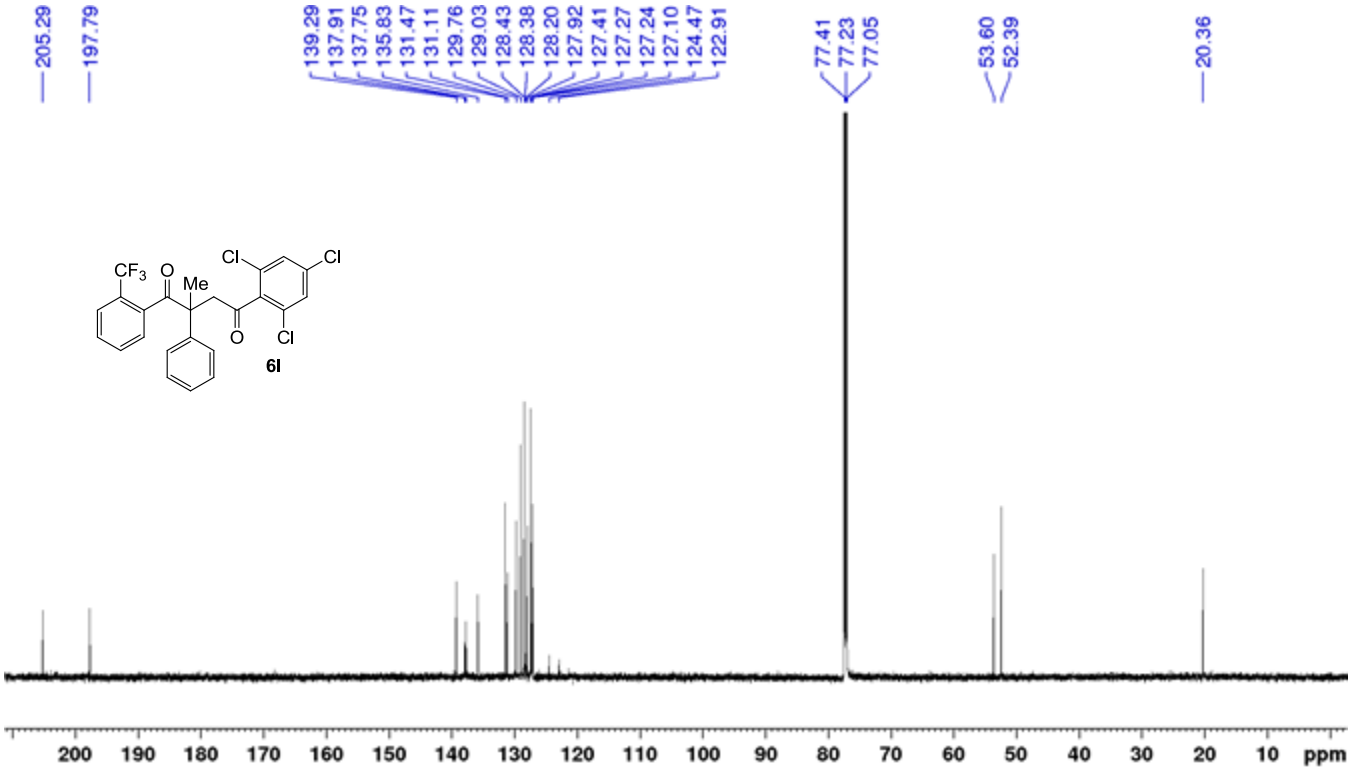
2D COESY ($CDCl_3$, 25 ºC) of (6k)



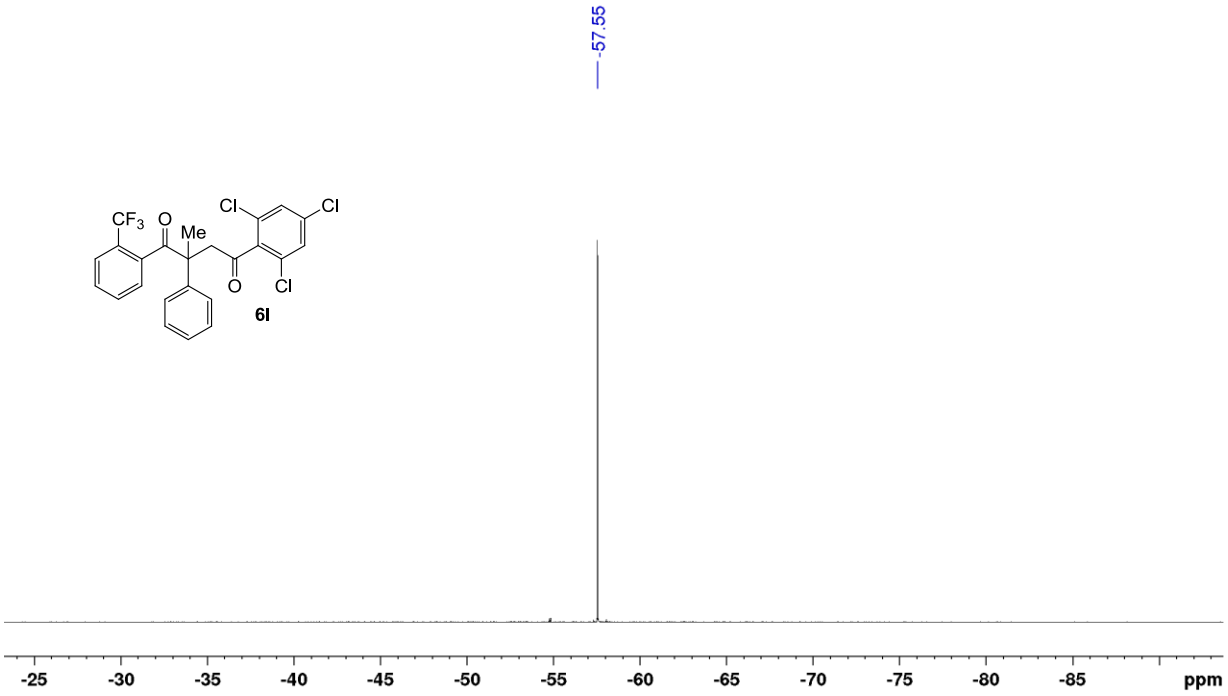
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6l)



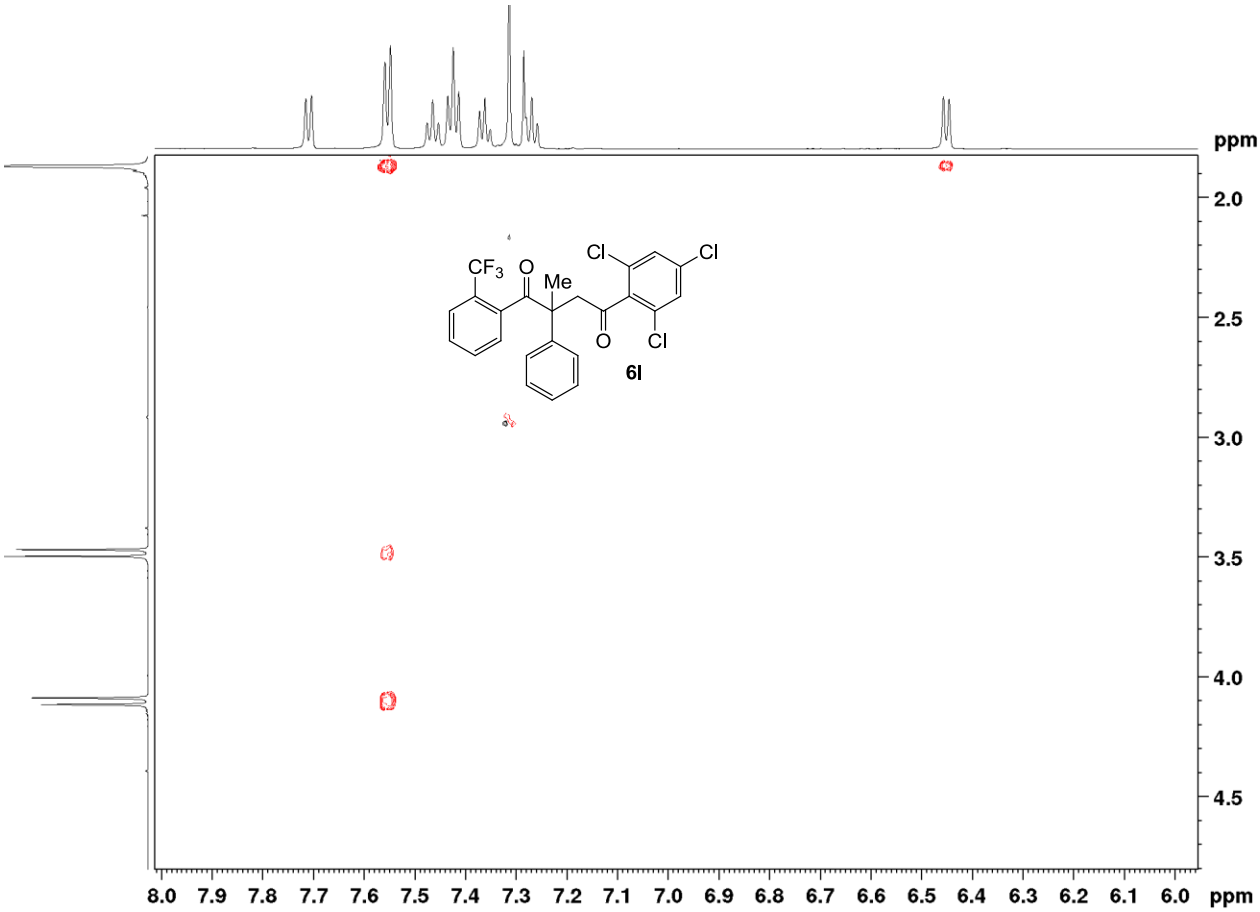
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6l)



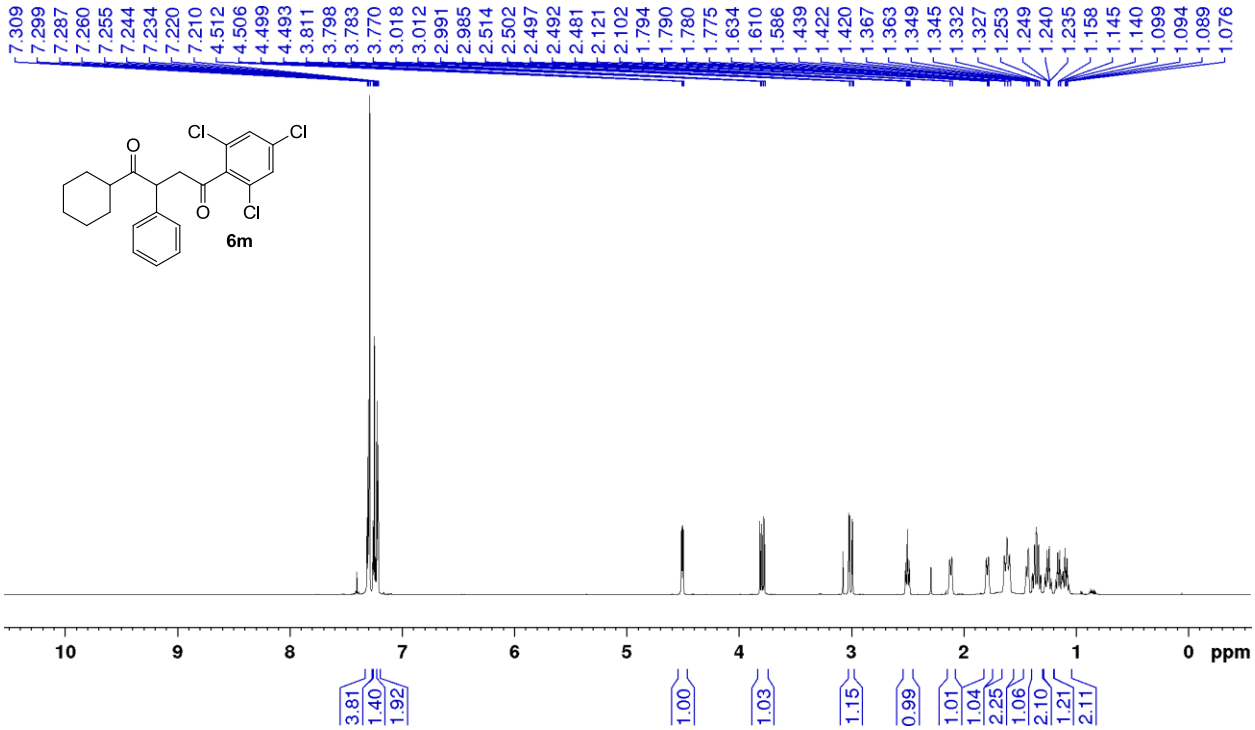
^{19}F NMR (175 MHz, $CDCl_3$, 25 °C) of (6l)



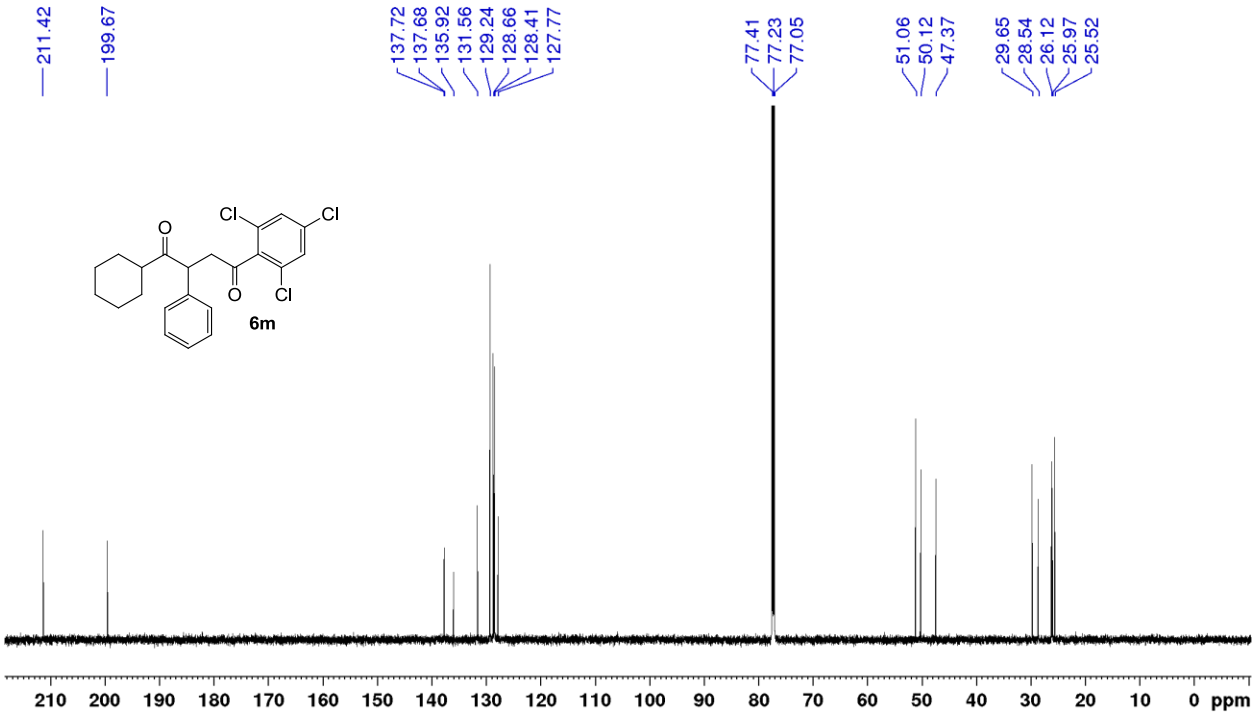
2D COESY ($CDCl_3$, 25 °C) of (6l)



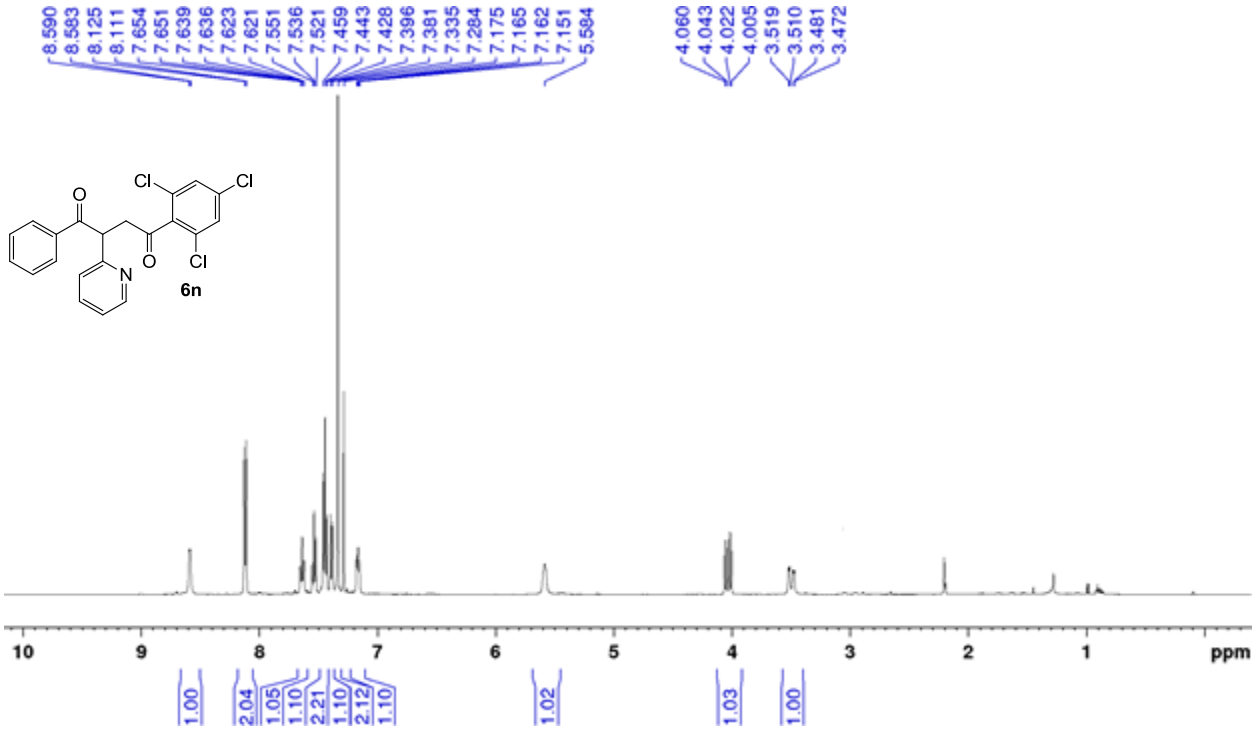
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (6m)



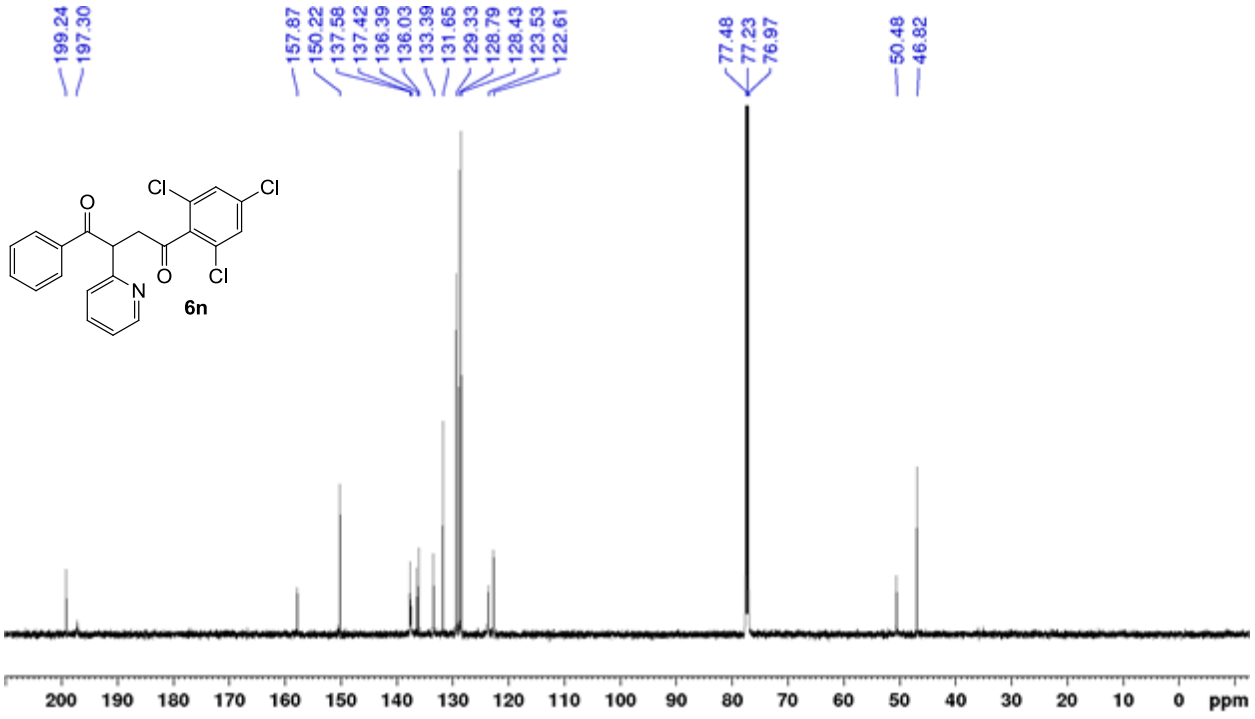
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (6m)



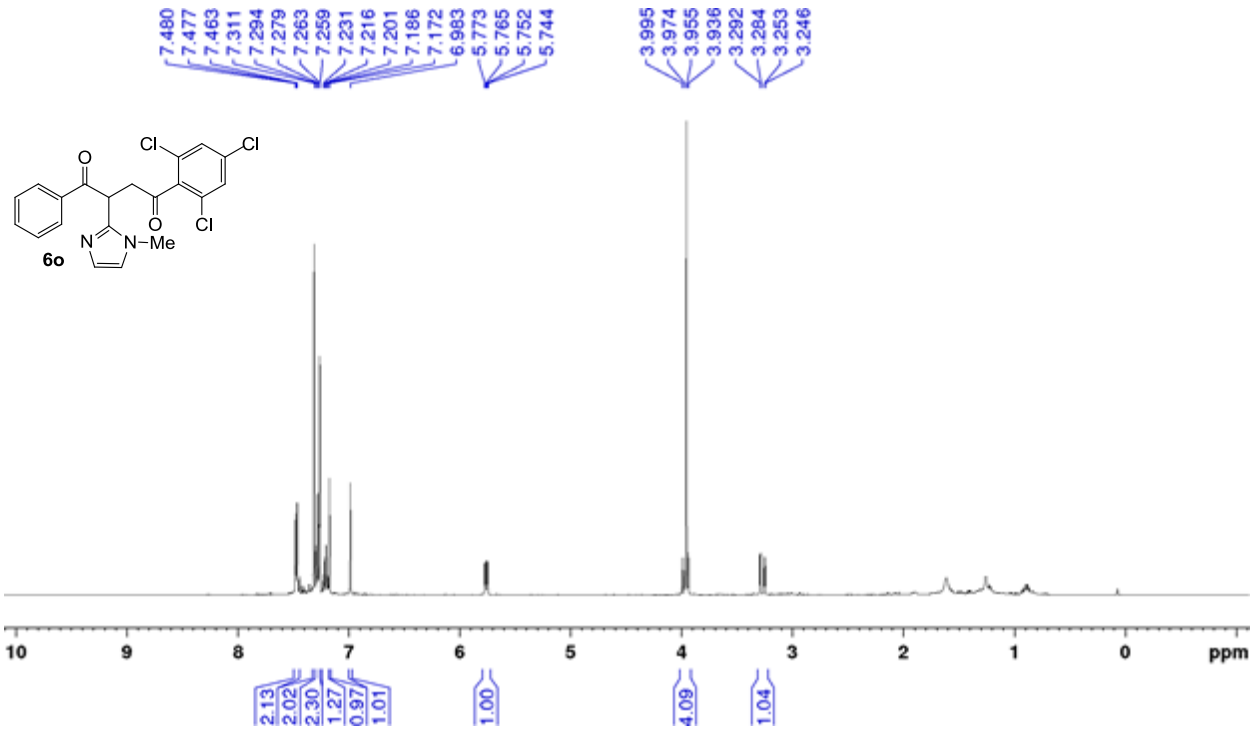
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (6n)



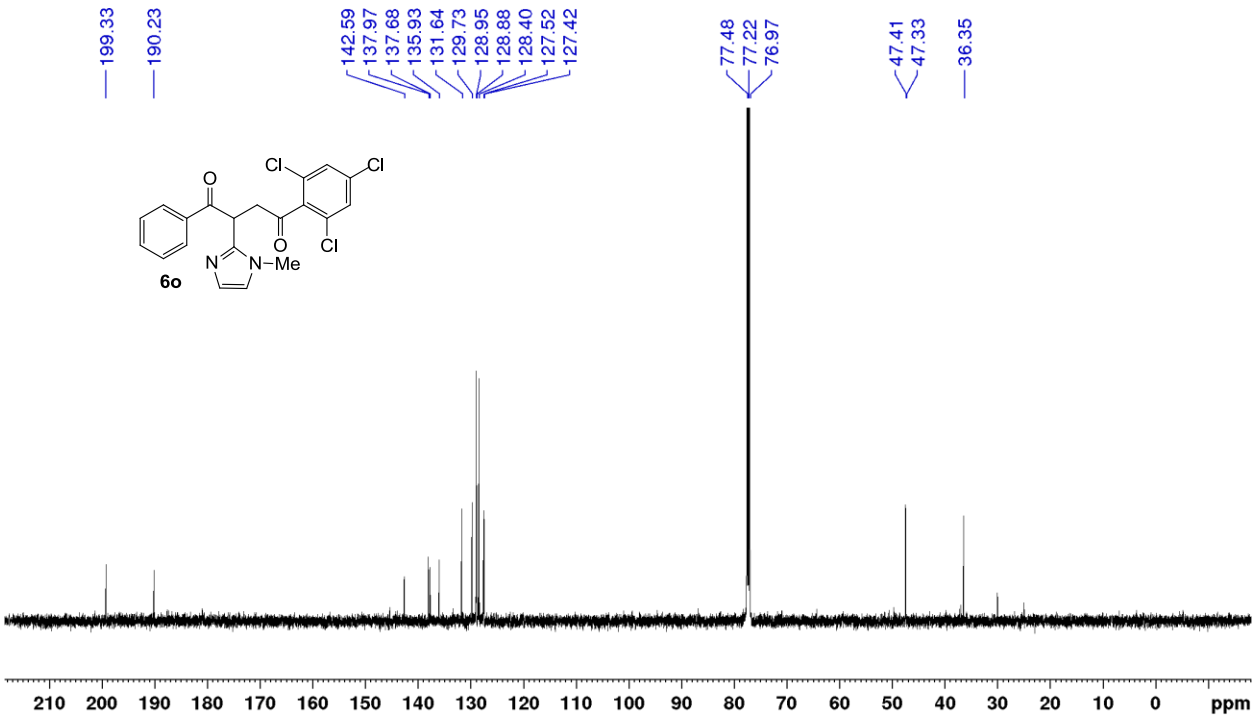
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (6n)



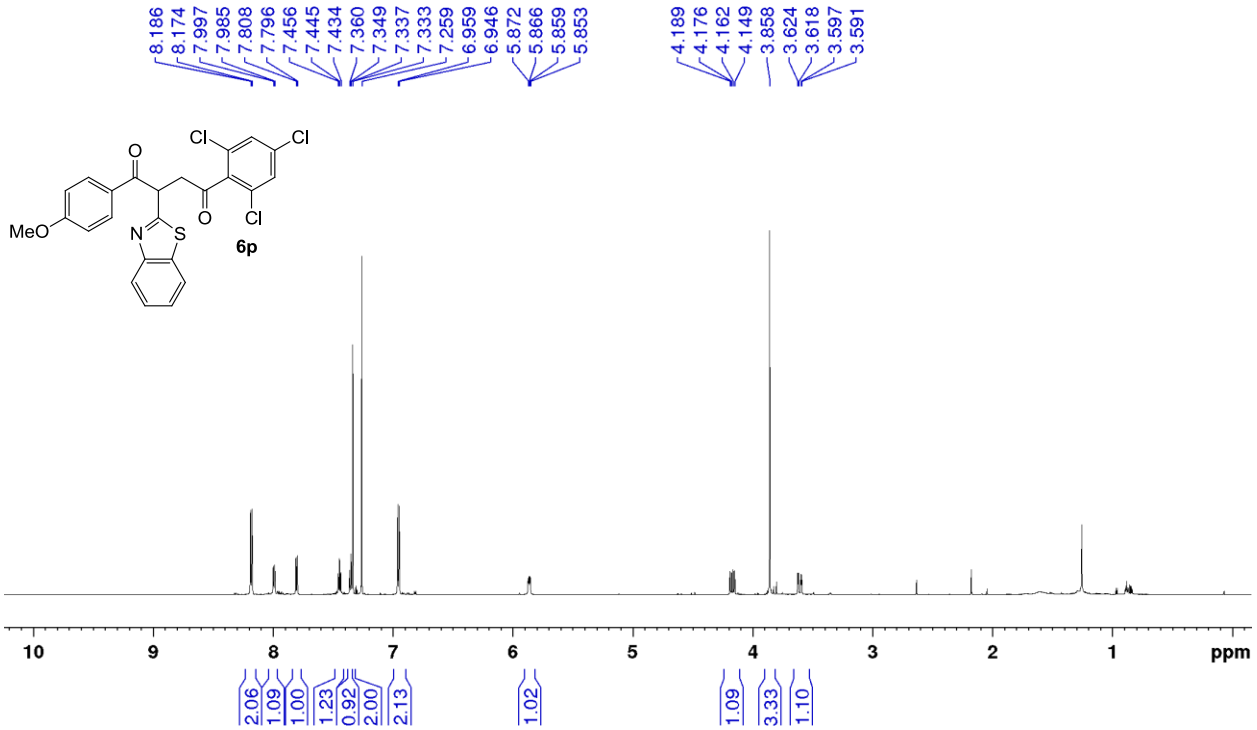
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (6o)



