Supporting Information

Ruthenium(II)-Catalyzed Regioselective C–H Olefination of Aromatic Ketones and Amides with Allyl Sulfones

Suman Dana, Chandan Kumar Giri, and Mahiuddin Baidya*

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, Tamil Nadu, India

mbaidya@iitm.ac.in

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General information

[Ru(*p*-cymene)Cl_2]$_2$ was purchased from Alfa Aesar. Acetophenones, benzoic acids, amines, DCE, 1,4-dioxane, and inorganic bases were purchased from Avra chemicals, Spectrochem, and Sigma-Aldrich. $AgSbF_6$, KPF_6, $KSbF_6$, and $AgBF_4$ were purchased from Alfa Aesar and Sigma-Aldrich. All the compounds were utilized without further purification.

All reactions were monitored by thin layer chromatography (TLC) on Merck 60 F 254 precoated silica plates and visualized using a UV lamp (366 or 254 nm) or by use of potassium permanganate, 5 g K_2CO_3, / 100 mL water. Products were isolated by column chromatography (Merck silica gel 100-200 μm).

^{13}C and ^{1}H NMR spectra were recorded on a Bruker 400 or Bruker 500 MHz spectrometers. Chemical shift values (δ) are reported in ppm and calibrated to the residual solvent peak- $CDCl_3$ δ = 7.26 ppm for ^{1}H, δ = 77.16 ppm for ^{13}C; DMSO-d_6 δ = 2.51 ppm for ^{1}H, δ = 39.5 ppm for ^{13}C; or calibrated to tetramethylsilane (δ = 0.00). All NMR spectra were recorded at ambient temperature (290 K) unless otherwise noted. ^{1}H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constant, integration). The following abbreviations are used to indicate multiplicities: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublet; dt, doublet of triplet; dq, doublet of quartet; td, triplet of doublet; tt, triplet of triplet; dq, doublet of quartet; br, broad.

Mass spectra were recorded by electron spray ionization (ESI) method on a Q-TOF Micro with lock spray source.

X-ray data of the crystals were collected and integrated using a Bruker Axs (Kappa Apex 2) CCD diffractometer equipped with graphite monochromatic Mo (Kα) radiation. The crystal sample was prepared through solvent evaporation method in ethyl acetate: hexane (9:1) solvent mixture at room temperature.

References:

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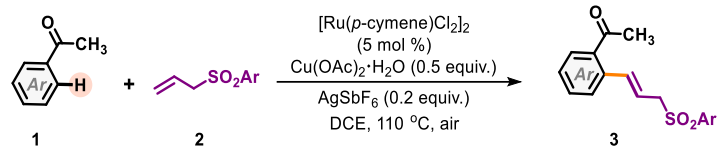
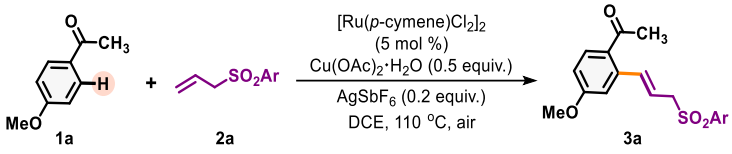
Typical Ru(II)-catalyzed C–H olefination of aromatic ketones (1) with allyl sulfones (2):



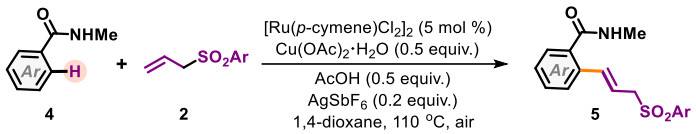
To an oven dried screw cap reaction tube (10×1.5 cm) corresponding aromatic ketone **1** (0.3 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (0.5 equiv.), and olefin **2** (1.5 equiv.) were added. Then the reaction tube was flushed with nitrogen gas for 2-3 minutes and $AgSbF_6$ (0.2 equiv.) was added in it. Next 0.3 mL DCE was added into the reaction mixture. After stirring the reaction mixture under inert atmosphere for 5 minutes at room temperature, the cap was opened and stirred at room temperature for the next 5 minutes under air. Then the reaction tube was capped, placed in a pre-heated oil bath, and it was stirred at 110 ^oC for 24 h. After completion (monitored by TLC), the crude reaction mixture was diluted with ethyl acetate and filtered through a celite pad. In order to get pure products **3**, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate.

Typical scaled-up Ru(II)-catalyzed C–H olefination of aromatic ketones (1a) with allyl sulfones (2a):



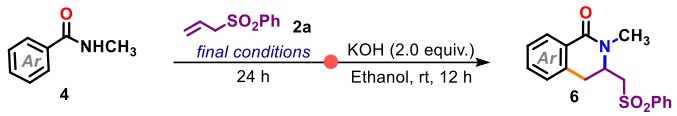
To an oven dried screw cap reaction tube (10×1.5 cm) corresponding aromatic ketone **1a** (450 mg, 3.0 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (0.5 equiv.), and olefin **2a** (1.5 equiv.) were added. Then the reaction tube was flushed with nitrogen gas for 2-3 minutes and $AgSbF_6$ (0.2 equiv.) was added in it. Next 3.0 mL DCE was added into the reaction mixture. After stirring the reaction mixture under inert atmosphere for 5 minutes at room temperature, the cap was opened and stirred at room temperature for the next five minutes under air. Then the reaction tube was capped, placed in a pre-heated oil bath and it was stirred at 110 ^oC for 24 h. After completion (monitored by TLC), the crude reaction mixture was diluted with ethyl acetate and filtered through a celite pad. In order to get pure products **3a**, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. Yield obtained= 65% (0.6435 gm).

Typical Ru(II)-catalyzed C–H olefination of aromatic amides (4) with allyl sulfones (2):



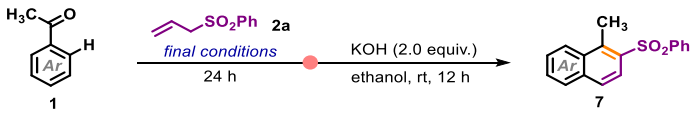
To an oven dried screw cap reaction tube (10×1.5 cm) corresponding aromatic amide **4** (0.3 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (0.5 equiv.), AcOH (0.5 equiv.), and olefin **2** (1.5 equiv.) were added. Then the reaction tube was flushed with nitrogen gas for 2-3 minutes and $AgSbF_6$ (0.2 equiv.) was added in it. Next 0.5 mL 1,4-dioxane was added into the reaction mixture. After stirring the reaction mixture under air atmosphere for 5 minutes at room temperature, it was capped. Then the reaction tube was placed in a pre-heated oil bath and stirred at 110 ^oC for 24 h. After completion (monitored by TLC), the crude reaction mixture was diluted with ethyl acetate and filtered through a celite pad. In order to get pure products **5**, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate.

Typical formal 1,2-carboamination of allyl sulfones (6):



To an oven dried screw cap reaction tube (10×1.5 cm) corresponding aromatic amide **4** (0.3 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol %), Cu(OAc)$_2$·H_2O (0.5 equiv.), AcOH (0.5 equiv.), and olefin **2a** (1.5 equiv.) were added. Then the reaction tube was flushed with nitrogen gas for 2-3 minutes and $AgSbF_6$ (0.2 equiv.) was added in it. Next 0.5 mL 1,4-dioxane was added into the reaction mixture. After stirring the reaction mixture under air atmosphere for 5 minutes at room temperature, it was capped. Then the reaction tube was placed in a pre-heated oil bath and stirred at 110 ^oC for 24 h. After completion (monitored by TLC), the solvent was evaporated and to the crude reaction mixture KOH (2.0 equiv.) was added along with the addition of 0.5 mL EtOH. The reaction mixture was stirred at room temperature for another 12 h under air. After completion (monitored by TLC), the reaction mixture was diluted with ethyl acetate and filtered through a celite pad. In order to get pure product **6**, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane-ethyl acetate mixture.

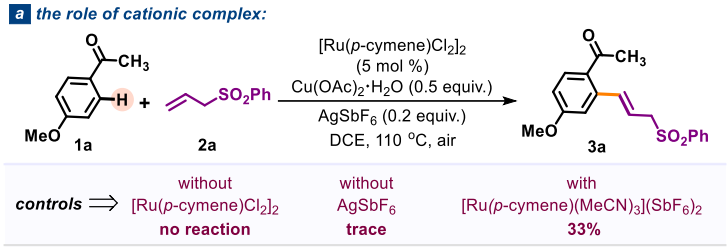
Typical intramolecular aldol reaction (synthesis of 7):



To an oven dried screw cap reaction tube (10 × 1.5 cm) corresponding product **3** (0.3 mmol, 1.0 equiv.) and KOH (2.0 equiv.) was added followed by the addition of 0.5 mL EtOH. The reaction tube was capped and then the reaction mixture was stirred at room temperature for 12 h under air. After completion (monitored by TLC), the reaction mixture was diluted with ethyl acetate and filtered through a celite pad. In order to get pure product **7**, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane-ethyl acetate mixture.

Mechanistic Studies:

a) The role of cationic complex:



To three separate oven dried screw cap reaction tubes (10×1.5 cm) corresponding aromatic ketone **1a** (0.3 mmol, 1.0 equiv.), $Cu(OAc)_2 \cdot H_2O$ (0.5 equiv.), and olefin **2a** (1.5 equiv.) were added.

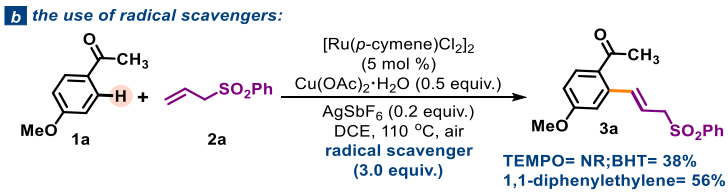
In reaction tube 1, $[Ru(p\text{-cymene})Cl_2]_2$ was not added. However, $AgSbF_6$ (0.2 equiv.) was added in it.

In reaction tube 2, $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol %) was added. However, $AgSbF_6$ was excluded.

In reaction tube 3, both $[Ru(p\text{-cymene})Cl_2]_2$ and $AgSbF_6$ were not added. Instead, $[Ru(p\text{-cymene})(MeCN)_3]$ SbF_6 (10 mol %) was added in it.

Next 0.3 mL DCE was added in each of them. Then the reaction tube was capped following the standard method, placed in a pre-heated oil bath and it was stirred at 110 °C for 24 h under air. After completion (monitored by TLC), the crude reaction mixture was diluted with ethyl acetate and filtered through a celite pad. While in reaction tubes 1 and 2, almost no product formation was observed, from reaction tube 3, 33% of the product **3a** was isolated.

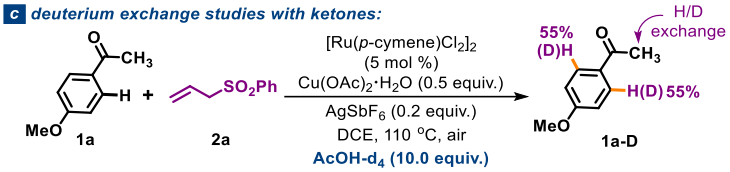
b) Radical Scavengers Study:



To an oven dried screw cap reaction tube (10×1.5 cm) corresponding aromatic ketone **1a** (0.3 mmol, 1.0 equiv.), $[Ru(p\text{-cymene})Cl_2]_2$ (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (0.5 equiv.), olefin **2a** (1.5 equiv.), and radical scavengers (3.0 equiv.) were added. Then the reaction tube was flushed with nitrogen gas for 2-3 minutes and $AgSbF_6$ (0.2 equiv.) was added in it. Next 0.3 mL DCE was added into reaction mixture. After stirring the reaction mixture under inert atmosphere for 5 minutes at room temperature, the cap was opened and stirred at room temperature for the next

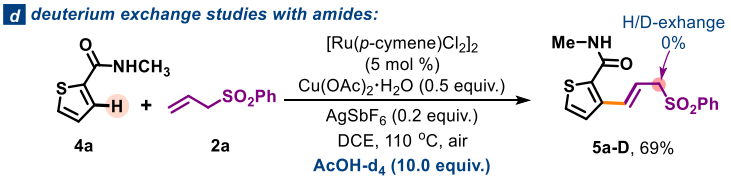
5 minutes. Then the reaction tube was capped, placed in a pre-heated oil bath and it was stirred at 110 °C for 24 h under air. After completion (monitored by TLC), the crude reaction mixture was diluted with ethyl acetate and filtered through a celite pad. In order to get pure products **3**, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate.

c) Deuterium exchange studies with ketone:



In an oven dried screw cap reaction tubes (10×1.5 cm) corresponding aromatic ketone **1a** (0.3 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (0.5 equiv.), olefin **2a** (1.5 equiv.), and radical scavengers (3.0 equiv.) were added. Then the reaction tubes were flushed with nitrogen gas for 2-3 minutes and $AgSbF_6$ (0.2 equiv.) was added in it. Next 0.3 mL DCE was added in each of them. After stirring the reaction mixture under inert atmosphere for 5 minutes at room temperature, the cap was opened and stirred at room temperature for the next 5 minutes. In the reaction tube, CD_3COOD (10.0 equiv.) was added. Then the reaction tube was capped, placed in a pre-heated oil bath and it was stirred at 110 °C for 12 h under air. After completion (monitored by TLC), the crude reaction mixture was diluted with ethyl acetate and filtered through a celite pad. The deuterium incorporation was studied from isolated ketone **1a**.

d) Deuterium exchange studies with amide:



To an oven dried screw cap reaction tube (10×1.5 cm) corresponding aromatic amide **4a** (0.3 mmol, 1.0 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (5 mol %), $Cu(OAc)_2 \cdot H_2O$ (0.5 equiv.), and olefin **2a** (1.5 equiv.) were added. Then the reaction tube was flushed with nitrogen gas for 2-3 minutes and $AgSbF_6$ (0.2 equiv.) was added in it. Next 0.5 mL 1,4-dioxane and CD_3COOD (10.0 equiv.) were added into reaction mixture. After stirring the reaction mixture under air atmosphere for 5 minutes at room temperature, it was capped. Then the reaction tube was placed in a pre-heated oil bath and stirred at 110 °C for 10 h under air. After completion (monitored by TLC),

the crude reaction mixture was diluted with ethyl acetate and filtered through a celite pad. In order to get pure product **5a**, the resulting residue was purified by column chromatography on silica gel with a gradient eluent of hexane and ethyl acetate. The deuterium incorporation was studied from isolated product **5a**.

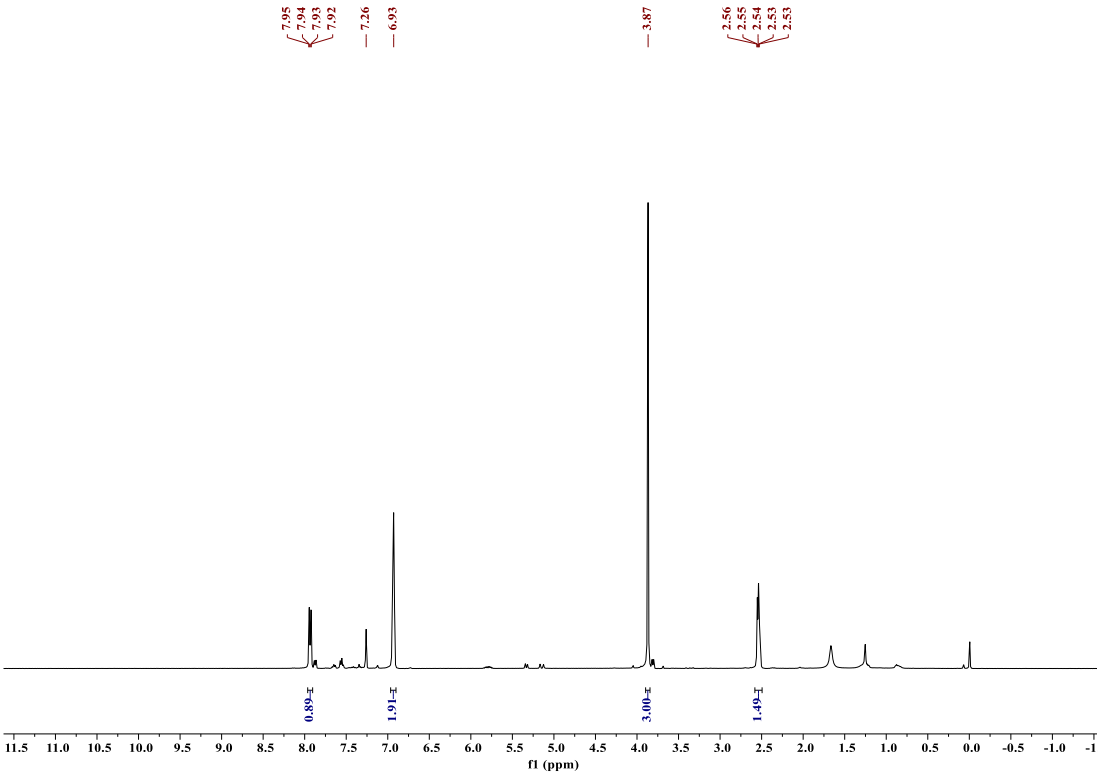


Figure S1. Deuterium exchange experiment with **1a** using CD_3CO_2D.

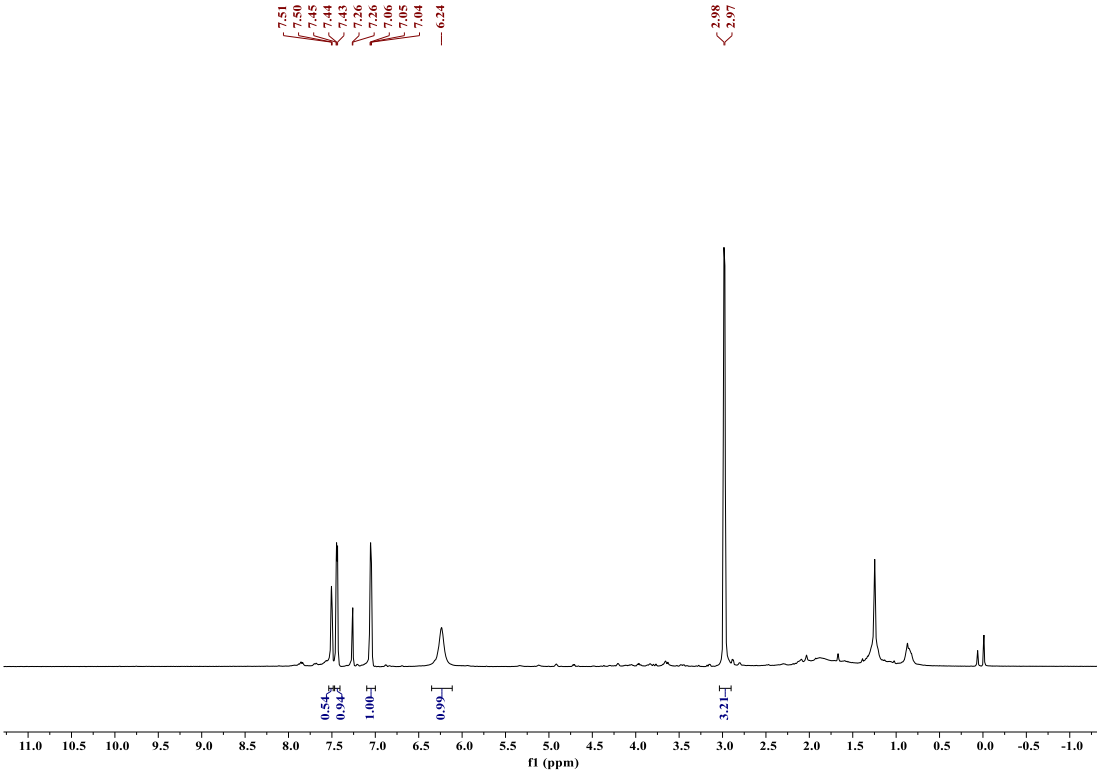


Figure S2. Deuterium exchange experiment with **4e**.

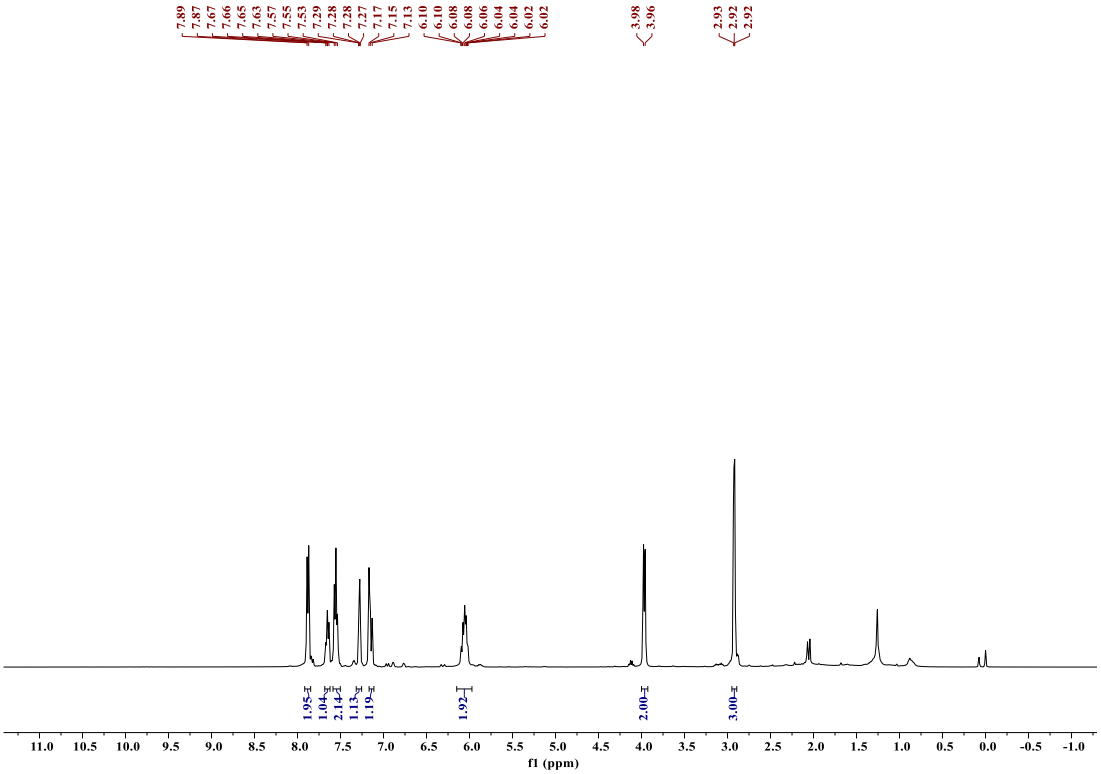
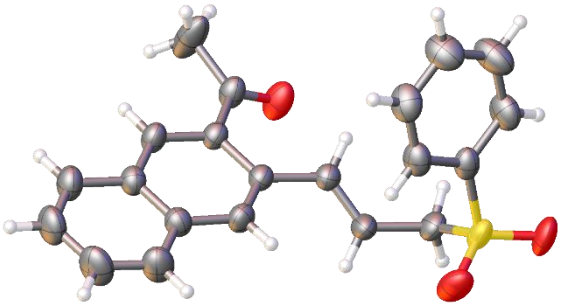


Figure S3. NMR Spectra of isolated **5e** after deuterium exchange experiment.

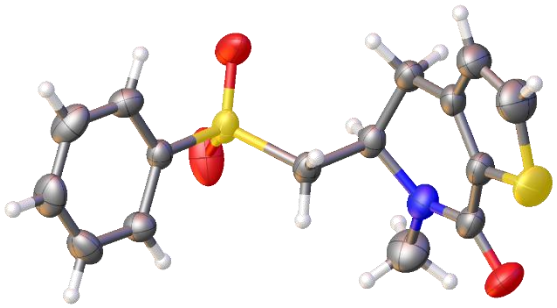
Crystal data and structure refinement for 3l (CCDC No 2070584):



Identification code	**3l**
Empirical formula	$C_{21}H_{18}O_3S$
Formula weight	350.41
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 7.7123(4) A alpha = 105.665(2) deg.
	b = 10.2924(5) A beta = 95.392(2) deg.
	c = 11.6131(6) A gamma = 91.621(2) deg.
Volume	882.27(8) A^3
Z, Calculated density	2, 1.319 Mg/m^3
Absorption coefficient	0.200 mm^-1
F(000)	368
Crystal size	0.250 x 0.220 x 0.100 mm
Theta range for data collection	1.831 to 24.999 deg.
Limiting indices	-8<=h<=9, -12<=k<=12, -13<=l<=13
Reflections collected / unique	11705 / 3104 [R(int) = 0.0201]
Completeness to theta = 24.999	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3104 / 0 / 228
Goodness-of-fit on F^2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0922
R indices (all data)	R1 = 0.0414, wR2 = 0.0982
Extinction coefficient	0.067(4)
Largest diff. peak and hole	0.227 and -0.261 e.A^-3

Ellipsoid contour % probability levels = 50%

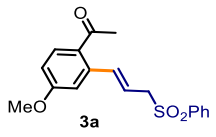
Crystal data and structure refinement for 6a (CCDC No 2080954):



Identification code	**6a**
Empirical formula	$C_{15}H_{15}NO_3S_2$
Formula weight	321.40
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 8.3007(6) A alpha = 67.294(3) deg.
	b = 9.6260(7) A beta = 73.333(3) deg.
	c = 10.5879(6) A gamma = 89.438(3) deg.
Volume	742.76(9) A^3
Z, Calculated density	2, 1.437 Mg/m^3
Absorption coefficient	0.367 mm^-1
F(000)	336
Crystal size	0.250 x 0.220 x 0.160 mm
Theta range for data collection	2.191 to 24.977 deg.
Limiting indices	-9<=h<=9, -11<=k<=11, -12<=l<=12
Reflections collected / unique	10065 / 2610 [R(int) = 0.0282]
Completeness to theta = 24.977	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2610 / 0 / 192
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0366, wR2 = 0.0907
R indices (all data)	R1 = 0.0416, wR2 = 0.0952
Extinction coefficient	0.035(3)
Largest diff. peak and hole	0.387 and -0.376 e.A^-3

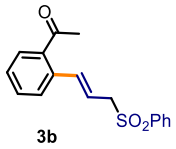
Ellipsoid contour % probability levels = 50%

NMR spectroscopic data of synthesized compounds:



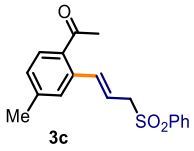
3a

(E)-1-(4-methoxy-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3a): Pale yellow liquid; yield 72% (71 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.70 (d, *J* = 8.6 Hz, 1H), 7.66 – 7.59 (m, 1H), 7.54 (dd, *J* = 8.3, 7.0 Hz, 2H), 7.08 (d, *J* = 15.7 Hz, 1H), 6.90 (d, *J* = 2.6 Hz, 1H), 6.84 (dd, *J* = 8.7, 2.7 Hz, 1H), 5.99 – 5.89 (m, 1H), 4.00 (d, *J* = 7.6 Hz, 2H), 3.87 (s, 3H), 2.47 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.2, 162.4, 139.3, 139.2, 138.6, 133.9 (2C), 132.4, 129.2, 128.5, 117.6, 113.7, 113.1, 60.6, 55.6, 29.0 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{18}O_4SNa$ 353.0823; Found 353.0829.



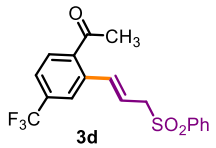
3b

(E)-1-(2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3b): Pale yellow liquid; yield 75% (68 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 – 7.84 (m, 2H), 7.68 – 7.57 (m, 2H), 7.58 – 7.50 (m, 2H), 7.49 – 7.43 (m, 2H), 7.41 – 7.31 (m, 1H), 6.94 (d, *J* = 15.7 Hz, 1H), 6.05 – 5.88 (m, 1H), 3.99 (d, *J* = 7.6 Hz, 2H), 2.49 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.3, 138.5, 138.3, 136.9, 135.9, 133.9, 132.0, 129.3, 129.2, 128.4, 128.2, 128.1, 117.8, 60.5, 29.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{17}H_{16}O_3SNa$ 323.0718; Found 323.0725.



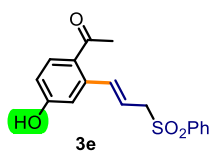
3c

(E)-1-(4-methyl-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3c): Pale yellow liquid; yield 68% (64 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.94 – 7.87 (m, 2H), 7.68 – 7.50 (m, 4H), 7.27 (s, 1H), 7.17 (d, *J* = 7.8 Hz, 1H), 7.00 (d, *J* = 15.7 Hz, 1H), 6.06 – 5.93 (m, 1H), 4.01 (d, *J* = 7.6 Hz, 2H), 2.49 (s, 3H), 2.40 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.7, 142.8, 138.8, 138.6, 136.4, 134.0, 133.9, 129.8, 129.2, 128.9 (2C), 128.5, 117.3, 60.6, 29.3, 21.6 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{18}O_3SNa$ 337.0874; Found 337.0882.



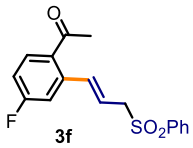
3d

(E)-1-(2-(3-(phenylsulfonyl)prop-1-en-1-yl)-4-(trifluoromethyl)phenyl)ethan-1-one (3d): Pale yellow liquid; yield 63% (70 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.72 (d, *J* = 8.1 Hz, 1H), 7.67 – 7.53 (m, 5H), 6.93 (d, *J* = 15.8 Hz, 1H), 6.14 – 5.96 (m, 1H), 4.00 (d, *J* = 7.6 Hz, 2H), 2.51 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.7, 140.0, 138.6, 136.7, 136.4, 134.1, 133.4 (q, *J* = 33.3 Hz, 1C), 129.4, 129.3, 128.5, 125.0 – 124.8 (m, 2C), 124.8 (q, *J* = 273.7 Hz, 1C), 119.9, 60.4, 29.8 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{18}H_{16}O_3F_3S$ 369.0772; Found 369.0748.



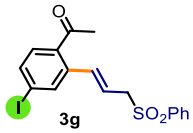
3e

(E)-1-(4-hydroxy-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3e): Pale yellow liquid; yield 71% (67 mg); Eluent- 35-40% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.42 (s, 1H), 7.88 (d, *J* = 7.7 Hz, 2H), 7.77 – 7.68 (m, 2H), 7.69 – 7.58 (m, 2H), 7.01 (d, *J* = 15.6 Hz, 1H), 6.85 – 6.73 (m, 2H), 5.88 – 5.74 (m, 1H), 4.27 (d, *J* = 7.5 Hz, 2H), 2.39 (s, 3H) ppm; **^{13}C NMR** (101 MHz, DMSO) δ 199.1, 160.7, 138.7, 138.1 (2C), 134.0, 133.0, 129.4, 128.1, 127.9, 118.0, 115.0, 114.1, 59.0, 29.2 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{17}H_{16}O_4SNa$ 339.0667; Found 339.0647.



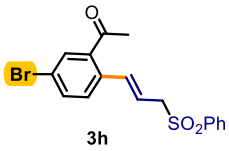
3f

(E)-1-(4-fluoro-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3f): Pale yellow liquid; yield 70% (67 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.92 – 7.85 (m, 2H), 7.73 – 7.59 (m, 2H), 7.58 – 7.50 (m, 2H), 7.15 – 7.07 (m, 1H), 7.07 – 6.95 (m, 2H), 6.04 – 5.92 (m, 1H), 3.99 (d, *J* = 7.6 Hz, 2H), 2.49 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.6, 164.5 (d, *J* = 253.9 Hz), 139.5 (d, *J* = 8.8 Hz), 138.6, 137.5, 134.0, 133.0 (d, *J* = 3.2 Hz), 132.1 (d, *J* = 9.4 Hz), 129.3, 128.4, 119.1, 115.1 (d, *J* = 9.5 Hz), 114.9 (d, *J* = 10.1 Hz), 60.4, 29.4 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{17}H_{15}FO_3SNa$ 341.0624; Found 341.0630.



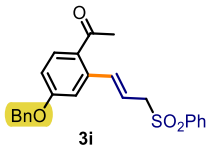
3g

(E)-1-(4-iodo-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3g): Pale yellow liquid; yield 60% (77 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.92 – 7.85 (m, 2H), 7.77 (s, 1H), 7.73 – 7.61 (m, 2H), 7.59 – 7.50 (m, 2H), 7.36 (d, *J* = 8.2 Hz, 1H), 6.88 (d, *J* = 15.7 Hz, 1H), 6.03 – 5.88 (m, 1H), 3.97 (d, *J* = 7.6 Hz, 2H), 2.46 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.4, 138.6, 137.7, 137.2, 137.1, 137.0, 135.9, 134.0, 130.5, 129.3, 128.4, 119.1, 99.3, 60.4, 29.4 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{17}H_{15}IO_3SNa$ 448.9684; Found 448.9662.



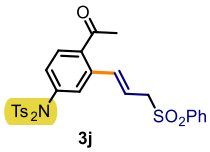
3h

(E)-1-(5-bromo-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3h): Pale yellow liquid; yield 61% (69 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 – 7.84 (m, 2H), 7.74 – 7.71 (m, 1H), 7.65 – 7.59 (m, 1H), 7.59 – 7.47 (m, 3H), 7.31 (d, *J* = 8.2 Hz, 1H), 6.84 (d, *J* = 15.7 Hz, 1H), 6.06 – 5.91 (m, 1H), 3.96 (d, *J* = 7.6 Hz, 2H), 2.46 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.9, 138.6, 138.4, 137.0, 134.8, 134.6, 133.9, 131.9, 129.5, 129.3, 128.4, 122.0, 118.6, 60.4, 29.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{17}H_{15}BrO_3SNa$ 400.9823; Found 400.9831.



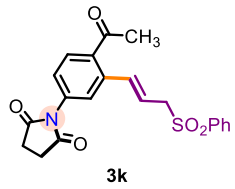
3i

(E)-1-(4-(benzyloxy)-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)ethan-1-one (3i): Pale yellow liquid; yield 67% (82 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.5 Hz, 2H), 7.69 (d, *J* = 8.6 Hz, 1H), 7.63 – 7.57 (m, 1H), 7.54 – 7.46 (m, 2H), 7.46 – 7.31 (m, 5H), 7.07 (d, *J* = 15.7 Hz, 1H), 7.00 (s, 1H), 6.91 (d, *J* = 8.6 Hz, 1H), 6.01 – 5.88 (m, 1H), 5.13 (s, 2H), 3.99 (d, *J* = 7.4 Hz, 2H), 2.45 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.1, 161.4, 139.2, 139.0, 138.5, 136.1, 133.8, 132.3, 129.3, 129.1, 128.8, 128.4 (2C), 127.5, 117.7, 114.5, 113.9, 70.2, 60.4, 28.9 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{24}H_{22}O_4SNa$ 429.1136; Found 429.1142.



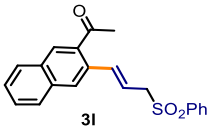
3j

(E)-N-(4-acetyl-3-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)-4-methyl-N-tosylbenzenesulfonamide (3j): Pale yellow liquid; yield 37% (69 mg); Eluent- 40-45% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.86 – 7.81 (m, 4H), 7.77 (d, *J* = 7.4 Hz, 2H), 7.69 – 7.59 (m, 2H), 7.56 – 7.49 (m, 2H), 7.43 – 7.36 (m, 4H), 7.10 (d, *J* = 8.1 Hz, 1H), 6.91 – 6.80 (m, 2H), 5.67 – 5.53 (m, 1H), 3.92 (d, *J* = 7.3 Hz, 2H), 2.51 (s, 9H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.3, 145.9, 138.4, 137.7, 137.5, 137.4, 137.0, 136.3, 134.1, 131.5, 131.0, 130.1, 130.0, 129.4, 128.7, 128.4, 119.7, 60.5, 29.6, 21.9 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{31}H_{29}NO_7S_3Na$ 646.1004; Found 646.0994.



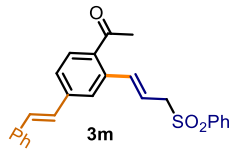
3k

(E)-1-(4-acetyl-3-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)pyrrolidine-2,5-dione (3k): Pale yellow liquid; yield 49% (58 mg); Eluent- 35-40% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 7.9 Hz, 2H), 7.75 (d, *J* = 8.2 Hz, 1H), 7.63 (t, *J* = 7.4 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.45 (s, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 6.92 (d, *J* = 15.7 Hz, 1H), 6.08 – 5.95 (m, 1H), 3.98 (d, *J* = 7.6 Hz, 2H), 2.94 (s, 4H), 2.49 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.3, 175.8, 138.4, 137.4, 137.3, 136.3, 135.0, 134.0, 130.1, 129.3, 128.5, 126.1, 125.8, 119.2, 60.5, 29.6, 28.6 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{21}H_{20}O_5S$ 398.1062; Found 398.1065.



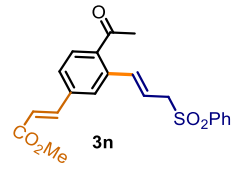
3l

(E)-1-(3-(3-(phenylsulfonyl)prop-1-en-1-yl)naphthalen-2-yl)ethan-1-one (3l): Pale yellow solid; yield 57% (60 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.20 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 2H), 7.91 –7.81 (m, 3H), 7.66 – 7.48 (m, 5H), 7.08 (d, *J* = 15.5 Hz, 1H), 6.15 – 6.00 (m, 1H), 4.04 (d, *J* = 7.5 Hz, 2H), 2.63 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.8, 139.0, 138.7, 134.8, 134.7, 133.9, 133.1, 132.1, 130.9, 129.2, 128.9, 128.8, 128.5, 128.0, 127.7, 127.3, 117.0, 60.6, 29.3 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{21}H_{18}O_3SNa$ 373.0874; Found 373.0882.



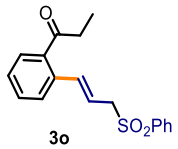
3m

1-(2-((E)-3-(phenylsulfonyl)prop-1-en-1-yl)-4-((E)-styryl)phenyl)ethan-1-one (3m): Pale yellow liquid; yield 69% (83 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 (d, *J* = 7.7 Hz, 2H), 7.71 – 7.61 (m, 2H), 7.59 – 7.51 (m, 5H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.43 – 7.36 (m, 2H), 7.32 (dd, *J* = 8.2, 6.4 Hz, 1H), 7.23 (s, 1H), 7.13 – 7.01 (m, 2H), 6.13 – 5.99 (m, 1H), 4.03 (d, *J* = 7.5 Hz, 2H), 2.50 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.3, 141.1, 138.8, 138.7, 136.9, 136.6, 135.1, 133.9, 131.7, 130.2, 129.2, 128.9, 128.5 (2C), 127.0, 126.9, 126.3, 125.8, 117.8, 60.6, 29.3 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{25}H_{22}O_3SNa$ 425.1187; Found 425.1190.



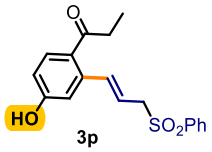
3n

Methyl (E)-3-(4-acetyl-3-((E)-3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)acrylate (3n): Pale yellow liquid; yield 62% (71 mg); Eluent- 35-40% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.94 – 7.84 (m, 2H), 7.71 – 7.60 (m, 3H), 7.58 – 7.44 (m, 4H), 6.97 (d, *J* = 15.7 Hz, 1H), 6.55 – 6.42 (m, 1H), 6.04 – 5.90 (m, 1H), 3.99 (d, *J* = 7.5 Hz, 2H), 3.81 (s, 3H), 2.48 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 200.4, 166.9, 142.9, 138.6, 137.8, 137.7, 136.7, 133.9, 129.9, 129.3, 128.4 (2C), 127.7, 127.3, 120.6, 118.6, 60.4, 52.0, 29.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{21}H_{20}O_5SNa$ 407.0929; Found 407.0931.