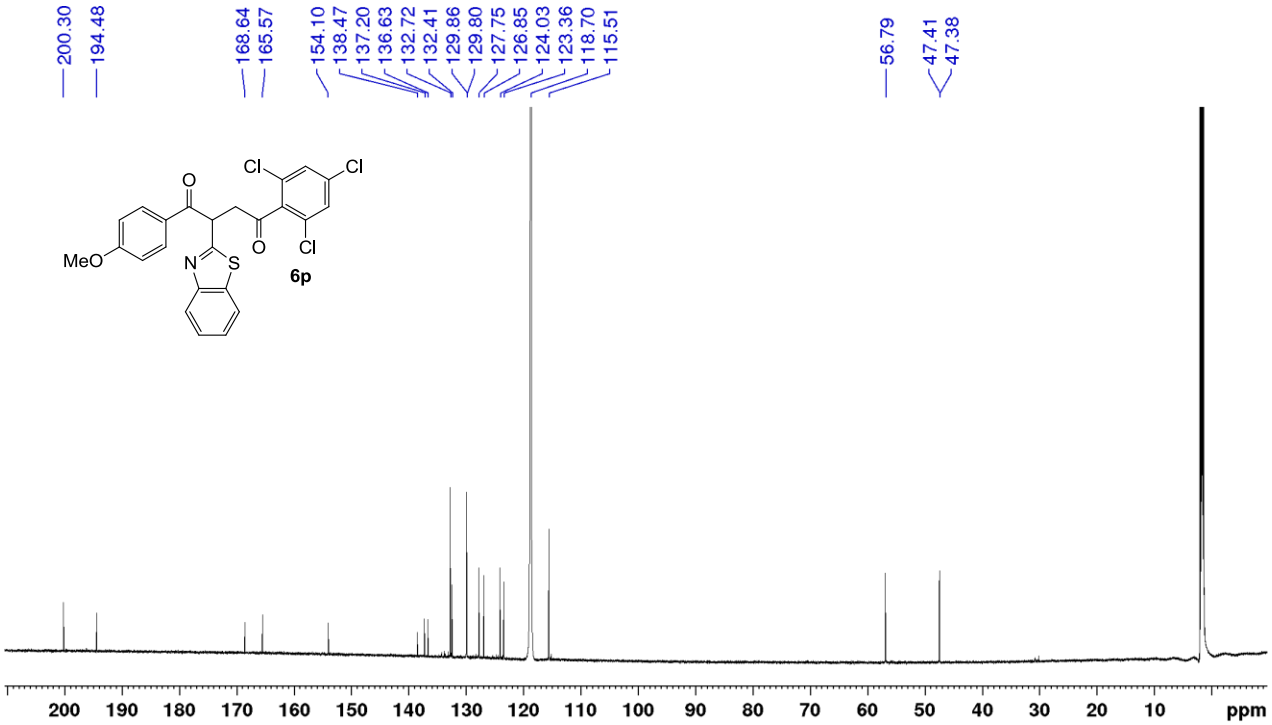
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (6o)



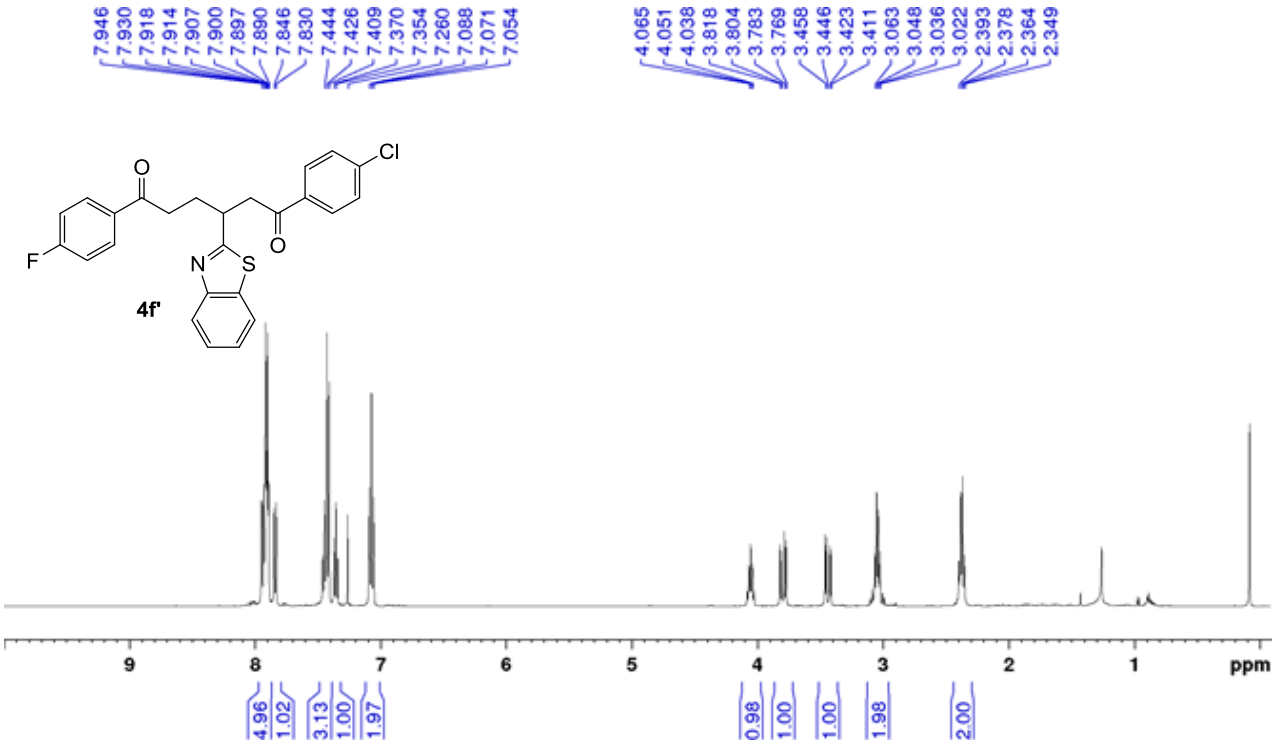
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (6p)



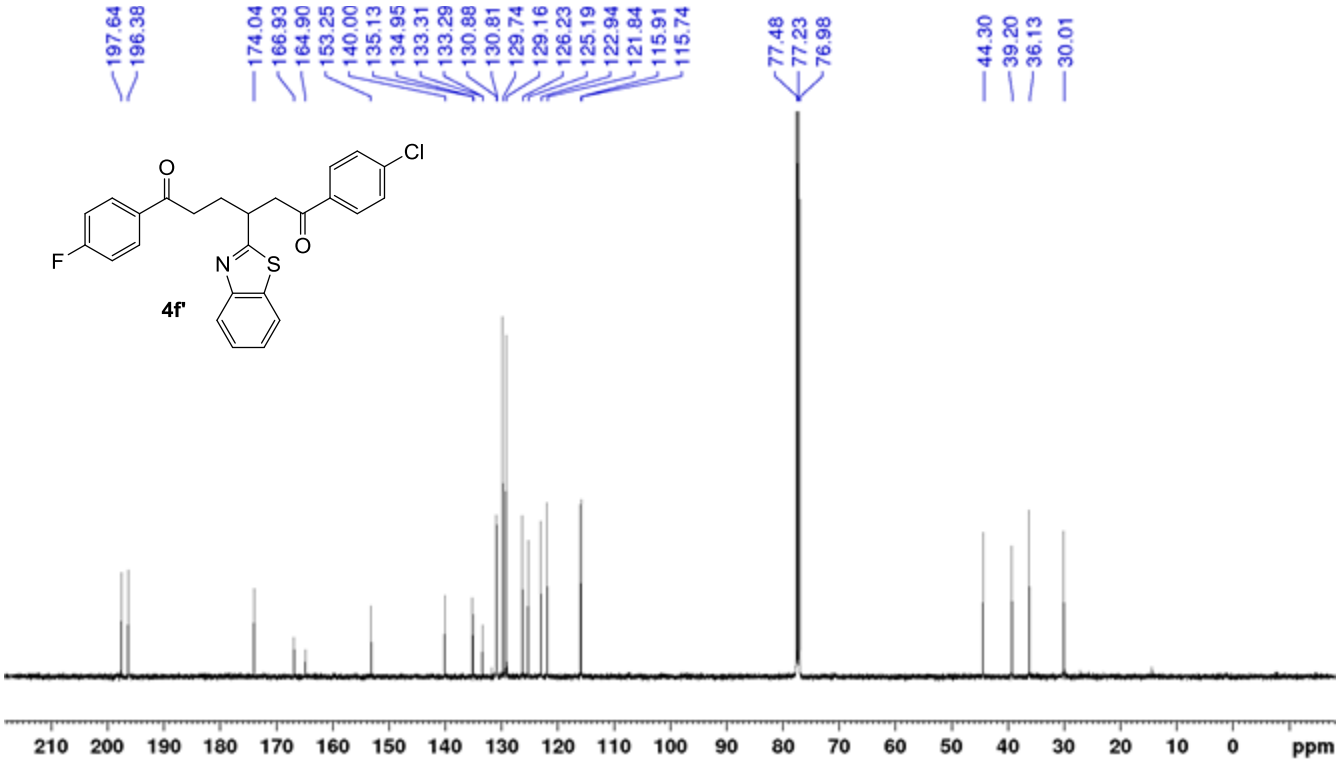
^{13}C NMR (175 MHz, CD_3CN, 25 ºC) of (6p)



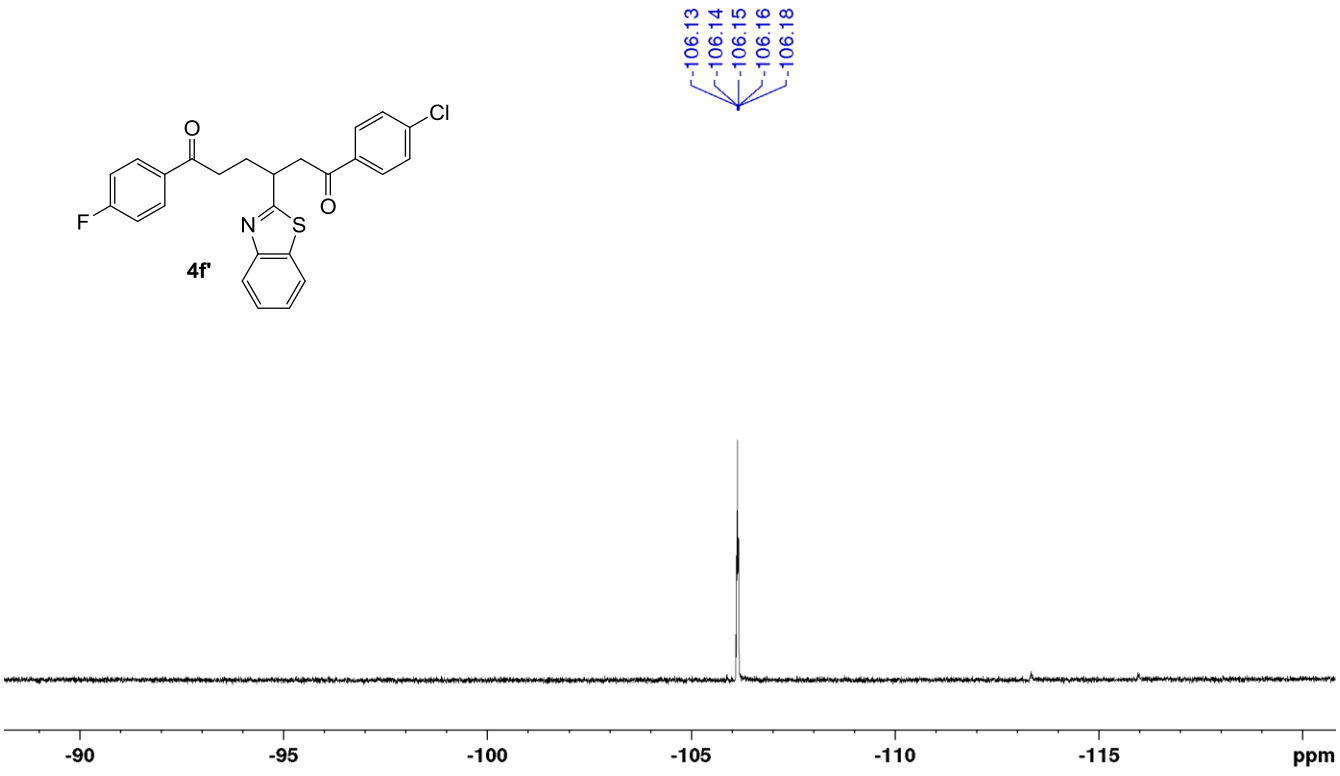
^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) of (4f')



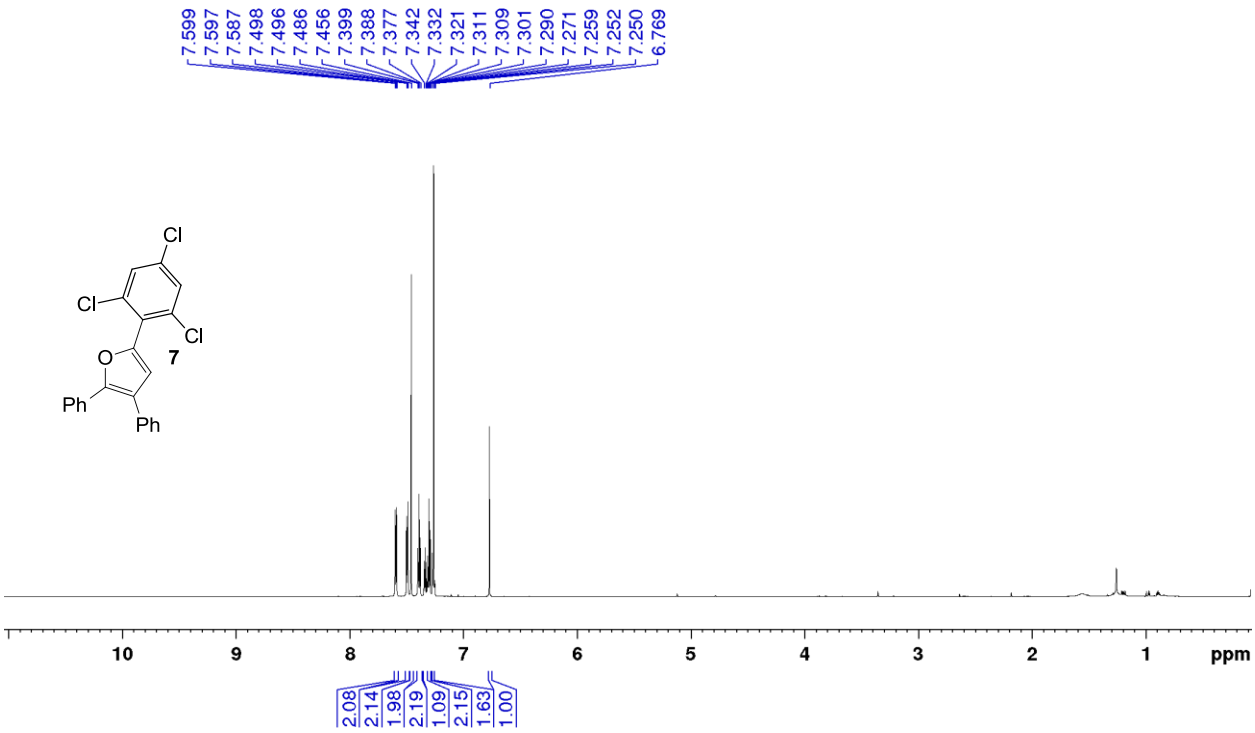
^{13}C NMR (125 MHz, $CDCl_3$, 25 °C) of (4f')



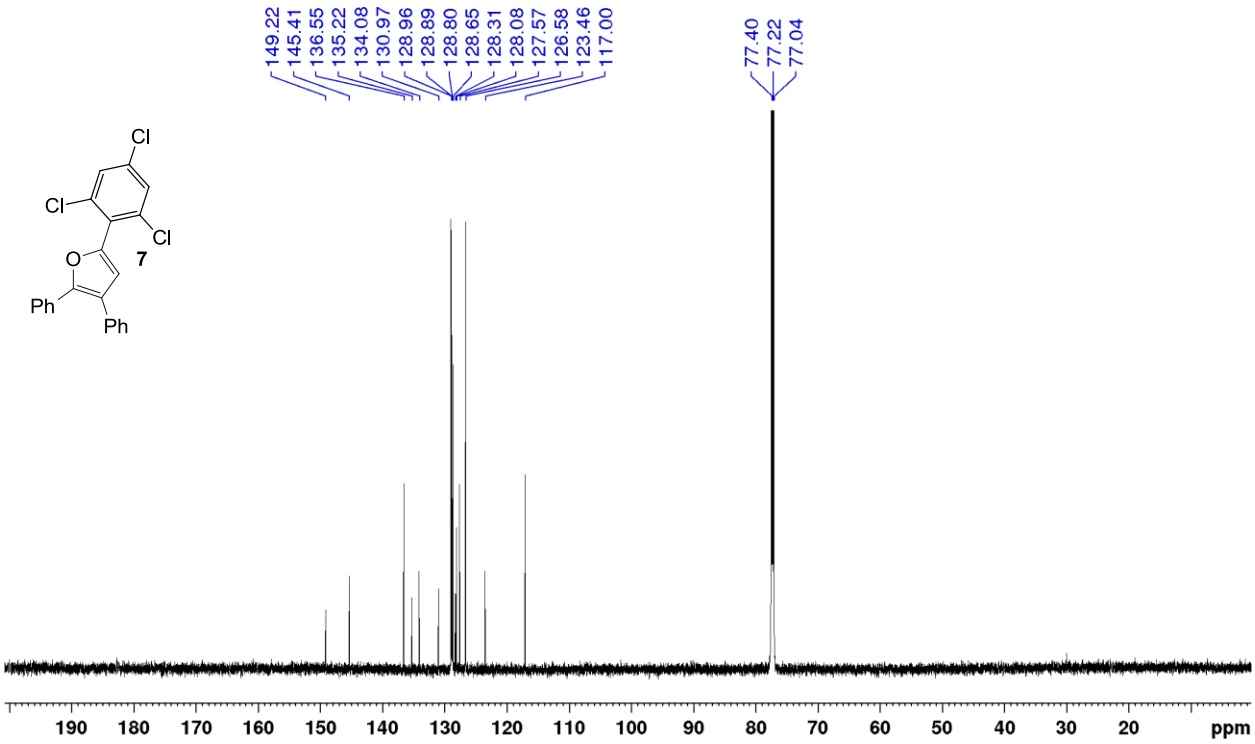
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (4f')



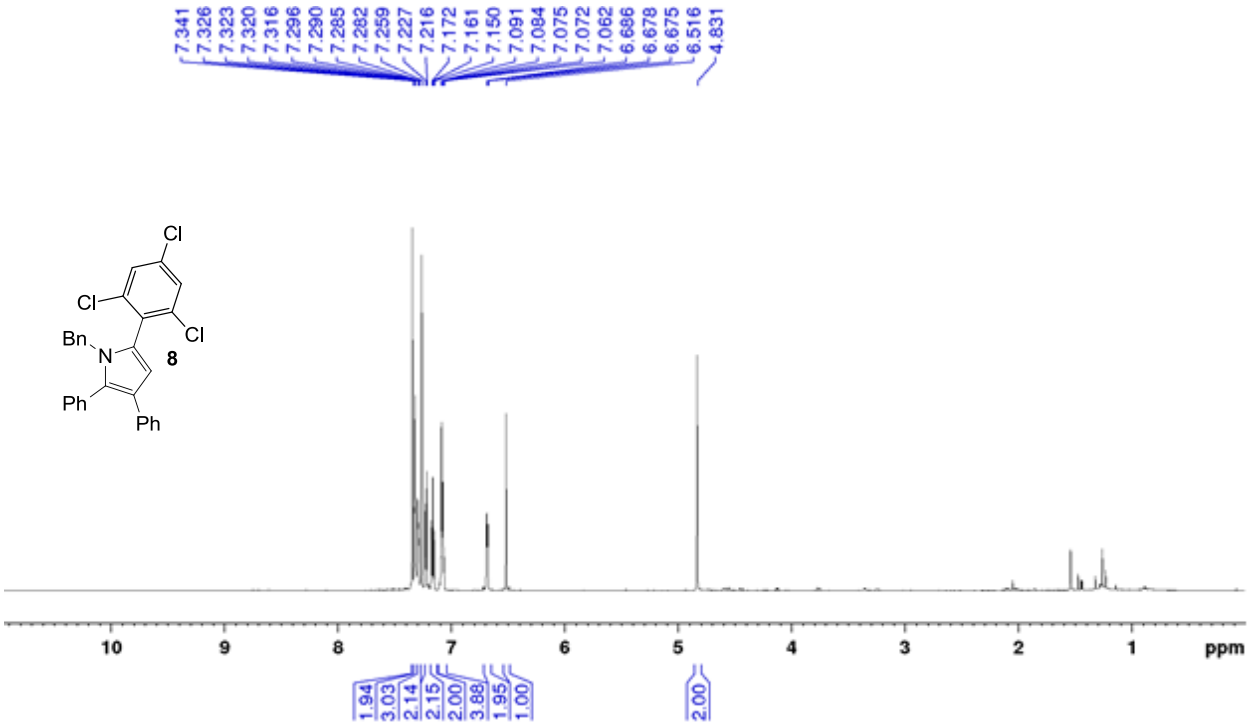
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (7)



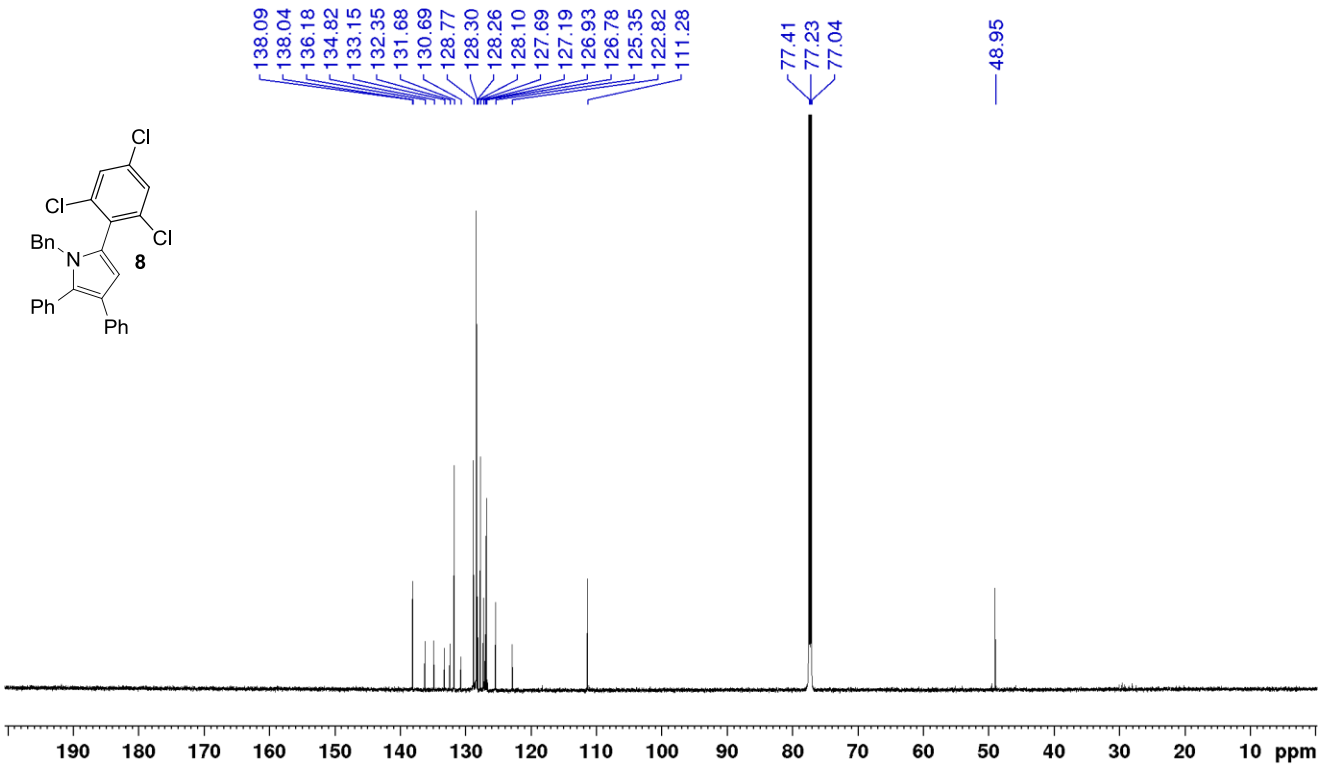
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (7)



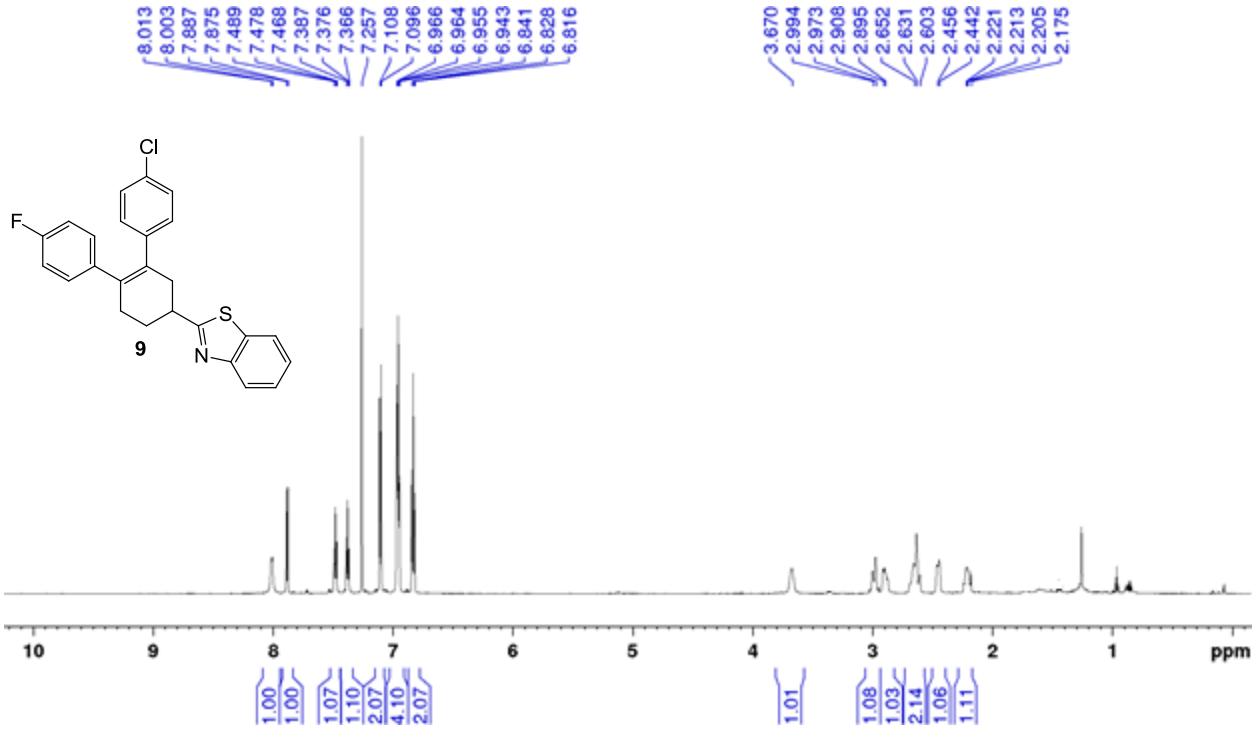
^{1}H NMR (700 MHz, $CDCl_3$, 25 °C) of (8)



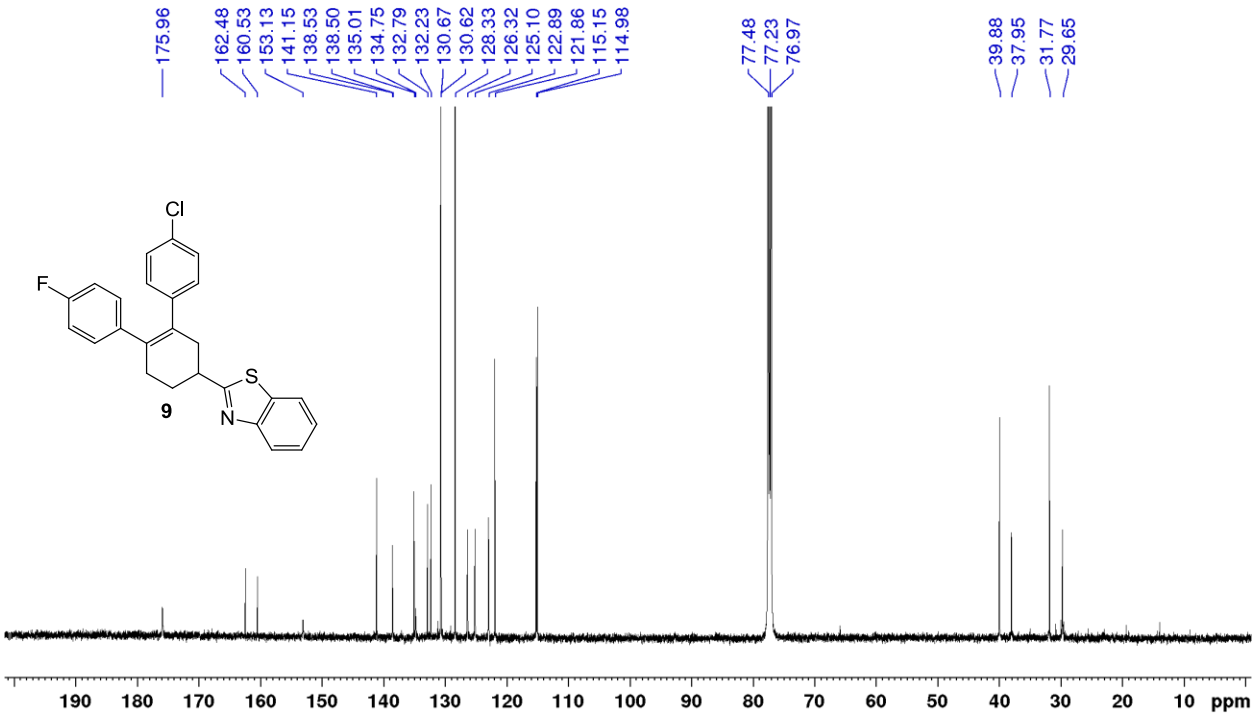
^{13}C NMR (175 MHz, $CDCl_3$, 25 °C) of (8)