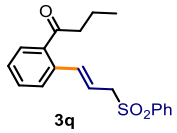
3o

(E)-1-(2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)propan-1-one (3o): Pale yellow liquid; yield 53% (50 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.91 – 7.86 (m, 2H), 7.65 – 7.57 (m, 2H), 7.56 – 7.50 (m, 2H), 7.48 – 7.41 (m, 2H), 7.38 – 7.31 (m, 1H), 6.91 – 6.81 (m, 1H), 6.07 – 5.92 (m, 1H), 3.99 (d, *J* = 7.5 Hz, 2H), 2.83 (q, *J* = 7.2 Hz, 2H), 1.11 (t, *J* = 7.2 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 204.7, 138.6, 138.2, 137.3, 135.6, 133.9, 131.6, 129.2, 128.5, 128.4, 128.3, 127.9, 117.7, 60.6, 34.8, 8.4 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{18}O_3SNa$ 337.0874; Found 337.0855.



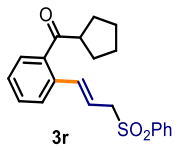
3p

(E)-1-(4-hydroxy-2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)propan-1-one (3p): Pale yellow liquid; yield 62% (61 mg); Eluent- 35-40% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.92 – 7.87 (m, 2H), 7.65 – 7.58 (m, 2H), 7.56 – 7.50 (m, 2H), 7.06 – 6.99 (m, 1H), 6.96 (s, 1H), 6.88 – 6.76 (m, 1H), 5.99 – 5.86 (m, 1H), 3.99 (d, *J* = 7.5 Hz, 2H), 2.83 (q, *J* = 7.3 Hz, 2H), 1.10 (t, *J* = 7.3 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 203.0, 159.6, 139.6, 139.3, 138.2, 134.1, 131.8, 129.4, 128.6, 128.4, 116.8, 115.3, 115.1, 60.6, 33.8, 8.7 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{18}O_4SNa$ 353.0823; Found 353.0805.



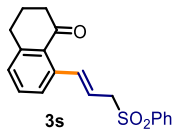
3q

(E)-1-(2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)butan-1-one (3q): Pale yellow liquid; yield 51% (50 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.65 – 7.57 (m, 2H), 7.57 – 7.50 (m, 2H), 7.49 – 7.41 (m, 2H), 7.38 – 7.31 (m, 1H), 6.86 (d, *J* = 15.7 Hz, 1H), 6.06 – 5.93 (m, 1H), 3.98 (d, *J* = 7.6 Hz, 2H), 2.78 (t, *J* = 7.3 Hz, 2H), 1.71 – 1.59 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 204.4, 138.7, 138.1, 137.6, 135.6, 133.9, 131.6, 129.2, 128.5, 128.4, 128.2, 127.9, 117.7, 60.6, 43.6, 17.9, 13.9 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{19}H_{20}O_3SNa$ 351.1031; Found 351.1031.



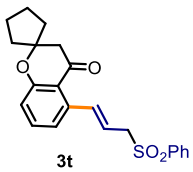
3r

(E)-cyclopentyl(2-(3-(phenylsulfonyl)prop-1-en-1-yl)phenyl)methanone (3r): Pale yellow liquid; yield 46% (49 mg); Eluent- 20-25% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.94 – 7.84 (m, 2H), 7.66 – 7.40 (m, 6H), 7.37 – 7.32 (m, 1H), 6.78 (d, *J* = 15.7 Hz, 1H), 6.07 – 5.97 (m, 1H), 3.98 (d, *J* = 7.6 Hz, 2H), 3.55 – 3.37 (m, 1H), 1.82 – 1.72 (m, 4H), 1.68 – 1.56 (m, 4H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 207.1, 138.7, 138.2, 137.9, 135.6, 133.9, 131.3, 129.2, 128.5, 128.3, 128.2, 127.7, 117.6, 60.6, 49.6, 29.9, 26.3 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{21}H_{22}O_3SNa$ 377.1187; Found 377.1190.



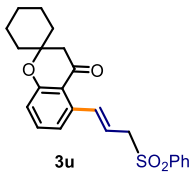
3s

(E)-8-(3-(phenylsulfonyl)prop-1-en-1-yl)-3,4-dihydronaphthalen-1(2H)-one (3s): Pale yellow liquid; yield 84% (82 mg); Eluent- 25-30% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 7.7 Hz, 2H), 7.65 – 7.58 (m, 1H), 7.57 – 7.49 (m, 2H), 7.43 – 7.34 (m, 1H), 7.33 – 7.15 (m, 3H), 5.95 – 5.82 (m, 1H), 4.03 (d, *J* = 7.5 Hz, 2H), 2.93 (t, *J* = 6.1 Hz, 2H), 2.59 (t, *J* = 6.6 Hz, 2H), 2.11 – 1.99 (m, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.7, 145.6, 140.4, 138.6 (2C), 133.8, 132.7, 130.1, 129.1 (2C), 128.4, 127.0, 116.8, 60.6, 40.6, 30.6, 22.8 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{19}H_{18}O_3SNa$ 349.0874; Found 349.0862.

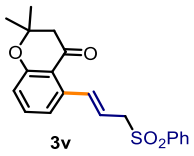


3t

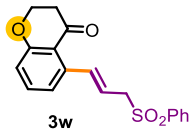
(E)-5-(3-(phenylsulfonyl)prop-1-en-1-yl)spiro[chromane-2,1'-cyclopentan]-4-one (3t): Pale yellow liquid; yield 65% (74 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 7.8 Hz, 2H), 7.69 – 7.49 (m, 3H), 7.44 – 7.33 (m, 2H), 6.98 – 6.85 (m, 2H), 6.03 – 5.90 (m, 1H), 4.03 (d, *J* = 7.6 Hz, 2H), 2.75 (s, 2H), 2.14 – 1.95 (m, 2H), 1.91 – 1.79 (m, 2H), 1.76 – 1.55 (m, 4H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.9, 161.1, 139.3, 138.6, 135.0, 133.8, 129.2 (2C), 128.5 (2C), 120.5, 118.9, 117.9, 89.4, 60.6, 48.3, 37.3, 23.9 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{22}H_{22}O_4SNa$ 405.1136; Found 405.1144.



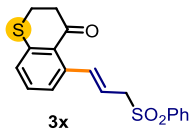
(E)-5-(3-(phenylsulfonyl)prop-1-en-1-yl)spiro[chromane-2,1'-cyclohexan]-4-one (3u): Pale yellow liquid; yield 70% (83 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 – 7.84 (m, 2H), 7.67 – 7.58 (m, 1H), 7.57 – 7.48 (m, 2H), 7.41 – 7.30 (m, 2H), 6.97 – 6.85 (m, 2H), 5.99 – 5.86 (m, 1H), 4.00 (d, *J* = 7.5 Hz, 2H), 2.61 (s, 2H), 1.97 – 1.82 (m, 2H), 1.74 – 1.55 (m, 3H), 1.53 – 1.39 (m, 4H), 1.37 – 1.21 (m, 1H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.8, 160.4, 139.2, 138.6, 138.4, 135.1, 133.8, 129.1, 128.5, 120.4, 118.8, 117.9, 117.7, 79.4, 60.6, 49.3, 34.6, 25.2, 21.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{23}H_{24}O_4SNa$ 419.1293; Found 419.1294.



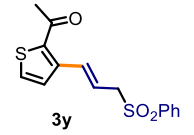
(E)-2,2-dimethyl-5-(3-(phenylsulfonyl)prop-1-en-1-yl)chroman-4-one (3v): Pale yellow liquid; yield 68% (73 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 – 7.84 (m, 2H), 7.64 – 7.56 (m, 1H), 7.56 – 7.49 (m, 2H), 7.40 – 7.31 (m, 2H), 6.96 – 6.84 (m, 2H), 6.02 – 5.83 (m, 1H), 4.00 (d, *J* = 7.7 Hz, 2H), 2.63 (s, 2H), 1.39 (s, 6H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.7, 160.7, 139.2, 138.6, 138.4, 135.1, 133.8, 129.1, 128.5, 120.4, 118.7, 117.9, 117.1, 78.6, 60.6, 50.1, 26.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{20}H_{20}O_4SNa$ 379.0980; Found 379.0985.



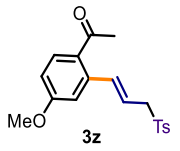
(E)-5-(3-(phenylsulfonyl)prop-1-en-1-yl)chroman-4-one (3w): Pale yellow liquid; yield 71% (70 mg); Eluent- 30-40% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 7.8 Hz, 2H), 7.67 – 7.57 (m, 1H), 7.57 – 7.48 (m, 2H), 7.42 – 7.32 (m, 2H), 7.00 – 6.88 (m, 2H), 6.01 – 5.86 (m, 1H), 4.45 (t, *J* = 6.5 Hz, 2H), 4.02 (d, *J* = 7.7 Hz, 2H), 2.73 (t, *J* = 6.5 Hz, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 193.0, 162.7, 139.3, 139.2, 138.6, 135.1, 133.8, 129.2, 128.5, 121.2, 118.4, 118.3, 118.0, 66.5, 60.6, 39.0 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{16}O_4SNa$ 351.0667; Found 351.0674.



(E)-5-(3-(phenylsulfonyl)prop-1-en-1-yl)thiochroman-4-one (3x): Pale yellow liquid; yield 38% (39 mg); Eluent- 35-40% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.97 – 7.86 (m, 2H), 7.69 – 7.61 (m, 1H), 7.61 – 7.51 (m, 2H), 7.35 – 7.21 (m, 2H), 7.13 – 7.03 (m, 2H), 5.94 – 5.78 (m, 1H), 4.02 (d, *J* = 7.5 Hz, 2H), 3.23 – 3.11 (m, 2H), 3.02 – 2.88 (m, 2H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 195.9, 143.4, 140.5, 140.4, 138.8, 133.9, 132.4, 129.2, 129.0, 128.5, 128.0, 126.0, 117.0, 60.6, 41.2, 26.3 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{16}O_3S_2Na$ 367.0439; Found 367.0437.

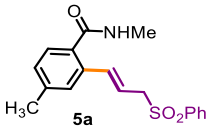


(E)-1-(3-(3-(phenylsulfonyl)prop-1-en-1-yl)thiophen-2-yl)ethan-1-one (3y): Pale yellow liquid; yield 73% (67 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.82 – 7.78 (m, 2H), 7.60 – 7.53 (m, 1H), 7.49 – 7.44 (m, 2H), 7.36 – 7.32 (m, 1H), 7.24 – 7.18 (m, 2H), 6.18 – 6.03 (m, 1H), 3.93 (d, *J* = 7.7 Hz, 2H), 2.39 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 191.1, 142.3, 138.5, 136.2, 133.9, 132.8, 130.1, 129.2, 128.4, 127.5, 120.2, 60.7, 30.0 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{15}H_{14}O_3S_2Na$ 329.0282; Found 329.0287.



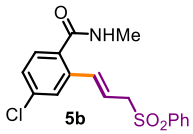
3z

(E)-1-(4-methoxy-2-(3-tosylprop-1-en-1-yl)phenyl)ethan-1-one (3z): Pale yellow liquid; yield 67% (69 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.79 – 7.73 (m, 2H), 7.72 – 7.67 (m, 1H), 7.32 (d, *J* = 7.8 Hz, 2H), 7.09 (d, *J* = 15.6 Hz, 1H), 6.92 – 6.88 (m, 1H), 6.87 – 6.80 (m, 1H), 6.03 – 5.85 (m, 1H), 3.98 (d, *J* = 7.0 Hz, 2H), 3.87 (s, 3H), 2.47 (s, 3H), 2.41 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 199.2, 162.4, 144.8, 139.4, 139.0, 135.8, 132.3, 129.8, 129.3, 128.5, 117.9, 113.7, 113.1, 60.6, 55.6, 29.0, 21.7 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{19}H_{20}O_4SNa$ 367.0980; Found 367.0982.



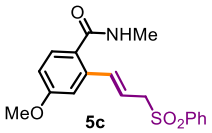
5a

(E)-N,4-dimethyl-2-(3-(phenylsulfonyl)prop-1-en-1-yl)benzamide (5a): White solid; yield 73% (72 mg); Eluent- 60-65% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, DMSO) δ 8.14 – 8.07 (m, 1H), 7.94 – 7.87 (m, 2H), 7.77 – 7.70 (m, 1H), 7.68 – 7.61 (m, 2H), 7.38 (s, 1H), 7.26 – 7.22 (m, 1H), 7.13 (d, *J* = 7.6 Hz, 1H), 6.85 – 6.77 (m, 1H), 6.12 – 6.01 (m, 1H), 4.27 (d, *J* = 7.5 Hz, 2H), 2.70 (d, *J* = 4.4 Hz, 3H), 2.33 (s, 3H) ppm; **^{13}C NMR** (101 MHz, DMSO) δ 168.8, 139.2, 138.7, 135.8, 133.8, 133.6, 133.6, 129.3, 128.5, 128.0, 127.5, 126.2, 117.4, 59.0, 26.1, 20.8 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{18}H_{20}NO_3S$ 330.1164; Found 330.1151.



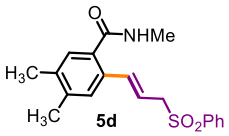
5b

(E)-4-chloro-N-methyl-2-(3-(phenylsulfonyl)prop-1-en-1-yl)benzamide (5b): White solid; yield 39% (41 mg); Eluent- 60-65% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 7.5 Hz, 2H), 7.72 – 7.65 (m, 1H), 7.61 – 7.56 (m, 2H), 7.46 (d, *J* = 8.3 Hz, 1H), 7.41 (d, *J* = 2.0 Hz, 1H), 7.32 – 7.27 (m, 1H), 6.90 (d, *J* = 15.7 Hz, 1H), 6.13 – 5.93 (m, 2H), 3.97 (d, *J* = 7.6 Hz, 2H), 2.97 (d, *J* = 4.8 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 168.4, 138.9, 136.7, 136.6, 136.1, 134.2, 133.6, 129.6, 129.5, 128.6, 128.4, 126.9, 119.3, 60.4, 27.2 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{17}H_{17}ClNO_3S$ 350.0618; Found 350.0606.



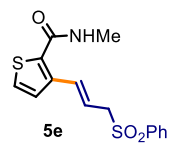
5c

(E)-4-methoxy-N-methyl-2-(3-(phenylsulfonyl)prop-1-en-1-yl)benzamide (5c): White solid; yield 69% (71 mg); Eluent- 65-70% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.94 – 7.86 (m, 2H), 7.70 – 7.63 (m, 1H), 7.61 – 7.53 (m, 2H), 7.52 – 7.44 (m, 1H), 6.97 (d, *J* = 15.7 Hz, 1H), 6.91 (s, 1H), 6.87 – 6.81 (m, 1H), 6.08 – 5.89 (m, 2H), 3.97 (d, *J* = 7.6 Hz, 2H), 3.84 (s, 3H), 2.94 (d, *J* = 4.7 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.1, 161.1, 138.9, 138.1, 136.3, 134.0, 130.0, 129.4, 128.4, 127.9, 118.0, 113.9, 112.2, 60.5, 55.6, 27.1 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{18}H_{20}NO_4S$ 346.1113; Found 346.1102.



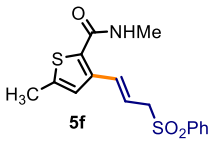
5d

(E)-N,4,5-trimethyl-2-(3-(phenylsulfonyl)prop-1-en-1-yl)benzamide (5d): White solid; yield 52% (54 mg); Eluent- 60-65% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.93 – 7.85 (m, 2H), 7.68 – 7.61 (m, 1H), 7.59 – 7.50 (m, 2H), 7.27 (d, *J* = 1.7 Hz, 1H), 7.22 (s, 1H), 6.84 (s, 1H), 6.07 – 5.95 (m, 1H), 5.90 (s, 1H), 3.95 (d, *J* = 7.6 Hz, 2H), 2.93 (d, *J* = 4.8 Hz, 3H), 2.27 (s, 3H), 2.25 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 169.6, 139.3, 138.9, 137.8, 137.4, 134.0, 132.8, 131.8, 129.3, 129.2, 128.4, 127.9, 116.6, 60.6, 27.0, 19.8, 19.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{19}H_{22}NO_3S$ 344.1320; Found 344.1313.



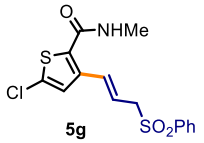
5e

(E)-N-methyl-3-(3-(phenylsulfonyl)prop-1-en-1-yl)thiophene-2-carboxamide (5e): Pale yellow solid; yield 92% (89 mg); Eluent- 60-65% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.80 (d, *J* = 7.8 Hz, 2H), 7.61 – 7.54 (m, 1H), 7.52 – 7.43 (m, 2H), 7.20 (d, *J* = 5.3 Hz, 1H), 7.12 – 7.00 (m, 2H), 6.08 – 5.90 (m, 2H), 3.89 (d, *J* = 7.5 Hz, 2H), 2.84 (d, *J* = 4.8 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.1, 139.6, 138.7, 134.0, 133.0, 132.7, 129.3, 128.4, 127.2, 126.8, 118.6, 60.5, 27.0 ppm; HRMS (ESI) m/z: [M + Na]+ Calcd. For $C_{15}H_{15}NO_3S_2Na$ 344.0386; Found 344.0390.



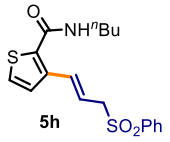
5f

(E)-N,5-dimethyl-3-(3-(phenylsulfonyl)prop-1-en-1-yl)thiophene-2-carboxamide (5f): Pale yellow solid; yield 89% (89 mg); Eluent- 60-65% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 7.3 Hz, 2H), 7.67 – 7.59 (m, 1H), 7.58 – 7.50 (m, 2H), 7.10 (d, *J* = 15.8 Hz, 1H), 6.84 (s, 1H), 6.05 – 5.93 (m, 1H), 5.89 – 5.82 (m, 1H), 3.93 (d, *J* = 7.7 Hz, 2H), 2.87 (d, *J* = 4.4 Hz, 3H), 2.42 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.1, 141.9, 139.9, 138.7, 134.0, 132.8, 130.6, 129.3, 128.4, 125.2, 118.3, 60.6, 26.9, 15.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{16}H_{17}NO_3S_2Na$ 358.0548; Found 358.0547.



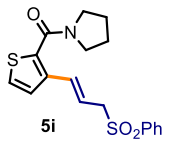
5g

(E)-5-chloro-N-methyl-3-(3-(phenylsulfonyl)prop-1-en-1-yl)thiophene-2-carboxamide (5g): Pale yellow solid; yield 72% (77 mg); Eluent- 60-65% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.86 (d, *J* = 7.9 Hz, 2H), 7.69 – 7.63 (m, 1H), 7.61 – 7.52 (m, 2H), 7.02 (d, *J* = 15.9 Hz, 1H), 6.95 (s, 1H), 6.19 – 5.88 (m, 2H), 3.94 (d, *J* = 7.6 Hz, 2H), 2.90 (d, *J* = 4.9 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.0, 138.7 (2C), 134.2, 133.0, 132.1, 131.9, 129.5, 128.4, 126.0, 119.8, 60.3, 27.1 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{15}H_{14}ClNO_3S_2Na$ 378.0001; Found 378.0001.



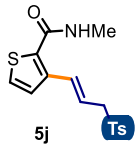
5h

(E)-N-butyl-3-(3-(phenylsulfonyl)prop-1-en-1-yl)thiophene-2-carboxamide (5h): Pale yellow solid; yield 83% (90 mg); Eluent- 55-60% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.92 – 7.82 (m, 2H), 7.70 – 7.60 (m, 1H), 7.59 – 7.50 (m, 2H), 7.27 (d, *J* = 5.4 Hz, 1H), 7.21 – 7.12 (m, 2H), 6.14 – 6.00 (m, 1H), 6.02 – 5.94 (m, 1H), 3.96 (d, *J* = 7.6 Hz, 2H), 3.36 (q, *J* = 6.7 Hz, 2H), 1.59 – 1.51 (m, 2H), 1.40 – 1.32 (m, 2H), 0.94 (t, *J* = 7.3 Hz, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 162.3, 139.7, 138.7, 134.0, 133.1, 132.6, 129.3, 128.4, 127.0, 126.9, 118.4, 60.6, 40.0, 31.7, 20.2, 13.9 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{21}NO_3S_2Na$ 386.0861; Found 386.0862.