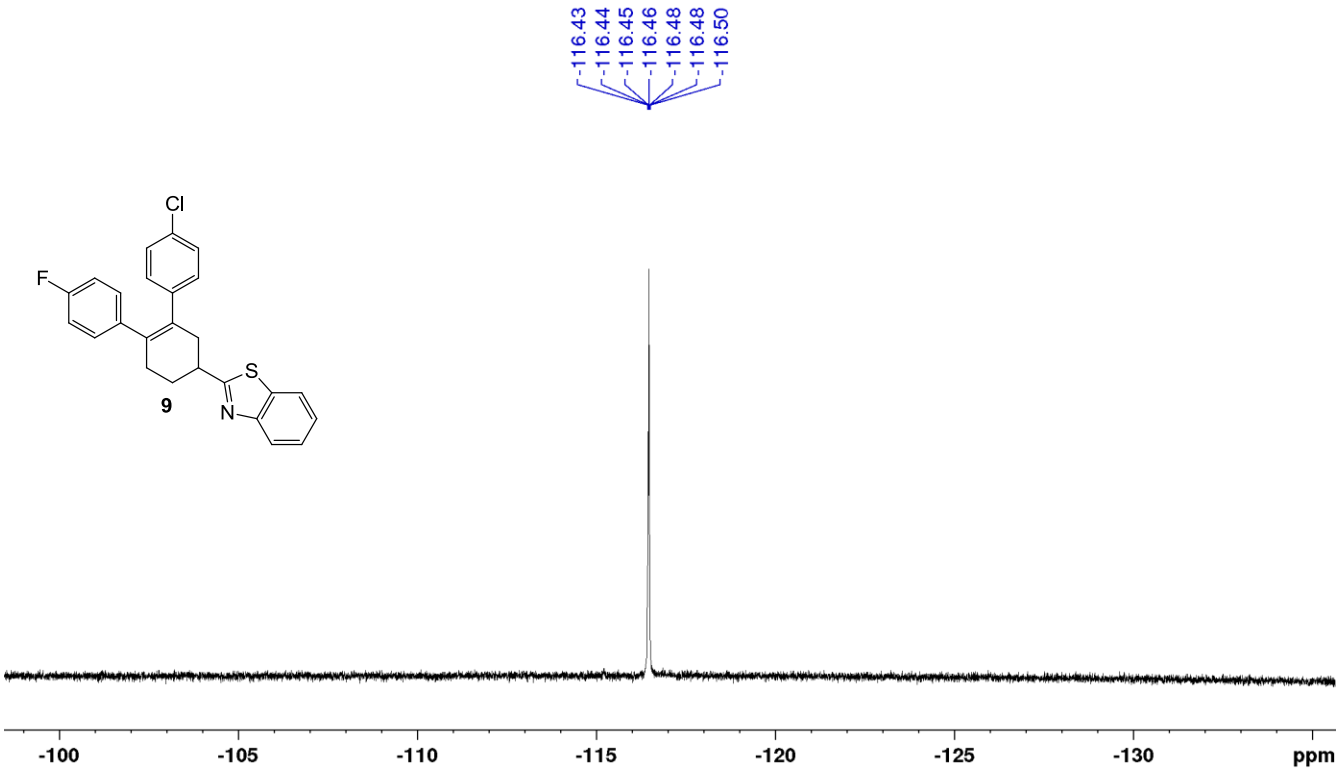
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (9)



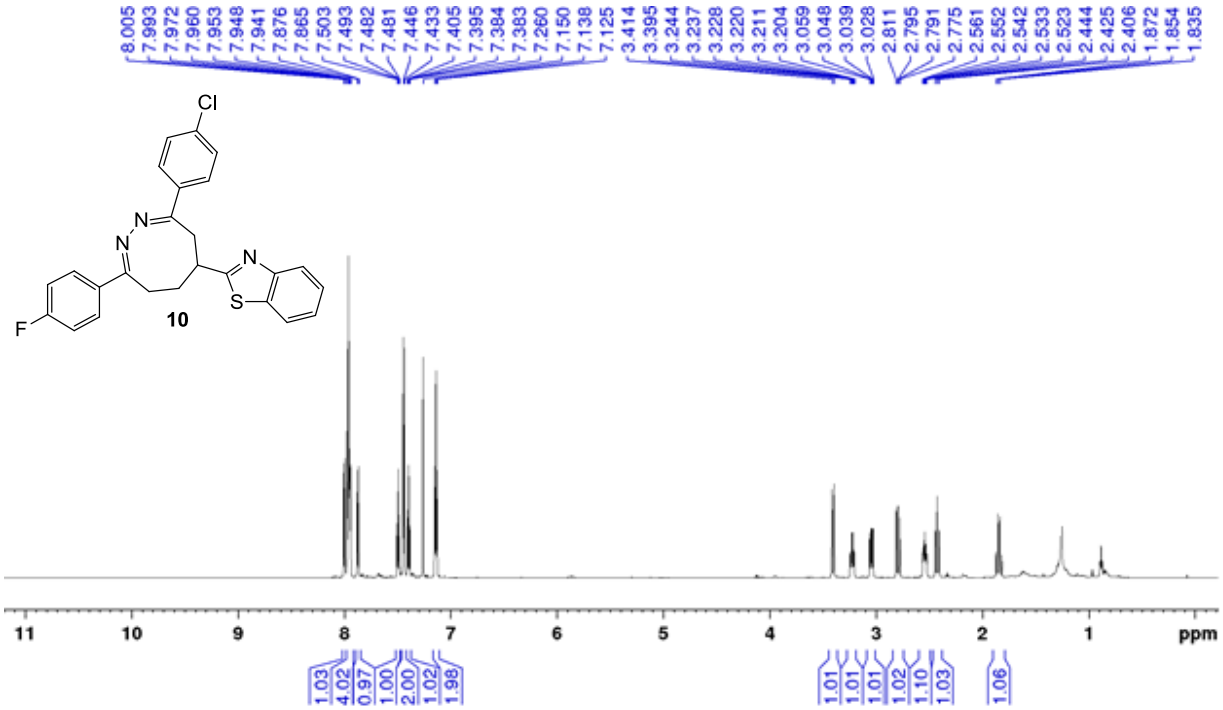
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (9)



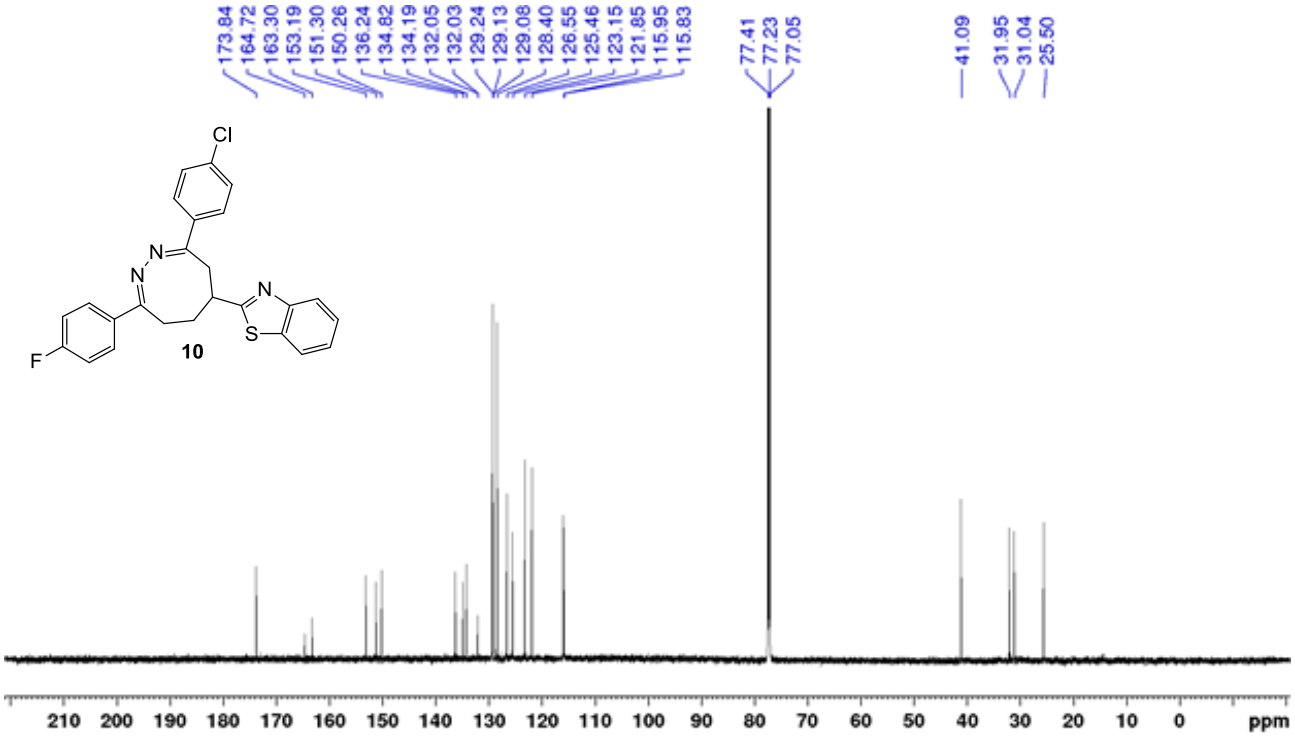
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (9)



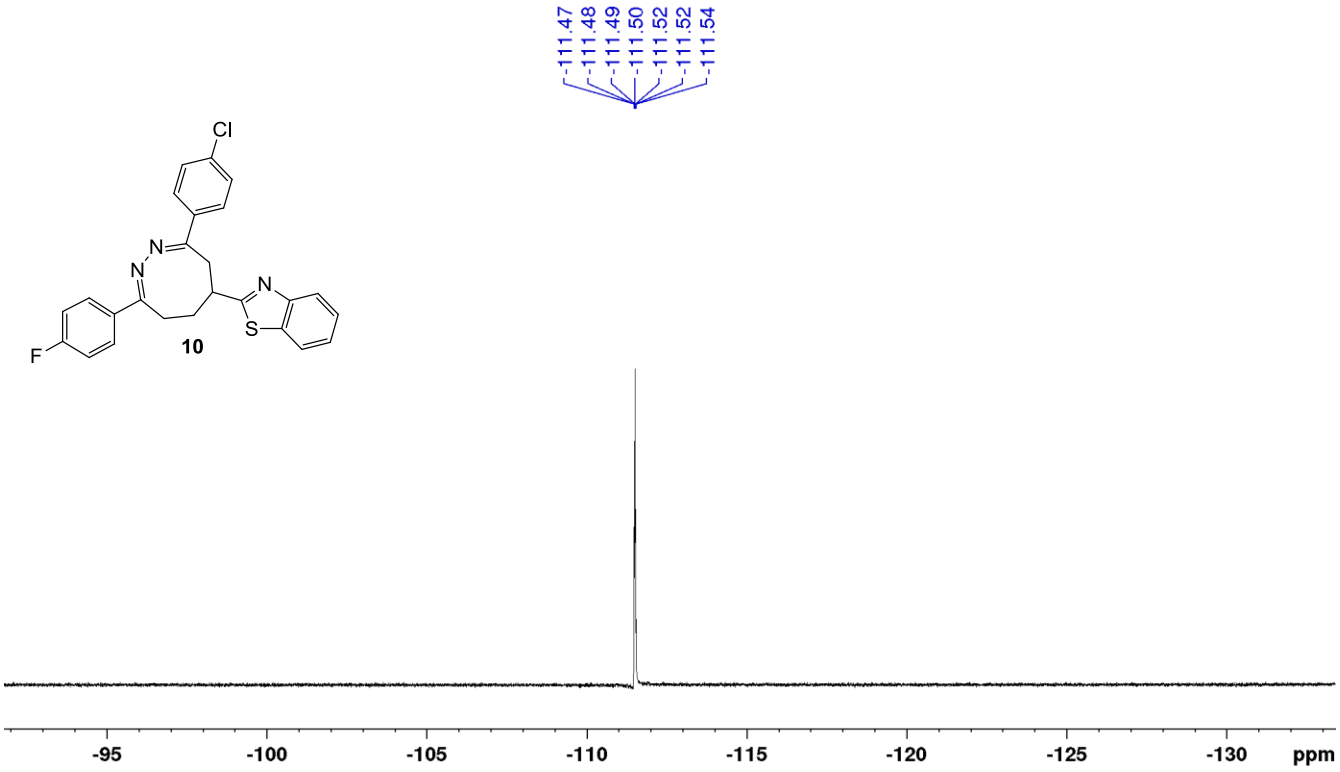
^{1}H NMR (700 MHz, $CDCl_3$, 25 ºC) of (10)



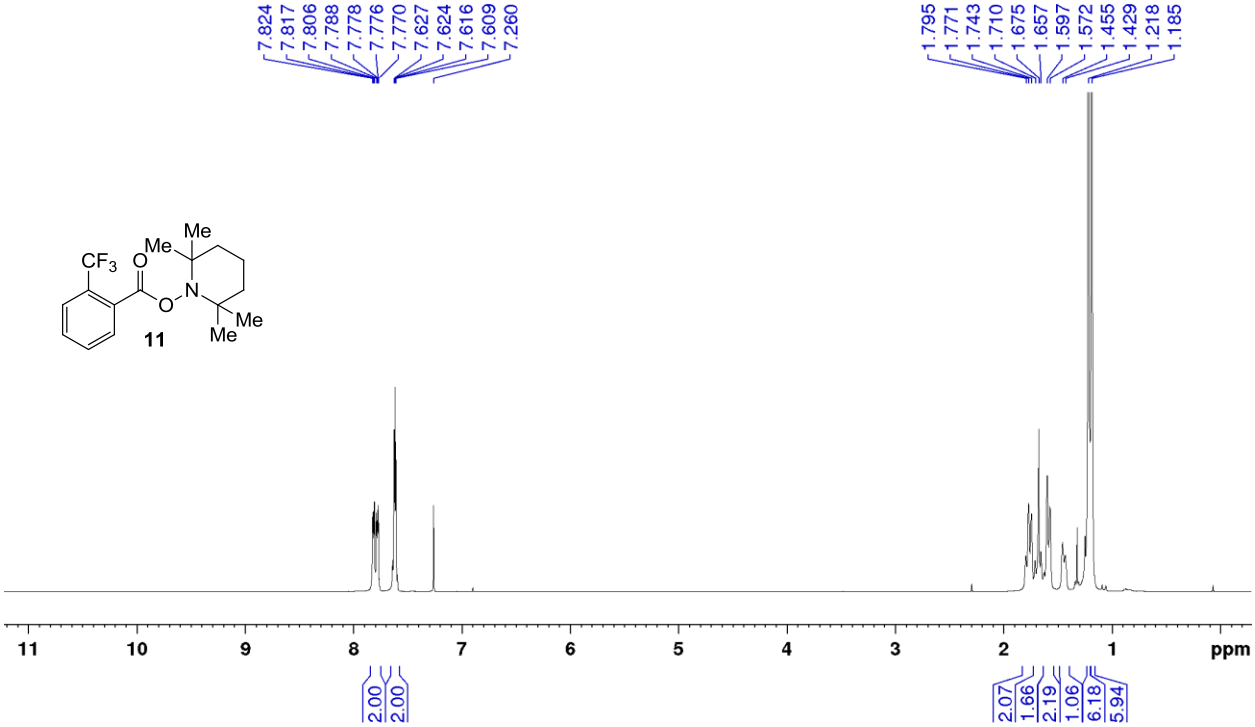
^{13}C NMR (175 MHz, $CDCl_3$, 25 ºC) of (10)



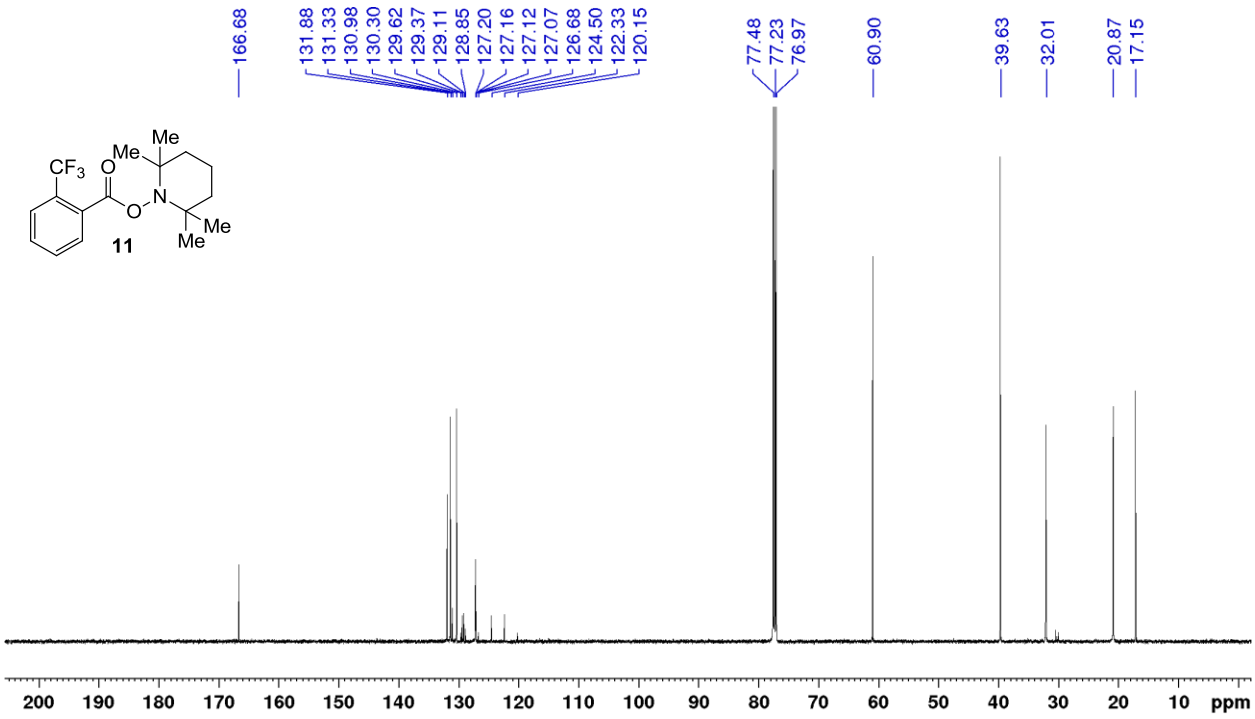
^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (10)



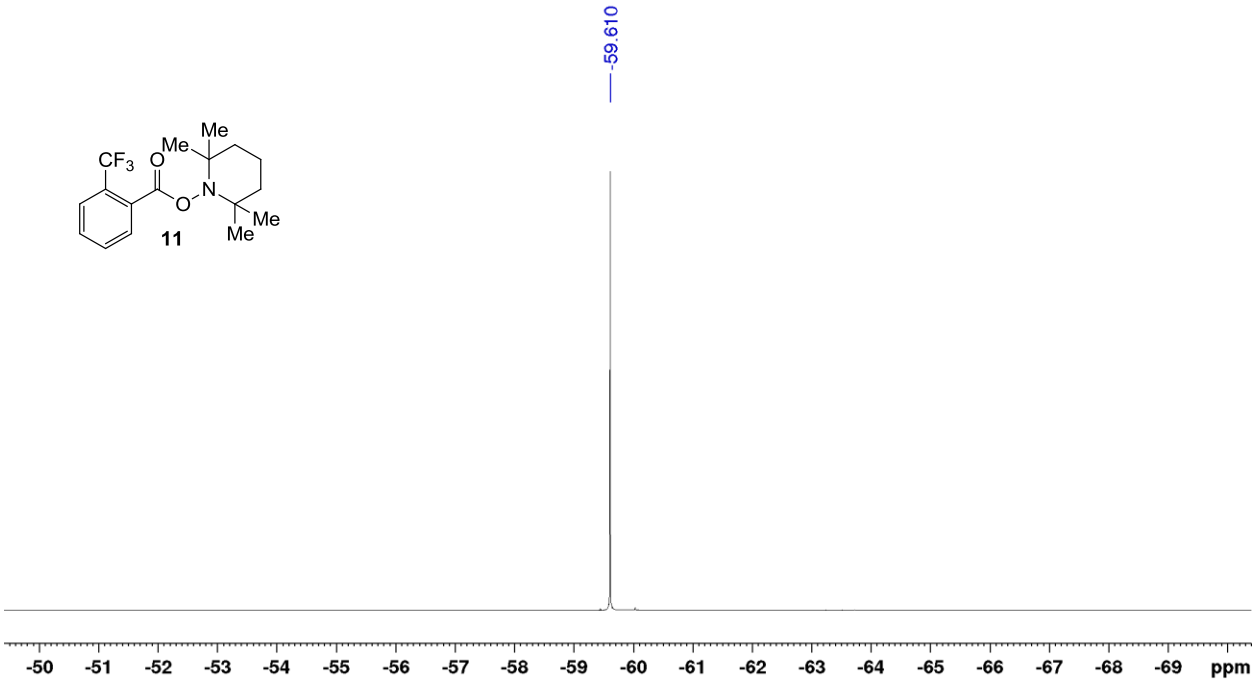
^{1}H NMR (500 MHz, $CDCl_3$, 25 ºC) of (11)



^{13}C NMR (125 MHz, $CDCl_3$, 25 ºC) of (11)



^{19}F NMR (376 MHz, $CDCl_3$, 25 ºC) of (11)



Cartesian Coordinates

For each species, the following are provided:

UMN15/def2-TZVP//UMN15/def2-SVP + SMD electronic energies

UMN15/def2-SVP + SMD Gibbs free energy correction (298 K, 1 M)

UMN15/def2-SVP + SMD stationary point Cartesian coordinates.

*Stationary Points for Shift of Radical **5a***

5a (extended conformation)

E(UMN15) = -2868.19176498

Thermal correction to Gibbs Energy= 0.257942

C,0,1.7446552191,-0.2305187585,0.8184355721

C,0,0.6516127647,-1.133234993,0.3199212887

H,0,0.8581209539,-2.1707003121,0.0595687384

C,0,-0.7478506697,-0.6630631257,0.409443726

H,0,-0.9735813633,0.1373376297,-0.3288443753

H,0,-0.9449856156,-0.1912691093,1.3926948267

C,0,-1.7817845593,-1.7363783265,0.1937592547

O,0,1.5257948419,0.0728486933,2.1757207381

H,0,1.4690400054,1.0489636769,2.2354836134

O,0,-1.5201976386,-2.8837170657,-0.0857598135

C,0,3.133703298,-0.8347916065,0.6011552889

C,0,4.1282231451,-0.6409704799,1.5643566794

C,0,3.4391290369,-1.5408274475,-0.5697908316

C,0,5.4131388912,-1.1502515545,1.3620620045

H,0,3.8781920731,-0.0976798585,2.4768059891

C,0,4.7246209936,-2.0459516511,-0.773385183

H,0,2.6697029555,-1.6979824669,-1.3317078566

C,0,5.7151303563,-1.8528512809,0.1932650644

H,0,6.1818224257,-0.9981785577,2.1231164089

H,0,4.9512415969,-2.5960891104,-1.6891891933

C,0,-3.21749441,-1.2821343772,0.3433269149

C,0,-3.9494707619,-0.822055404,-0.7546629807
C,0,-3.8538152703,-1.3136655865,1.5872624902
C,0,-5.2783758123,-0.4199401904,-0.6362897124
C,0,-5.1811465512,-0.9206112447,1.7450319719
C,0,-5.880289327,-0.4795649103,0.6210575205
H,0,-5.830979395,-0.0660558914,-1.506573789
H,0,-5.6583501337,-0.9566854766,2.7242711713
C,0,1.6718576472,1.0937394083,0.0584341993
S,0,1.7089877419,1.1755406044,-1.6753927781
C,0,1.4761833943,3.2798709113,-0.2069978847
C,0,1.5515729212,2.9017904269,-1.5667362707
N,0,1.5425047316,2.2170916304,0.6812680287
C,0,1.3440225389,4.6344782762,0.1337718873
C,0,1.2907168328,5.5778001669,-0.8853406307
H,0,1.2863680425,4.9216021481,1.1850328874
C,0,1.498483654,3.8505231511,-2.5938532267
C,0,1.3670773863,5.1891991239,-2.2363026014
H,0,1.1882732302,6.6358999006,-0.6368769748
H,0,1.5578878609,3.5507508657,-3.64133437
H,0,1.3227309867,5.9497579178,-3.0183328375
Cl,0,-2.9548795803,-1.8467390551,2.9648357837
Cl,0,-3.1691055997,-0.7376520022,-2.2954321816
Cl,0,-7.5251575728,0.0102549858,0.7911826887
H,0,6.7196501751,-2.2515189339,0.0359089841

5a (folded conformation)
E(UMN15) = -2868.20448080
Thermal correction to Gibbs Energy= 0.266607
C,0,-2.433207208,-0.250170979,-1.0205203238
C,0,-1.9454268022,-1.6337021356,-0.6687891856
H,0,-2.4448390347,-2.2146020823,0.1064921344
C,0,-0.8794643909,-2.2670139245,-1.4931727911
H,0,-0.4760592289,-1.5363887468,-2.2116147247
H,0,-1.2565099618,-3.1466476411,-2.0413645022

C,0,0.2319570178,-2.7502849628,-0.5867821605
O,0,-2.7465166164,-0.1961569237,-2.3914626915
H,0,-1.9750771257,0.2099526774,-2.833912001
O,0,0.4050683085,-3.9177798047,-0.3181654701
C,0,-3.6260800049,0.1648905216,-0.17068137
C,0,-4.6894293853,0.8617936949,-0.7517156879
C,0,-3.6506600016,-0.1107504225,1.2040186743
C,0,-5.7680828178,1.2775332459,0.0324219376
H,0,-4.6613467408,1.0658547347,-1.8227216078
C,0,-4.725526997,0.3137070158,1.9873952099
H,0,-2.8205237395,-0.6517951075,1.6688716341
C,0,-5.7885809064,1.0064613836,1.4025730113
H,0,-6.5975851383,1.8166342251,-0.4306319049
H,0,-4.7335825603,0.0964795009,3.0575663278
C,0,1.1240429382,-1.7059690432,0.0594684787
C,0,1.0386125271,-1.4317327894,1.430471733
C,0,2.1587146394,-1.0892575638,-0.653791756
C,0,1.9481156459,-0.5984622712,2.0773912052
C,0,3.0982698581,-0.2631040335,-0.0389315648
C,0,2.983072163,-0.0348679665,1.330900323
H,0,1.850710141,-0.3950118008,3.1437949206
H,0,3.8966485491,0.1972020597,-0.6214094626
C,0,-1.2591183702,0.6982764123,-0.7964924601
S,0,-0.8593395023,1.3881807426,0.7452505309
C,0,0.6047340496,1.7564673552,-1.343674701
C,0,0.5550378901,2.0921342157,0.0285172051
N,0,-0.4494678684,0.9669192587,-1.7703856577
C,0,1.6775385423,2.1981667553,-2.1326492662
C,0,2.6733756774,2.9619986817,-1.5350836329
H,0,1.7175537719,1.9239642448,-3.1881163963
C,0,1.5491242601,2.8736950798,0.6270243452
C,0,2.6083022136,3.2984416519,-0.1691083896
H,0,3.5194588799,3.3081683242,-2.1320524067
H,0,1.5090140586,3.1217145602,1.6891998927

H,0,3.4065316056,3.8950424491,0.2767590965
Cl,0,2.2947425645,-1.3721389326,-2.3549435332
Cl,0,-0.257946218,-2.1124581487,2.3511187676
Cl,0,4.1334348541,0.9805080476,2.1188487367
H,0,-6.6325345363,1.3325624416,2.0141994833

5a (TS1)

E(UMN15) = -2868.18487200

Thermal correction to Gibbs Energy= 0.265403

C,0,2.1814461541,-1.0590743219,0.9394924845
C,0,1.018103019,-1.2991113131,0.0442327592
H,0,1.2165543888,-1.5230360146,-1.0040688985
C,0,-0.3654997117,-1.4669312628,0.5664010155
H,0,-0.5025598383,-0.82231435,1.4518993002
H,0,-0.5681520487,-2.5084391862,0.867746771
C,0,-1.3999693496,-1.0699742992,-0.4613483426
O,0,1.9300279018,-1.2324180543,2.2916172237
H,0,1.5334973093,-0.3932140895,2.605038237
O,0,-2.3064903303,-1.793747592,-0.8034945389
C,0,3.5364785382,-1.5754153369,0.5138104449
C,0,4.498372651,-1.826571165,1.4990078097
C,0,3.8687455449,-1.7801675125,-0.8330381683
C,0,5.772967388,-2.2730980551,1.1450249758
H,0,4.2308497261,-1.6730989488,2.5449329702
C,0,5.1462195004,-2.2202334161,-1.1851312869
H,0,3.1408316268,-1.5949798709,-1.6275570543
C,0,6.1020231597,-2.4697721718,-0.197848731
H,0,6.5124682921,-2.4688973822,1.9246220772
H,0,5.3912870926,-2.3731501982,-2.238173696
C,0,-1.2739891142,0.3129293472,-1.0787298938
C,0,-0.7453143007,0.500302572,-2.3614594191
C,0,-1.7970966093,1.4363158743,-0.429596866
C,0,-0.7281375014,1.7482771695,-2.9801973528
C,0,-1.8170535524,2.6967500126,-1.0237840371

C,0,-1.277602435,2.8355865298,-2.3011391451
H,0,-0.3019468615,1.8660424137,-3.9764625451
H,0,-2.2359648634,3.5522472617,-0.4940049747
C,0,1.8304697895,0.3448168246,0.5043410293
S,0,2.4894953046,1.1895049232,-0.8971941221
C,0,1.0187500393,2.3852390793,0.871655061
C,0,1.6733003146,2.6293106188,-0.3666469578
N,0,1.1338019376,1.1079064491,1.3444291074
C,0,0.3252860691,3.4372875679,1.5016499116
C,0,0.287587066,4.6827235034,0.8873958482
H,0,-0.1792324059,3.2487098893,2.4507179127
C,0,1.6320280993,3.8819042932,-0.9823327515
C,0,0.9312799532,4.9049192446,-0.3449070093
H,0,-0.2520127281,5.5030789147,1.3652680436
H,0,2.1274795554,4.0542548277,-1.9396595033
H,0,0.8787042344,5.8900765922,-0.8120368895
Cl,0,-2.4456261024,1.2571851597,1.1637071748
Cl,0,-0.0882216855,-0.8543205582,-3.2162618061
Cl,0,-1.2843693002,4.3854388669,-3.058043666
H,0,7.0989867529,-2.8186091861,-0.4750938717