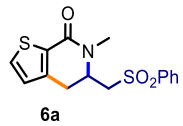
5i

(E)-(3-(3-(phenylsulfonyl)prop-1-en-1-yl)thiophen-2-yl)(pyrrolidin-1-yl)methanone (5i): Pale yellow solid; yield 80% (87 mg); Eluent- 50-55% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.87 (d, *J* = 7.7 Hz, 2H), 7.72 – 7.59 (m, 1H), 7.59 – 7.48 (m, 2H), 7.28 (d, *J* = 5.2 Hz, 1H), 7.13 (d, *J* = 5.2 Hz, 1H), 6.63 (d, *J* = 15.8 Hz, 1H), 6.09 – 5.98 (m, 1H), 3.93 (d, *J* = 7.6 Hz, 2H), 3.59 – 3.52 (m, 2H), 3.37 – 3.27 (m, 2H), 2.10-1.73 (m, 4H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.2, 138.8, 137.8, 133.9, 133.6, 131.9, 129.3, 128.4, 126.8, 125.1, 117.2, 60.5, 49.4, 46.7, 26.2, 24.5 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{18}H_{19}NO_3S_2Na$ 384.0704; Found 384.0707.



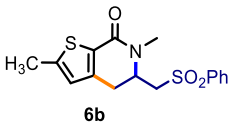
5j

(E)-N-methyl-3-(3-tosylprop-1-en-1-yl)thiophene-2-carboxamide (5j): Pale yellow solid; yield 85% (85 mg); Eluent- 60-65% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.34 (d, *J* = 7.9 Hz, 2H), 7.28 (d, *J* = 4.4 Hz, 1H), 7.20 – 7.09 (m, 2H), 6.12 – 5.96 (m, 2H), 3.94 (d, *J* = 7.5 Hz, 2H), 2.92 (d, *J* = 4.4 Hz, 3H), 2.43 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 163.1, 145.1, 139.6, 135.8, 133.1, 132.5, 130.0, 128.4, 127.2, 126.9, 118.9, 60.6, 27.0, 21.7 ppm; HRMS (ESI/TOF-Q) m/z: [M + Na]+ Calcd. For $C_{16}H_{17}NO_3S_2Na$ 358.0548; Found 358.0551.



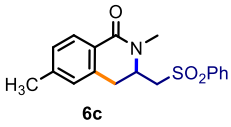
6a

(R)-6-methyl-5-((phenylsulfonyl)methyl)-5,6-dihydrothieno[2,3-c]pyridin-7(4H)-one (6a): White solid; yield 72% (69 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.89 (d, *J* = 8.3 Hz, 2H), 7.71 – 7.65 (m, 1H), 7.61 – 7.54 (m, 2H), 7.50 – 7.46 (m, 1H), 6.93 – 6.89 (m, 1H), 4.35 – 4.18 (m, 1H), 3.41 – 3.32 (m, 2H), 3.31 – 3.24 (m, 1H), 3.13 (d, *J* = 14.0 Hz, 1H), 2.98 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.7, 141.0, 139.4, 134.4, 131.9, 131.3, 129.7, 127.9, 127.6, 56.2, 54.8, 32.9, 29.1 ppm; HRMS (ESI) m/z: [M + Na]+ Calcd. For $C_{15}H_{15}NO_3S_2Na$ 344.0391; Found 344.0398.



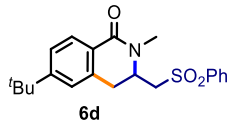
6b

(R)-2,6-dimethyl-5-((phenylsulfonyl)methyl)-5,6-dihydrothieno[2,3-c]pyridin-7(4H)-one (6b): White solid; yield 65% (65 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.90 (d, *J* = 7.4 Hz, 2H), 7.74 – 7.64 (m, 1H), 7.63 – 7.53 (m, 2H), 6.59 (s, 1H), 4.27 – 4.14 (m, 1H), 3.50 – 3.32 (m, 1H), 3.27 – 3.19 (m, 2H), 3.12 (d, *J* = 14.0 Hz, 1H), 2.95 (s, 3H), 2.48 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 160.8, 147.7, 141.5, 139.5, 134.3, 129.7, 128.9, 127.9, 126.2, 56.2, 54.7, 32.8, 29.2, 16.0 ppm; HRMS (ESI) m/z: [M + Na]+ Calcd. For $C_{16}H_{17}NO_3S_2Na$ 358.0548; Found 358.0551.



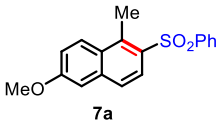
6c

(R)-2,6-dimethyl-3-((phenylsulfonyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one (6c): White solid; yield 52% (51 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.87 – 7.84 (m, 3H), 7.68 – 7.63 (m, 1H), 7.59 – 7.51 (m, 2H), 7.12 (d, *J* = 7.9 Hz, 1H), 6.93 (s, 1H), 4.24 – 4.12 (m, 1H), 3.39 (dd, *J* = 16.1, 5.7 Hz, 1H), 3.27 – 3.16 (m, 1H), 3.16 – 3.06 (m, 2H), 3.02 (s, 3H), 2.34 (s, 3H) ppm; **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.0, 143.0, 139.4, 134.8, 134.2, 129.6, 129.0, 128.4, 128.2, 127.8, 126.1, 56.2, 53.5, 33.7, 32.1, 21.6 ppm; HRMS (ESI) m/z: [M + Na]+ Calcd. For $C_{18}H_{19}NO_3SNa$ 352.0983; Found 352.0980.



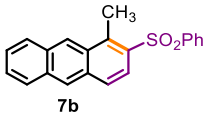
6d

(R)-6-(tert-butyl)-2-methyl-3-((phenylsulfonyl)methyl)-3,4-dihydroisoquinolin-1(2H)-one (6d): White solid; yield 53% (59 mg); Eluent- 30-35% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.94 – 7.84 (m, 3H), 7.73 – 7.63 (m, 1H), 7.64 – 7.55 (m, 2H), 7.36 (d, *J* = 8.3 Hz, 1H), 7.11 (s, 1H), 4.37 – 3.95 (m, 1H), 3.51 – 3.34 (m, 1H), 3.32 – 3.22 (m, 1H), 3.13 (d, *J* = 16.0 Hz, 2H), 3.02 (s, 3H), 1.32 (s, 9H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 164.1, 156.2, 139.5, 134.6, 134.3, 129.7, 128.1, 127.9, 126.1, 125.2, 124.9, 56.4, 53.6, 35.1, 33.7, 32.5, 31.3 ppm; HRMS (ESI) m/z: [M + Na]+ Calcd. For $C_{21}H_{25}NO_3SNa$ 394.1453; Found 394.1454.



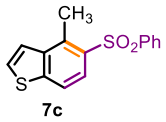
7a

6-methoxy-1-methyl-2-(phenylsulfonyl)naphthalene (7a): White solid; yield 89% (83 mg); Eluent- 20-25% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.26 (d, *J* = 8.9 Hz, 1H), 8.01 (d, *J* = 9.4 Hz, 1H), 7.88 (d, *J* = 7.7 Hz, 2H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.51 – 7.44 (m, 2H), 7.24 – 7.18 (m, 1H), 7.14 (d, *J* = 2.6 Hz, 1H), 3.94 (s, 3H), 2.81 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 159.7, 142.6, 137.4, 137.0, 134.0, 132.9, 129.1, 128.3, 127.4, 126.9, 125.8, 125.4, 120.2, 106.4, 55.6, 15.5 ppm; HRMS (ESI) m/z: [M + Na]+ Calcd. For $C_{18}H_{16}O_3SNa$ 335.0718; Found 335.0697; HRMS (ESI) m/z: [M + H]+ Calcd. For $C_{18}H_{17}O_3S$ 313.0898; Found 313.0885.



7b

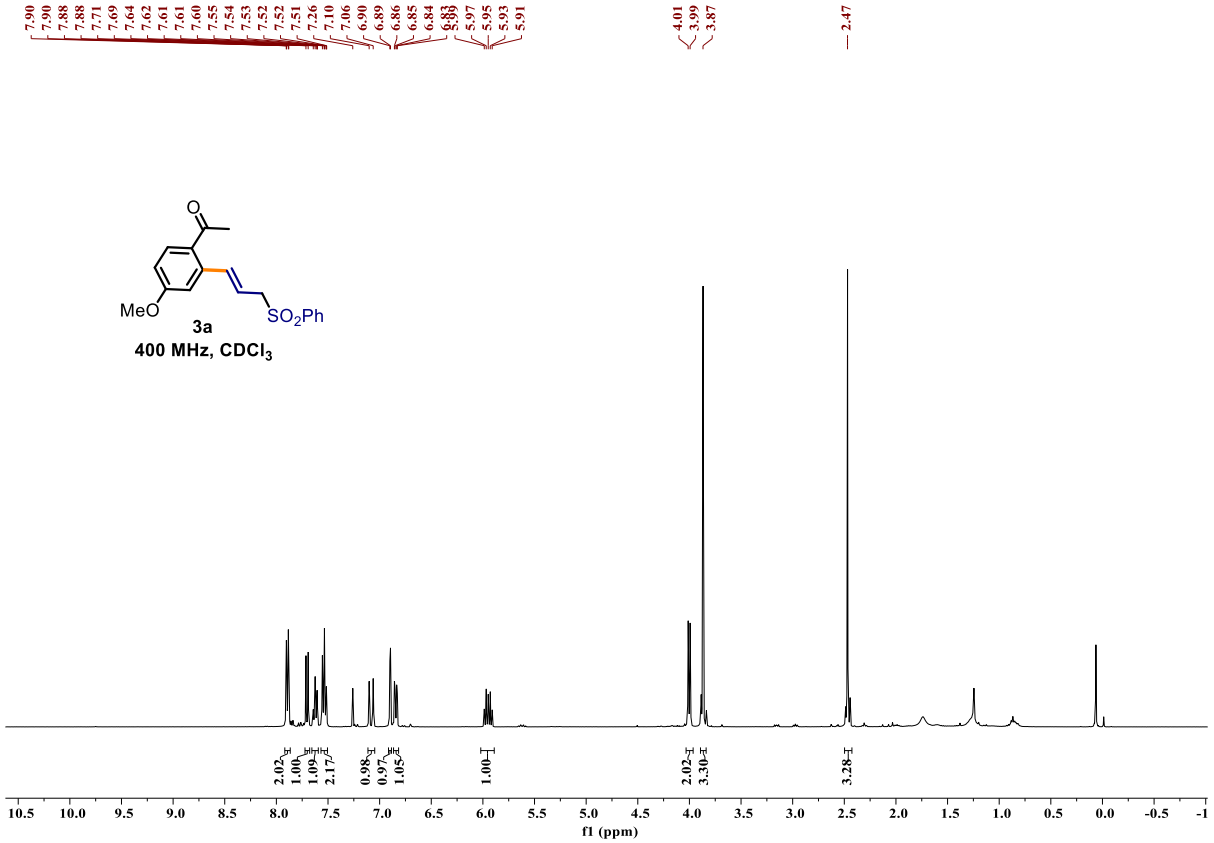
1-methyl-2-(phenylsulfonyl)anthracene (7b): Pale yellow solid; yield 92% (92 mg); Eluent- 20-25% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.70 (s, 1H), 8.43 (s, 1H), 8.21 (d, *J* = 9.1 Hz, 1H), 8.06 – 7.98 (m, 3H), 7.97 – 7.90 (m, 2H), 7.61 – 7.45 (m, 5H), 3.03 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.6, 138.2, 135.7, 133.1 (2C), 132.4, 132.2, 131.0, 129.2, 129.0, 127.9, 127.6, 127.5, 127.3, 127.2, 126.4, 125.1, 123.1, 15.8 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{21}H_{17}O_2S$ 333.0949; Found 333.0936.



7c

4-methyl-5-(phenylsulfonyl)benzo[*b*]thiophene (7c): Off-white solid; yield 84% (73 mg); Eluent- 20-25% ethyl acetate in hexane; **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.27 – 8.21 (m, 1H), 7.92 – 7.87 (m, 2H), 7.85 – 7.80 (m, 1H), 7.66 – 7.62 (m, 1H), 7.58 – 7.52 (m, 1H), 7.52 – 7.45 (m, 2H), 7.43 – 7.38 (m, 1H), 2.74 (s, 3H) ppm; **^{13}C NMR** (101 MHz, $CDCl_3$) δ 143.1, 142.8, 142.2, 134.0, 133.2, 133.1, 130.9, 129.2, 127.6, 125.5, 124.8, 121.6, 18.7 ppm; HRMS (ESI/TOF-Q) m/z: [M + H]+ Calcd. For $C_{15}H_{13}O_2S_2$ 289.0357; Found 289.0347.

NMR Spectra of Synthesized Compounds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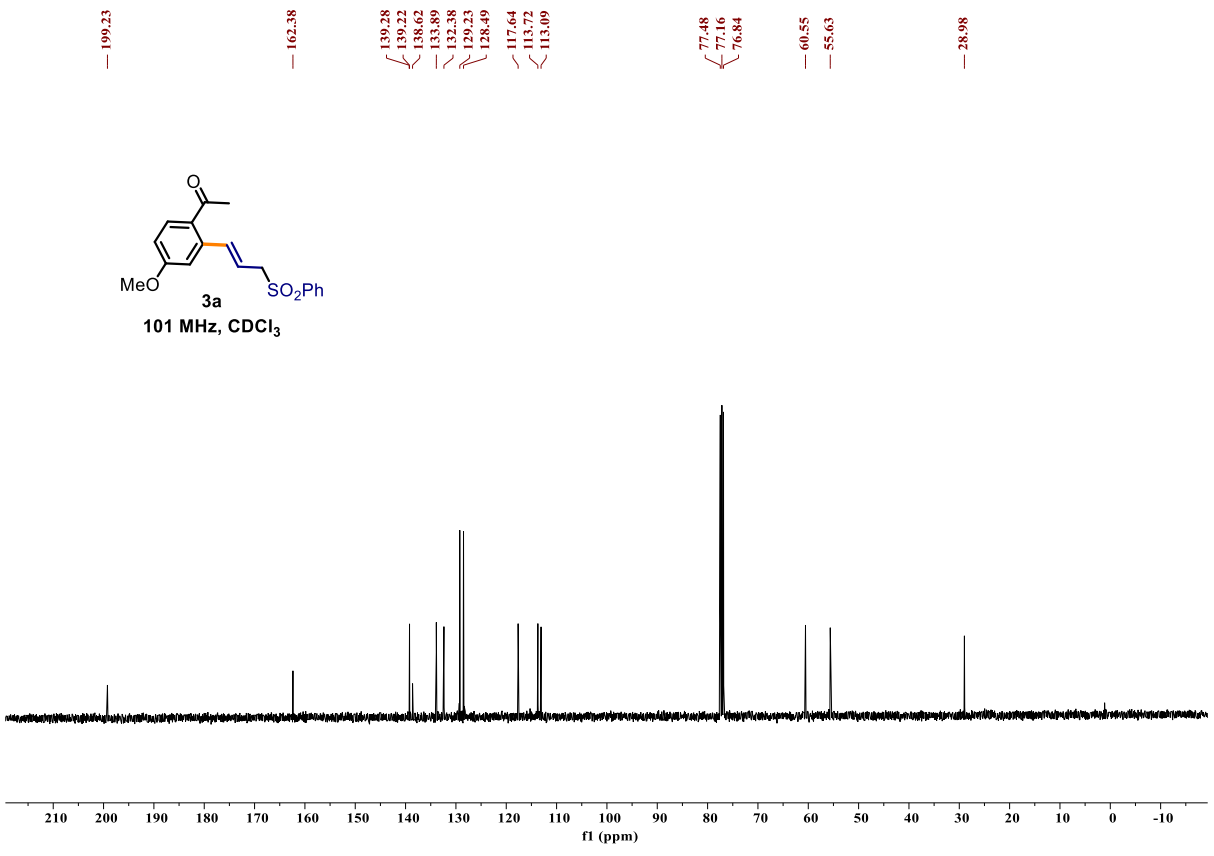
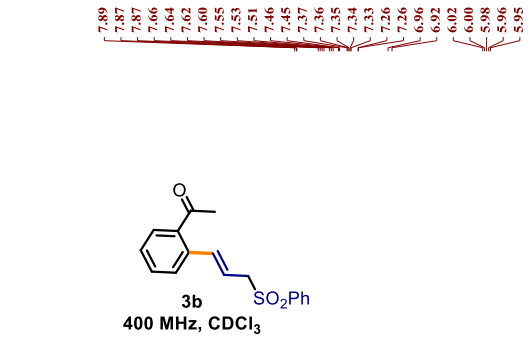
7.90
7.88
7.88
7.71
7.69
7.64
7.62
7.61
7.61
7.60
7.55
7.54
7.53
7.52
7.52
7.51
7.26
7.10
7.06
6.90
6.89
6.86
6.85
6.84
5.97
5.95
5.93
5.91
4.01
3.99
3.87
2.47
MeO
SO2Ph
3a
400 MHz, CDCl3
2.02
1.00
1.09
2.17
0.98
0.97
1.05
1.00
2.02
3.30
3.28
f1 (ppm)


199.23
162.38
139.28
139.22
138.62
133.89
132.38
129.23
128.49
117.64
113.72
113.09
77.48
77.16
76.84
60.55
55.63
28.98
MeO
SO2Ph
3a
101 MHz, CDCl3
f1 (ppm)


7.89
7.87
7.87
7.66
7.64
7.62
7.60
7.55
7.53
7.51
7.46
7.45
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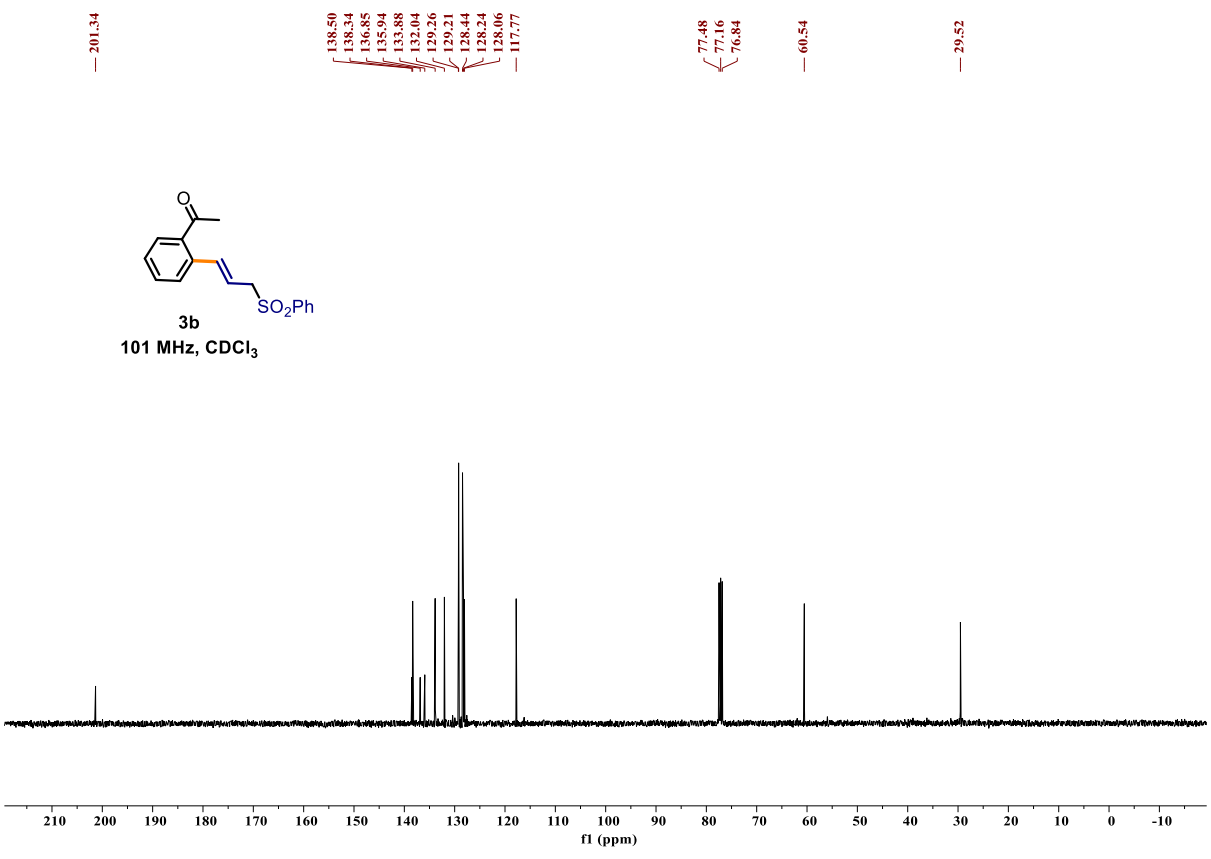
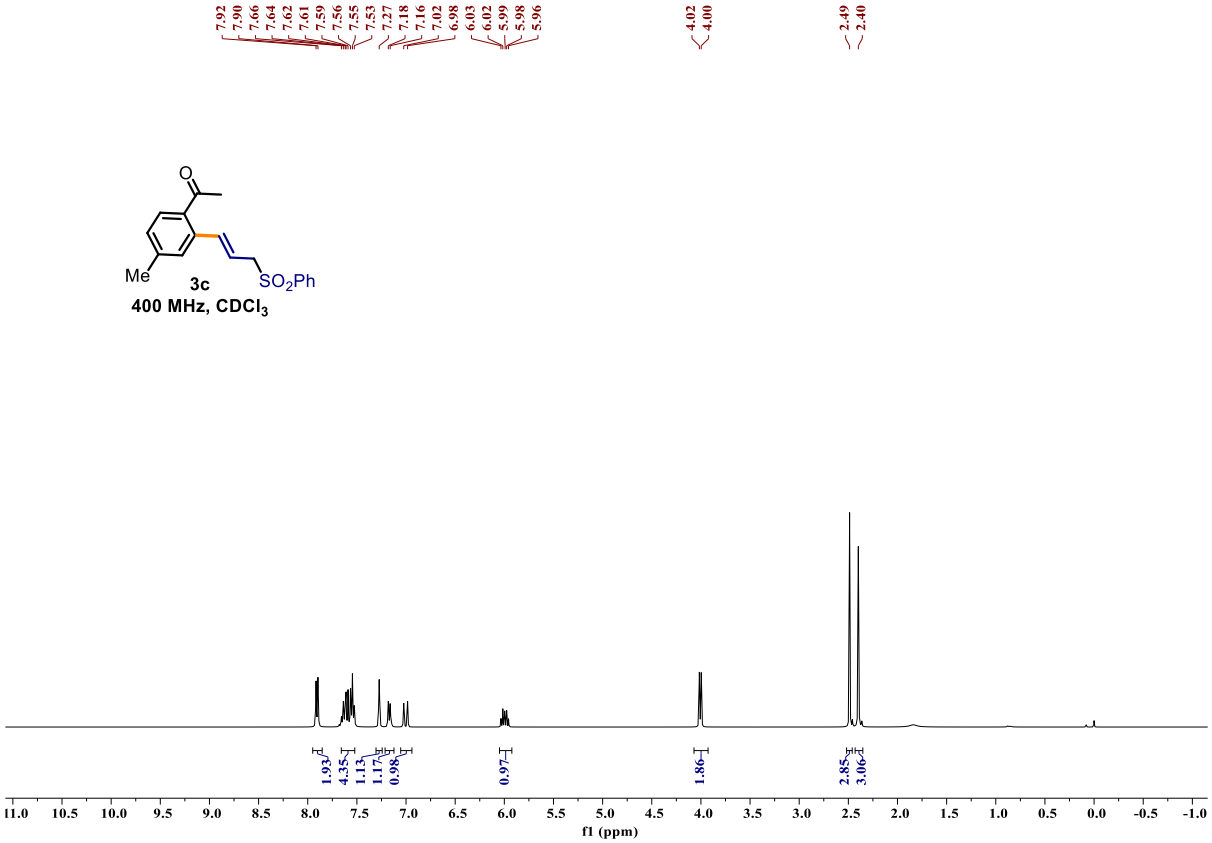
7.36
7.35
7.34
7.33
7.26
7.26
6.96
6.92
6.02
6.00
5.98
5.96
5.95
4.00
3.98
2.49
O
SO2Ph
3b
400 MHz, CDCl3
2.01
2.13
2.20
2.10
1.18
0.99
1.00
2.02
3.23
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


201.34
138.50
138.34
136.85
135.94
133.88
132.04
129.26
129.21
128.44
128.24
128.06
117.77
77.48
77.16
76.84
60.54
29.52
O
SO2Ph
3b
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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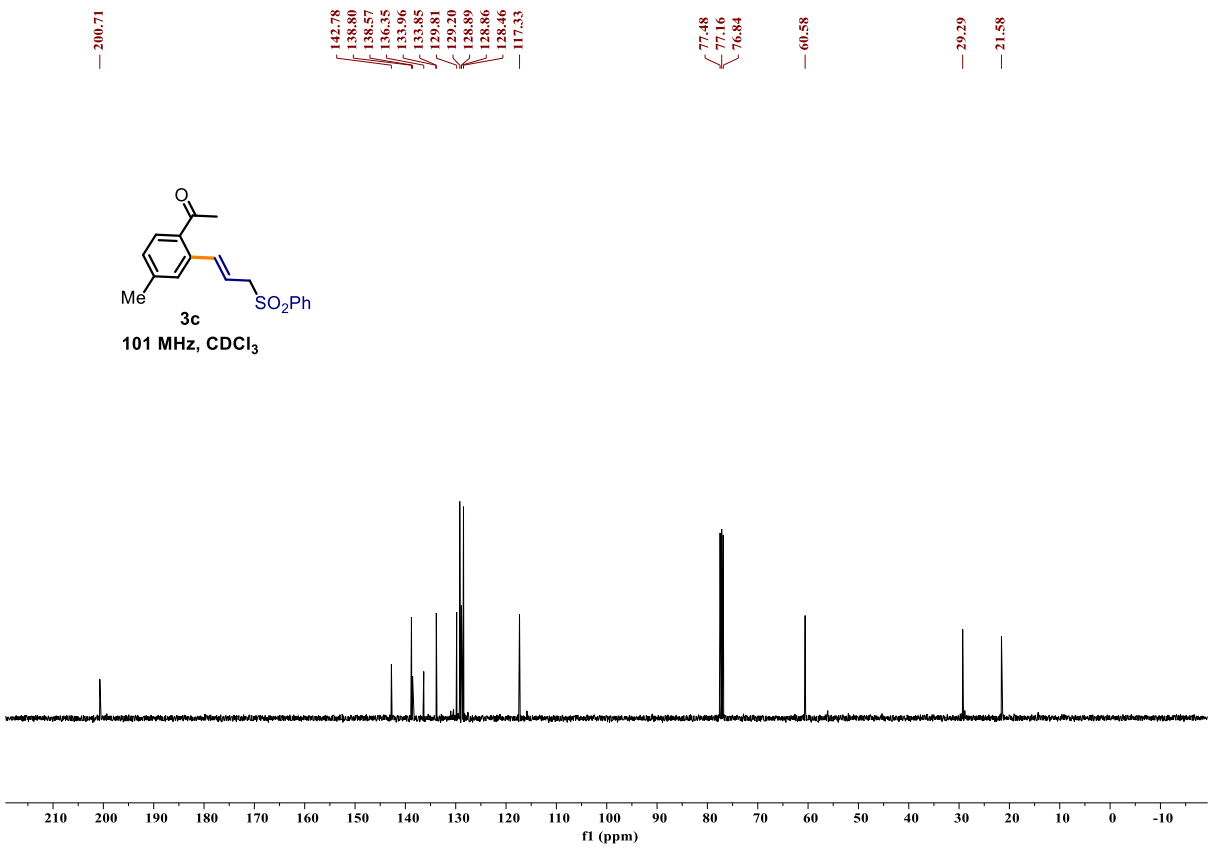
7.90
7.66
7.64
7.62
7.61
7.59
7.56
7.55
7.53
7.27
7.18
7.16
7.02
6.98
6.03
6.02
5.99
5.98
5.96
4.02
4.00
2.49
2.40
O
Me
SO2Ph
3c
400 MHz, CDCl3
1.93
4.35
1.13
1.17
0.98
0.97
1.86
2.85
3.06
f1 (ppm)


200.71
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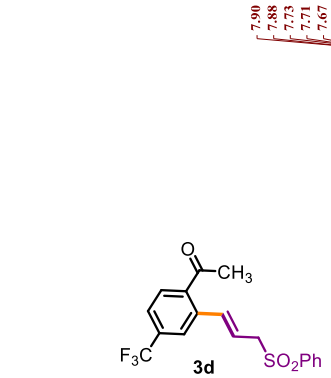
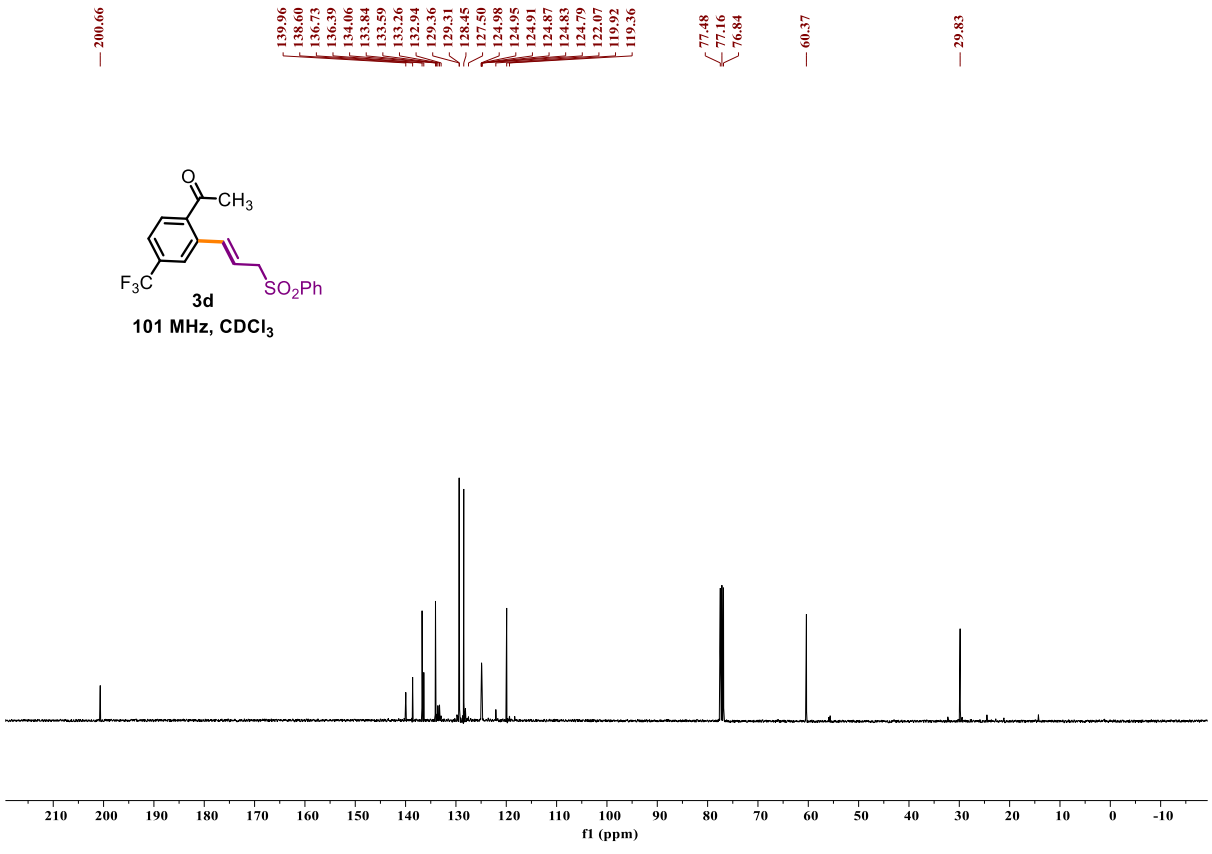
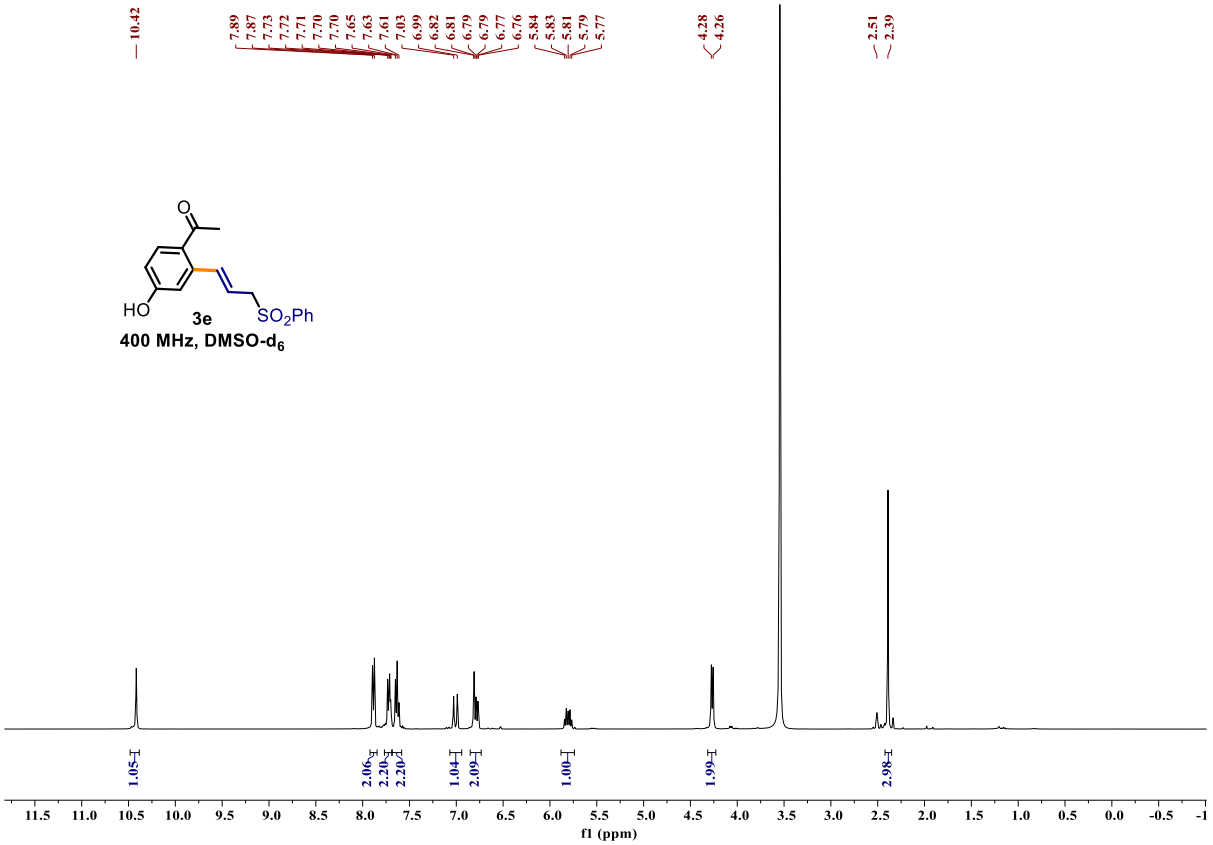
138.80
138.57
136.35
133.96
133.85
129.81
129.20
128.89
128.86
128.46
117.33
77.48
77.16
76.84
60.58
29.29
21.58
O
Me
SO2Ph
3c
101 MHz, CDCl3
f1 (ppm)


7.90
7.88
7.73
7.71
7.67
7.64
7.61
7.57
7.55
7.53
7.26
6.95
6.91
6.08
6.07
6.05
6.03
6.01
4.01
3.99
2.51
O
CH3
F3C
SO2Ph
3d
400 MHz, CDCl3
2.06
1.01
5.34
0.98
1.00
2.02
3.30
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


200.66
139.96
138.60
136.73
136.39
134.06
133.84
133.59
133.26
132.94
129.36
129.31
128.45
127.50
124.98
124.95
124.91
124.87
124.83
124.79
122.07
119.92
119.36
77.48
77.16
76.84
60.37
29.83
O
CH3
F3C
SO2Ph
3d
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


10.42
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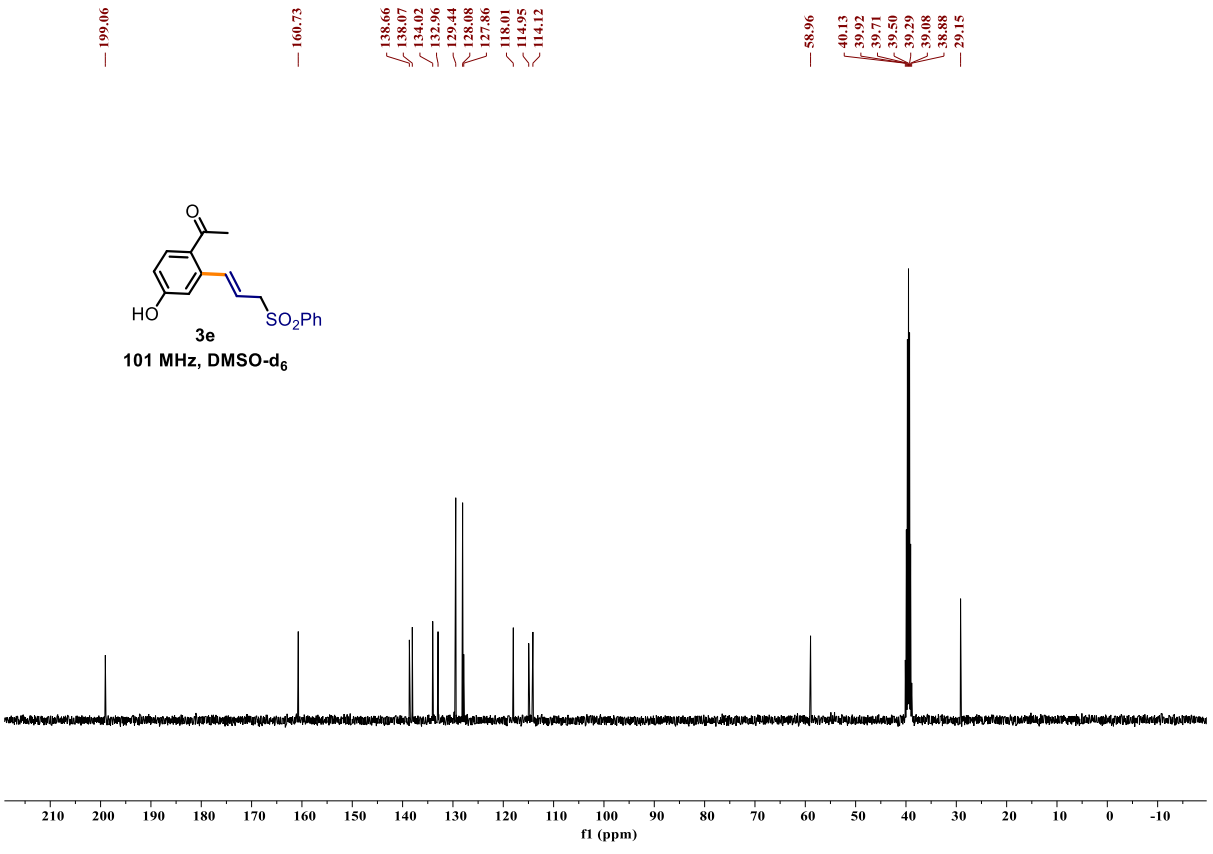
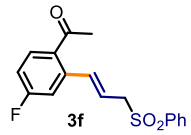
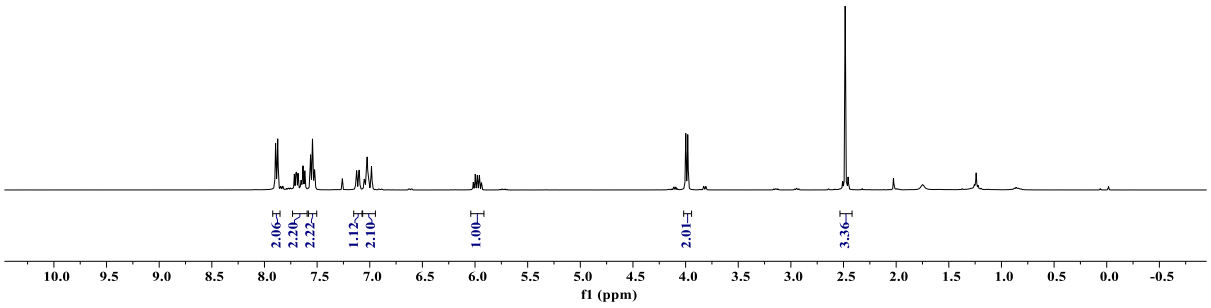
7.87
7.73
7.72
7.71
7.70
7.70
7.65
7.63
7.61
7.03
6.99
6.82
6.81
6.79
6.79
6.77
6.76
5.84
5.83
5.81
5.79
5.77
4.28
4.26
2.51
2.39
O
HO
SO2Ph
3e
400 MHz, DMSO-d6
1.05
2.06
2.20
2.20
1.04
2.09
1.00
1.99
2.98
f1 (ppm)