5a (cyclic intermediate)
E(UMN15) = -2868.19726531
Thermal correction to Gibbs Energy= 0.266597
C,0,-2.5609394155,-0.1966676812,-0.9363265538
C,0,-1.5994559246,-1.2001680714,-0.3840729506
H,0,-1.8196586104,-1.5452392894,0.6295430495
C,0,-0.9263355845,-2.21484902,-1.2741199139
H,0,-0.6500530804,-1.7328765871,-2.2261650944
H,0,-1.5873504634,-3.065598155,-1.4911727065
C,0,0.3434577266,-2.7620755135,-0.6653674177
O,0,-2.7084770738,-0.1373194542,-2.3056429083
H,0,-1.8717116499,0.2243275238,-2.662610571

O,0,0.5965850153,-3.9447914915,-0.6224533165
C,0,-3.7725174336,0.2205701837,-0.167815325
C,0,-4.8148336522,0.8638760566,-0.8493386012
C,0,-3.896606077,0.0098718001,1.2147793803
C,0,-5.9544634489,1.289645782,-0.1647109149
H,0,-4.7199583503,1.0206812244,-1.924216728
C,0,-5.0336886364,0.4419807616,1.8980250806
H,0,-3.1056152965,-0.4916392115,1.7793939662
C,0,-6.0683652138,1.0827789629,1.2115469491
H,0,-6.7585603451,1.7863197023,-0.7123039787
H,0,-5.1116320156,0.2714544376,2.9738153946
C,0,1.3422131632,-1.7659548913,-0.0999863222
C,0,1.4001075665,-1.4903268467,1.2705025929
C,0,2.2911512811,-1.1485157599,-0.9208490301
C,0,2.3525943245,-0.630394619,1.8141027099
C,0,3.2687072553,-0.2950699736,-0.4134673966
C,0,3.2832309918,-0.0428154618,0.9577824155
H,0,2.3656359174,-0.4244221833,2.8843795197
H,0,3.9930865436,0.1751800946,-1.0785039765
C,0,-1.1498958669,0.2604285658,-0.4493129499
S,0,-0.8427400206,1.1861318454,1.0652374132
C,0,0.5704488386,1.5774235908,-1.0901228116
C,0,0.47938344,1.9870977875,0.2828200163
N,0,-0.3114815017,0.6525028207,-1.485173362
C,0,1.5830830802,2.141750039,-1.9117910693
C,0,2.4691725638,3.050437617,-1.3609871582
H,0,1.6530320687,1.8222769561,-2.9530312489
C,0,1.3727890155,2.910512699,0.8224859195
C,0,2.3697851948,3.4316982942,-0.004819662
H,0,3.259829461,3.4792481345,-1.9798025774
H,0,1.3022365749,3.2125804887,1.8688245338
H,0,3.0859761547,4.1454567873,0.4061464447
Cl,0,2.230975892,-1.4241042599,-2.6265718035
Cl,0,0.2448117143,-2.2265901096,2.3283246238

Cl,0,4.4744202592,1.0233377386,1.605850043
H,0,-6.9592033817,1.4165626858,1.7476832961

5a (TS2)

E(UMN15) = -2868.19465920
Thermal correction to Gibbs Energy= 0.263891
C,0,2.5183065746,0.5784338728,-0.8782752005
C,0,1.5129923019,1.3639383937,-0.1173575914
H,0,1.8017684737,1.5888342116,0.9137712696
C,0,0.7684212562,2.4877706792,-0.8121783375
H,0,0.507157611,2.163409339,-1.8324804742
H,0,1.3906843085,3.3903638197,-0.8812182306
C,0,-0.5264439035,2.8702151256,-0.1321777686
O,0,2.4884714372,0.6365566728,-2.2364675959
H,0,1.5887593785,0.3463716297,-2.5139875055
O,0,-0.8114105978,4.0162881391,0.1325800029
C,0,3.7446394969,0.0316770695,-0.2805485016
C,0,4.6860910986,-0.5928767649,-1.119274143
C,0,4.0042980606,0.0885223681,1.1021498653
C,0,5.8530720337,-1.1412107664,-0.5907884717
H,0,4.4867236586,-0.6347998306,-2.1905365561
C,0,5.1699962714,-0.4674512238,1.6259766895
H,0,3.2978109343,0.5655546232,1.7856958716
C,0,6.1004875598,-1.0834859646,0.7838412199
H,0,6.5751113413,-1.6181850449,-1.2571295476
H,0,5.3542510053,-0.4150869135,2.7009916152
C,0,-1.5043330729,1.7569624185,0.1977450281
C,0,-1.5692598839,1.2135794643,1.4836164074
C,0,-2.391099813,1.2556609273,-0.7608703276
C,0,-2.4658242858,0.1987025263,1.815620077
C,0,-3.3140946853,0.2564555452,-0.4631560375
C,0,-3.3326500883,-0.26906621,0.828932408
H,0,-2.4801776704,-0.2208955437,2.8215910084

H,0,-3.9878862444,-0.1224550841,-1.2315839509
C,0,0.980972295,-0.0343346485,-0.2829382328
S,0,0.8654095426,-1.1810489439,1.0667989443
C,0,-0.5149416634,-1.4799188109,-1.1119740628
C,0,-0.3011190557,-2.0925625792,0.1575471096
N,0,0.1936578352,-0.3464103545,-1.3392611026
C,0,-1.4580075434,-2.0455377689,-1.9983197622
C,0,-2.1623034177,-3.17448106,-1.6048264109
H,0,-1.6324842875,-1.5627216838,-2.9621338708
C,0,-1.0006534128,-3.2374474663,0.5407036922
C,0,-1.9362798766,-3.7689239096,-0.3476953324
H,0,-2.9044945389,-3.6094954997,-2.2773229292
H,0,-0.8301828475,-3.6984220948,1.5153110797
H,0,-2.5055750545,-4.6547983281,-0.0599482636
Cl,0,-2.308770945,1.8588760024,-2.3788728866
Cl,0,-0.4710647013,1.7911728539,2.6906504395
Cl,0,-4.443681723,-1.5335090684,1.2067115373
H,0,7.0140698377,-1.5150331189,1.1978448288

5a (shifted product)
E(UMN15) = -2868.22516075
Thermal correction to Gibbs Energy= 0.264966
C,0,-2.9550284573,-0.0303979943,-0.8153622248
C,0,-1.7042724221,-0.4187866556,-0.0723929602
H,0,-1.9197864943,-0.5580845591,0.9943064366
C,0,-1.158603733,-1.7363082036,-0.685222328
H,0,-0.878127589,-1.5171786093,-1.7300165161
H,0,-1.9527290627,-2.4957296707,-0.6972752067
C,0,0.0422090891,-2.3746190817,-0.0244357912
O,0,-2.7787643121,0.3124324379,-2.1066679522
H,0,-1.8313720719,0.5379212102,-2.2590758888
O,0,0.0722308757,-3.5596798345,0.2254412816
C,0,-4.2798482007,-0.1114988002,-0.3118309491

C,0,-5.374897823,0.2370578633,-1.1556089169
C,0,-4.5815534764,-0.5408024321,1.0122316754
C,0,-6.6823233681,0.1624775382,-0.695519446
H,0,-5.164894601,0.5666532104,-2.1739313638
C,0,-5.8956193897,-0.6094116587,1.456468076
H,0,-3.7790147411,-0.8242024321,1.695802701
C,0,-6.9598449142,-0.260051986,0.6128143658
H,0,-7.5024749801,0.4369446441,-1.3635188138
H,0,-6.0970276597,-0.9420709791,2.4774824199
C,0,1.2466556164,-1.521011821,0.3289644478
C,0,1.5005260079,-1.1849807898,1.6633173063
C,0,2.1631425566,-1.0779155227,-0.6320984906
C,0,2.6096633544,-0.4326590064,2.0423113293
C,0,3.279052111,-0.3138440132,-0.2931082794
C,0,3.4862776256,0.0030132705,1.0488881753
H,0,2.7665239264,-0.1643340512,3.0870237232
H,0,3.9633831234,0.0376999908,-1.0659836825
C,0,-0.6870123799,0.6804907408,-0.2357228307
S,0,-0.0934818593,1.6267682017,1.0872768106
C,0,0.8332935725,1.8899350986,-1.2989632279
C,0,1.0371395791,2.3812291442,0.0109635774
N,0,-0.1708246572,0.9435929307,-1.3985953347
C,0,1.6802424737,2.3008816402,-2.3394759695
C,0,2.714700362,3.181237841,-2.0466992398
H,0,1.5282408777,1.9042590454,-3.3447838574
C,0,2.07058043,3.2781405765,0.3040289505
C,0,2.9077968804,3.6647583081,-0.7377524505
H,0,3.3922880134,3.5012432616,-2.8406496259
H,0,2.2303186186,3.6423953122,1.3202375085
H,0,3.7328290359,4.3503706255,-0.5347815028
Cl,0,1.9037183234,-1.4692638334,-2.2944519604
Cl,0,0.3306675836,-1.6108533663,2.863991402
Cl,0,4.8372359446,0.9825820586,1.4835814384
H,0,-7.9898527887,-0.3172686496,0.9697581837

*Stationary Points for Shift of Radical **5b***

5b (extended conformation)

E(UMN15) = -2907.47203692

Thermal correction to Gibbs Energy= 0.288075

C,0,-3.2990234449,-1.7676255223,-0.3595908419
C,0,-2.2945652069,-2.9240896208,-0.0708563519
H,0,-2.8994087975,-3.8474009349,-0.0944242666
H,0,-1.8824928084,-2.8195876181,0.9451488694
C,0,-1.1983978661,-2.9615744575,-1.0721111954
H,0,-1.4233983838,-3.1880113733,-2.1140815194
C,0,0.1793315645,-2.5505501596,-0.7152395368
H,0,0.6433397647,-3.2184393514,0.0405070276
H,0,0.2066799945,-1.5526162897,-0.2222226696
C,0,1.1393118358,-2.4643661224,-1.8714860185
O,0,-3.8330599543,-1.9507628878,-1.6399590173
H,0,-3.3830817996,-1.303391491,-2.2196069889
O,0,0.8266078766,-2.6181101934,-3.030110895
C,0,-4.4187807508,-1.7113843823,0.6769997958
C,0,-4.1593763161,-1.8393252067,2.0496567833
C,0,-5.7365793104,-1.5020593353,0.254183332
C,0,-5.1980038181,-1.7522074422,2.9789479233
H,0,-3.1419676306,-2.0070925769,2.4122798335
C,0,-6.7757157498,-1.4195600123,1.1837235472
H,0,-5.9337072535,-1.4104862316,-0.8142485172
C,0,-6.5104388281,-1.5430729479,2.54918053
H,0,-4.9783990768,-1.8532920381,4.0439604815
H,0,-7.7990840947,-1.2580312216,0.8373586271
H,0,-7.3228535144,-1.4790175686,3.2762375252
C,0,2.5749956536,-2.1659136591,-1.4913630004
C,0,3.4735134852,-3.2031097497,-1.2251205189
C,0,3.0475863581,-0.8538570124,-1.4000062069
C,0,4.805244884,-2.9590684105,-0.8960082294

C,0,4.3724259998,-0.5697899708,-1.0735013673
C,0,5.2393656403,-1.634867833,-0.828465515
H,0,5.4879639778,-3.784563852,-0.6949893103
H,0,4.7192341435,0.4615571099,-1.0097287543
C,0,-2.5168571101,-0.4635100849,-0.3801741181
S,0,-1.8120594025,0.2539623621,1.0376047151
C,0,-1.4429910219,1.2307932948,-1.3164130454
C,0,-1.0785332786,1.4621904689,0.0288000022
N,0,-2.2514732607,0.1216538025,-1.5016616961
C,0,-0.9801538953,2.09320263,-2.3222070655
C,0,-0.1616537116,3.1578939963,-1.9644862946
H,0,-1.2636888322,1.9103556598,-3.3600031717
C,0,-0.2569228905,2.5352222961,0.3913587026
C,0,0.1977526168,3.3756478064,-0.6202886812
H,0,0.2104976391,3.8355698547,-2.7353102651
H,0,0.0206233857,2.7062240532,1.4326571958
H,0,0.8441830717,4.2180072454,-0.3662441126
Cl,0,1.9465286153,0.4485601417,-1.6859521771
Cl,0,2.9013280603,-4.8337823516,-1.2940527044
Cl,0,6.8839939508,-1.3067844319,-0.4246541488

5b (folded conformation)

E(UMN15) = -2907.47674692

Thermal correction to Gibbs Energy= 0.290924

C,0,2.4824532439,0.7161661622,-0.6164611168
C,0,2.2933409869,1.9865918278,0.2305999291
H,0,3.0504084446,2.7179591243,-0.1109759614
H,0,2.5161030231,1.76957284,1.2880791693
C,0,0.9114369293,2.5119086461,0.0932238471
H,0,0.5419714083,2.6969148866,-0.9157835287
C,0,0.0816796407,2.8851099323,1.2708014074
H,0,0.3229310129,3.8833714482,1.6828677043
H,0,0.2540367942,2.1571007843,2.0883471983
C,0,-1.4014451292,2.8691304681,0.9915326457

O,0,2.1841381599,1.0047085757,-1.9570662497
H,0,1.5150561134,0.3520429226,-2.2423585845
O,0,-2.1483419299,3.7731801701,1.2899997221
C,0,3.889644283,0.1156028451,-0.5079926004
C,0,4.8022411918,0.4600138623,0.494121914
C,0,4.2526177157,-0.8498107737,-1.4578453103
C,0,6.0603765854,-0.1504451209,0.5418119221
H,0,4.5511174699,1.2095796776,1.2466081196
C,0,5.5048992945,-1.4591459041,-1.4102032403
H,0,3.5366817714,-1.1154051676,-2.2395243639
C,0,6.4150979549,-1.1093953405,-0.4070573629
H,0,6.7659115282,0.1312365605,1.3265058215
H,0,5.773810409,-2.2089938556,-2.1574825456
H,0,7.3980286126,-1.5837298134,-0.3672284982
C,0,-1.9644865584,1.6347050875,0.3072447578
C,0,-2.2860875591,1.6492361224,-1.0550388345
C,0,-2.3016050107,0.488345847,1.0359840192
C,0,-2.9102021546,0.5719173004,-1.6800017542
C,0,-2.9465755712,-0.599802134,0.4499994415
C,0,-3.2478394294,-0.5402543468,-0.9097387408
H,0,-3.1469227529,0.6104561479,-2.7432514114
H,0,-3.203278672,-1.4770488357,1.045096505
C,0,1.5011664737,-0.344576647,-0.1500136078
S,0,1.292184164,-0.7333871797,1.529557802
C,0,0.0404722462,-1.9921580039,-0.3357722405
C,0,0.1704458437,-1.9750825465,1.0720504092
N,0,0.8096843082,-1.0417158653,-0.9901971591
C,0,-0.8148389908,-2.9238559259,-0.9414212614
C,0,-1.5252503497,-3.8047884152,-0.133993204
H,0,-0.9217266152,-2.9308553455,-2.0276449073
C,0,-0.5514596211,-2.8519284303,1.8877679966
C,0,-1.3974442354,-3.7679639055,1.2671666429
H,0,-2.2018607324,-4.5285914347,-0.5922822296
H,0,-0.4541726674,-2.8195435748,2.9741335216

H,0,-1.9699976879,-4.4681294786,1.87877589
Cl,0,-1.9493443373,0.4290697318,2.7303627276
Cl,0,-1.9185835243,3.0540255275,-1.9964700673
Cl,0,-4.0651660806,-1.862347453,-1.6587863332

5b (TS1)

E(UMN15) = -2907.45182173

Thermal correction to Gibbs Energy= 0.292130

C,0,-2.6464239617,-0.9130229817,-0.6907276906
C,0,-2.4088825284,-2.2023814306,0.0867677054
H,0,-2.8777676556,-3.093556583,-0.3573410092
H,0,-2.7409414617,-2.0999781705,1.1324824084
C,0,-0.9081526102,-2.1410604777,0.0136950742
H,0,-0.4996271346,-2.278210564,-0.9911776363
C,0,-0.0832714452,-2.5894364758,1.1765678636
H,0,-0.4076299557,-3.5881268062,1.5178273742
H,0,-0.2371343009,-1.8963381541,2.0272997185
C,0,1.3953636891,-2.6581812742,0.9020065474
O,0,-2.4514084183,-1.1536204923,-2.0605402436
H,0,-1.7810996164,-0.5037411432,-2.3574430382
O,0,2.0606251253,-3.6458706425,1.1180882654
C,0,-3.9284917588,-0.1390050281,-0.4489922969
C,0,-4.9744088945,-0.6334119789,0.3335358859
C,0,-4.0582853423,1.1198522582,-1.0536392276
C,0,-6.1401006263,0.1208586817,0.5098957062
H,0,-4.8923427424,-1.6153951072,0.8053929092
C,0,-5.2155933323,1.8744685566,-0.8744192236
H,0,-3.2364572081,1.5024142272,-1.6666416856
C,0,-6.2618568763,1.3742126838,-0.0901201033
H,0,-6.9548508085,-0.2765716446,1.1191255048
H,0,-5.3057432301,2.8555205063,-1.3460408806
H,0,-7.1705927439,1.9634314397,0.0508470677
C,0,2.0705094774,-1.4216769424,0.3398024755
C,0,2.4432244585,-1.3526071651,-1.0076769317

C,0,2.4761086213,-0.3759347861,1.1765897386
C,0,3.1972664743,-0.2958532481,-1.5124157322
C,0,3.2502250438,0.68571685,0.7126956059
C,0,3.607269505,0.7067119515,-0.6341172718
H,0,3.4713329366,-0.2645115934,-2.5668825347
H,0,3.5620152876,1.4812799314,1.3894710975
C,0,-1.3853899577,-0.1617709514,-0.2032500464
S,0,-1.3357952607,0.5226718576,1.4342080584
C,0,0.0390276255,1.5386878254,-0.5070532239
C,0,-0.1739518627,1.6897439633,0.891225569
N,0,-0.6771913692,0.5326631149,-1.0931260104
C,0,0.9005855676,2.4358299927,-1.1702119591
C,0,1.5274867705,3.4358881809,-0.4390773733
H,0,1.0616689443,2.3247338602,-2.2443722508
C,0,0.4826524286,2.6757057044,1.6307034896
C,0,1.3309859837,3.5493852729,0.9508263829
H,0,2.1971107403,4.1339391909,-0.9447224886
H,0,0.3245266027,2.7686872366,2.7065672148
H,0,1.8445265546,4.3375761262,1.5051010415
Cl,0,2.0360533186,-0.4107344345,2.8498600055
Cl,0,1.9684696238,-2.6223832918,-2.0830905551
Cl,0,4.5638343238,2.0098709547,-1.2335962964

5b (cyclic intermediate)

E(UMN15) = -2907.47464459

Thermal correction to Gibbs Energy= 0.293597

C,0,2.6743094733,1.0505298063,-0.7522495841
C,0,2.5124586391,2.3828082329,-0.0081800742
H,0,2.9549577276,3.263224491,-0.4911569562
H,0,2.8489739203,2.3137404398,1.0382175141
C,0,0.9863384707,2.1973565894,-0.0921867237
H,0,0.6358320862,2.5257684615,-1.0807240865
C,0,0.1374919705,2.7903583699,1.0225187805
H,0,0.3951897395,3.8503241721,1.1640051971

H,0,0.3492999194,2.2634217593,1.970341107
C,0,-1.3521169254,2.7298272862,0.8053137807
O,0,2.5385846721,1.2652797607,-2.1330454582
H,0,1.7830046735,0.7195209768,-2.4280923479
O,0,-2.0738640593,3.6926082941,0.9456049191
C,0,3.7882958641,0.0857948179,-0.4427365474
C,0,4.7567462638,0.3287620066,0.5358801331
C,0,3.82184924,-1.1242592074,-1.1523175429
C,0,5.7467568085,-0.6222102499,0.8015918459
H,0,4.7481279179,1.2676503972,1.0944150198
C,0,4.8012794043,-2.0785066783,-0.8800747681
H,0,3.071095107,-1.3100337605,-1.9257681446
C,0,5.7688478086,-1.8280890658,0.0988416112
H,0,6.5034892952,-0.4179548088,1.5623160098
H,0,4.8146132444,-3.0192089699,-1.4350957922
H,0,6.5402800675,-2.5718653308,0.310032814
C,0,-1.9733933154,1.4052233795,0.4025949227
C,0,-2.3778200336,1.1818172595,-0.9196885747
C,0,-2.2804236141,0.4203920734,1.3466854903
C,0,-3.0685111385,0.0340418696,-1.2982130906
C,0,-2.9659375722,-0.7452270779,1.0039505564
C,0,-3.3616852804,-0.9177788517,-0.3207864057
H,0,-3.3712595903,-0.1150210166,-2.3346640504
H,0,-3.1925124883,-1.4970981616,1.7601580526
C,0,1.2274069159,0.6580797371,-0.2143802737
S,0,1.2718306978,-0.1786472828,1.4179881769
C,0,0.1087911478,-1.2917837241,-0.6295212485
C,0,0.4097044586,-1.5199459681,0.7609692305
N,0,0.5041688337,-0.1258947486,-1.1352476894
C,0,-0.5803002734,-2.3059619154,-1.3568399723
C,0,-0.9675931572,-3.4606531407,-0.7063788307
H,0,-0.7983629147,-2.1355018162,-2.4126536129
C,0,0.0028265999,-2.6853597994,1.406531855
C,0,-0.6909210682,-3.6473966997,0.6679069485

H,0,-1.5058204123,-4.2369144152,-1.2529577859
H,0,0.2229546766,-2.8446193911,2.4633633511
H,0,-1.0167680874,-4.5657213515,1.1598616931
Cl,0,-1.8328043827,0.6585997505,2.9997906857
Cl,0,-2.0011132848,2.3630981051,-2.1249307052
Cl,0,-4.2275390457,-2.3415846044,-0.7630464293

5b (TS2)
E(UMN15) = -2907.46467386
Thermal correction to Gibbs Energy= 0.292420
C,0,-2.6364128757,-1.365570842,-0.8262365986
C,0,-2.1691081603,-2.6560898691,-0.1799704073
H,0,-2.5262838736,-3.5684323867,-0.6788576375
H,0,-2.4295886786,-2.6968741928,0.8878135386
C,0,-0.6839097663,-2.3180955012,-0.3525817414
H,0,-0.3843173583,-2.5294726944,-1.3896652678
C,0,0.2960478291,-2.9604284732,0.6289866787
H,0,0.1532379607,-4.0505691346,0.6376965031
H,0,0.1010669551,-2.5823073191,1.6482729343
C,0,1.7530401307,-2.7127006025,0.3132057682
O,0,-2.4936246839,-1.3783947861,-2.1900517904
H,0,-1.7632169955,-0.756222868,-2.4153100981
O,0,2.5463918176,-3.6133768756,0.1509760335
C,0,-3.6748338392,-0.4740167161,-0.2940122728
C,0,-4.229618564,-0.6336172354,0.9899373089
C,0,-4.0673346659,0.6368655411,-1.066582627
C,0,-5.1572547591,0.2846093281,1.478359036
H,0,-3.9416216465,-1.4834099023,1.6118413221
C,0,-4.986148209,1.5591246029,-0.5696107569
H,0,-3.6462042233,0.7607501091,-2.0659603733
C,0,-5.5364792296,1.3859015642,0.704169038
H,0,-5.5869521108,0.1411930331,2.47208731
H,0,-5.2791621953,2.4157339698,-1.1805453805
H,0,-6.2603396815,2.105580926,1.0923366066

C,0,2.2249606478,-1.2756292801,0.1890204903
C,0,2.5054626929,-0.7186457221,-1.0645709598
C,0,2.4626064043,-0.481083105,1.315867456
C,0,2.9833515802,0.5824212055,-1.2049007569
C,0,2.93422157,0.8267033261,1.2147610322
C,0,3.1863545448,1.345072224,-0.0548395609
H,0,3.1793926455,0.9969234037,-2.1938452363
H,0,3.1043808907,1.4252373489,2.1097118118
C,0,-0.8781490951,-0.7958177601,-0.2816570913
S,0,-0.8956743691,-0.0518186417,1.3401050064
C,0,-0.2898424111,1.3137047427,-0.7719836786
C,0,-0.4711155655,1.4697462638,0.632787442
N,0,-0.4607813917,0.0521016435,-1.2450995158
C,0,0.0923398208,2.4335618479,-1.5449501737
C,0,0.301604642,3.6497366521,-0.9142127891
H,0,0.2316812328,2.312225086,-2.6208363847
C,0,-0.2663484926,2.7002730538,1.2617690128
C,0,0.1281784204,3.7840524566,0.478876989
H,0,0.6114057775,4.51689832,-1.5008265365
H,0,-0.4030461979,2.8074756356,2.3392341579
H,0,0.3048594529,4.7515443976,0.9527836974
Cl,0,2.1841483935,-1.1450718902,2.8889149254
Cl,0,2.216499087,-1.6573104006,-2.4868116245
Cl,0,3.7626315429,2.9635335167,-0.2056698392

5b (shifted product)
E(UMN15) = -2907.49762382
Thermal correction to Gibbs Energy= 0.291181
C,0,-3.0567524209,-0.7320325475,-0.6376943942
C,0,-2.2466388043,-1.5918507242,0.2943470475
H,0,-2.5333038812,-2.6546702133,0.1717456815
H,0,-2.47840276,-1.3387844068,1.3438037812
C,0,-0.7336569282,-1.4745557827,0.0738725684
H,0,-0.530643486,-1.6742729887,-0.990946653

C,0,0.0443987262,-2.4910178747,0.924798548
H,0,-0.4816784168,-3.4555474868,0.9551988211
H,0,0.1265326346,-2.1347523076,1.968309373
C,0,1.4504993233,-2.7726964108,0.4294825268
O,0,-2.4983592358,-0.2714079826,-1.780798139
H,0,-1.5821496253,0.0598423775,-1.6485183757
O,0,1.9190764516,-3.8866744222,0.3968315705
C,0,-4.4586388129,-0.5490114811,-0.4766448419
C,0,-5.1772830015,-1.140930113,0.60065357
C,0,-5.1972822173,0.2347131844,-1.4085336858
C,0,-6.5468735911,-0.9454502092,0.7362964321
H,0,-4.6542171962,-1.7618046887,1.3309282159
C,0,-6.5649912359,0.4197907476,-1.2596640587
H,0,-4.6626281264,0.6921360598,-2.2421001852
C,0,-7.2556604748,-0.1650909948,-0.1873110291
H,0,-7.0736324042,-1.4106297236,1.5730952175
H,0,-7.1072731935,1.0289489399,-1.9872173666
H,0,-8.3313825756,-0.0164995168,-0.074721494
C,0,2.2486565839,-1.5711276931,-0.0347899358
C,0,2.3493575415,-1.2462845519,-1.3906732906
C,0,2.8493167945,-0.7067433432,0.8875745171
C,0,2.9821552601,-0.0834359593,-1.8248569382
C,0,3.4794348227,0.4713247748,0.4925761793
C,0,3.525176305,0.7740729746,-0.8690364821
H,0,3.0284137747,0.1588654731,-2.886500098
H,0,3.9228734433,1.1388206183,1.231749946
C,0,-0.2979316403,-0.0511777017,0.2977990324
S,0,-0.155375446,0.6238153515,1.8954392143
C,0,0.3042067301,2.0213546431,-0.2150131074
C,0,0.320791685,2.1351471469,1.1933042201
N,0,-0.0680168113,0.7709473795,-0.6800312823
C,0,0.6826119556,3.1151801915,-1.0085297153
C,0,1.0699769742,4.292028242,-0.3804576438
H,0,0.679534535,3.0180618424,-2.095700472

C,0,0.7077722356,3.3213783624,1.8272300104
C,0,1.0808828597,4.3947395797,1.0238968309
H,0,1.3748422939,5.1501738562,-0.9825520906
H,0,0.7206412,3.4005910557,2.915450578
H,0,1.3905508941,5.3310486498,1.4922720072
Cl,0,2.8075048704,-1.1190100675,2.5660578974
Cl,0,1.6109632752,-2.282861602,-2.5616947208
Cl,0,4.2628601152,2.246223343,-1.3786767863

*Stationary Points for Shift of Radical **1a***

1a (extended conformation)
E(UMN15) = -2946.74128748
Thermal correction to Gibbs Energy= 0.309429
C,0,-3.0426795558,-1.4736723253,-0.1729456016
C,0,-1.7113561758,-2.1128273442,0.2468209816
H,0,-1.8778918035,-3.19662681,0.3597368652
H,0,-1.4109021335,-1.7286025666,1.2355346776
C,0,0.6714270202,-2.5478241148,-0.4181603922
H,0,0.8243692456,-2.9782356379,0.5730467369
C,0,1.801550514,-2.5725245758,-1.3743378395
H,0,2.1824800844,-1.5555287796,-1.6150266824
H,0,1.5102820963,-2.9769905765,-2.3657427766
C,0,3.0006689924,-3.359028858,-0.9152583348
O,0,-3.4002361685,-1.9201221369,-1.4551848902
H,0,-3.4192815382,-1.1294442207,-2.0307641201
O,0,3.0890360704,-3.9023471131,0.162306274
C,0,-4.1837240429,-1.7599809,0.8101308026
C,0,-5.4936152202,-1.5433438319,0.3600857756
C,0,-3.9790361588,-2.18594917,2.1266540011
C,0,-6.5803935922,-1.7481679764,1.2081949612
H,0,-5.6465828185,-1.2171062944,-0.6712964908
C,0,-5.069795465,-2.392496782,2.978368472