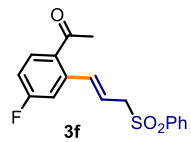

199.06
160.73
138.66
138.07
134.02
132.96
129.44
128.08
127.86
118.01
114.95
114.12
58.96
40.13
39.92
39.71
39.50
39.29
39.08
38.88
29.15
O
HO
SO2Ph
3e
101 MHz, DMSO-d6
f1 (ppm)



3f

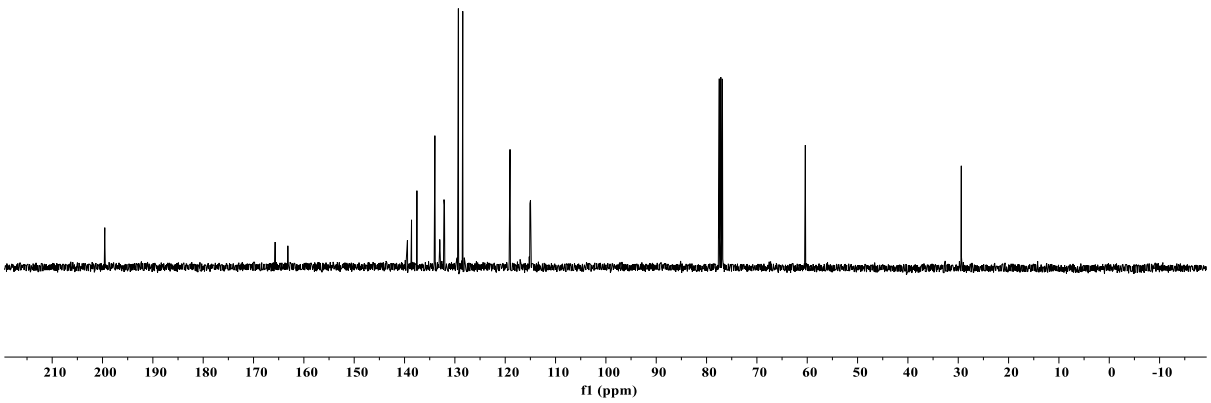
400 MHz, $CDCl_3$

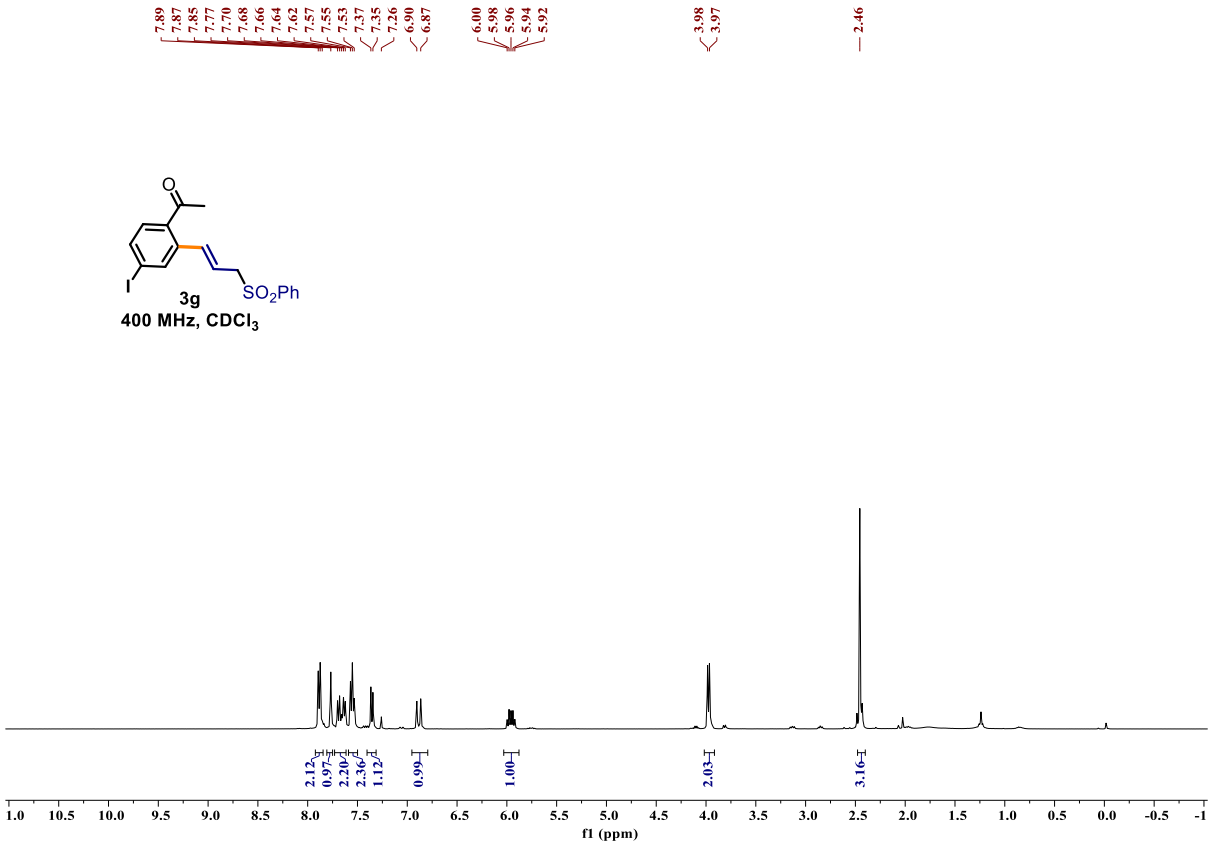


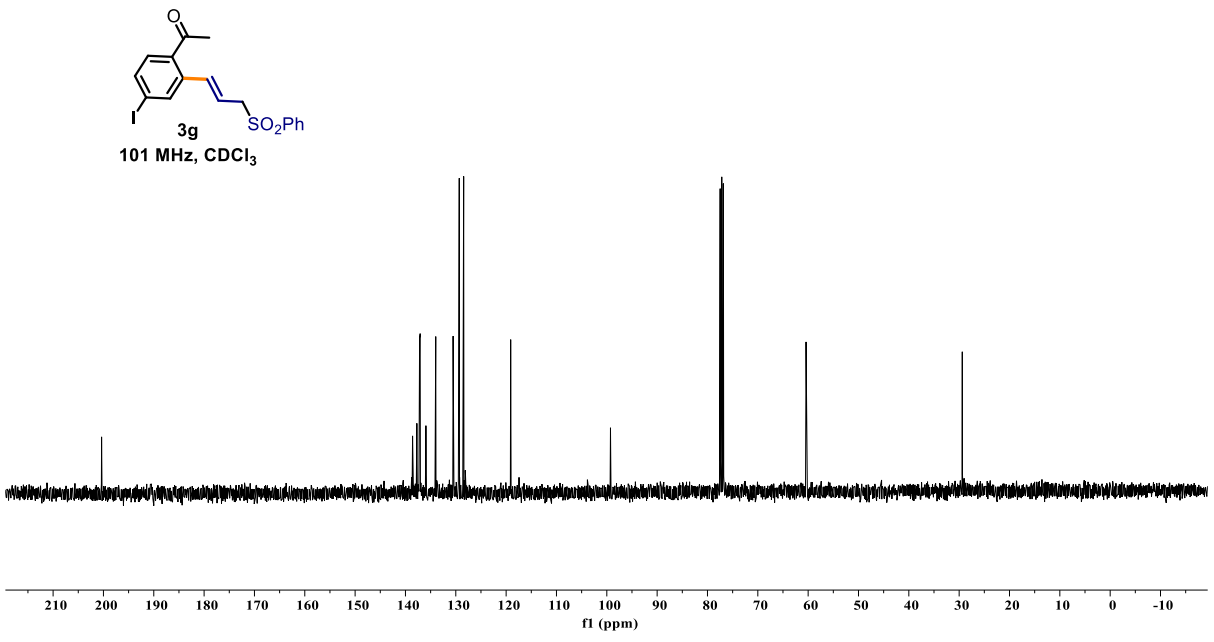


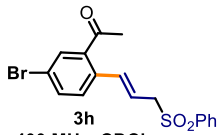
3f

101 MHz, $CDCl_3$

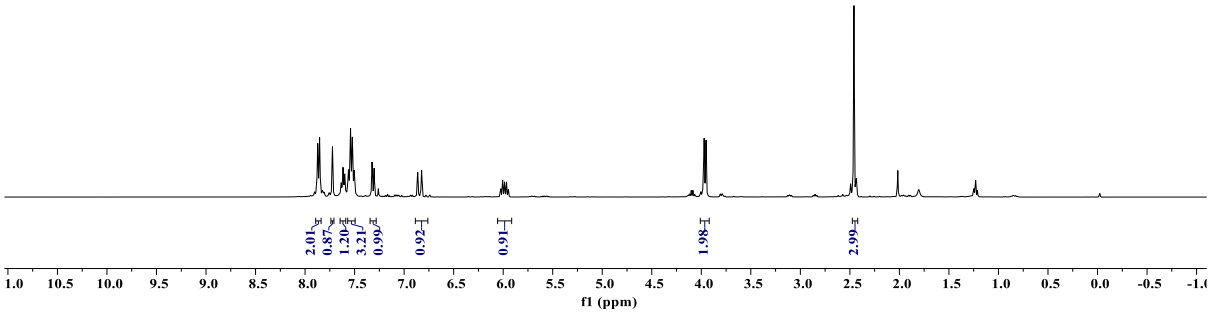


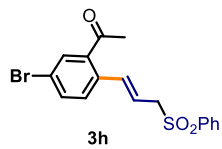

7.89
7.87
7.85
7.77
7.70
7.68
7.66
7.64
7.62
7.57
7.55
7.53
7.37
7.35
7.26
6.90
6.87
6.00
5.98
5.96
5.94
5.92
3.98
3.97
2.46
O
I
SO2Ph
3g
400 MHz, CDCl3
2.12
0.97
2.20
2.36
1.12
0.99
1.00
2.03
3.16
f1 (ppm)


200.37
138.59
137.73
137.19
137.08
136.98
135.94
133.98
130.53
129.31
128.43
119.09
99.27
77.48
77.16
76.84
60.42
29.38
O
I
SO2Ph
3g
101 MHz, CDCl3
f1 (ppm)

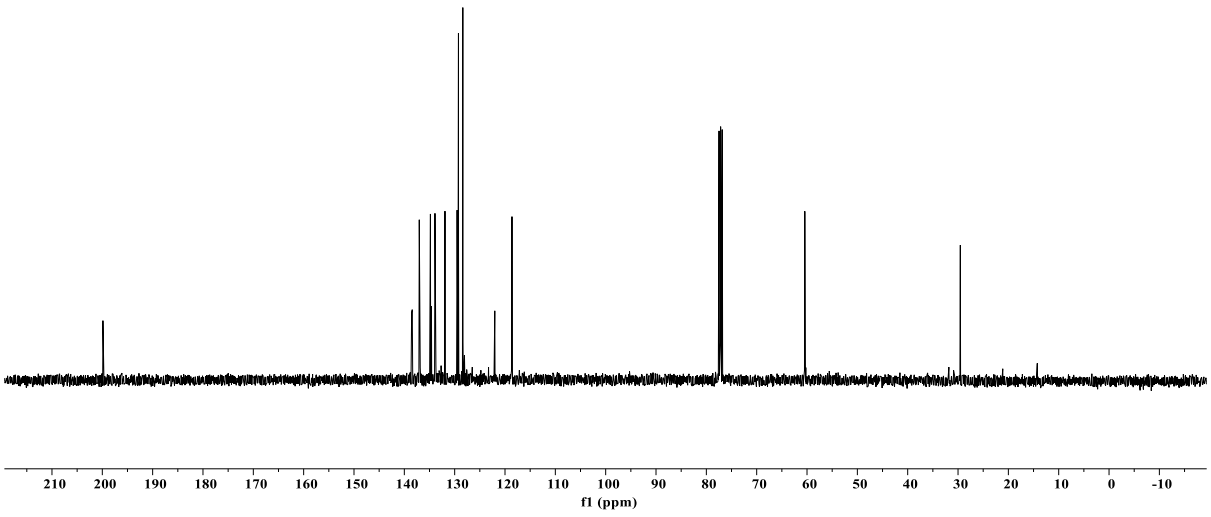


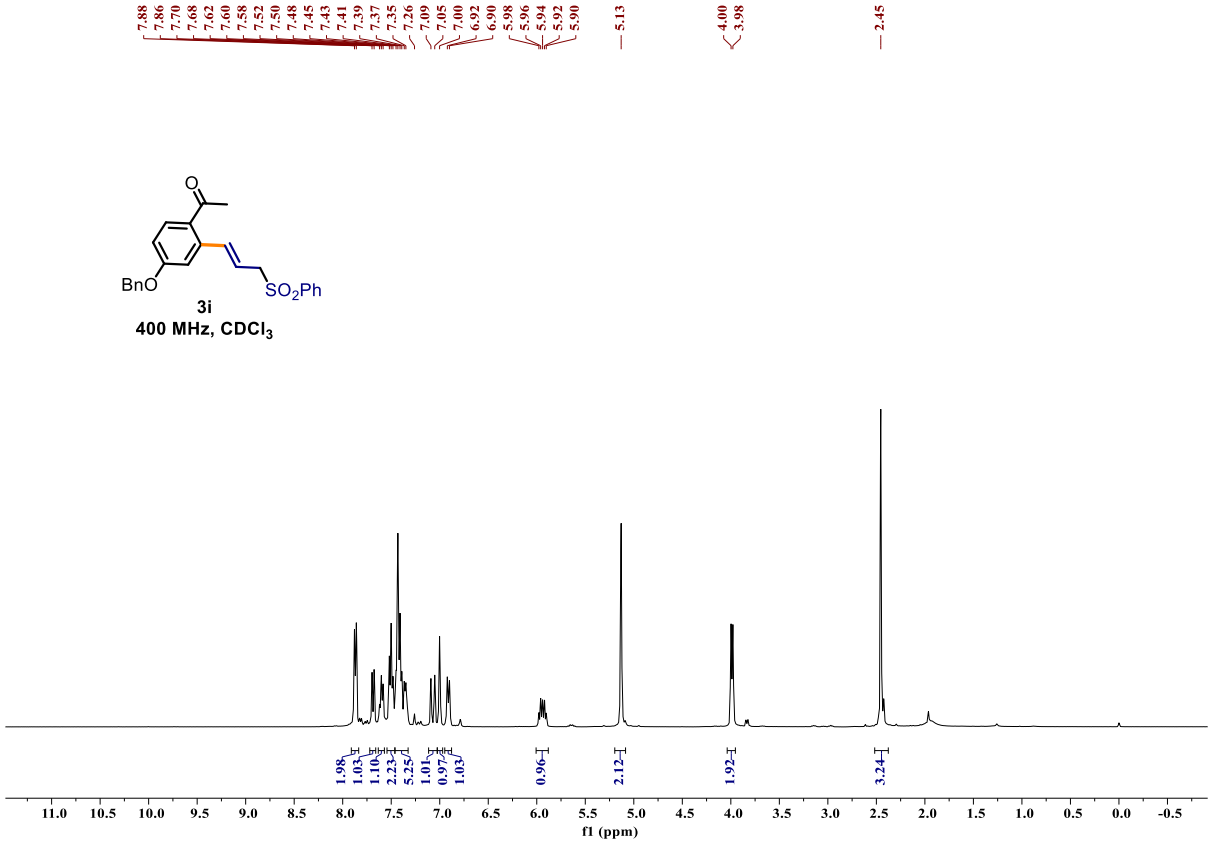
3h
400 MHz, $CDCl_3$

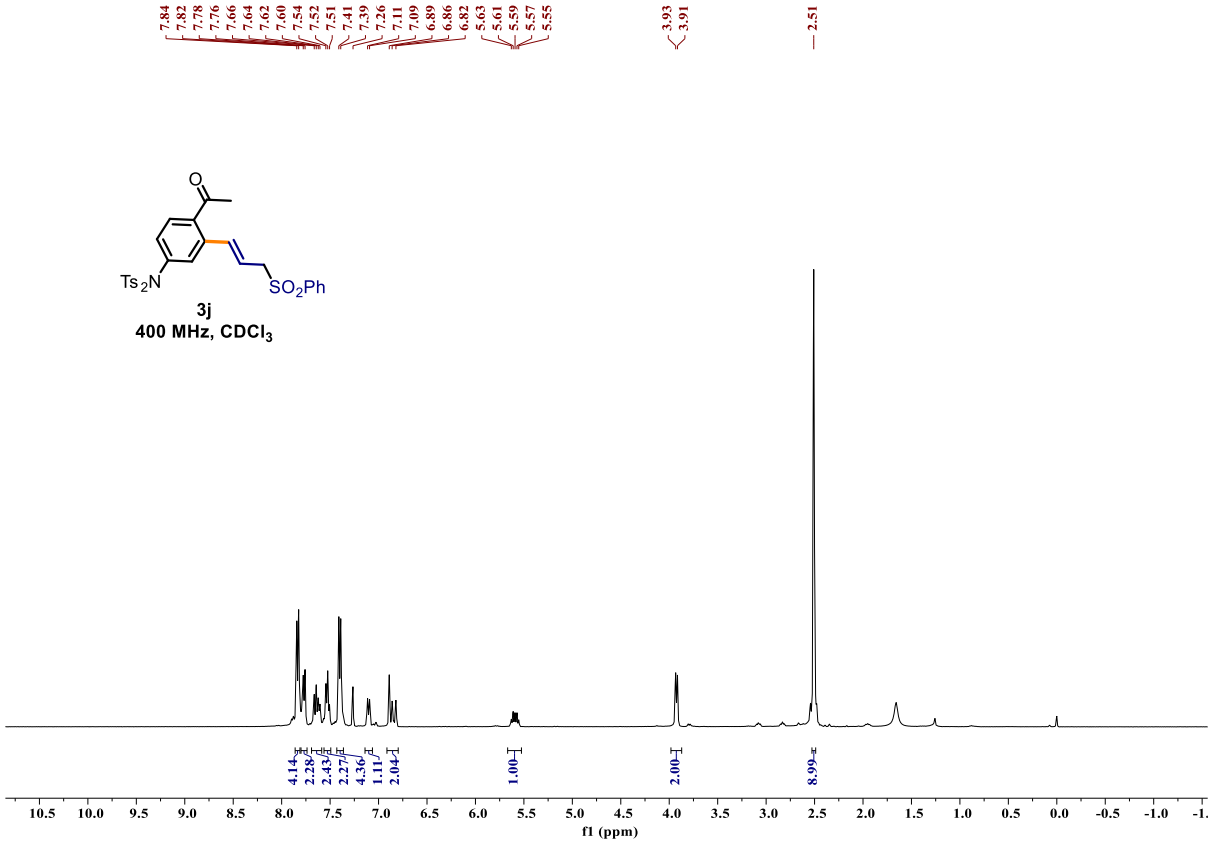


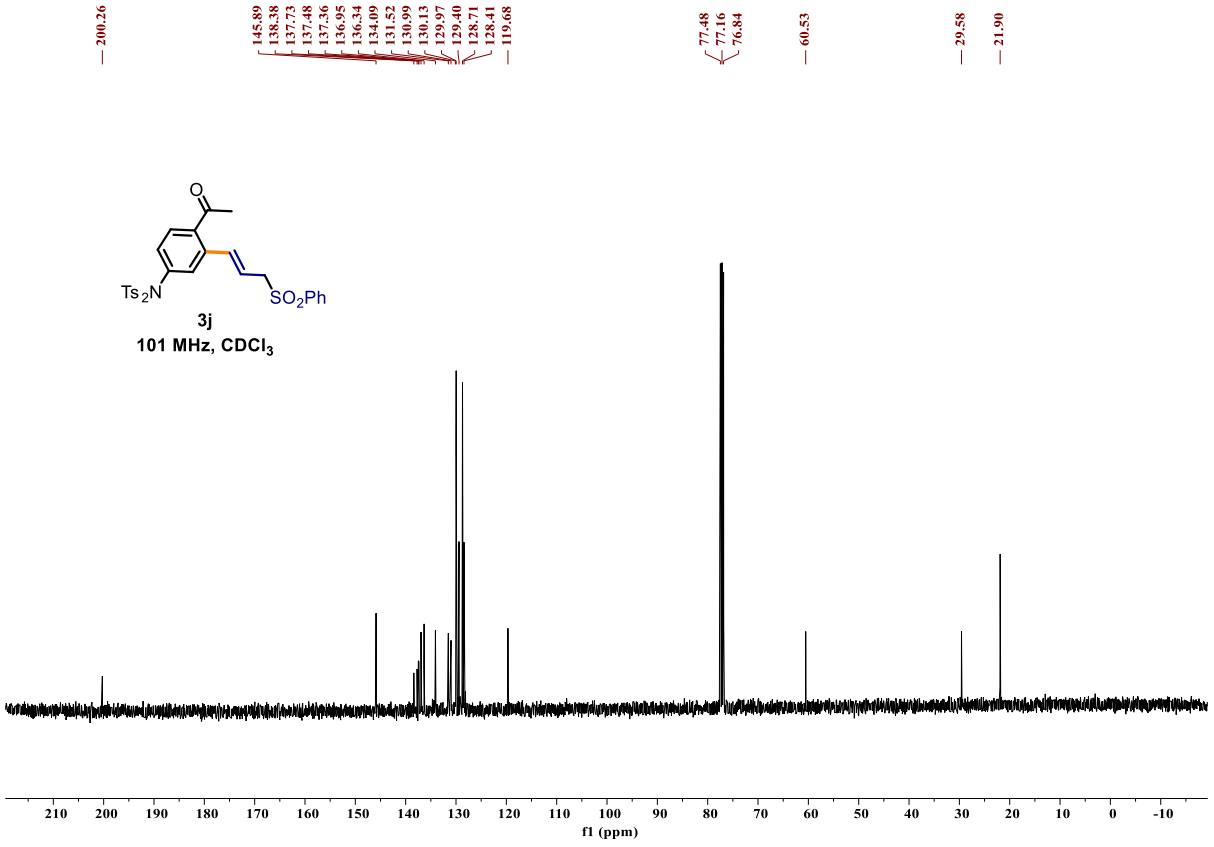


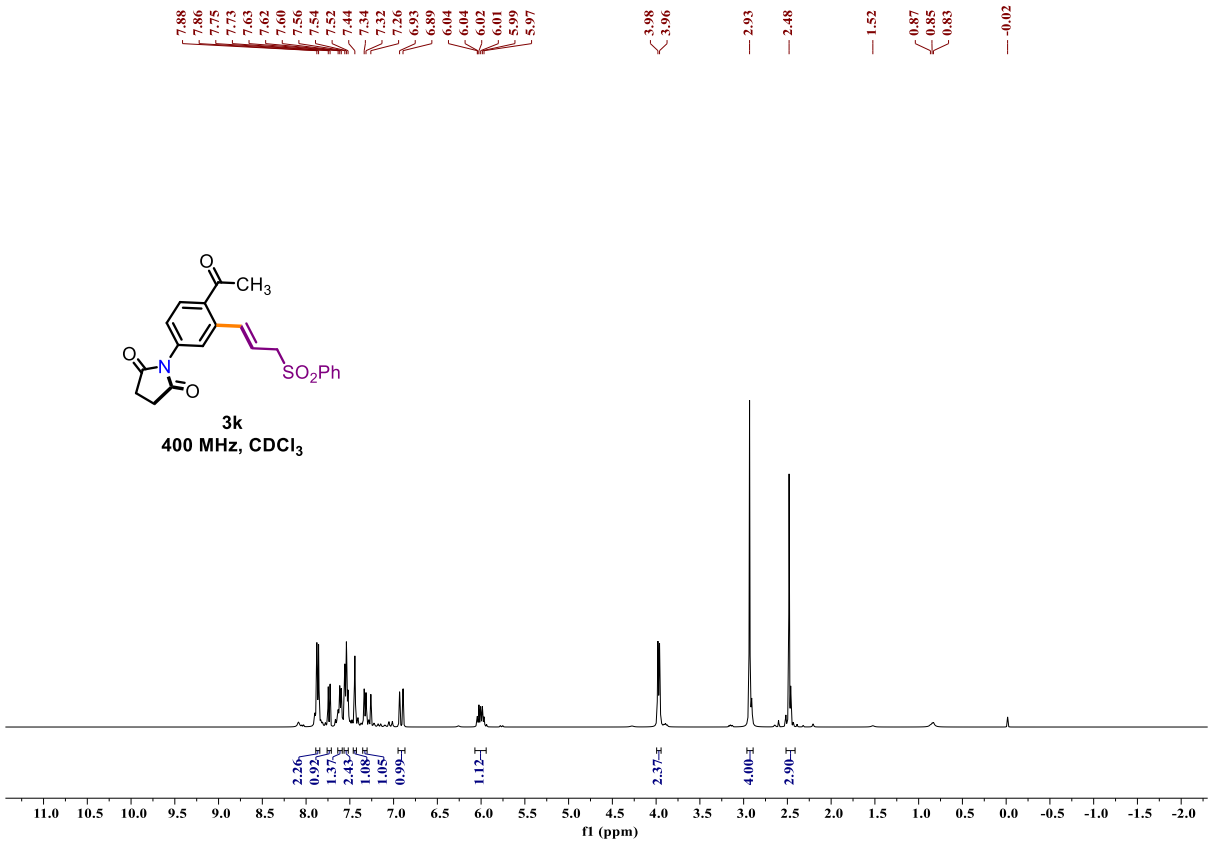
3h
101 MHz, $CDCl_3$



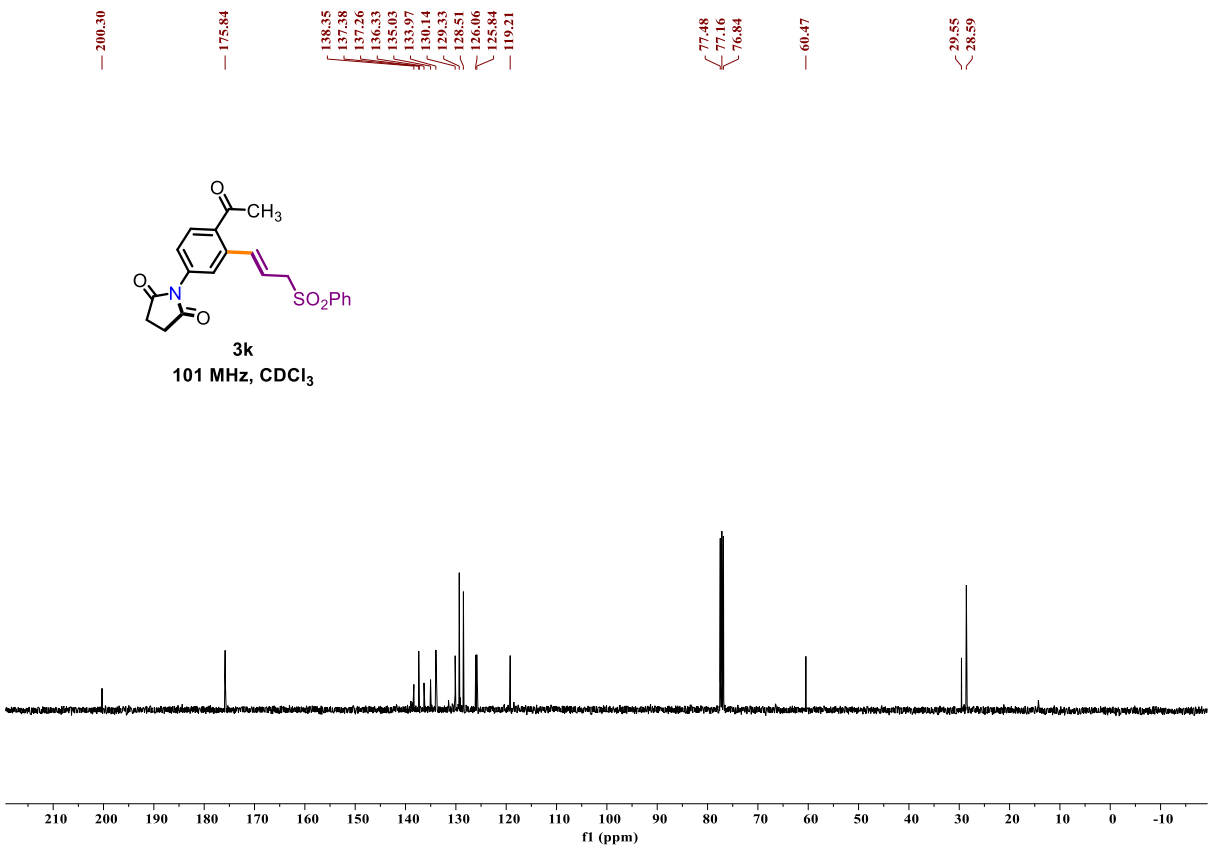

7.88
7.86
7.70
7.68
7.62
7.60
7.58
7.52
7.50
7.48
7.45
7.43
7.41
7.39
7.37
7.35
7.26
7.09
7.05
7.00
6.92
6.90
5.98
5.96
5.94
5.92
5.90
5.13
4.00
3.98
2.45
O
BnO
SO2Ph
3i
400 MHz, CDCl3
1.98
1.03
1.16
2.23
5.25
1.01
0.97
1.03
0.96
2.12
1.92
3.24
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
199.14
161.41
139.16
139.01
138.54
136.09
133.78
132.31
129.32
129.14
128.80
128.39
128.35
127.50
117.68
114.51
113.90
77.48
77.16
76.84
70.21
60.44
28.91
O
BnO
SO2Ph
3i
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.84
7.82
7.78
7.76
7.66
7.64
7.62
7.60
7.54
7.52
7.51
7.41
7.39
7.26
7.11
7.09
6.89
6.86
6.82
5.63
5.61
5.59
5.57
5.55
3.93
3.91
2.51
O
Ts2N
SO2Ph
3j
400 MHz, CDCl3
4.14
2.28
2.43
2.27
4.36
1.11
2.04
1.00
2.00
8.99
f1 (ppm)

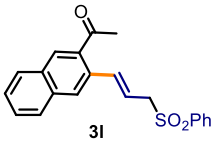

200.26
145.89
138.38
137.73
137.48
137.36
136.95
136.34
134.09
131.52
130.99
130.13
129.97
129.40
128.71
128.41
119.68
77.48
77.16
76.84
60.53
29.58
21.90
O
Ts2N
SO2Ph
3j
101 MHz, CDCl3
f1 (ppm)