H,0,-2.9712126613,-2.3666124689,2.5045945106
C,0,-6.3705421755,-2.1748737614,2.5238021564
H,0,-7.5953785772,-1.57622508,0.8429966093
H,0,-4.8966473002,-2.7297155728,4.0026915541
H,0,-7.2198223572,-2.338180243,3.1907550092
C,0,4.1421251852,-3.4287744913,-1.9084806082
C,0,4.2002465132,-4.4421823097,-2.8692459667
C,0,5.1750944407,-2.4873637726,-1.8898345958
C,0,5.2522173024,-4.5369931648,-3.7780417082
C,0,6.2433842992,-2.5482775073,-2.7825306312
C,0,6.2679583774,-3.5824769336,-3.7186373268
H,0,5.2772951841,-5.3377762788,-4.5170122587
H,0,7.0383025315,-1.8033327194,-2.7487342903
C,0,-2.8794260249,0.0351957195,-0.2505257322
S,0,-2.3881123834,0.9881129102,1.11546946
C,0,-2.881679214,2.0399378062,-1.1837992806
C,0,-2.4775428855,2.408269243,0.1195965276
N,0,-3.0972507445,0.6801872366,-1.3486393021
C,0,-3.0271822585,3.0252807576,-2.1720220159
C,0,-2.7680145686,4.3497198618,-1.8398505085
H,0,-3.3390147776,2.736572723,-3.1772168254
C,0,-2.2164988589,3.7411435999,0.4556675917
C,0,-2.3665096311,4.704223107,-0.538072797
H,0,-2.8769152316,5.1277283325,-2.5979648019
H,0,-1.9054989418,4.0170801795,1.4645405439
H,0,-2.1691398121,5.7517845037,-0.3021176236
Cl,0,5.109217863,-1.2040608888,-0.7323744956
Cl,0,2.9182576009,-5.6015745598,-2.9310183889
Cl,0,7.5811236666,-3.6796027851,-4.8329354838
C,0,-0.5952795886,-1.8510745503,-0.7560713248
H,0,-0.4179825384,-0.7552047455,-0.8283091028
H,0,-0.9412075037,-2.1426249029,-1.7648532529

1a (folded conformation)

E(UMN15) = -2946.74939838

Thermal correction to Gibbs Energy= 0.318375

C,0,-2.8922445779,0.8642736288,0.2682847368

C,0,-2.8419404403,2.0331951833,-0.7270151999

H,0,-3.8491028842,2.47217099,-0.7979762131

H,0,-2.60009948,1.6416023583,-1.7298212788

C,0,-0.4587017606,2.5629548816,-0.1371701666

H,0,0.0155124829,2.0661272542,-0.9860281069

C,0,0.2512421063,2.5854824775,1.1736564937

H,0,0.0126982674,1.6745833523,1.764980517

H,0,-0.0411408957,3.4593080013,1.7768931451

C,0,1.7457111735,2.6248157779,0.9652986287

O,0,-2.847961794,1.3740342741,1.5732315158

H,0,-2.3526365525,0.7209457881,2.1070050443

O,0,2.4415098973,3.5751058466,1.2425494242

C,0,-4.1592711447,0.0210010669,0.0439189674

C,0,-4.9502905416,-0.3439642804,1.1377892979

C,0,-4.5353002961,-0.4040715695,-1.2386741451

C,0,-6.0971506699,-1.1217081228,0.9556152747

H,0,-4.6679542226,-0.0023029962,2.134482979

C,0,-5.6808981082,-1.1798005125,-1.4207649243

H,0,-3.9317223757,-0.1355711908,-2.1095852423

C,0,-6.4661487179,-1.5428775694,-0.3229422581

H,0,-6.7061080726,-1.3965976483,1.8198694076

H,0,-5.9612698835,-1.5011398952,-2.4262696785

H,0,-7.3626401744,-2.15008366,-0.4655596187

C,0,2.3633376371,1.3866579242,0.3415920635

C,0,2.7614785133,1.3505865516,-0.9997912579

C,0,2.6375461487,0.2607691444,1.1266102472

C,0,3.3729559944,0.2286258649,-1.5571680804

C,0,3.2812536932,-0.862669718,0.614284725

C,0,3.631876825,-0.8669054976,-0.7348881864

H,0,3.65815038,0.2197545654,-2.6091178987

H,0,3.498070023,-1.7174593343,1.2542304945

C,0,-1.7158589711,-0.0986251292,0.1292762837
S,0,-1.0862148263,-0.6605924654,-1.3933167934
C,0,-0.3001955532,-1.6427489859,0.8526294813
C,0,-0.0864921797,-1.7927068814,-0.5369196978
N,0,-1.2228911181,-0.6645860183,1.1843197654
C,0,0.3629909397,-2.4908115556,1.7528812431
C,0,1.2117080544,-3.4696650729,1.2489969209
H,0,0.195143927,-2.3724358607,2.8244993105
C,0,0.7817647578,-2.7656560555,-1.0449304004
C,0,1.4202613174,-3.6051410824,-0.136600551
H,0,1.7266941416,-4.1434660749,1.936919357
H,0,0.948155937,-2.8688926876,-2.1187205065
H,0,2.1000936283,-4.3747109702,-0.5070421303
Cl,0,2.1991335251,0.279339828,2.8011955691
Cl,0,2.497112294,2.7328663143,-2.0059277329
Cl,0,4.4048265326,-2.257113653,-1.402179245
C,0,-1.8293983651,3.1076179585,-0.3187024946
H,0,-2.1693432844,3.5817509198,0.6127320743
H,0,-1.8349773065,3.886107536,-1.1035291601

1a (TS1)

E(UMN15) = -2946.73714152

Thermal correction to Gibbs Energy= 0.319658

C,0,2.9100530124,-1.0622138886,0.2564350819
C,0,2.8509151234,-2.2689857198,-0.6733269898
H,0,3.8125797324,-2.802384695,-0.6903215347
H,0,2.6384468621,-1.9240835607,-1.6994041907
C,0,0.504973083,-2.2592677623,0.0248400808
H,0,0.0191548063,-1.9418349678,-0.9008701514
C,0,-0.391844473,-2.4408351561,1.2134238001
H,0,-0.2796678635,-1.5754425102,1.8971833339
H,0,-0.1404159905,-3.3549099929,1.771963737
C,0,-1.8374622202,-2.5170571968,0.7815372988
O,0,3.0489435949,-1.5150479965,1.5798833316

H,0,2.460043448,-0.95291915,2.1226224282
O,0,-2.5125381582,-3.5173628919,0.863924218
C,0,4.0074385929,-0.053611083,-0.0865732696
C,0,4.3242938205,0.926536727,0.8645803371
C,0,4.6884147923,-0.0541237875,-1.3089885666
C,0,5.2994408669,1.8874743988,0.6007276397
H,0,3.7955941821,0.9295904378,1.8209407874
C,0,5.6679004363,0.9080967646,-1.574798262
H,0,4.466223353,-0.8064256182,-2.0682761559
C,0,5.9759336742,1.8811150923,-0.6233059511
H,0,5.5343065451,2.6439671688,1.3528880853
H,0,6.1938262055,0.8919824146,-2.5319920294
H,0,6.7415340108,2.6314701337,-0.8322390376
C,0,-2.4153383392,-1.2446649289,0.1906891338
C,0,-2.6357368155,-1.0917529302,-1.1831923073
C,0,-2.8173475909,-0.1971993426,1.0287691682
C,0,-3.1871898637,0.0723153078,-1.7164947128
C,0,-3.4019248784,0.9656145981,0.5355265875
C,0,-3.5655578263,1.0904821054,-0.8432456468
H,0,-3.3272716767,0.1751857017,-2.7925029021
H,0,-3.7096523447,1.7618320103,1.2129685117
C,0,1.551733839,-0.3428950755,0.1939879338
S,0,1.0580459525,0.4885813456,-1.2966933265
C,0,0.2963933486,1.3119823719,1.0322205093
C,0,0.1298697291,1.60602327,-0.3485560353
N,0,1.1244330384,0.2533164661,1.298455355
C,0,-0.3288044715,2.1324310822,1.9912313183
C,0,-1.0861729902,3.2149155832,1.562217354
H,0,-0.2016974842,1.9058127845,3.0510370741
C,0,-0.645936036,2.6866826833,-0.7772864779
C,0,-1.2431233888,3.4923299944,0.1905073268
H,0,-1.5683612417,3.8614597684,2.2984340914
H,0,-0.7770874896,2.8978342795,-1.840396401
H,0,-1.8503763896,4.3438028024,-0.1228093717

Cl,0,-2.6146292805,-0.3650464909,2.7390849712
Cl,0,-2.2134370741,-2.374438554,-2.2652502572
Cl,0,-4.2347159366,2.5456055689,-1.4820395891
C,0,1.70587941,-3.1333536851,-0.1612162073
H,0,1.9917483887,-3.5877554341,0.7961521377
H,0,1.478104975,-3.943839443,-0.8743762591

1a (cyclic intermediate)
E(UMN15) = -2946.77284381
Thermal correction to Gibbs Energy= 0.323968
C,0,-2.7883423852,1.1855021817,0.3243906367
C,0,-3.0329018197,2.4324929776,-0.5142951729
H,0,-4.0395099057,2.8427431564,-0.3484397935
H,0,-2.9275096892,2.1862301376,-1.5832737384
C,0,-0.6661296417,2.4196510123,-0.0055360095
H,0,-0.1561398136,2.4834335435,-0.9779953583
C,0,0.3279253595,2.8235868439,1.0929037656
H,0,0.099908344,2.2706736579,2.0193500953
H,0,0.2438830916,3.8993715704,1.3045700396
C,0,1.7765862432,2.5814783829,0.7471233457
O,0,-2.9259469434,1.55397333,1.6776574164
H,0,-2.2441751021,1.0554750293,2.1685603074
O,0,2.6206446996,3.4471696334,0.8296916474
C,0,-3.6182145148,-0.0446993129,0.006262624
C,0,-3.7356426705,-1.052615337,0.9744637532
C,0,-4.2475834376,-0.2307961474,-1.2323873322
C,0,-4.4438558677,-2.2257516136,0.706517301
H,0,-3.2696420866,-0.9129977805,1.9521476578
C,0,-4.9657009937,-1.3979546874,-1.4997231505
H,0,-4.1778157475,0.5384292777,-2.004099286
C,0,-5.0611913481,-2.4026427005,-0.5336410806
H,0,-4.5186042858,-3.0007056046,1.4726762241
H,0,-5.4528425203,-1.5223479607,-2.4694084137
H,0,-5.6201652399,-3.3169605095,-0.744738171

C,0,2.1911532542,1.2009786101,0.2694224019
C,0,2.4367065171,0.9380489527,-1.0839223407
C,0,2.4501525188,0.1715214798,1.180333356
C,0,2.8732845983,-0.3084624477,-1.5285286693
C,0,2.9054456016,-1.0816630467,0.7767299636
C,0,3.098847062,-1.3099441035,-0.5848823047
H,0,3.0346293427,-0.491486393,-2.5908425958
H,0,3.0907501383,-1.8665986856,1.5098948226
C,0,-1.2281021054,0.9585198015,0.1073283504
S,0,-0.896225397,0.0409166342,-1.4621206961
C,0,-0.4425214474,-1.069569947,0.8448574045
C,0,-0.4490765207,-1.3621774139,-0.5674819462
N,0,-0.7722285799,0.1676447801,1.1950091419
C,0,-0.0792707455,-2.1016283512,1.7600963152
C,0,0.2715255279,-3.3446542795,1.271693293
H,0,-0.076075455,-1.8747886893,2.8275413548
C,0,-0.0942671929,-2.6236439903,-1.0419564325
C,0,0.2687832992,-3.6066170622,-0.1188529711
H,0,0.5540444289,-4.1402754889,1.9637797093
H,0,-0.0941557434,-2.8375728788,-2.1120953454
H,0,0.5551733732,-4.596811331,-0.4776710118
Cl,0,2.1807560514,0.4511871974,2.8649636226
Cl,0,2.1830091185,2.1877044133,-2.2529941305
Cl,0,3.6249502969,-2.8660669092,-1.1102923038
C,0,-1.8997428113,3.34352038,-0.0634029881
H,0,-2.123530652,3.7281489389,0.9406500179
H,0,-1.7310812033,4.1973297491,-0.733390325

1a (TS2)

E(UMN15) = -2946.75680805

Thermal correction to Gibbs Energy= 0.322722

C,0,2.7081004531,-1.6399948356,0.3457633192
C,0,2.6815810834,-2.854224614,-0.5365640503
H,0,3.5785119688,-3.4770836908,-0.3790409627

H,0,2.6659862175,-2.5487237934,-1.5941945246
C,0,0.2440774783,-2.5790979025,-0.2622271091
H,0,-0.1499045719,-2.6175232855,-1.2909521103
C,0,-0.8848753424,-2.9392987399,0.7158275777
H,0,-0.6060513122,-2.5690884379,1.7172665368
H,0,-1.0015672744,-4.0314120372,0.7707078301
C,0,-2.2563478905,-2.3962285807,0.3873714327
O,0,2.5693906193,-1.9529084597,1.6680724321
H,0,1.8576096572,-1.3704401614,2.0259405077
O,0,-3.233654338,-3.1122061256,0.3399910916
C,0,3.4762409468,-0.4270275983,0.0426754024
C,0,3.6861238415,0.5242062877,1.0618555845
C,0,3.9308084487,-0.1252417392,-1.2575279897
C,0,4.3004151072,1.7450408641,0.7876340323
H,0,3.3576247165,0.296313567,2.0774338666
C,0,4.5524770117,1.0916889062,-1.5270371156
H,0,3.7919426788,-0.8443966683,-2.066795405
C,0,4.730304999,2.0366472303,-0.5099244983
H,0,4.445742013,2.4710546857,1.5906784046
H,0,4.8994946438,1.3077161156,-2.5398316546
H,0,5.2118367564,2.9923335175,-0.7280914058
C,0,-2.4338758715,-0.9132333515,0.1115660286
C,0,-2.5892378351,-0.4387985746,-1.1955623944
C,0,-2.5447149159,0.0183387128,1.149354076
C,0,-2.804121813,0.9095508271,-1.4753775605
C,0,-2.7712167514,1.3720847595,0.9110371302
C,0,-2.8852105677,1.8044968105,-0.4094783658
H,0,-2.8964511706,1.2530345966,-2.5056978996
H,0,-2.8374538475,2.0764597786,1.7401847775
C,0,0.750938926,-1.1436240966,-0.0574792729
S,0,0.7213873875,-0.1158880888,-1.5079915613
C,0,0.5243128546,0.8912099228,0.8582818352
C,0,0.6410580678,1.2898452144,-0.5054180768
N,0,0.509801983,-0.4502966799,1.0741272508

C,0,0.4031930763,1.8809638645,1.8579739951
C,0,0.4031603693,3.2174691348,1.4861136564
H,0,0.3012339698,1.5717049307,2.9002262419
C,0,0.6500543565,2.6376405355,-0.8721189523
C,0,0.5268553608,3.5956922702,0.133302752
H,0,0.3070225073,3.991192547,2.250730894
H,0,0.7426226454,2.932468163,-1.9190034757
H,0,0.5214509927,4.6547157923,-0.1319236823
Cl,0,-2.3673361217,-0.515593688,2.7835806716
Cl,0,-2.4717399911,-1.5521293296,-2.5151874764
Cl,0,-3.1226808785,3.4836224121,-0.7287804284
C,0,1.4019666153,-3.5934500523,-0.1710638933
H,0,1.4877471579,-3.9580936953,0.8624466988
H,0,1.2148165826,-4.45859122,-0.8217921606

1a (shifted product)
E(UMN15) = -2946.77739278
Thermal correction to Gibbs Energy= 0.319660
C,0,3.1620656069,-1.5319219429,0.4576666043
C,0,2.6819100605,-2.6894731045,-0.3698941178
H,0,3.4487930399,-3.4865055953,-0.3546216669
H,0,2.5677635457,-2.391715865,-1.4235032278
C,0,0.1087714676,-2.465017684,-0.1580209469
H,0,-0.131620943,-2.5624988107,-1.2303824885
C,0,-1.0541110132,-3.0010055309,0.6942168327
H,0,-0.8851321039,-2.6679041239,1.7342881395
H,0,-1.0612606006,-4.1006699209,0.6961916317
C,0,-2.4499862746,-2.5579456657,0.3150889846
O,0,3.0350352818,-1.6658948322,1.8081341006
H,0,2.1097201456,-1.4403765842,2.058487797
O,0,-3.4012452441,-3.3048036519,0.3691401595
C,0,3.7306784914,-0.3263406825,-0.0432123072
C,0,4.0706532067,0.7200311121,0.8634514232
C,0,3.9399262587,-0.0820457055,-1.4304014539

C,0,4.557878904,1.9367204569,0.4072336617
H,0,3.9196326141,0.5487131219,1.9301971802
C,0,4.4283572352,1.141189964,-1.873647217
H,0,3.7076199643,-0.8576392305,-2.1626857622
C,0,4.7378799531,2.1637063432,-0.9654060761
H,0,4.7968401726,2.7246673401,1.1260425492
H,0,4.5723853879,1.3038137689,-2.9445917442
H,0,5.1185305193,3.1225505382,-1.3230377488
C,0,-2.6334104762,-1.1232626375,-0.1381981476
C,0,-2.7815779461,-0.8192722635,-1.4949572613
C,0,-2.630725372,-0.0575603415,0.77028664
C,0,-2.8914233496,0.4931319485,-1.9506601394
C,0,-2.7088431536,1.2678954863,0.3493817485
C,0,-2.8272366768,1.5260697612,-1.0167900282
H,0,-2.9798378243,0.7046519627,-3.0162038262
H,0,-2.6672782281,2.0822763884,1.0736693591
C,0,0.3525066495,-1.0076299582,0.1286924193
S,0,0.45959647,0.1396503407,-1.1680240839
C,0,0.7062097588,0.8449916022,1.2864856659
C,0,0.7160585646,1.4014881907,-0.0141167722
N,0,0.5073506285,-0.5242681943,1.3258734896
C,0,0.8725337811,1.6830454844,2.4004526379
C,0,1.0527913856,3.044700905,2.1914847198
H,0,0.8558829994,1.2530776652,3.4036736009
C,0,0.8917521191,2.7732842277,-0.2263632693
C,0,1.0631893918,3.585184733,0.8903303871
H,0,1.1841687303,3.70935648,3.0477551397
H,0,0.8899149972,3.1915762433,-1.2344673294
H,0,1.2026848119,4.65979321,0.7561948937
Cl,0,-2.5180103132,-0.3883383979,2.4617678684
Cl,0,-2.7275554664,-2.1035060811,-2.6527782819
Cl,0,-2.8590507134,3.1623417716,-1.5593582896
C,0,1.3727146405,-3.2935241062,0.1479593889
H,0,1.4486650264,-3.4230097526,1.2401756691

H,0,1.2299158888,-4.2989023829,-0.2749425056

*Stationary Points for Shift of Radical **5c***

5c (extended conformation)

E(UMN15) = -2986.01481571

Thermal correction to Gibbs Energy= 0.335665

C,0,3.6954189946,-0.9423268418,0.2255015067

C,0,2.7375575166,-1.9701618388,-0.4058844992

H,0,3.2402273722,-2.9502467641,-0.3451737282

H,0,2.5995895012,-1.7478721074,-1.4767215041

C,0,-0.8077818784,-3.2478207391,0.4694000227

H,0,-0.9888694178,-2.6925412807,1.3915203246

C,0,-1.8633280193,-4.1682805258,-0.0110445097

H,0,-1.5481974166,-5.2345709756,0.0150759412

H,0,-2.118811576,-4.0045284737,-1.078816659

C,0,-3.1561908018,-4.1031323543,0.7579982627

O,0,3.8946120013,-1.2756970398,1.5722580447

H,0,3.5816440853,-0.5117401056,2.0978636399

O,0,-3.347264835,-3.3859727725,1.7137402029

C,0,5.0376560733,-0.8907418919,-0.5153679575

C,0,5.1101352338,-0.8524132742,-1.9157083592

C,0,6.2262280092,-0.8576240834,0.2223896521

C,0,6.3458527894,-0.7811216736,-2.5614824001

H,0,4.2009640114,-0.8750013984,-2.5219371828

C,0,7.4631439649,-0.7888980644,-0.4233739635

H,0,6.1666718162,-0.8950891268,1.310502745

C,0,7.5279585747,-0.7501892879,-1.8174467753

H,0,6.3830976068,-0.7528086273,-3.6526561752

H,0,8.3811802276,-0.7666434498,0.1683474338

H,0,8.4944521771,-0.6973254091,-2.3232920144

C,0,-4.2494362686,-5.0254949707,0.2592536257

C,0,-4.3892714871,-6.3200246675,0.7674039814

C,0,-5.1587238151,-4.6057153034,-0.7156298216
C,0,-5.4038520883,-7.1739719799,0.3393896671
C,0,-6.186695025,-5.4300818859,-1.1687802237
C,0,-6.2967928606,-6.7112426139,-0.6275132541
H,0,-5.4942760997,-8.1790541693,0.7512216679
H,0,-6.8855231159,-5.0798131361,-1.9283677357
C,0,3.0545871729,0.4377120964,0.1969537685
S,0,2.5492580296,1.2205953246,-1.2698192408
C,0,2.1871484254,2.2900553545,1.0440162171
C,0,1.9508308841,2.5483521874,-0.3248537082
N,0,2.8106906733,1.0776304445,1.292815193
C,0,1.79094222,3.2294140686,2.0082086971
C,0,1.1717543457,4.400050453,1.5867420495
H,0,1.9745939159,3.0258387662,3.0645336622
C,0,1.3294223537,3.7272561731,-0.7513658043
C,0,0.9431879044,4.6465752959,0.2196515031
H,0,0.8574575891,5.1404817985,2.3248975196
H,0,1.1524841006,3.9195233262,-1.8108029524
H,0,0.4548977661,5.5741085304,-0.0857450028
Cl,0,-4.9877126805,-3.0184123152,-1.3809905462
Cl,0,-3.2574308707,-6.8744448888,1.9518602772
Cl,0,-7.5626459225,-7.7494910653,-1.1708708154
C,0,1.384432069,-2.0243128073,0.2878053385
H,0,0.8444301241,-1.0740671767,0.1285515411
H,0,1.5447576668,-2.1154592659,1.3741297987
C,0,0.5152381209,-3.1781788029,-0.2020740807
H,0,1.0667731072,-4.1323428951,-0.0593725924
H,0,0.3778413146,-3.1076701991,-1.2994513975

5c (folded conformation)
E(UMN15) = -2986.01884341
Thermal correction to Gibbs Energy= 0.343806
C,0,-3.1340418268,0.3472254077,0.513552563
C,0,-3.8654861947,1.5874440422,-0.0318758625

H,0,-4.8665499889,1.5753937411,0.4269764198
H,0,-4.0328802403,1.4477581243,-1.1148170125
C,0,-0.7479957474,2.5732005012,-0.0105967174
H,0,-0.7858438724,2.0750531591,0.9589683791
C,0,0.533259743,2.5912064947,-0.7786640454
H,0,0.5880208493,3.4984225544,-1.4041518774
H,0,0.6219106708,1.7173578452,-1.4546600253
C,0,1.694663601,2.6147730171,0.1899781028
O,0,-2.6523192527,0.6213216549,1.8027496138
H,0,-1.8769663384,0.0410608512,1.9370357877
O,0,2.0311550547,3.6143477795,0.7846707291
C,0,-4.1173102506,-0.8383965054,0.5356756151
C,0,-4.7464598972,-1.2794252556,-0.6377957224
C,0,-4.4056317905,-1.4817831623,1.7428180379
C,0,-5.6462296654,-2.3453365014,-0.6019329352
H,0,-4.5301311845,-0.7956344134,-1.5942242486
C,0,-5.3053865155,-2.551251669,1.7780288252
H,0,-3.925446665,-1.1321416724,2.6575334553
C,0,-5.9283491945,-2.9868348032,0.6076375281
H,0,-6.1278026724,-2.6770261425,-1.5244717472
H,0,-5.5208669468,-3.044076908,2.728901197
H,0,-6.6311423436,-3.8223365944,0.635669438
C,0,2.4083710445,1.3074095579,0.4602030364
C,0,3.2950829141,0.780060661,-0.4843593865
C,0,2.2763123065,0.6280931668,1.6767834801
C,0,4.0549759094,-0.3591989594,-0.2338094969
C,0,3.0060921087,-0.5263802837,1.9552510552
C,0,3.8912413703,-1.0047814252,0.9899129783
H,0,4.7367382594,-0.7495301545,-0.9894904412
H,0,2.8722127159,-1.0510739457,2.9013418765
C,0,-1.9467636586,-0.1169144046,-0.32204132
S,0,-1.8151233252,0.0910544799,-2.0445616037
C,0,-0.0748153708,-1.2365188223,-0.6899623615
C,0,-0.3405903748,-0.8260452896,-2.0176704475

N,0,-1.0031186373,-0.8018252647,0.2392706773
C,0,1.0384487764,-2.0482282069,-0.4265684871
C,0,1.8805984449,-2.3951546464,-1.4762148924
H,0,1.2261432094,-2.3885066238,0.593505152
C,0,0.5164918541,-1.1585615123,-3.0726301103
C,0,1.6315714685,-1.9417504757,-2.784851523
H,0,2.7588507009,-3.0138454721,-1.2756544901
H,0,0.3131297068,-0.8232238662,-4.091017405
H,0,2.3154990916,-2.2164266999,-3.5902864186
Cl,0,1.1552423308,1.2027815576,2.8622269109
Cl,0,3.4515783579,1.5711632516,-2.0152900525
Cl,0,4.7471724028,-2.4739868677,1.2823298111
C,0,-3.2356370044,2.952296398,0.239830626
H,0,-3.0490030842,3.0436482722,1.321479535
H,0,-3.9938901884,3.7095478662,-0.0114850816
C,0,-1.9524511011,3.2760914912,-0.5209711352
H,0,-1.7762575288,4.3709825953,-0.4782896248
H,0,-2.0848140307,3.0610970778,-1.6007843588

5c (TS1)

E(UMN15) = -2986.00875476

Thermal correction to Gibbs Energy= 0.348357

C,0,3.2230795682,-0.6296972045,0.4675750819
C,0,3.9918886811,-1.7667915583,-0.211985799
H,0,5.0153733247,-1.7561005634,0.1940504043
H,0,4.0820187224,-1.533694542,-1.2869071238
C,0,0.9896177141,-2.3928911593,0.0847970029
H,0,1.0915861171,-2.3551551588,1.1717177362
C,0,-0.3965317816,-2.253244274,-0.4548146148
H,0,-0.6732453794,-3.1761511877,-0.9988615833
H,0,-0.471636749,-1.4521705047,-1.2088400939
C,0,-1.4228930832,-2.0818624277,0.6466521733
O,0,2.9617710241,-0.9810550648,1.8014872355
H,0,2.1796698778,-0.458672765,2.0676569594

O,0,-1.3696345172,-2.7657432368,1.6476609155
C,0,4.0390677057,0.6758563178,0.4080325053
C,0,4.6471780568,1.1162304501,-0.7768981875
C,0,4.1778392357,1.456597867,1.561568776
C,0,5.3698510357,2.3103010971,-0.8069610371
H,0,4.5569245256,0.5314442196,-1.6948978392
C,0,4.898347404,2.6534014708,1.5322984062
H,0,3.729876604,1.116310053,2.4959222191
C,0,5.496507507,3.0862419796,0.3478612709
H,0,5.8370120805,2.6340798773,-1.7397041257
H,0,4.9951527404,3.2470273998,2.4442398695
H,0,6.0613432791,4.0207148918,0.3242752009
C,0,-2.49890321,-1.0310829456,0.5239400499
C,0,-3.2844302317,-0.8626166264,-0.6281675046
C,0,-2.7797637191,-0.1794636196,1.6098772603
C,0,-4.2989498693,0.0895778738,-0.7100114374
C,0,-3.7866817025,0.78139167,1.5570223165
C,0,-4.536488078,0.908384103,0.3902271799
H,0,-4.8882777733,0.1877694028,-1.6215436847
H,0,-3.959587786,1.4415778481,2.4070303723
C,0,1.8650087382,-0.3261991029,-0.1876301454
S,0,1.7238965577,-0.1370455643,-1.9388448628
C,0,0.1284298734,1.0700261329,-0.3062328556
C,0,0.3353531286,0.8787285055,-1.6987624048
N,0,1.0144962476,0.4124999248,0.5070540819
C,0,-0.9183889794,1.911169941,0.1184609796
C,0,-1.7532138112,2.4875277402,-0.8302674258
H,0,-1.0593463185,2.0782438977,1.1877551408
C,0,-0.5169999302,1.4422943651,-2.652075415
C,0,-1.5645475862,2.2459384959,-2.2044845448
H,0,-2.5795634776,3.1249059143,-0.5058262192
H,0,-0.3603328827,1.2667531833,-3.7177895448
H,0,-2.240393846,2.7014465228,-2.9309210158
Cl,0,-1.8003410828,-0.1921142043,3.0335406416

Cl,0,-3.0553839507,-1.8759452943,-2.0122225408
Cl,0,-5.7497407708,2.1280909202,0.2924637059
C,0,3.3736659414,-3.1470297127,-0.0357977372
H,0,3.3272556904,-3.3833070618,1.038805452
H,0,4.0342274299,-3.8923384172,-0.5029879239
C,0,1.9745793654,-3.2513113573,-0.62977569
H,0,1.6206253273,-4.3002782507,-0.5779413406
H,0,1.9827790124,-2.9964612613,-1.7066372404

5c (cyclic intermediate)
E(UMN15) = -2986.05141135
Thermal correction to Gibbs Energy= 0.351520
C,0,-3.1686201333,0.8263517631,0.4465502364
C,0,-4.0723779236,1.8652953036,-0.2167671634
H,0,-5.0764837891,1.7786801118,0.2272793003
H,0,-4.1694405676,1.6206875124,-1.2867692376
C,0,-1.1825018448,2.376676685,0.0078130029
H,0,-1.2069268587,2.5797709001,1.0907614141
C,0,0.2771334515,2.4600199898,-0.4562433486
H,0,0.4909062228,3.4851604649,-0.7999780973
H,0,0.4481952508,1.7917727022,-1.3110028511
C,0,1.2427936394,2.1872893995,0.6830275063
O,0,-3.0426559108,1.1707621294,1.8077066555
H,0,-2.2126363303,0.7670781331,2.1222084554
O,0,1.1854117975,2.8430385075,1.702970938
C,0,-3.7001473522,-0.6029402308,0.3028717333
C,0,-4.4294756834,-1.0300331692,-0.8166601903
C,0,-3.4433072028,-1.5353477827,1.3186860636
C,0,-4.8752122762,-2.3498018347,-0.9228140981
H,0,-4.6525850122,-0.3340218148,-1.6265770445
C,0,-3.8819745605,-2.8565388013,1.2138086491
H,0,-2.8953834691,-1.2254952044,2.2100057985
C,0,-4.6001079089,-3.2702843858,0.0899129135
H,0,-5.4425656903,-2.6568932301,-1.8042362527

H,0,-3.665450535,-3.563167814,2.0181507111
H,0,-4.947717377,-4.3023578423,0.0063392194
C,0,2.2544711334,1.072596746,0.5640504015
C,0,3.046360981,0.8802812838,-0.5816092222
C,0,2.4527271865,0.1664919373,1.6237300334
C,0,3.9444656227,-0.1781256838,-0.7060579524
C,0,3.3551542998,-0.8923561317,1.5332519503
C,0,4.0803526729,-1.0662325225,0.3579399773
H,0,4.5363256269,-0.2931092594,-1.6140138819
H,0,3.4623057959,-1.5910943739,2.3631861164
C,0,-1.7167586809,0.9339954924,-0.1560931521
S,0,-1.7187057768,0.458775637,-1.9508983708
C,0,-0.3581472784,-0.9231400617,-0.2050407899
C,0,-0.6567606289,-0.8599135203,-1.6142878574
N,0,-0.8827750081,0.0268999808,0.5589919025
C,0,0.4803179691,-1.9756717379,0.2706319697
C,0,1.0305571344,-2.8660802557,-0.6288711537
H,0,0.6731553968,-2.0367345897,1.3427477503
C,0,-0.1015400725,-1.7735810682,-2.5078891584
C,0,0.7497792975,-2.7641796434,-2.0117469466
H,0,1.6961955769,-3.6557469449,-0.2737379223
H,0,-0.3234923161,-1.7143880557,-3.5746078161
H,0,1.1983045899,-3.4789989077,-2.7040159682
Cl,0,1.5147657369,0.2449764532,3.0715595496
Cl,0,3.0031829927,2.0209521145,-1.8838985076
Cl,0,5.1515680006,-2.4079661465,0.2140088899
C,0,-3.5176388021,3.2774838441,-0.0744413839
H,0,-3.4754795677,3.538245886,0.9945293933
H,0,-4.1946250935,3.994265919,-0.5618983726
C,0,-2.1158331887,3.3764094622,-0.6669551564
H,0,-1.708338489,4.3908494628,-0.536442168
H,0,-2.1418540474,3.1833081915,-1.7556524672

5c (TS2)

E(UMN15) = -2986.03141339

Thermal correction to Gibbs Energy= 0.351737

C,0,3.2280746167,-0.706848269,0.2633709281

C,0,3.896880462,-1.6525311689,-0.6916042608

H,0,4.9900961651,-1.518206856,-0.596431486

H,0,3.6344942713,-1.363417875,-1.7217832669

C,0,1.0846341812,-2.5470980408,0.1894264493

H,0,1.3489220837,-2.7463665959,1.240729553

C,0,-0.3442559862,-3.0620921791,-0.087717486

H,0,-0.341524151,-4.1500203543,0.0762726695

H,0,-0.560223446,-2.8750408824,-1.1462247742

C,0,-1.4423872021,-2.5214670904,0.8065082879

O,0,3.2864743017,-1.1215557313,1.5602053651

H,0,2.505569679,-0.7323580386,2.01366652

O,0,-1.6872375572,-3.0677857927,1.8632429051

C,0,3.3678009877,0.7432475272,0.0299422098

C,0,3.4858197434,1.2812860569,-1.267924473

C,0,3.3518604063,1.6328652896,1.1206419345

C,0,3.5410948084,2.659568671,-1.4637350641

H,0,3.5179095804,0.621243685,-2.1355923945

C,0,3.4089802078,3.0114482956,0.9225264911

H,0,3.2956614453,1.2382909269,2.1371146885

C,0,3.4914556609,3.5317103276,-0.371416776

H,0,3.6233314191,3.0571422322,-2.4776727972

H,0,3.3875871345,3.6829815441,1.7836546709

H,0,3.5302910511,4.6117812068,-0.5288770174

C,0,-2.2166447314,-1.2870374487,0.399337481

C,0,-2.7565661169,-1.0925873727,-0.8878114775

C,0,-2.4554432542,-0.2570373591,1.3318471268

C,0,-3.3902331543,0.0885226533,-1.2669353604

C,0,-3.0878292177,0.9347617794,0.9800078117

C,0,-3.5249274136,1.1085562387,-0.3286256077

H,0,-3.7839575644,0.1991170396,-2.2771514864

H,0,-3.2125850489,1.7241320745,1.7208857429

C,0,1.1607035495,-1.0339291728,0.0280722003
S,0,0.6915612302,-0.3736398737,-1.5621173681
C,0,0.3084823803,0.9556652417,0.6218237112
C,0,0.1671592757,1.0866452529,-0.7882408543
N,0,0.7630680205,-0.2547634651,1.0530362387
C,0,-0.0390406991,2.0474337054,1.4473705953
C,0,-0.5267425543,3.2088150622,0.8663107476
H,0,0.0772950793,1.9510176919,2.5283273431
C,0,-0.3181225987,2.2606945724,-1.3702623411
C,0,-0.6733630233,3.3161676132,-0.5315028969
H,0,-0.8023876754,4.0548882641,1.4996347111
H,0,-0.4201601782,2.3465173968,-2.4538098157
H,0,-1.0683030979,4.2373157166,-0.9643709915
Cl,0,-1.9163808897,-0.3651494652,2.9675696559
Cl,0,-2.7610880332,-2.3620296478,-2.0686118301
Cl,0,-4.2555401727,2.59975998,-0.7876928072
C,0,3.5055823122,-3.1018175263,-0.4566161431
H,0,3.7363311889,-3.3800647423,0.5833005631
H,0,4.1050794197,-3.7525207119,-1.1098457331
C,0,2.0277260981,-3.3236000534,-0.7329087532
H,0,1.7852635535,-4.3934773806,-0.642175241
H,0,1.7984904534,-3.0463369515,-1.7802600978

5c (shifted product)
E(UMN15) = -2986.05004832
Thermal correction to Gibbs Energy= 0.348710
C,0,3.7926033749,-0.6365519004,0.4135181218
C,0,4.3590883012,-1.7727756115,-0.3685094923
H,0,5.3954051374,-1.9598867295,-0.024502083
H,0,4.4429831929,-1.4989325837,-1.4297767704
C,0,1.0561444979,-2.4693321251,0.1359834011
H,0,1.2883605537,-2.6861004907,1.190856306
C,0,-0.2960689324,-3.1283568858,-0.2382418484
H,0,-0.2077438251,-4.2135273342,-0.0865764302

H,0,-0.4712271864,-2.9387601309,-1.30720979
C,0,-1.4989619005,-2.6910672201,0.5805914327
O,0,3.4614373186,-0.9529419075,1.6907180939
H,0,2.6027928563,-0.5302432769,1.9154667636
O,0,-1.9072513363,-3.3809666807,1.4908878934
C,0,3.6942708979,0.7157615649,-0.0307418343
C,0,3.8167486019,1.0889286723,-1.4004362397
C,0,3.4337426901,1.7573586122,0.9042835191
C,0,3.6545422134,2.4084530339,-1.7992146191
H,0,4.0112159168,0.3264724877,-2.1569212879
C,0,3.2776005761,3.075610727,0.4924232835
H,0,3.3598633823,1.5133226282,1.9667240962
C,0,3.3775718129,3.4153693252,-0.8617223419
H,0,3.7396082768,2.6609641128,-2.8590392405
H,0,3.0712170953,3.8491759387,1.2362943419
H,0,3.2471557985,4.450284569,-1.1844680876
C,0,-2.1839170067,-1.3698812685,0.2872136959
C,0,-2.7120826884,-1.0447810118,-0.9749335519
C,0,-2.3724940426,-0.4192668778,1.3077823185
C,0,-3.3191408087,0.1802423715,-1.2411988926
C,0,-2.9743174145,0.816842479,1.0713172815
C,0,-3.4254579662,1.1127249332,-0.2110159027
H,0,-3.7091311665,0.3950067513,-2.2360125453
H,0,-3.0692925823,1.5416672329,1.879675386
C,0,0.8877207413,-0.9786559414,0.0498832688
S,0,0.5576904832,-0.2229447538,-1.4883603521
C,0,0.3689156905,1.0678940321,0.7256373171
C,0,0.1841561063,1.2538451456,-0.6618631625
N,0,0.78181026,-0.2030584892,1.0868080162
C,0,0.0815417762,2.114534453,1.6147372133
C,0,-0.3833266328,3.3184189568,1.1004780281
H,0,0.2133406073,1.9573753538,2.687136905
C,0,-0.268359944,2.4712733584,-1.1831563433
C,0,-0.5553342348,3.4958961067,-0.2862676839

H,0,-0.6223469756,4.1400415882,1.7789672921
H,0,-0.4083037853,2.606752514,-2.2571355471
H,0,-0.9274308246,4.4502170836,-0.6644358295
Cl,0,-1.8118111662,-0.7107508465,2.9133878193
Cl,0,-2.6868298025,-2.1987391352,-2.266261031
Cl,0,-4.1361295721,2.6510475675,-0.525794614
C,0,3.574430018,-3.0780000276,-0.2263126731
H,0,3.5500360633,-3.370396664,0.8357653609
H,0,4.1362207905,-3.8649580753,-0.7521551765
C,0,2.1459997002,-3.0676227539,-0.7740530091
H,0,1.854605203,-4.1112972881,-0.9684682364
H,0,2.1148088595,-2.5616675895,-1.7572115395

*Stationary Points for Shift of Radical **5d***

5d (extended conformation)
E(UMN15) = -3025.28868391
Thermal correction to Gibbs Energy= 0.361642
C,0,-4.3847242927,-1.1640969757,-0.5717989237
C,0,-3.0948330271,-1.5878505949,0.1466418465
H,0,-2.9853580325,-2.6780611669,0.0181252347
H,0,-3.197949765,-1.4017601821,1.2288904802
C,0,1.9450007422,-1.1481772031,0.2815053574
H,0,1.9616983894,-2.0294120951,0.9253212489
C,0,3.2336713694,-0.4999647728,-0.0524494373
H,0,3.2464560934,0.581416997,0.2007795427
H,0,3.4476388631,-0.5077479268,-1.143402044
C,0,4.4401133719,-1.1075681065,0.6124071682
O,0,-4.2490011654,-1.3671688007,-1.9546885822
H,0,-4.3071076621,-0.485179332,-2.3731880702
O,0,4.4029076022,-2.0596634709,1.3583214338
C,0,-5.6298854215,-1.9017609467,-0.0656422233
C,0,-5.6816807481,-2.5836026569,1.1544518852

C,0,-6.7796213761,-1.8506333864,-0.866505918
C,0,-6.8663554977,-3.204853571,1.5652771498
H,0,-4.8018925291,-2.6440737729,1.797422812
C,0,-7.9600538651,-2.4680879011,-0.4575699485
H,0,-6.729909094,-1.3220197309,-1.8213709529
C,0,-8.0064761935,-3.1493550724,0.76344693
H,0,-6.892207465,-3.738086535,2.5181492445
H,0,-8.8475452736,-2.4201467866,-1.0925605866
H,0,-8.9292392469,-3.6361324532,1.0865016986
C,0,5.7595202118,-0.4404513436,0.2822611784
C,0,6.2432886031,0.6223153249,1.0503317361
C,0,6.5366534327,-0.8725786423,-0.7961322964
C,0,7.4640690858,1.2351693198,0.7749041463
C,0,7.7624617856,-0.2852842457,-1.1032176522
C,0,8.2130280079,0.7663022514,-0.3047348216
H,0,7.8215676057,2.0615555029,1.3891608807
H,0,8.3518971969,-0.640075034,-1.9486129621
C,0,-4.6180938499,0.3215257556,-0.3553300832
S,0,-4.797782871,1.0115434664,1.2282010786
C,0,-4.8924258756,2.444406951,-0.9105125662
C,0,-4.9804688006,2.5751064849,0.4941010162
N,0,-4.6841500437,1.1452616688,-1.3483463316
C,0,-5.0135183252,3.5809008389,-1.7243118169
C,0,-5.2191549372,4.8166018177,-1.1222106123
H,0,-4.9445886191,3.4755601659,-2.8083651699
C,0,-5.1876063374,3.8182706449,1.1017582575
C,0,-5.3053422134,4.9340495917,0.2778455902
H,0,-5.3154376372,5.7100319883,-1.742219372
H,0,-5.2549813224,3.9105640536,2.1869190834
H,0,-5.467387837,5.9159829433,0.726810119
Cl,0,5.9447490019,-2.1647490307,-1.7816217007
Cl,0,5.2858156902,1.1948999639,2.3720622492
Cl,0,9.7281645613,1.5081498091,-0.6644754561
C,0,-1.8633849981,-0.8638722127,-0.3785426593

H,0,-1.9558044859,0.2187846297,-0.173815699
H,0,-1.8300371263,-0.9700104154,-1.4751263113
C,0,-0.5665665511,-1.3785124167,0.2319790204
H,0,-0.4641546052,-2.4581732418,0.0251255335
H,0,-0.608304825,-1.2829637112,1.3310453828
C,0,0.6676583223,-0.6497819406,-0.289178297
H,0,0.5659627582,0.4378752347,-0.095401177
H,0,0.6916496465,-0.7220421859,-1.3973678154

5d (folded conformation)

E(UMN15) = -3025.28229931

Thermal correction to Gibbs Energy= 0.372848

C,0,2.8031577611,0.2772773943,-0.3800677776
C,0,3.7405898092,1.2641631613,0.3760055418
H,0,4.7533071137,0.8388149271,0.3618440522
H,0,3.4544961198,1.3191117211,1.4394871648
C,0,0.8856847167,2.4527778487,1.3084765326
H,0,1.5265778268,2.235049509,2.1672994923
C,0,-0.5324257451,2.0110550851,1.4821947338
H,0,-0.9956554506,2.5704571725,2.3222435732
H,0,-0.584261737,0.9529080233,1.7909099968
C,0,-1.4463314907,2.2691472575,0.304671988
O,0,2.0805642051,0.950568859,-1.372940878
H,0,1.2152180951,0.5033052822,-1.452130435
O,0,-1.5303153181,3.3603437506,-0.2170689282
C,0,3.612934721,-0.8796739299,-0.9996958466
C,0,4.4832237493,-1.6515398341,-0.2157599249
C,0,3.4612698685,-1.194209209,-2.3526545064
C,0,5.190608751,-2.7147964145,-0.7765279299
H,0,4.6087420595,-1.4242908258,0.8472625601
C,0,4.1731068607,-2.2577599867,-2.9168443051
H,0,2.789344406,-0.590842858,-2.9643776529
C,0,5.0381905754,-3.0215020125,-2.132478844
H,0,5.864491125,-3.3058130808,-0.1523422359

H,0,4.0498701888,-2.4872295006,-3.9778167564
H,0,5.5931919325,-3.8523855224,-2.5733837709
C,0,-2.3070108906,1.1447565449,-0.2335902735
C,0,-2.1957156705,0.730770028,-1.5691819993
C,0,-3.3171959081,0.5533000339,0.5347710688
C,0,-3.0491318817,-0.220657806,-2.1235995187
C,0,-4.2078499416,-0.3797776424,0.0057827215
C,0,-4.0615625536,-0.757690659,-1.3269799263
H,0,-2.9292050386,-0.5319954896,-3.1612417528
H,0,-4.9909836612,-0.8106674872,0.6297514172
C,0,1.7759015823,-0.3984144075,0.5228420732
S,0,2.0477707012,-0.7722235647,2.2003109407
C,0,-0.0946201177,-1.492246337,0.9735482443
C,0,0.5065572637,-1.5679191349,2.2510592791
N,0,0.6560251994,-0.8174639501,0.0265727902
C,0,-1.3567054334,-2.0669891979,0.7663131177
C,0,-2.0038464405,-2.6723519411,1.8367097884
H,0,-1.8084601903,-2.0161159315,-0.2262968677
C,0,-0.1399670189,-2.1818197949,3.3294949563
C,0,-1.4015973634,-2.7274763778,3.1078095269
H,0,-2.9932790959,-3.1111141597,1.689396619
H,0,0.3278845702,-2.2282894921,4.3142193106
H,0,-1.9295467593,-3.2079068226,3.9338672097
Cl,0,-3.4862517052,0.9791420758,2.2019157773
Cl,0,-0.9554765097,1.3888134547,-2.579636758
Cl,0,-5.1346912614,-1.9273804883,-1.9986904979
C,0,3.8039751718,2.6846622505,-0.203637093
H,0,3.6440938531,2.639683931,-1.2907617335
H,0,4.8319265462,3.0525961556,-0.0600412369
C,0,2.8691668397,3.7257520925,0.41706537
H,0,3.0868377839,4.6938583714,-0.0615994531
H,0,3.1367445046,3.850895255,1.482509558
C,0,1.3640304181,3.4666726503,0.3296196131
H,0,1.0812533575,3.1729053176,-0.6963357729

H,0,0.8238125061,4.4191317062,0.5051896579

5d (TS1)

E(UMN15) = -3025.26776141

Thermal correction to Gibbs Energy= 0.376456

C,0,-2.7679805386,-0.4918630991,-0.4937251682

C,0,-3.8265622429,-1.456548171,0.0899816947

H,0,-4.8141431505,-1.0865827987,-0.2189521478

H,0,-3.812987286,-1.3892257343,1.1937699019

C,0,-0.9515613625,-2.1387704502,1.2029490969

H,0,-1.6279285382,-2.0724235522,2.0616012588

C,0,0.4746580838,-1.8440410033,1.5917399151

H,0,0.72079304,-2.4887312626,2.4562473835

H,0,0.584720414,-0.8077432421,1.9442547836

C,0,1.5072658262,-2.1890382598,0.537829381

O,0,-2.1585320577,-1.0573664005,-1.6216115695

H,0,-1.2602497087,-0.6715733071,-1.6707759765

O,0,1.7054041591,-3.3373603342,0.1997326815

C,0,-3.4214821237,0.8563018973,-0.8667654334

C,0,-4.3930362586,1.4537663311,-0.0508550968

C,0,-3.0196406613,1.5228764033,-2.0292823019

C,0,-4.9501370466,2.687509011,-0.3904843492

H,0,-4.7206018125,0.9555984345,0.8653313302

C,0,-3.5769820474,2.7576718554,-2.3724935465

H,0,-2.2730742304,1.0631022995,-2.678633083

C,0,-4.5436398968,3.3452600087,-1.554533817

H,0,-5.7073886387,3.135177768,0.2570461781

H,0,-3.2546600819,3.2598987243,-3.2875687012

H,0,-4.9807310395,4.30953109,-1.822952396

C,0,2.3486925644,-1.1096969515,-0.1051223046

C,0,2.2978179202,-0.8799776242,-1.487072825

C,0,3.3060558636,-0.4009596239,0.6279924176

C,0,3.1657928075,0.0067559231,-2.1198381288

C,0,4.2088340196,0.4741851799,0.0257455138

C,0,4.1274500175,0.6662861552,-1.3515007013
H,0,3.0966854221,0.1757857479,-3.1944032176
H,0,4.9498776351,1.0031151001,0.6251431436
C,0,-1.625983593,-0.1164865695,0.4742795307
S,0,-1.9910165484,0.5662925687,2.0756293466
C,0,0.0819928568,1.3092172089,0.7298356572
C,0,-0.5419231723,1.5137407215,1.9907180022
N,0,-0.5567789335,0.4235768262,-0.0958020904
C,0,1.2575254278,2.0205873861,0.4256716628
C,0,1.8099254231,2.861233252,1.3831255904
H,0,1.7188810278,1.8851220007,-0.5545377714
C,0,0.0187708159,2.3533505861,2.9565221273
C,0,1.2014253489,3.021894893,2.6421120288
H,0,2.7305146599,3.4036046502,1.1559882531
H,0,-0.4601711525,2.4878542543,3.9278564767
H,0,1.6549540198,3.6855486095,3.3808509828
Cl,0,3.3778128986,-0.6021716753,2.3439793724
Cl,0,1.1146383737,-1.6910490844,-2.4523066493
Cl,0,5.2198491868,1.7562887321,-2.1201931335
C,0,-3.7253837632,-2.913575057,-0.3603715482
H,0,-3.5483471976,-2.9282073484,-1.4458420561
H,0,-4.7122844134,-3.3756123596,-0.1996711909
C,0,-2.6862875051,-3.774572979,0.34476573
H,0,-2.7300803849,-4.7890426768,-0.0817088089
H,0,-2.9656805477,-3.8803866211,1.4088660643
C,0,-1.2462980301,-3.2787909479,0.2799506484
H,0,-0.9443739485,-3.036784702,-0.7522517419
H,0,-0.5688168992,-4.0998137831,0.5819946005

5d (cyclic intermediate)
E(UMN15) = -3025.30961228
Thermal correction to Gibbs Energy= 0.380973
C,0,2.7354197246,0.6240947511,-0.4003801577
C,0,3.9170686311,1.5097966406,0.0370110071

H,0,4.8389978082,1.0482752645,-0.3476043956
H,0,3.9971296883,1.4801643516,1.1391708723
C,0,1.1244342234,2.1392974023,1.0953173864
H,0,1.7585777015,2.3325887332,1.9778563102
C,0,-0.3276115027,2.1034604736,1.6369929337
H,0,-0.4315982849,2.9028252729,2.3860812633
H,0,-0.5064687417,1.1403687716,2.1368145748
C,0,-1.3983433226,2.3868792871,0.6019186195
O,0,2.245854268,1.0936947657,-1.632838513
H,0,1.303709337,0.8364711442,-1.6783420559
O,0,-1.631155926,3.5205820298,0.2337818271
C,0,3.1608068707,-0.8449501259,-0.53434188
C,0,4.1324236757,-1.4174504968,0.3010395542
C,0,2.5346632332,-1.6657765225,-1.4806940808
C,0,4.4363842009,-2.7771823684,0.2204455771
H,0,4.6451610707,-0.8018439183,1.0428014441
C,0,2.8308393158,-3.0290340519,-1.5620976779
H,0,1.7924139345,-1.2351503421,-2.1554852884
C,0,3.7773623927,-3.5918641463,-0.7044478188
H,0,5.1907742593,-3.2025846219,0.8861062519
H,0,2.3194411811,-3.6504757935,-2.3007706192
H,0,4.0099667087,-4.6575002705,-0.7630734188
C,0,-2.2365229113,1.2717298467,0.0124761024
C,0,-2.2625288181,1.041292264,-1.3718432413
C,0,-3.1136811426,0.518163364,0.7997625858
C,0,-3.1117608212,0.1017765912,-1.9498245024
C,0,-3.9781136516,-0.4327422114,0.2553506787
C,0,-3.9667447602,-0.6290554155,-1.1227454609
H,0,-3.0987242795,-0.064602195,-3.0270440955
H,0,-4.6515053157,-0.9989239431,0.8987298672
C,0,1.5127593845,0.708470076,0.6213561221
S,0,1.8879911054,-0.2501881802,2.1686267976
C,0,0.151929887,-1.1426188708,0.4501664089
C,0,0.8764216543,-1.5381847912,1.6336087808

N,0,0.4355541879,0.0549384389,-0.0471577989
C,0,-0.7738353501,-2.062564967,-0.1261640175
C,0,-0.9382450738,-3.3076597772,0.4462617737
H,0,-1.3135599531,-1.765218051,-1.0266869261
C,0,0.7057838234,-2.802775859,2.1921718168
C,0,-0.2014854366,-3.6815932235,1.594860691
H,0,-1.6368949114,-4.0200383509,0.0034420776
H,0,1.2690478472,-3.1007328062,3.0779669295
H,0,-0.3427405733,-4.6762525718,2.0215673087
Cl,0,-3.1795748981,0.7912020598,2.5083613578
Cl,0,-1.182887121,1.898531653,-2.4147028087
Cl,0,-5.0146658355,-1.8069843925,-1.8216991978
C,0,3.8600012946,2.9481024066,-0.4694571761
H,0,3.7062646695,2.9204499591,-1.5579786302
H,0,4.8488850603,3.4040975683,-0.3025286711
C,0,2.8045877215,3.8361601542,0.175503059
H,0,2.8345035694,4.8247747145,-0.3098977792
H,0,3.0772283026,4.0094478955,1.2329399018
C,0,1.3690195923,3.3169665813,0.1447942514
H,0,1.0445627917,3.0743404264,-0.8774437267
H,0,0.7066515135,4.1279503768,0.4835808061

5d (TS2)

E(UMN15) = -3025.28969721

Thermal correction to Gibbs Energy= 0.378551

C,0,-2.9362789782,-0.4451726088,-0.576231019
C,0,-3.9000615033,-1.4524337255,0.0209540895
H,0,-4.9096273719,-1.0122734079,-0.063756739
H,0,-3.7258935494,-1.5474089963,1.1072780286
C,0,-1.0465471138,-2.1926102467,0.656123557
H,0,-1.8475430061,-2.3256176069,1.4026006858
C,0,0.2206979501,-2.6159150601,1.4411959839
H,0,0.052257309,-3.6370241425,1.8145025452
H,0,0.3462447617,-1.9440127026,2.2995599845

C,0,1.5025612784,-2.6768344367,0.6481439983
O,0,-2.6054348401,-0.7278368134,-1.8688567932
H,0,-1.6537332615,-0.4774801802,-1.9739026012
O,0,1.9574504101,-3.7379521561,0.2690015833
C,0,-3.1915704531,0.9875645208,-0.2971746322
C,0,-3.789808518,1.4092923597,0.9057371867
C,0,-2.79916353,1.9647981829,-1.228712454
C,0,-3.9586687189,2.7652454637,1.1766077658
H,0,-4.1094095227,0.6699176197,1.6433086375
C,0,-2.9628429747,3.3230542628,-0.9546742909
H,0,-2.3633229208,1.6503203875,-2.1786886134
C,0,-3.5356223414,3.7281044941,0.2527832521
H,0,-4.4210721046,3.0757161535,2.1161967785
H,0,-2.6422317576,4.0658680934,-1.6887359289
H,0,-3.6643963797,4.7904586659,0.4716257795
C,0,2.2254588479,-1.3996181877,0.2820176063
C,0,2.5010313008,-1.1152046877,-1.0686471509
C,0,2.7020586235,-0.485501385,1.2318320867
C,0,3.1942084143,0.0260010852,-1.4576049088
C,0,3.3861768848,0.677536271,0.8716655936
C,0,3.6224042402,0.9209890517,-0.4765916694
H,0,3.3734721109,0.2279215081,-2.5136944575
H,0,3.7383312171,1.3679867004,1.6380669099
C,0,-1.0666707087,-0.7068980525,0.3157286222
S,0,-0.9547164529,0.3288709647,1.7737454187
C,0,0.0319283994,1.0881781122,-0.4839929955
C,0,-0.2031307236,1.5698826341,0.8371182091
N,0,-0.3604461495,-0.1899269151,-0.7195283308
C,0,0.6203961569,1.951629089,-1.4368094334
C,0,0.9623926456,3.2409249119,-1.060809541
H,0,0.7871211656,1.5828989662,-2.4511544805
C,0,0.1441153631,2.8696276535,1.2102782488
C,0,0.7335834195,3.6966308477,0.2541528027
H,0,1.4204083065,3.9135163084,-1.7887904068

H,0,-0.046125589,3.2305605978,2.222644031
H,0,1.0146871187,4.7158700877,0.5267288717
Cl,0,2.5364259076,-0.7981192604,2.9276511246
Cl,0,1.9072236528,-2.1462367794,-2.3205380554
Cl,0,4.4382732735,2.3633613056,-0.9493038408
C,0,-3.911141577,-2.8134643188,-0.6791248145
H,0,-3.9844886439,-2.6260785411,-1.7601767165
H,0,-4.838521029,-3.3324149458,-0.3908766211
C,0,-2.7373289554,-3.7557141391,-0.4089397955
H,0,-2.8183015394,-4.6088610307,-1.1012003445
H,0,-2.8372904286,-4.1816026345,0.6059742064
C,0,-1.3396148153,-3.1453330788,-0.5155883785
H,0,-1.193781366,-2.6334314819,-1.4770977935
H,0,-0.5980279336,-3.9596097776,-0.4917977813

5d (shifted product)

E(UMN15) = -3025.32241033

Thermal correction to Gibbs Energy= 0.375964

C,0,-3.7969594542,-0.5100394736,-0.9060253016
C,0,-4.5546685888,-1.7506032962,-0.5469957857
H,0,-5.5887154135,-1.6505332663,-0.9323137202
H,0,-4.6607689316,-1.8211320651,0.5468060182
C,0,-1.2018019652,-1.6796035866,0.4911939483
H,0,-2.1430063822,-1.5241022222,1.0513366981
C,0,-0.2064407868,-2.2719687421,1.5234673719
H,0,-0.5918822002,-3.2457388911,1.8600005695
H,0,-0.1325183998,-1.606255645,2.3965053041
C,0,1.1798812283,-2.5226656953,0.9588244365
O,0,-3.2852296913,-0.4914456276,-2.1623348716
H,0,-2.3746885832,-0.1234465761,-2.1401889229
O,0,1.5631025304,-3.6384522581,0.6788839517
C,0,-3.7101659795,0.6605976269,-0.0955210008
C,0,-4.087442184,0.6788022047,1.279127567
C,0,-3.2099027205,1.8773264092,-0.6454125706

C,0,-3.9458496268,1.8287072861,2.0454915518
H,0,-4.4859498965,-0.2229234118,1.7481938091
C,0,-3.07275483,3.0190245327,0.1336581149
H,0,-2.9412811473,1.9154609782,-1.7035375204
C,0,-3.4334731537,3.0090879686,1.4877243443
H,0,-4.237056649,1.8070277382,3.0985241616
H,0,-2.6776260945,3.931723735,-0.3203236646
H,0,-3.3227547321,3.9074123759,2.0980518376
C,0,2.0799052644,-1.3314178075,0.685678327
C,0,2.431645767,-0.9780880106,-0.6260063521
C,0,2.602028323,-0.5419980242,1.7197436708
C,0,3.2046425261,0.1497589625,-0.905279148
C,0,3.3895579617,0.5803772407,1.4775903498
C,0,3.6660184379,0.926066164,0.1549660235
H,0,3.4313964398,0.4188201107,-1.9371338677
H,0,3.7718087568,1.1763384681,2.3062107262
C,0,-0.7504843828,-0.312733734,0.0467391345
S,0,-0.3625951989,0.8824044074,1.2611619306
C,0,0.0070831199,1.3284197732,-1.2368314821
C,0,0.212651514,1.9391746362,0.0200879287
N,0,-0.5619597567,0.0668984954,-1.1791787208
C,0,0.4261751999,1.9813803331,-2.4054161796
C,0,1.0477325091,3.220430618,-2.292872196
H,0,0.2752891963,1.5003710684,-3.3737311177
C,0,0.8233194976,3.1920663441,0.1351716874
C,0,1.2430677078,3.8201635995,-1.0343383802
H,0,1.3913032337,3.7362045498,-3.1917207182
H,0,0.9809882222,3.6547641518,1.1110338412
H,0,1.7385327175,4.7911683646,-0.9726195847
Cl,0,2.2614654666,-0.9598848734,3.3634985349
Cl,0,1.879119106,-1.92227116,-1.961221139
Cl,0,4.597168143,2.3391957732,-0.1742057247
C,0,-3.9744010092,-3.0571543892,-1.0969970049
H,0,-3.8089440432,-2.9365923534,-2.1798720903

H,0,-4.7433310479,-3.8375527682,-0.9850750406
C,0,-2.6814463129,-3.5602664395,-0.4521434729
H,0,-2.4704278005,-4.5550156019,-0.8739443055
H,0,-2.8410550561,-3.7247034217,0.6300212387
C,0,-1.4535735775,-2.6637438742,-0.6640069013
H,0,-1.5542044822,-2.115248836,-1.6099748672
H,0,-0.5563317904,-3.2906308651,-0.7813984261

*Stationary Points for Shifts of Radical **5j***

5j Ph pathway (extended conformation)
E(UMN15) = -2837.42621
Thermal correction to Gibbs Free Energy= 0.24928
C 0.00000000 0.00000000 0.00000000
C 1.18934000 -0.28817900 0.86473100
H 1.05270800 -0.31765400 1.94569400
C 2.55071800 -0.09500600 0.32220900
H 2.69188800 0.92456800 -0.10065700
H 2.75848300 -0.75756500 -0.53939100
C 3.64876000 -0.28922300 1.33173000
O 3.46761800 -0.55320100 2.49850700
C 5.05396300 -0.12158200 0.79082500
C 5.69162100 1.12187100 0.80760100
C 6.99202400 1.29229500 0.33767400
C 7.66327500 0.17776800 -0.16480000
C 7.06314600 -1.08037500 -0.21075200
C 5.76123400 -1.20770400 0.26837700
Cl 4.98583800 -2.75486400 0.21169100
H 7.59568000 -1.94360200 -0.61147300
Cl 9.27802400 0.36168300 -0.74961400
H 7.46900700 2.27269500 0.36225500
Cl 4.82866200 2.49085800 1.42358200
O 0.38604400 -0.24492000 -1.33541700

H -0.32846400 0.06441200 -1.91756300
C -1.22448200 -0.85173200 0.36443200
C -1.16923700 -1.85086100 1.34413900
C -2.28135200 -2.63414600 1.66107100
C -3.48833200 -2.43523600 0.99241400
C -3.57343400 -1.45583200 0.00239100
C -2.45213600 -0.68468700 -0.29795900
Cl -2.62616300 0.50778700 -1.56213000
H -4.50259000 -1.28407800 -0.54431300
H -4.36506600 -3.04046300 1.23212400
H -2.19845600 -3.40239500 2.43265000
H -0.22840700 -2.02528700 1.86938000
C -0.27458700 1.49541100 0.24269500
C 0.25195100 2.45466800 -0.63127500
C 0.06846200 3.81637000 -0.37627200
C -0.63945600 4.23275200 0.75326100
C -1.16023100 3.27741400 1.63198300
C -0.97684900 1.91737800 1.38050600
H -1.38297400 1.17427200 2.07332800
H -1.71484800 3.59375800 2.51874900
H -0.78541200 5.29743500 0.94983800
H 0.47896700 4.55563100 -1.06851600
H 0.79850100 2.12907500 -1.51933900

5j Ph pathway (folded conformation)

E(UMN15) = -2837.43158

Thermal correction to Gibbs Free Energy= 0.25341

C 0.00000000 0.00000000 0.00000000
C 0.70790100 -1.14109300 0.67229200
H 0.63971300 -1.19457300 1.75881500
C 1.59503200 -2.08831100 -0.05222800
H 1.69143000 -1.76395800 -1.10012300
H 1.19994800 -3.12001400 -0.04053000
C 2.97573500 -2.14648600 0.56739700

O	3.45550900	-3.14802800	1.04711500
C	3.75468000	-0.84418900	0.58786900
C	3.87411600	-0.07951100	1.75497300
C	4.60380000	1.10565500	1.79047000
C	5.23713900	1.52955900	0.62333300
C	5.16452400	0.79372400	-0.55692000
C	4.41832000	-0.38328400	-0.55293800
Cl	4.31047100	-1.30278200	-2.01848100
H	5.66495800	1.13323200	-1.46450000
Cl	6.08472100	3.03401100	0.63177600
H	4.66079800	1.69581000	2.70580000
Cl	3.07626800	-0.59835400	3.20086400
O	0.05483100	-0.21928000	-1.39010500
H	-0.30879600	0.56425100	-1.83638800
C	-1.46718600	0.11666300	0.45651200
C	-2.04843800	-0.80886500	1.33263700
C	-3.38383400	-0.71158700	1.73009700
C	-4.18101600	0.32596900	1.24951800
C	-3.63670000	1.25760900	0.36535400
C	-2.30174000	1.14287700	-0.01834700
Cl	-1.70125300	2.33402400	-1.14590900
H	-4.23972800	2.07442500	-0.03573200
H	-5.22623400	0.41349700	1.55319000
H	-3.79800700	-1.45325600	2.41619500
H	-1.44136900	-1.63313400	1.71161500
C	0.78957500	1.25887600	0.40764600
C	1.69347800	1.84749400	-0.48542800
C	2.41909000	2.97960000	-0.10768700
C	2.26445000	3.52422200	1.16971000
C	1.38296000	2.92241500	2.07284800
C	0.64860600	1.79680700	1.69381200
H	-0.04468700	1.33252400	2.40196900
H	1.26076500	3.33518700	3.07726600
H	2.83947900	4.40561000	1.46414600

H 3.12331200 3.43070100 -0.81187600

H 1.82316100 1.41869500 -1.48227600

5j Ph pathway (TS1)

E(UMN15) = -2837.41436

Thermal correction to Gibbs Free Energy= 0.25186

C 0.00000000 0.00000000 0.00000000

C -0.03069100 -1.83643500 -0.37117500

C 1.02901500 -0.80059000 -0.69449400

H 0.10389800 0.12109400 1.07901200

C -0.91834400 0.91185800 -0.74668200

H -1.10808000 0.50413400 -1.75228200

H -0.47040100 1.91335000 -0.87056000

C -2.23926300 1.09737200 -0.03775900

O -2.60591400 2.15673500 0.41783500

C -3.12740900 -0.12553900 0.09945500

C -3.23457700 -0.82511800 1.30626100

C -4.09034400 -1.91421600 1.45674900

C -4.86204100 -2.30675900 0.36466300

C -4.79944800 -1.63403300 -0.85411000

C -3.92550300 -0.55537000 -0.96523400

Cl -3.81854700 0.27642100 -2.48167100

H -5.40622300 -1.94894500 -1.70387400

Cl -5.89698300 -3.68135300 0.51732600

H -4.14218700 -2.45228700 2.40395100

Cl -2.26938800 -0.34104600 2.65913600

O 1.13952600 -0.47810100 -2.04588700

H 1.48178900 -1.26010600 -2.51328300

C 2.37005900 -0.98885000 -0.02009800

C 2.86278600 -0.08219400 0.92367500

C 4.11539100 -0.26188800 1.51475500

C 4.89825400 -1.36362200 1.16749300

C 4.43209500 -2.28166200 0.22434700

C 3.18137900 -2.08257700 -0.35546400

Cl 2.62436600 -3.23244200 -1.54259900
H 5.02978000 -3.14789400 -0.06547600
H 5.87750700 -1.51386800 1.62693900
H 4.47907800 0.46156500 2.24727600
H 2.25097800 0.78179700 1.19505300
C -0.94489400 -2.26203900 -1.39168400
C -1.81246800 -3.31833100 -1.15919600
C -1.79751500 -4.01752300 0.05907600
C -0.86859700 -3.64647800 1.05096500
C 0.01047500 -2.59905700 0.84582300
H 0.73605600 -2.32571100 1.61714600
H -0.83062400 -4.19961300 1.99310100
H -2.49489000 -4.83996800 0.23219500
H -2.51095400 -3.61639000 -1.94614500
H -0.94834400 -1.74652800 -2.35460200

5j Ph pathway (cyclic intermediate)
E(UMN15) = -2837.42431
Thermal correction to Gibbs Free Energy= 0.25454
C 0.00000000 0.00000000 0.00000000
C -0.11609200 -1.52123700 -0.22104900
C 1.08521900 -0.65543000 -0.76620300
H 0.25316200 0.24553800 1.03621500
C -0.91299600 1.00042400 -0.67268500
H -1.09567500 0.69350700 -1.71536500
H -0.44525900 1.99585800 -0.69271100
C -2.25313300 1.14360300 0.00992800
O -2.68396000 2.19561700 0.42362100
C -3.06810100 -0.12903600 0.13950900
C -3.03659600 -0.89896400 1.30604200
C -3.72189100 -2.10634200 1.41386400
C -4.47624600 -2.53772600 0.32301500
C -4.56986700 -1.78514300 -0.84625200
C -3.85340600 -0.59293600 -0.91901500

Cl -3.90159600 0.32497500 -2.38793500
H -5.16572700 -2.12952100 -1.69223200
Cl -5.29419200 -4.05615200 0.41759200
H -3.66050700 -2.70106700 2.32608900
Cl -2.10132400 -0.34696800 2.65368300
O 1.07969100 -0.41246900 -2.12659400
H 1.33536100 -1.23305800 -2.58413000
C 2.43080700 -0.89952200 -0.15698200
C 3.01758600 -0.01098700 0.75124500
C 4.27635000 -0.26684400 1.29931400
C 4.96915900 -1.42582700 0.94438500
C 4.40462000 -2.33104700 0.04318800
C 3.14699700 -2.05929600 -0.49014300
Cl 2.43573900 -3.20324800 -1.59625500
H 4.92838900 -3.24510300 -0.24265600
H 5.95355600 -1.63310200 1.36944600
H 4.71676500 0.44203600 2.00349900
H 2.47450200 0.89653100 1.02728400
C -0.98999100 -2.09056800 -1.25713600
C -1.45352400 -3.38114000 -1.16394900
C -1.14143500 -4.20318800 -0.05508000
C -0.35434700 -3.67121800 0.99622800
C 0.13226700 -2.38896800 0.94070100
H 0.72702500 -1.98031900 1.76268500
H -0.13657100 -4.28888600 1.87175100
H -1.52192700 -5.22444800 -0.00005900
H -2.09028300 -3.77502800 -1.96140700
H -1.25028400 -1.47734900 -2.12270300

5j Ph pathway (TS2)

E(UMN15) = -2837.42162

Thermal correction to Gibbs Free Energy= 0.25381

C 0.00000000 0.00000000 0.00000000
C -1.14082700 0.54500900 -0.76415600

O	-1.07373100	0.41130900	-2.11855700
H	-1.45016600	1.20503800	-2.54100600
C	-2.44698300	0.83546900	-0.13265000
C	-2.99217600	0.00419300	0.85880200
C	-4.21607000	0.30010100	1.45873900
C	-4.92259000	1.44456500	1.08067200
C	-4.39735000	2.29909800	0.10967800
C	-3.17020600	1.99256200	-0.47283100
Cl	-2.49096000	3.10608900	-1.62854700
H	-4.92406800	3.20771300	-0.18796900
H	-5.88212900	1.68127600	1.54509900
H	-4.62219600	-0.36906900	2.22010700
H	-2.44628900	-0.89669600	1.14977300
C	0.20737300	1.49933200	-0.09834200
C	0.96982900	2.11729400	-1.15890900
C	1.27518600	3.46530700	-1.11714500
C	0.88479000	4.27149000	-0.03069500
C	0.18998000	3.67939000	1.04475800
C	-0.12467400	2.33541900	1.03352500
H	-0.64397900	1.87794100	1.88071000
H	-0.08999000	4.28727800	1.90944000
H	1.13519400	5.33386600	-0.01105200
H	1.84660800	3.90558000	-1.93939200
H	1.29630900	1.51359900	-2.00882600
H	-0.26169200	-0.29455400	1.02256400
C	0.93612700	-0.98521100	-0.67752400
H	1.13686600	-0.65418400	-1.70957400
H	0.47024300	-1.97990600	-0.72779200
C	2.26527500	-1.13748900	0.02624100
O	2.68946400	-2.19551400	0.43094000
C	3.06989100	0.13803500	0.18744700
C	3.00794500	0.89161600	1.36321100
C	3.64241200	2.12503100	1.48592900
C	4.38610800	2.59591300	0.40380300

C 4.51701300 1.85759000 -0.77125000
C 3.84465600 0.64093600 -0.86076900
Cl 3.93436000 -0.25767800 -2.33967500
H 5.10702400 2.23053700 -1.60923400
Cl 5.14738200 4.14175300 0.51905000
H 3.55274400 2.70782800 2.40348900
Cl 2.08060500 0.29230000 2.69578700

5j Ph pathway (shifted product)

E(UMN15) = -2837.45315

Thermal correction to Gibbs Free Energy= 0.25337

C 0.00000000 0.00000000 0.00000000
C 1.34117300 0.31477600 -0.61577100
O 1.22718600 1.30974000 -1.51009500
H 2.07009000 1.49656500 -1.96075900
C 2.54047200 -0.40405500 -0.34954600
C 2.52542000 -1.49791500 0.58034800
C 3.64707300 -2.24720400 0.88688700
C 4.88322000 -1.96699500 0.28683500
C 4.95476800 -0.91333700 -0.62542700
C 3.82835000 -0.16025600 -0.93395100
Cl 4.10330900 1.12989700 -2.09255900
H 5.89843200 -0.66080500 -1.11376500
H 5.77333800 -2.55278600 0.52120800
H 3.55796200 -3.06526300 1.60507600
H 1.58903700 -1.75944600 1.07178300
H 0.14389900 -0.59670200 0.90850200
C -0.67814400 1.32490000 0.41775400
H -0.91074900 1.92095100 -0.47847600
H 0.02438600 1.90643700 1.03209100
C -1.94221300 1.17319700 1.22989000
O -2.03943900 1.55575800 2.37460800
C -3.11742500 0.51030600 0.53988400
C -3.44014300 -0.82572600 0.79943100

C -4.43881200 -1.49510200 0.09674300
C -5.15436100 -0.78870200 -0.86992300
C -4.90344000 0.55837400 -1.12660000
C -3.88170700 1.18462900 -0.41664000
Cl -3.53654800 2.84970500 -0.75026400
H -5.47929300 1.10598300 -1.87357100
Cl -6.37617700 -1.60725300 -1.77459600
H -4.64920500 -2.54653000 0.29570500
Cl -2.53918400 -1.69219300 1.99595300
C -0.78134400 -0.85632300 -0.99254500
C -1.44067100 -0.29319800 -2.09461500
C -2.14496200 -1.10042700 -2.99084400
C -2.18825200 -2.48582400 -2.80796500
C -1.51143500 -3.05860100 -1.72818700
C -0.81168700 -2.24881500 -0.83060900
H -0.29744100 -2.69892300 0.02294300
H -1.53323700 -4.14075000 -1.57819100
H -2.74592300 -3.11526400 -3.50549800
H -2.66791900 -0.64228100 -3.83414800
H -1.42363500 0.78938000 -2.24772300

5j 2-ClPh pathway (extended conformation)

E(UMN15) = -2837.41994

Thermal correction to Gibbs Free Energy= 0.24982

C 0.00000000 0.00000000 0.00000000
C 1.04670400 -0.86853700 -0.62886200
H 0.84919600 -1.36458500 -1.57849500
C 2.44397600 -0.74492100 -0.15242200
H 2.71662300 -1.53476100 0.58187300
H 2.60766800 0.19855000 0.39888800
C 3.47028600 -0.88416100 -1.25061500
O 3.24329200 -1.38955600 -2.32607000
C 4.85167000 -0.36465400 -0.91991900

C 5.88386800 -1.21004700 -0.50599400
C 7.15881900 -0.72638500 -0.21827600
C 7.39486700 0.64140200 -0.35504500
C 6.39311400 1.52244600 -0.76331000
C 5.13138500 0.99996600 -1.03671100
Cl 3.85605900 2.05881400 -1.53949500
H 6.58972300 2.59028800 -0.86625600
Cl 8.96893400 1.26160100 -0.00582400
H 7.94940000 -1.40330200 0.10743100
Cl 5.56175300 -2.90086900 -0.32724400
O 0.18644700 -0.09943700 1.39479000
H -0.36950800 0.56289100 1.83712300
C 0.26998800 1.41160300 -0.57692900
C 0.77790600 2.53568900 0.08812100
C 1.01957500 3.73989900 -0.58992600
C 0.78161900 3.84228500 -1.95465500
C 0.29048500 2.73104800 -2.64857500
C 0.04275500 1.54964400 -1.96139700
H -0.34518000 0.68321800 -2.50499500
H 0.09933500 2.78700900 -3.72215600
H 0.97978100 4.78289200 -2.47281400
H 1.40910800 4.58804800 -0.02348100
Cl 1.17201500 2.56560100 1.78979300
C -1.43073700 -0.44112900 -0.32559600
C -1.72682600 -1.77750700 -0.61751400
C -3.05045500 -2.18840600 -0.79664700
C -4.09434300 -1.26846600 -0.67716300
C -3.80791500 0.06568300 -0.37444400
C -2.48474100 0.47508100 -0.20220600
H -2.26730400 1.52215700 0.03028900
H -4.61816800 0.79204600 -0.27585100
H -5.12894400 -1.58972300 -0.81868200
H -3.26557700 -3.23408500 -1.02943800
H -0.91729900 -2.50731300 -0.69902500

5j 2-ClPh pathway (folded conformation)

E(UMN15) = -2837.42405

Thermal correction to Gibbs Free Energy= 0.25231

C 0.00000000 0.00000000 0.00000000
C 0.64000100 -0.55951900 1.23763400
H 0.78818600 0.14559500 2.05731500
C 1.18244400 -1.94417300 1.33660800
H 1.10326200 -2.46178700 0.36830000
H 0.62731100 -2.53136300 2.09135700
C 2.62640200 -1.91259100 1.80156100
O 2.93798500 -1.99248600 2.96802200
C 3.68680200 -1.71682800 0.73993600
C 4.40616400 -0.52015300 0.63702800
C 5.40583700 -0.34241600 -0.31693800
C 5.69023000 -1.39360100 -1.18643200
C 5.01535800 -2.61051500 -1.10935000
C 4.02068900 -2.74839200 -0.14411900
Cl 3.17884700 -4.25892100 -0.02574400
H 5.25105400 -3.43056100 -1.78855300
Cl 6.88213700 -1.16535900 -2.41541600
H 5.93558500 0.60789900 -0.39244900
Cl 4.02563300 0.79645400 1.68878000
O -0.73360200 1.13256600 0.41265100
H -1.07852900 1.57740200 -0.37935700
C 1.17608100 0.35308300 -0.93671800
C 1.89019200 1.56540700 -0.89077900
C 2.97095500 1.80650400 -1.74714600
C 3.39067700 0.83406100 -2.65018100
C 2.73247100 -0.39701600 -2.68231800
C 1.64981200 -0.62264800 -1.83573700
H 1.14090900 -1.58941300 -1.87394400
H 3.06188600 -1.18456700 -3.36386800
H 4.24355200 1.02863900 -3.30460200

H 3.48379200 2.76801500 -1.67970000
Cl 1.54504900 2.84123900 0.24001600
C -1.01403000 -0.94246200 -0.66792800
C -1.69172200 -1.91578500 0.07601600
C -2.72526800 -2.66130600 -0.49786600
C -3.10549300 -2.43329500 -1.82153100
C -2.45172500 -1.44691000 -2.56519600
C -1.41610500 -0.70804200 -1.99166600
H -0.91437400 0.06258500 -2.58403400
H -2.74845500 -1.25141400 -3.59839600
H -3.91230600 -3.01676400 -2.27111100
H -3.23794700 -3.42090100 0.09707100
H -1.42412200 -2.08690700 1.12137000

5j 2-ClPh pathway (TS1)

E(UMN15) = -2837.40594

Thermal correction to Gibbs Free Energy= 0.25203

C 0.00000000 0.00000000 0.00000000
C 0.30766100 0.46585200 -1.80810800
C -0.99938600 0.33742300 -1.03540500
H 0.31910400 0.85623500 0.59919400
C 0.34943100 -1.37851400 0.46052500
H 0.18582000 -2.11091900 -0.34639900
H -0.27902600 -1.67528800 1.31851100
C 1.78527500 -1.46780100 0.93079100
O 2.08634500 -1.59313800 2.09595200
C 2.87393000 -1.37668400 -0.11965900
C 3.64484100 -0.21932900 -0.27432400
C 4.68748900 -0.14458000 -1.19540100
C 4.96246000 -1.26358800 -1.97896400
C 4.23077000 -2.44309100 -1.85206300
C 3.19401900 -2.47591500 -0.92299600
Cl 2.26922100 -3.93231600 -0.75883500
H 4.45417600 -3.31472500 -2.46814600

Cl 6.22135000 -1.17458000 -3.15844500
H 5.26063400 0.77626900 -1.30952200
Cl 3.28383300 1.17646700 0.68007100
O -1.68468000 1.51381800 -0.73609000
H -2.09021200 1.84600000 -1.55467000
C 1.06533200 1.68454400 -1.95930900
C 2.14690300 1.76795900 -2.82442300
C 2.54316600 0.67342000 -3.60346300
C 1.83224100 -0.53200900 -3.48609700
C 0.75162100 -0.63281600 -2.63019100
H 0.20704400 -1.57744700 -2.56788000
H 2.12522400 -1.40205900 -4.07895400
H 3.40185900 0.75657000 -4.27228700
H 2.68840100 2.71493800 -2.88051300
Cl 0.73004100 3.09916500 -1.00941000
C -1.97899600 -0.70771900 -1.52891800
C -2.65137200 -1.53512200 -0.62160400
C -3.65709900 -2.39772600 -1.06445600
C -4.00694800 -2.43130100 -2.41644900
C -3.35302000 -1.59338000 -3.32429200
C -2.34518300 -0.73521000 -2.88172300
H -1.83163600 -0.08142000 -3.59318600
H -3.62822000 -1.60916000 -4.38144100
H -4.79261500 -3.10691600 -2.76270500
H -4.17237500 -3.04287200 -0.34896600
H -2.39609100 -1.49593000 0.44006200

5j 2-ClPh pathway (cyclic intermediate)

E(UMN15) = -2837.41709

Thermal correction to Gibbs Free Energy= 0.25424

C 0.00000000 0.00000000 0.00000000
C 0.38385800 0.28355100 -1.46411400
C -1.11210600 0.24634200 -0.94885500
H 0.18518400 0.87223600 0.63572000

C 0.24001100 -1.33035400 0.68548200
H -0.02199400 -2.16762500 0.01806100
H -0.39386600 -1.40769600 1.58107800
C 1.66930500 -1.53533700 1.13600500
O 1.98429000 -1.69267300 2.29329700
C 2.71861300 -1.55333200 0.04206200
C 3.48366400 -0.41859200 -0.24584800
C 4.40863000 -0.39533700 -1.28680700
C 4.57804500 -1.55283900 -2.04572600
C 3.86672300 -2.71991300 -1.77143200
C 2.94179800 -2.69618500 -0.73079700
Cl 2.00940700 -4.12102700 -0.40821800
H 4.01273900 -3.62201600 -2.36636700
Cl 5.68061200 -1.53113800 -3.37495300
H 4.97476800 0.51054300 -1.50744200
Cl 3.25286200 1.00826600 0.70209500
O -1.76780700 1.44956900 -0.77571900
H -2.22594000 1.67249800 -1.60357400
C 1.00710300 1.57724100 -1.82615600
C 1.78516400 1.72862800 -2.95252800
C 2.06985700 0.64005400 -3.80125000
C 1.57875600 -0.64280900 -3.45640900
C 0.80228700 -0.82801400 -2.34235900
H 0.45045700 -1.83273000 -2.09594000
H 1.83787100 -1.50611200 -4.07500200
H 2.68938400 0.78385100 -4.68735400
H 2.20119300 2.71586700 -3.16668100
Cl 0.80429800 2.95581800 -0.79745500
C -2.01394500 -0.83878000 -1.46307600
C -2.72198600 -1.66009000 -0.57534000
C -3.64651000 -2.58846000 -1.05974200
C -3.87691900 -2.69596400 -2.43371500
C -3.18493300 -1.86960900 -3.32380100
C -2.25771200 -0.94524400 -2.83992800

H -1.71011000 -0.29864400 -3.53218200
H -3.36707300 -1.94724300 -4.39819600
H -4.59980000 -3.42273500 -2.81180200
H -4.19204400 -3.22723000 -0.36117700
H -2.55388100 -1.56435900 0.50035200

5j 2-ClPh pathway (TS2)

E(UMN15) = -2837.41422

Thermal correction to Gibbs Free Energy= 0.25337

C 0.00000000 0.00000000 0.00000000
C -0.44412600 0.24486500 1.42590600
C -0.91899000 1.54204600 1.87276600
C -1.48352600 1.72448100 3.12424800
C -1.67143000 0.64362600 4.00020300
C -1.29770500 -0.64795700 3.57467000
C -0.72877100 -0.84809700 2.33502500
H -0.46228800 -1.86317700 2.02933300
H -1.47693300 -1.50933600 4.22355400
H -2.12346900 0.80379800 4.98021800
H -1.80403700 2.72969800 3.40789600
Cl -0.80962800 2.92460900 0.82790100
C 1.23581600 0.20084500 0.78609300
O 1.82481200 1.42121700 0.65832300
H 2.47141400 1.54112000 1.37538200
C 2.08269000 -0.87060200 1.37368200
C 2.60076700 -1.92423100 0.60601700
C 3.45032800 -2.86721200 1.19011600
C 3.79535900 -2.76294900 2.53973800
C 3.29079600 -1.71038300 3.30958000
C 2.43625200 -0.77277700 2.73058000
H 2.01942600 0.04116800 3.33327700
H 3.55634400 -1.62629300 4.36586400
H 4.46052900 -3.50187100 2.99258600
H 3.85189600 -3.68246100 0.58382400

H 2.35673000 -1.99555800 -0.45602300
H -0.19826000 0.87367500 -0.63237800
C -0.29645500 -1.31548800 -0.70853000
H -0.03927000 -2.16867200 -0.06044200
H 0.31169300 -1.38959600 -1.62153700
C -1.74484000 -1.47737200 -1.11562000
O -2.10285600 -1.57674300 -2.26670900
C -2.75110100 -1.52596400 0.01765100
C -3.49491700 -0.39488800 0.36896000
C -4.35174900 -0.38389300 1.46695700
C -4.48269500 -1.55418600 2.21444800
C -3.79550500 -2.71918000 1.87676400
C -2.93369000 -2.68066800 0.78330500
Cl -2.03141900 -4.10511700 0.38261100
H -3.91280000 -3.63228700 2.46122600
Cl -5.51405700 -1.55538100 3.59942000
H -4.90023600 0.52001800 1.73483800
Cl -3.31235500 1.04620100 -0.56604400

5j 2-ClPh pathway (shifted product)

E(UMN15) = -2837.44589

Thermal correction to Gibbs Free Energy= 0.25476

C 0.00000000 0.00000000 0.00000000
C -0.83458800 0.30001800 1.24413900
C 1.45285400 0.09698000 0.40306800
H -0.16073300 0.82915900 -0.70690900
C -0.40715100 -1.30417700 -0.70737800
H -0.35140900 -2.15078700 -0.01096600
H 0.28071500 -1.48946000 -1.54446000
C -1.80620600 -1.26199700 -1.28682500
O -2.02037900 -1.06748500 -2.46203600
C -2.95061900 -1.45785900 -0.31262800
C -3.81522900 -0.40061500 0.00252100
C -4.80249800 -0.51855900 0.97840100

C	-4.94851500	-1.74167100	1.63181100
C	-4.15040900	-2.83866100	1.31224000
C	-3.16372500	-2.67632500	0.34247400
Cl	-2.19088000	-4.04983700	-0.07369000
H	-4.29032500	-3.80067500	1.80644100
Cl	-6.15382200	-1.90268300	2.85704000
H	-5.44295300	0.32942400	1.22416900
Cl	-3.63890400	1.11395200	-0.80779200
O	1.79599200	1.39841100	0.54533200
H	2.74490900	1.48086500	0.74143300
C	-1.34462000	1.57680400	1.52535400
C	-2.13116100	1.81847700	2.65658700
C	-2.40168300	0.78386700	3.54911600
C	-1.86843400	-0.48776300	3.31680200
C	-1.09191000	-0.71346800	2.18261800
H	-0.67940000	-1.71227400	2.00936200
H	-2.06091000	-1.30454100	4.01593900
H	-3.02033900	0.97494200	4.42864000
H	-2.52451600	2.82291100	2.82468100
Cl	-1.04437800	2.92259600	0.46715100
C	2.33715800	-0.90778400	0.92227600
C	2.30391500	-2.28689500	0.56446900
C	3.22488500	-3.18875500	1.08394000
C	4.22175700	-2.77633300	1.97806600
C	4.27641600	-1.42788100	2.34672700
C	3.35891800	-0.51571600	1.83807100
H	3.40827900	0.51511100	2.19937700
H	5.03441600	-1.08259000	3.05423600
H	4.94193800	-3.49301800	2.37783700
H	3.17280400	-4.23493000	0.77208700
H	1.58729900	-2.65312000	-0.16667900

*Stationary Points for Shifts of Radical **5k***

5k Ph pathway (extended conformation)

E(UMN15) = -2714.82331

Thermal correction to Gibbs Free Energy= 0.26242

C	0.00000000	0.00000000	0.00000000
C	1.06082000	-0.60977400	0.86542200
H	0.85030200	-0.75856300	1.92422200
C	2.43188600	-0.81131300	0.34840500
H	2.60183200	-0.24022600	-0.58117500
H	2.62604300	-1.86580700	0.05404500
C	3.52346900	-0.45617200	1.32618300
O	3.33078500	-0.10596500	2.46907700
C	4.93063400	-0.55084600	0.77583600
C	5.50650400	0.53740500	0.11424300
C	6.80186100	0.49118200	-0.39535000
C	7.53088800	-0.68759400	-0.23648100
C	6.99264200	-1.80181600	0.40705000
C	5.69371400	-1.71392300	0.90364500
Cl	4.99281400	-3.08645500	1.69212800
H	7.57023000	-2.72003400	0.51946700
Cl	9.14103900	-0.77026100	-0.85636400
H	7.23078800	1.35450900	-0.90526800
Cl	4.56981400	1.98247000	-0.07897800
O	0.28919700	-0.35943700	-1.33882400
H	-0.30029200	0.13708900	-1.92995700
C	-1.35962800	-0.56457700	0.44743200
C	-1.85462900	-1.82018600	0.02651100
C	-3.09189600	-2.27444600	0.50236200
C	-3.83789500	-1.52720800	1.41194900
C	-3.33645200	-0.31018500	1.86544200
C	-2.11386100	0.15669900	1.38217000
H	-1.73239100	1.11482100	1.74087600

H -3.89430800 0.28449300 2.59208700
H -4.79873200 -1.90424000 1.76763000
H -3.47460000 -3.23681400 0.16215500
C -1.12982300 -2.75411100 -0.92401400
F -1.66220800 -3.98713600 -0.87423000
F -1.22098700 -2.37721500 -2.20460200
F 0.16335200 -2.90892200 -0.62640800
C 0.02389800 1.53903300 0.07138900
C 0.96522500 2.23696600 0.83256400
C 1.00636000 3.63589600 0.80233600
C 0.10238700 4.34860100 0.01528300
C -0.85018800 3.65730800 -0.74211400
C -0.88919600 2.26449200 -0.71106800
H -1.65141400 1.73649600 -1.29520100
H -1.56776000 4.20720500 -1.35559500
H 0.13442900 5.44035600 -0.00784600
H 1.75234600 4.16606700 1.39942200
H 1.67571700 1.68902400 1.45750000

5k Ph pathway (folded conformation)

E(UMN15) = -2714.82908

Thermal correction to Gibbs Free Energy= 0.26592

C 0.00000000 0.00000000 0.00000000
C 0.81124100 -1.10558800 0.62141500
H 0.76169100 -1.20162500 1.70613800
C 1.70320400 -2.00684400 -0.15185300
H 1.67963300 -1.71403500 -1.21357200
H 1.40014500 -3.06617400 -0.07507400
C 3.14395700 -1.93386700 0.31155700
O 3.79694500 -2.89766800 0.63910800
C 3.75441900 -0.54484000 0.35715900
C 3.87635500 0.15810200 1.56170200
C 4.44891400 1.42534100 1.62485000
C 4.91771300 1.99915800 0.44374400

C 4.83187700 1.33366900 -0.77672200
C 4.24711600 0.06825900 -0.79796900
Cl 4.12879600 -0.76823100 -2.31106900
H 5.20144800 1.79060900 -1.69522000
Cl 5.57868800 3.59414500 0.49336900
H 4.51267100 1.95938400 2.57362300
Cl 3.27766100 -0.55228100 3.02200400
O 0.11971300 -0.13420100 -1.39572100
H -0.38277300 0.57522800 -1.82425400
C -1.49096200 -0.09083100 0.41830900
C -1.94241200 -1.29344200 0.97624200
C -3.26843700 -1.49257000 1.36302000
C -4.19637100 -0.47018800 1.19573700
C -3.78341600 0.73009700 0.62057400
C -2.45517600 0.93105900 0.22462600
C -2.17339400 2.28327300 -0.39655000
F -1.60696500 3.15093500 0.44598500
F -3.29267600 2.86469400 -0.83515800
F -1.36165000 2.19883300 -1.47156900
H -4.51134700 1.52771700 0.46971500
H -5.23709100 -0.60031100 1.49828600
H -3.56729200 -2.44985500 1.79553100
H -1.22801500 -2.10815900 1.11150300
C 0.64584300 1.29319900 0.52247900
C 1.36718700 2.13216300 -0.33191300
C 1.93057200 3.31495100 0.15477600
C 1.80180700 3.65442500 1.50280200
C 1.11212500 2.79797500 2.36833700
C 0.53639700 1.62550200 1.88062500
H -0.01973500 0.96700900 2.55552100
H 1.01460600 3.05089400 3.42695700
H 2.24877200 4.57676800 1.88182600
H 2.48954000 3.96624600 -0.52215700
H 1.47657200 1.86260400 -1.38485300

5k Ph pathway (TS1)

E(UMN15) = -2714.81242

Thermal correction to Gibbs Free Energy= 0.26403

C	0.00000000	0.00000000	0.00000000
C	-0.12082400	-1.86146700	0.12573700
C	-1.13141200	-0.80177800	0.51746500
H	-0.01800100	0.26780600	-1.05680600
C	0.93259500	0.71819200	0.91878000
H	1.04771700	0.14092100	1.85067400
H	0.54420900	1.71458900	1.19272900
C	2.30111200	0.92352100	0.31456100
O	2.78517700	2.01687900	0.12778500
C	3.10011300	-0.31218400	-0.06381100
C	3.22491900	-0.72653900	-1.39424100
C	4.03222700	-1.80002900	-1.76507100
C	4.73888100	-2.47188400	-0.76952700
C	4.65457900	-2.09200300	0.56857900
C	3.82920300	-1.01964500	0.89758600
Cl	3.69446500	-0.55680800	2.56151800
H	5.20617900	-2.62623800	1.34299900
Cl	5.71640600	-3.82921700	-1.20150000
H	4.09731300	-2.11066900	-2.80848700
Cl	2.34128700	0.10577800	-2.62858100
O	-1.29830300	-0.61055900	1.88799100
H	-1.77891300	-1.37141100	2.25110900
C	-2.44356400	-0.74356600	-0.24766900
C	-2.77877500	0.45284600	-0.89119300
C	-3.99395900	0.61359400	-1.55795800
C	-4.90918900	-0.43647900	-1.59212500
C	-4.60157600	-1.63402300	-0.94829300
C	-3.38526900	-1.79458000	-0.27528600
C	-3.14856400	-3.14816400	0.35138100
F	-2.47148200	-3.97405500	-0.45242200

F -4.29769700 -3.76044400 0.64578300
F -2.45223900 -3.08133600 1.50291200
H -5.31730600 -2.45741300 -0.96525000
H -5.86266600 -0.32799600 -2.11259100
H -4.22229700 1.56200000 -2.04902600
H -2.06522800 1.27987200 -0.86316000
C 0.67558600 -2.49005900 1.13907700
C 1.54820700 -3.51534800 0.80653500
C 1.64398200 -3.98840300 -0.51195100
C 0.81445400 -3.42954500 -1.50509600
C -0.06488200 -2.40762600 -1.20296700
H -0.71359800 -1.98672600 -1.97670900
H 0.85917200 -3.81217400 -2.52815000
H 2.34838300 -4.78441000 -0.76318200
H 2.16471000 -3.96534300 1.58987100
H 0.58710700 -2.14922800 2.17267800

5k Ph pathway (cyclic intermediate)

E(UMN15) = -2714.82243

Thermal correction to Gibbs Free Energy= 0.26561

C 0.00000000 0.00000000 0.00000000
C 0.01113800 -1.53812600 0.11520200
C -1.14243400 -0.64738700 0.69184800
H -0.20973500 0.33350800 -1.02095600
C 0.95165900 0.89258600 0.76338700
H 1.09223800 0.49908600 1.78293200
H 0.53851000 1.90857300 0.84996100
C 2.31112500 1.01222200 0.11541400
O 2.80230500 2.06667000 -0.21713600
C 3.06452500 -0.28808000 -0.09124600
C 3.01974300 -0.97200700 -1.31014700
C 3.65304200 -2.19855300 -1.49331500
C 4.36810200 -2.73943500 -0.42511600
C 4.47483600 -2.07559700 0.79577100

C 3.81097200 -0.86007600 0.94239000
Cl 3.88022800 -0.04939200 2.47216200
H 5.04166100 -2.50365300 1.62336800
Cl 5.11880500 -4.28311700 -0.61602800
H 3.58140900 -2.72444600 -2.44618900
Cl 2.13774800 -0.28349600 -2.63065100
O -1.15462400 -0.48323300 2.06490800
H -1.46432900 -1.30765000 2.47529000
C -2.49865200 -0.66193100 0.03503100
C -2.92181000 0.50243100 -0.62219600
C -4.17897500 0.59499500 -1.21745900
C -5.05192000 -0.49261800 -1.16899500
C -4.65536300 -1.65768100 -0.51780900
C -3.39369100 -1.74865700 0.08393600
C -3.09183200 -3.08696500 0.71119000
F -2.85015600 -4.02332900 -0.21325900
F -4.13249600 -3.52699000 1.42908900
F -2.03581700 -3.07704600 1.53815700
H -5.33227900 -2.51409400 -0.47161700
H -6.03845900 -0.43545400 -1.63295900
H -4.47618300 1.51901900 -1.71811600
H -2.24203100 1.35721300 -0.65970300
C 0.84633600 -2.22373400 1.11487400
C 1.27593000 -3.51299200 0.91670600
C 0.95845200 -4.22730500 -0.26420800
C 0.20219300 -3.58565700 -1.27535000
C -0.25034700 -2.29949600 -1.11688600
H -0.82416000 -1.80653400 -1.90715600
H -0.02474400 -4.12253100 -2.20036700
H 1.31261300 -5.25015400 -0.40241500
H 1.88667300 -3.99398200 1.68615900
H 1.10441200 -1.69639300 2.03598400

5k Ph pathway (TS2)

E(UMN15) = -2714.82063

Thermal correction to Gibbs Free Energy= 0.26616

C 0.00000000 0.00000000 0.00000000
C -1.35983500 0.83863400 -0.75678100
C -1.22792300 -0.65182100 -0.51714200
H -1.08971700 -1.18805600 -1.46064100
C -2.13240800 -1.39652000 0.44734600
H -2.22660200 -0.82705900 1.38613900
H -1.69696200 -2.37593100 0.69309500
C -3.52091000 -1.63924600 -0.09901500
O -4.01261200 -2.73907100 -0.20734500
C -4.29443100 -0.39832800 -0.50199700
C -4.30690600 0.05586500 -1.82425800
C -4.91627100 1.25349500 -2.18986400
C -5.55464600 1.99929800 -1.19887000
C -5.60938400 1.56361100 0.12421900
C -4.96830000 0.37087000 0.45027400
Cl -4.96665800 -0.15474800 2.10162300
H -6.11807400 2.14969400 0.89042700
Cl -6.27900000 3.50894100 -1.62085800
H -4.88689800 1.59868300 -3.22401400
Cl -3.51001300 -0.87977700 -3.04286700
O 0.04598100 0.21459700 1.35086500
H 0.04222000 1.16670200 1.55518600
C 1.27513500 -0.02025200 -0.75608900
C 1.52369300 -1.05702800 -1.67266100
C 2.70183000 -1.11851400 -2.41479200
C 3.67476400 -0.13039900 -2.26690500
C 3.45077000 0.91483300 -1.37187900
C 2.27027600 0.98013700 -0.62700200
C 2.11765900 2.14646900 0.31205300
F 0.87734200 2.66638400 0.27693300
F 2.95751800 3.14068300 0.02009400
F 2.34887100 1.81514500 1.59204900

H 4.20017000 1.69912500 -1.25540700
H 4.60127800 -0.16747000 -2.84280400
H 2.85987800 -1.94950000 -3.10571000
H 0.78441200 -1.85122400 -1.78951500
C -2.02570700 1.72154900 0.17521700
C -2.30599100 3.03270800 -0.16658000
C -1.98440600 3.54072300 -1.43822200
C -1.38414700 2.68458500 -2.38673900
C -1.09554500 1.37249100 -2.07565100
H -0.64768800 0.70943400 -2.82142300
H -1.15754600 3.05961500 -3.38820100
H -2.21509000 4.57618200 -1.69511800
H -2.80738000 3.67557800 0.56227400
H -2.31775400 1.34970400 1.16031200

5k Ph pathway (shifted product)

E(UMN15) = -2714.85457

Thermal correction to Gibbs Free Energy= 0.26597

C 0.00000000 0.00000000 0.00000000
C 1.98565600 -0.37249800 -1.36011100
C 1.49587700 0.17833600 -0.02304500
H 1.73612200 1.25052800 -0.00153200
C 2.14378300 -0.47997300 1.20617400
H 2.11780500 -1.57810800 1.10269900
H 1.58244100 -0.23811800 2.11961000
C 3.58005500 -0.09166200 1.46980700
O 4.00702800 0.08791800 2.58842600
C 4.50374100 0.06001100 0.27768500
C 4.83850200 1.32343800 -0.21571900
C 5.65140900 1.49117900 -1.33474800
C 6.13255000 0.35188700 -1.97685700
C 5.83999400 -0.93039500 -1.51142300
C 5.03213900 -1.05356100 -0.38421800
Cl 4.66587100 -2.63640000 0.21301700

H 6.22887200 -1.81499700 -2.01730500
Cl 7.09647000 0.52971800 -3.39838600
H 5.88236500 2.48870300 -1.71009100
Cl 4.15636700 2.72940400 0.53381200
O -0.36826300 -1.13534900 0.61615300
H -1.32930900 -1.20789900 0.74235900
C -0.89516900 0.84558700 -0.72277600
C -0.50280300 2.19252900 -0.99127000
C -1.33886900 3.09666000 -1.62388500
C -2.61810000 2.71155100 -2.04887000
C -3.01583200 1.38956500 -1.85824800
C -2.18668600 0.46039000 -1.22693600
C -2.64940900 -0.96771500 -1.23251000
F -1.70241100 -1.80138500 -1.67960600
F -3.72973500 -1.15939000 -1.98367500
F -2.98581700 -1.41700200 0.00989800
H -3.98630200 1.06241500 -2.23393700
H -3.28483900 3.42141400 -2.54076600
H -0.99402000 4.12135400 -1.78027700
H 0.47049700 2.54295000 -0.64648400
C 1.88133600 -1.74149000 -1.64554600
C 2.33024500 -2.24478300 -2.86787700
C 2.87394700 -1.38427400 -3.82684200
C 2.95161300 -0.01424000 -3.56223000
C 2.50442700 0.48754800 -2.33747100
H 2.57639600 1.55868100 -2.12204900
H 3.37516800 0.66572900 -4.30588700
H 3.23036400 -1.78033600 -4.78065600
H 2.25559000 -3.31543500 -3.07330600
H 1.44986600 -2.41838600 -0.90241200

5k TFT pathway (extended conformation)

E(UMN15) = -2714.82114389

Thermal correction to Gibbs Free Energy= 0.26035

C	0.00000000	0.00000000	0.00000000
C	1.20355300	0.44275600	0.77464500
H	1.07411400	0.82305500	1.78774700
C	2.54856200	0.03162300	0.32022800
H	2.77556700	0.40378000	-0.69715100
H	2.63422600	-1.07144100	0.20825300
C	3.66604100	0.45731400	1.23147500
O	3.51028400	1.04580100	2.27713900
C	5.05618200	0.08882000	0.75568800
C	5.65818300	-1.11251800	1.13917800
C	6.94496500	-1.45706300	0.73144600
C	7.63882200	-0.56623000	-0.08715800
C	7.07350000	0.63849200	-0.50459800
C	5.78409100	0.94453800	-0.07528900
Cl	5.04938400	2.42659700	-0.58741500
H	7.62350000	1.32393400	-1.15039500
Cl	9.23801800	-0.96756700	-0.60181800
H	7.39410700	-2.40015000	1.04475700
Cl	4.76659800	-2.20783400	2.14088100
O	0.37450600	-0.02567000	-1.35715300
H	-0.41290500	-0.19390300	-1.89916500
C	-0.34589100	-1.39254000	0.58594700
C	-0.14807100	-2.65383000	-0.01516700
C	-0.43991800	-3.82230200	0.71091100
C	-0.92084400	-3.76943300	2.01404400
C	-1.12608400	-2.52613900	2.61421300
C	-0.83861100	-1.36711100	1.90309100
H	-0.99625900	-0.39481600	2.37787500
H	-1.50850000	-2.45734300	3.63486500
H	-1.13796900	-4.69392500	2.55252100
H	-0.28992600	-4.79311100	0.23929100
C	0.32782900	-2.86497200	-1.43753600
F	0.35905400	-4.16700800	-1.75321600

F -0.49537300 -2.29985600 -2.33977200
F 1.56164300 -2.40752500 -1.66386700
C -1.20695000 0.93088300 0.15015200
C -1.10436100 2.22494500 0.66719400
C -2.22392600 3.06340500 0.69586500
C -3.45031400 2.61790300 0.20082800
C -3.55728800 1.32652400 -0.32618600
C -2.44267100 0.48921500 -0.34672000
H -2.52933400 -0.52520400 -0.75220000
H -4.51323500 0.96997800 -0.71678200
H -4.32317000 3.27448900 0.22448600
H -2.13292300 4.07192600 1.10622400
H -0.14552900 2.58769100 1.04517600

5k TFT pathway (folded conformation)
E(UMN15) = -2714.82775
Thermal correction to Gibbs Free Energy= 0.26624
C 0.00000000 0.00000000 0.00000000
C 0.65958400 -0.45665800 1.27057400
H 0.70821600 0.27663800 2.07620100
C 1.31824400 -1.78274700 1.43576200
H 1.28480300 -2.35717100 0.49852000
H 0.81598600 -2.37249800 2.22454600
C 2.75388400 -1.59720800 1.89450300
O 3.06356100 -1.56559300 3.06376200
C 3.80164300 -1.38936300 0.82251900
C 4.43732400 -0.15357500 0.64875400
C 5.42617600 0.03789000 -0.31375200
C 5.78722800 -1.03970200 -1.12011500
C 5.19728300 -2.29348700 -0.97200300
C 4.21108700 -2.44442300 0.00002200
Cl 3.48011000 -4.00236000 0.20576100
H 5.49181600 -3.13390400 -1.60162800
Cl 6.96830000 -0.80274300 -2.35759000

H 5.88919300 1.01684200 -0.44360500
Cl 3.96545400 1.19386500 1.62154700
O -0.79077000 1.11764100 0.34177600
H -1.22353100 1.44422000 -0.46464700
C 1.15060700 0.37349000 -0.95785400
C 1.75584900 1.65102600 -1.02069900
C 2.81809900 1.87153100 -1.91022700
C 3.31218000 0.85488600 -2.72376200
C 2.74957100 -0.41705300 -2.63907300
C 1.68908400 -0.64378200 -1.76455000
H 1.25043200 -1.64345800 -1.71531400
H 3.13227500 -1.23668500 -3.25178400
H 4.14601400 1.05351800 -3.40059800
H 3.27227300 2.86082200 -1.96320800
C 1.33964000 2.85180700 -0.19007300
F 2.24703500 3.83707500 -0.28967800
F 0.18207400 3.38930600 -0.60671700
F 1.22952600 2.59694700 1.11333900
C -0.95386900 -1.03450000 -0.61714400
C -1.54878800 -2.03217200 0.16326100
C -2.52516600 -2.87289900 -0.37908700
C -2.92945000 -2.71684200 -1.70576900
C -2.35826200 -1.70752800 -2.48624900
C -1.37938900 -0.87370900 -1.94479900
H -0.93877300 -0.08749800 -2.56533100
H -2.67492700 -1.56932100 -3.52272900
H -3.69117600 -3.37513700 -2.12994800
H -2.97408900 -3.65056700 0.24332600
H -1.26158300 -2.15086100 1.21061200

5k TFT pathway (TS1)

E(UMN15) = -2714.80914

Thermal correction to Gibbs Free Energy= 0.26487

C 0.00000000 0.00000000 0.00000000

C 0.23500400 0.54778900 -1.79031900
C -1.04212500 0.36212400 -0.98317700
H 0.30193400 0.82989300 0.63997700
C 0.41426900 -1.38032200 0.39522800
H 0.27760500 -2.09376500 -0.43258400
H -0.19060100 -1.73514600 1.24763400
C 1.85631300 -1.41614100 0.85546300
O 2.16818900 -1.62350500 2.00591600
C 2.94385400 -1.16573800 -0.17231000
C 3.63786000 0.04819000 -0.22499300
C 4.70316600 0.25414600 -1.09925200
C 5.08049900 -0.78844900 -1.94302300
C 4.42221600 -2.01677600 -1.92536200
C 3.36022900 -2.18095000 -1.03971700
Cl 2.51960200 -3.69568800 -1.02064700
H 4.72077100 -2.82668500 -2.59187900
Cl 6.37105000 -0.53902900 -3.06379800
H 5.21611700 1.21605800 -1.12969300
Cl 3.15294100 1.35210300 0.80321500
O -1.71191900 1.52318100 -0.60238700
H -2.13750000 1.90569500 -1.38820000
C 0.95701400 1.79634900 -1.95650000
C 2.06357100 1.84361300 -2.80147100
C 2.49143700 0.73760300 -3.54355500
C 1.77122000 -0.46268800 -3.44512200
C 0.67556500 -0.55202100 -2.61065200
H 0.12233000 -1.49152400 -2.55888900
H 2.06879200 -1.33542800 -4.03178800
H 3.37013400 0.81495400 -4.18633900
H 2.60956800 2.78227500 -2.89944600
C 0.57509300 3.09800500 -1.29400000
F 1.50434500 4.04268100 -1.50352300
F -0.57004300 3.60820200 -1.78358500
F 0.43707200 3.01892300 0.03461100

C -2.02913000 -0.67021800 -1.48470600
C -2.64680500 -1.55508400 -0.59359000
C -3.65437700 -2.41444200 -1.03924200
C -4.05833000 -2.38710700 -2.37602700
C -3.45617900 -1.49341700 -3.26678400
C -2.44675500 -0.63865400 -2.82224500
H -1.97108000 0.05775700 -3.51969700
H -3.77339700 -1.46344700 -4.31173300
H -4.84549400 -3.05992800 -2.72427400
H -4.12800100 -3.10509000 -0.33765100
H -2.34714900 -1.56454100 0.45712000

5k TFT pathway (cyclic intermediate)

E(UMN15) = -2714.81837

Thermal correction to Gibbs Free Energy= 0.26755

C 0.00000000 0.00000000 0.00000000
C 0.33838200 0.37386800 -1.46914100
C -1.13258200 0.22955300 -0.92384500
H 0.13629800 0.83492000 0.68797600
C 0.34676000 -1.34064900 0.61612200
H 0.16742300 -2.16806200 -0.08861500
H -0.28214800 -1.51169100 1.50219700
C 1.78626900 -1.41039700 1.07619500
O 2.10787700 -1.55538800 2.23312700
C 2.83985200 -1.28969000 -0.00698400
C 3.48323700 -0.07554400 -0.26869100
C 4.41385000 0.06021400 -1.29561600
C 4.71365300 -1.06056500 -2.06914700
C 4.12450500 -2.29978100 -1.82319100
C 3.19017800 -2.39008800 -0.79448300
Cl 2.41191900 -3.91020300 -0.49922300
H 4.37207500 -3.17183700 -2.42960000
Cl 5.82620800 -0.90028600 -3.38014000
H 4.88492600 1.02369200 -1.49449900

Cl 3.09761000 1.30898000 0.69441800
O -1.81355400 1.40843100 -0.68198800
H -2.22236700 1.71251300 -1.51026200
C 0.88010800 1.70898300 -1.83941700
C 1.69054900 1.84635600 -2.95337400
C 2.05728500 0.76431200 -3.77163800
C 1.59392600 -0.53017000 -3.43804700
C 0.79279700 -0.72223900 -2.34519700
H 0.45540900 -1.73275400 -2.10650200
H 1.88674700 -1.38985600 -4.04598900
H 2.70550400 0.92402200 -4.63410400
H 2.06629100 2.83960500 -3.20635400
C 0.55754600 3.00228500 -1.13371300
F 1.55534400 3.89081200 -1.28196500
F -0.53282000 3.60412600 -1.64762700
F 0.35694000 2.89922300 0.18314500
C -2.00364400 -0.86306000 -1.47086600
C -2.64144000 -1.76846100 -0.61308900
C -3.52922300 -2.71724800 -1.12660900
C -3.79075100 -2.76176500 -2.49830300
C -3.16598500 -1.85326100 -3.35801800
C -2.27594300 -0.90851300 -2.84565800
H -1.77824600 -0.19884400 -3.51379300
H -3.37098200 -1.88363400 -4.43064000
H -4.48449700 -3.50476400 -2.89875300
H -4.02081800 -3.42227100 -0.45218700
H -2.44698400 -1.72412200 0.46145200

5k TFT pathway (TS2)

E(UMN15) = -2714.81588

Thermal correction to Gibbs Free Energy= 0.26654

C 0.00000000 0.00000000 0.00000000
C -1.66673900 0.13070200 0.64639400
C -1.23944800 -0.18431900 -0.77977100

H -1.39609200 0.65214100 -1.46306800
C -1.60780200 -1.50884100 -1.43665300
H -1.41025200 -2.35870100 -0.76486400
H -1.00333100 -1.64820900 -2.34433400
C -3.06317500 -1.56726400 -1.85007500
O -3.42370300 -1.66407000 -3.00030500
C -4.07141700 -1.50099100 -0.71966600
C -4.70628700 -0.30129000 -0.38242700
C -5.54975300 -0.19527900 0.72041500
C -5.78087800 -1.33733900 1.48744400
C -5.20733900 -2.56603700 1.16305800
C -4.35302000 -2.62275000 0.06461300
Cl -3.58192500 -4.12639000 -0.32100600
H -5.40337100 -3.45561000 1.76271200
Cl -6.79065900 -1.22065000 2.88319500
H -6.00966900 0.75953200 0.97868100
Cl -4.40092500 1.10577400 -1.33975200
O 0.58433300 1.22074500 -0.14819000
H 1.20228800 1.38076200 0.58668600
C -2.06270000 1.45306300 1.11312200
C -2.61477400 1.60818200 2.38554600
C -2.85759900 0.53040400 3.23936800
C -2.53558400 -0.76867300 2.79024200
C -1.98033000 -0.96064000 1.54703300
H -1.74572800 -1.97901900 1.22921700
H -2.74138600 -1.63583000 3.42304200
H -3.30233400 0.69264400 4.22218000
H -2.88277200 2.61546900 2.71455300
C -1.87113600 2.75628800 0.38262900
F -2.93887500 3.55924900 0.55244600
F -0.82576800 3.45304000 0.86867600
F -1.68802200 2.66546300 -0.93698000
C 0.83113000 -1.06650100 0.61213100
C 1.28091200 -2.17802600 -0.11552900

C 2.10766000 -3.12614600 0.49245300
C 2.49626400 -2.97013500 1.82497600
C 2.05707100 -1.86104000 2.55489000
C 1.22565600 -0.91767500 1.95303200
H 0.85770500 -0.06061400 2.52761500
H 2.35504400 -1.73750700 3.59851400
H 3.14338700 -3.71346100 2.29630900
H 2.45680600 -3.98699100 -0.08238500
H 1.00298800 -2.29175800 -1.16528700

5k TFT pathway (shifted product)
E(UMN15) = -2714.85171
Thermal correction to Gibbs Free Energy= 0.26638
C 0.00000000 0.00000000 0.00000000
C -1.50156400 -0.10620000 0.02586800
O -2.02148900 0.49487300 1.11752600
H -2.96036200 0.26453400 1.22563000
C -2.34605000 -0.73348600 -0.93168800
C -1.84371600 -1.62149600 -1.92580200
C -2.69508000 -2.23443800 -2.83566800
C -4.07636200 -1.99393300 -2.80524200
C -4.59170900 -1.11857000 -1.84035600
C -3.75224400 -0.49730000 -0.92395500
H -4.19238000 0.21145800 -0.21647300
H -5.66376900 -0.90845300 -1.81043900
H -4.73981200 -2.47982100 -3.52351300
H -2.27755600 -2.91917600 -3.57806800
H -0.77874100 -1.84972100 -1.95903800
H 0.19869900 0.77378800 0.75410200
C 0.66318700 -1.28641700 0.56252200
H 0.70192300 -2.08604300 -0.19378900
H 0.04844500 -1.64692700 1.39909300
C 2.04358000 -1.04785900 1.14036500
O 2.27323000 -1.14114700 2.32544600

C	3.15401600	-0.64690700	0.18810800
C	3.55873400	0.68657800	0.05929900
C	4.52847700	1.08012000	-0.85996200
C	5.12338700	0.10129900	-1.65573500
C	4.77572100	-1.24422000	-1.54106600
C	3.79143000	-1.59220100	-0.61968700
Cl	3.30260900	-3.25081300	-0.50518100
H	5.25077100	-2.00428800	-2.16228100
Cl	6.31567200	0.56787800	-2.81366200
H	4.80971400	2.12965500	-0.95432700
Cl	2.80044900	1.89870300	1.03171900
C	0.56736800	0.52389500	-1.31878500
C	0.44763900	1.88454000	-1.68631600
C	1.06984800	2.36937800	-2.84153800
C	1.80615200	1.52154600	-3.66859900
C	1.89651500	0.17018600	-3.34565100
C	1.28387700	-0.30968300	-2.18664300
H	1.38889000	-1.37102000	-1.95254300
H	2.45368100	-0.51857000	-3.98501900
H	2.29209100	1.91733600	-4.56243600
H	0.97372200	3.42430900	-3.09982300
C	-0.41023100	2.86029000	-0.91110500
F	-0.27324600	4.11096600	-1.36221900
F	-1.71303400	2.55751600	-1.02168800
F	-0.13659000	2.90233900	0.39883100