3k
400 MHz, $CDCl_3$

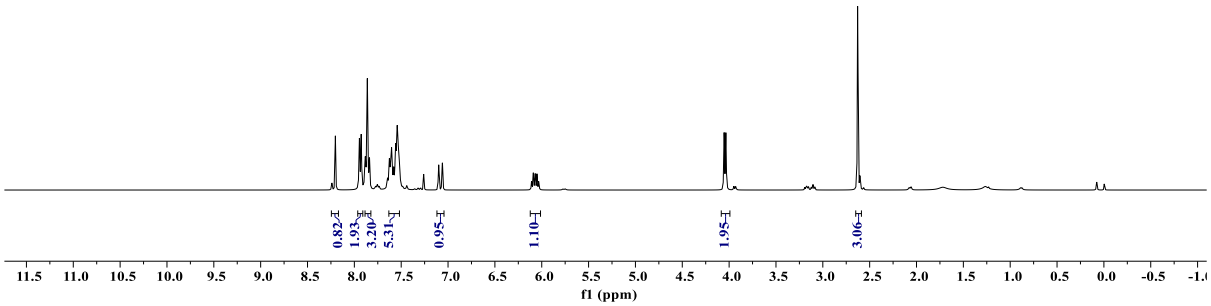


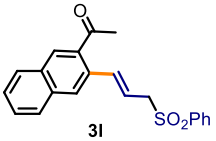
3k
101 MHz, $CDCl_3$



3l

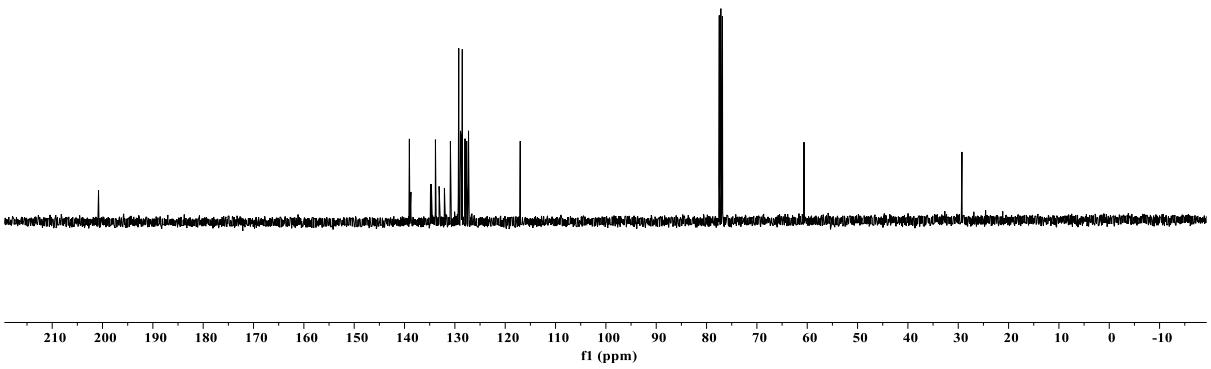
400 MHz, $CDCl_3$

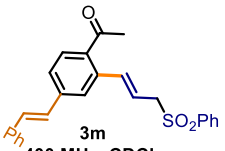




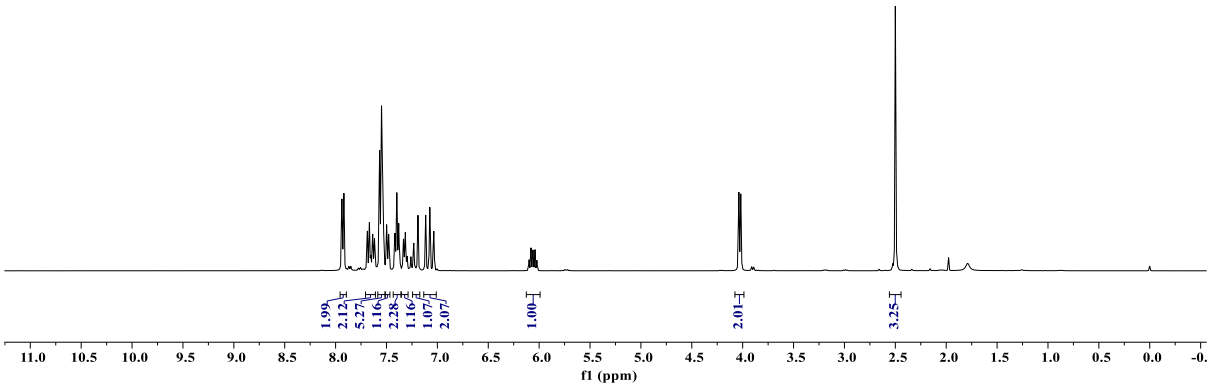
3l

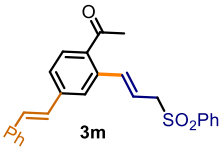
101 MHz, $CDCl_3$



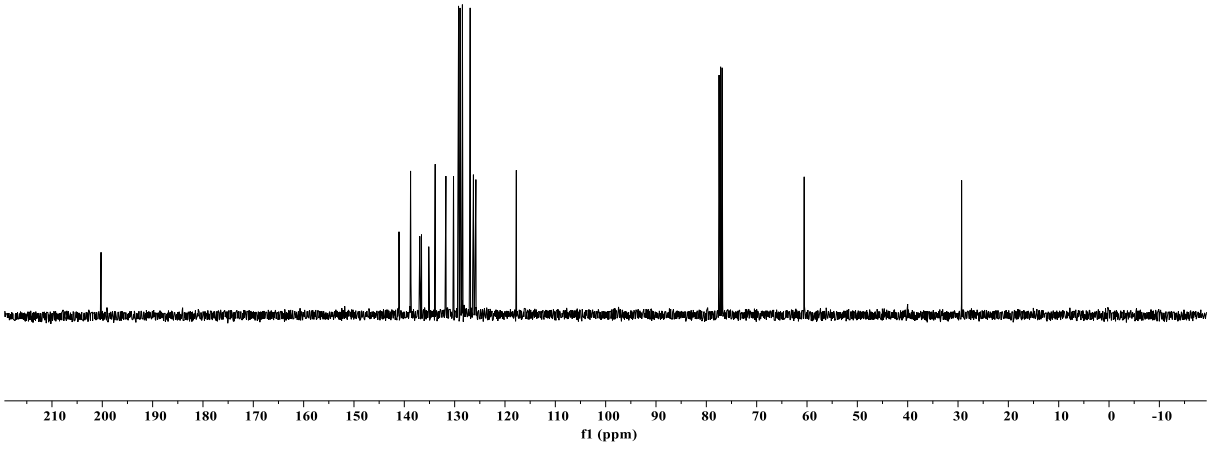


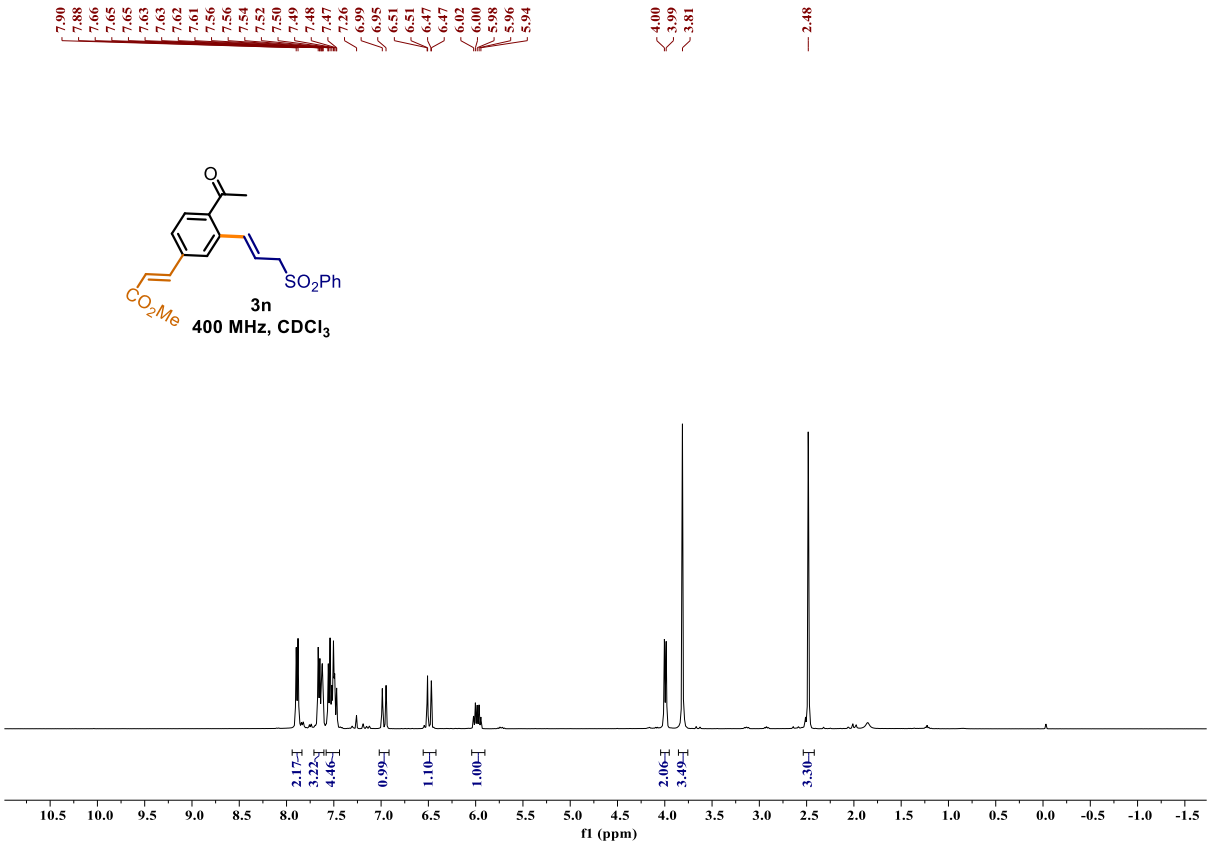
3m
400 MHz, $CDCl_3$

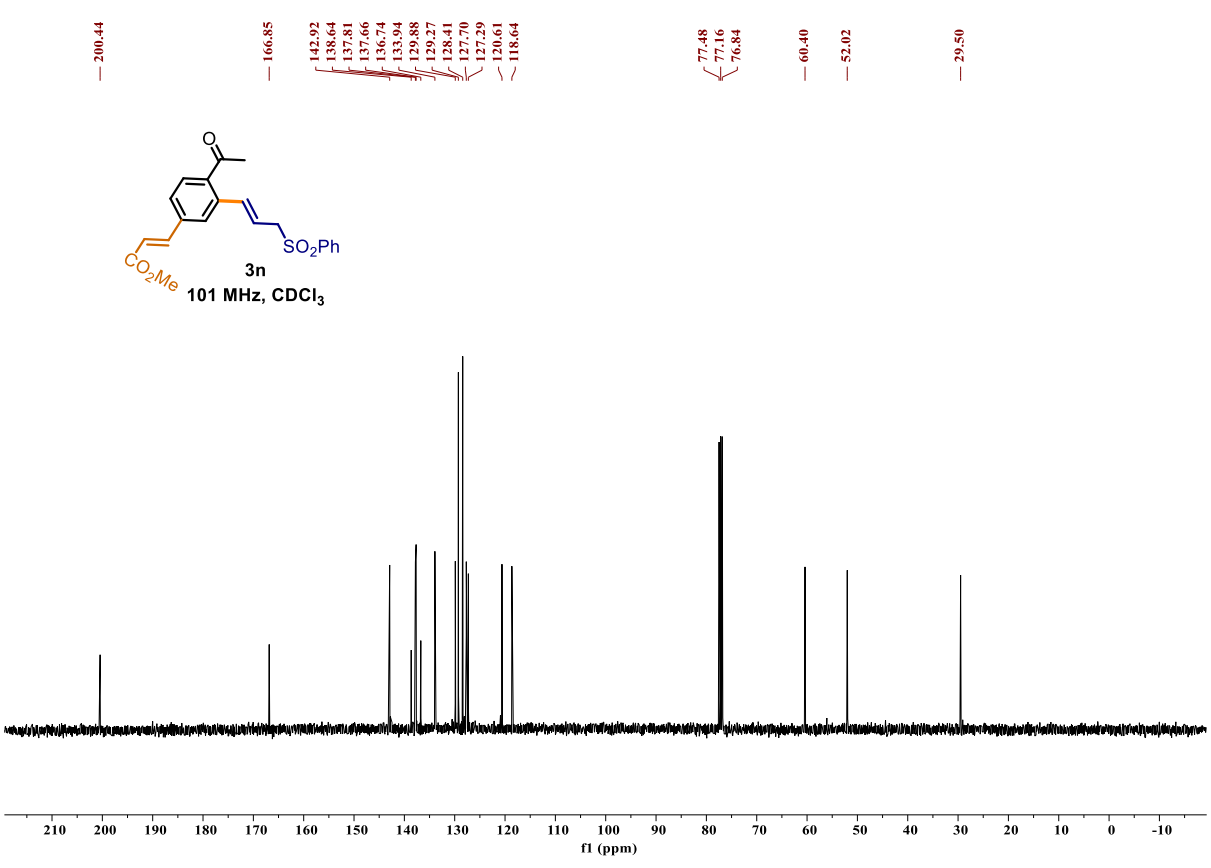


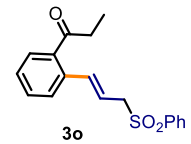


3m
101 MHz, $CDCl_3$



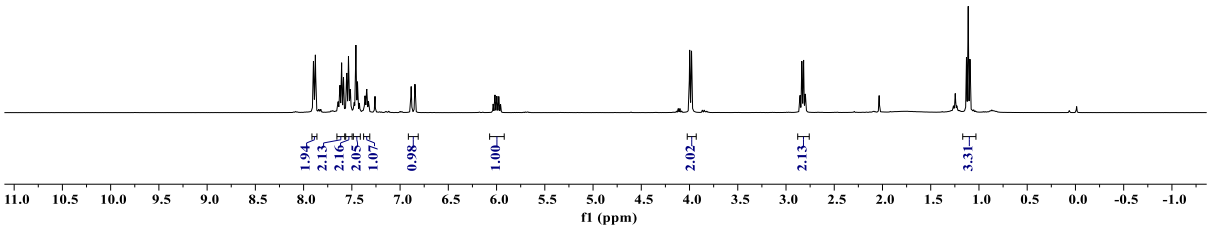

7.90
7.88
7.66
7.65
7.65
7.63
7.63
7.62
7.61
7.56
7.56
7.54
7.52
7.50
7.49
7.48
7.47
7.26
6.99
6.95
6.51
6.51
6.47
6.47
6.02
6.00
5.98
5.96
5.94
4.00
3.99
3.81
2.48
O
SO2Ph
CO2Me
3n
400 MHz, CDCl3
2.17
3.22
4.46
0.99
1.10
1.00
2.06
3.49
3.30
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

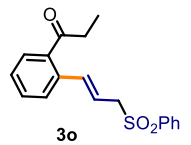

200.44
166.85
142.92
138.64
137.81
137.66
136.74
133.94
129.88
129.27
128.41
127.70
127.39
120.61
118.64
77.48
77.16
76.84
60.40
52.02
29.50
O
SO2Ph
CO2Me
3n
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



3o

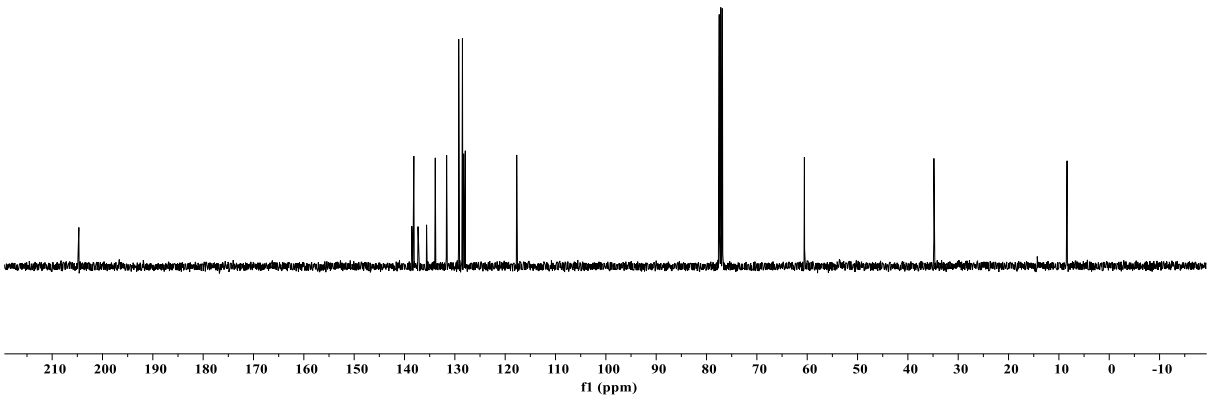
400 MHz, $CDCl_3$

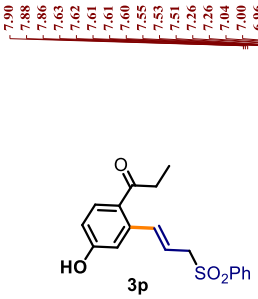




3o

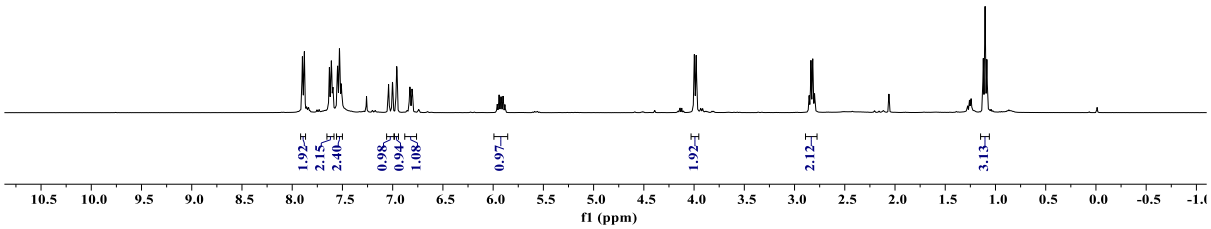
101 MHz, $CDCl_3$

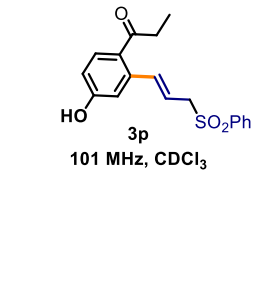




3p

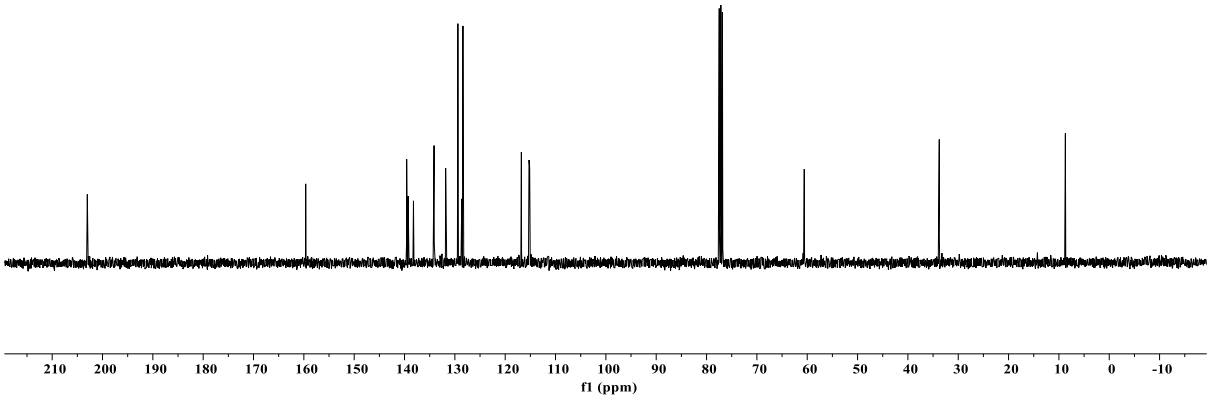
400 MHz, $CDCl_3$

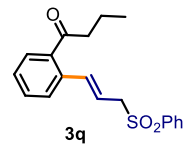




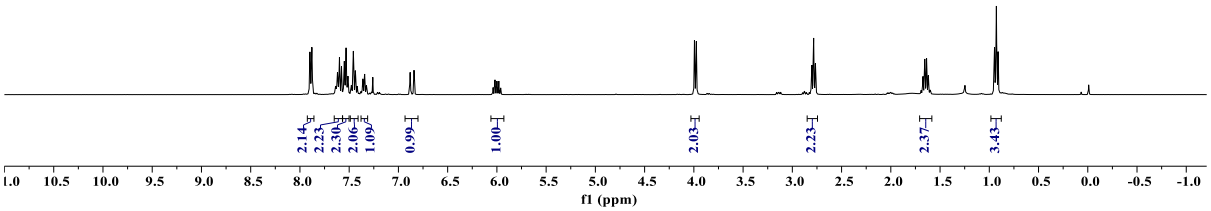
3p

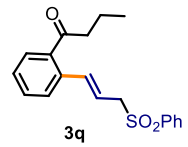
101 MHz, $CDCl_3$



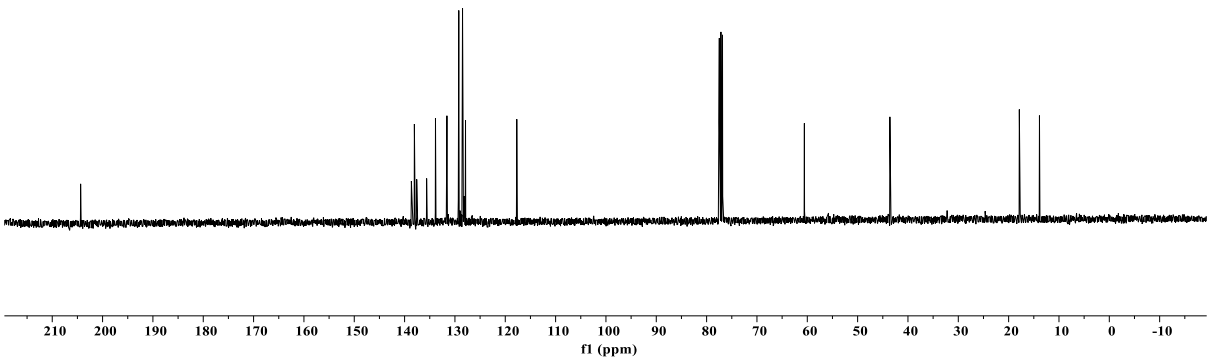


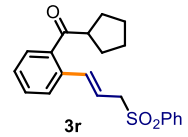
3q
400 MHz, $CDCl_3$





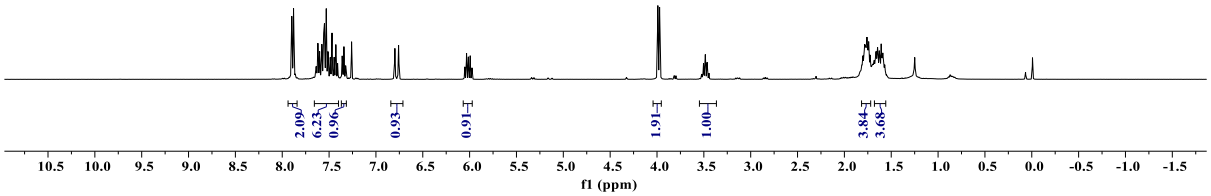
3q
101 MHz, $CDCl_3$

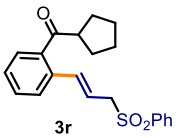




3r

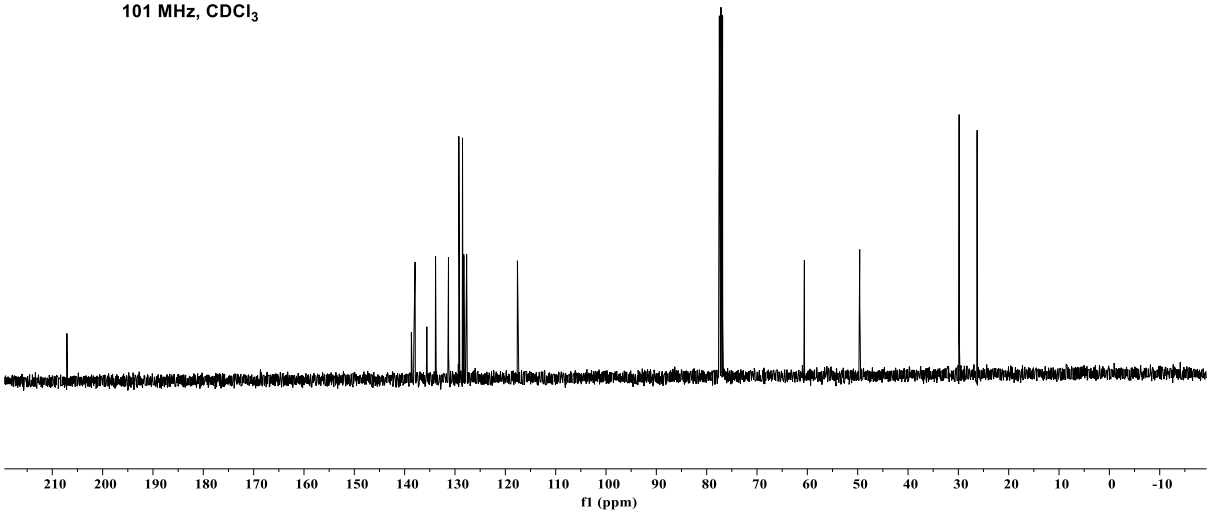
400 MHz, $CDCl_3$

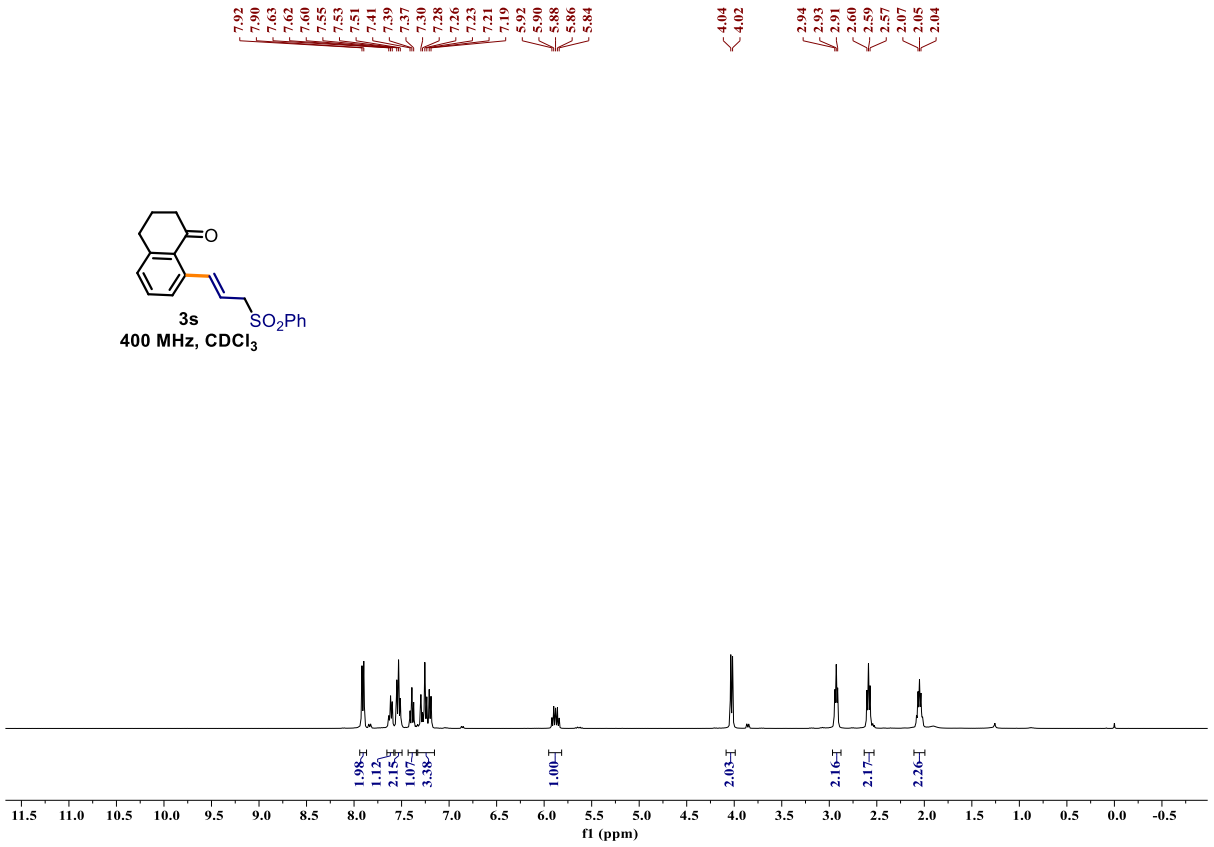


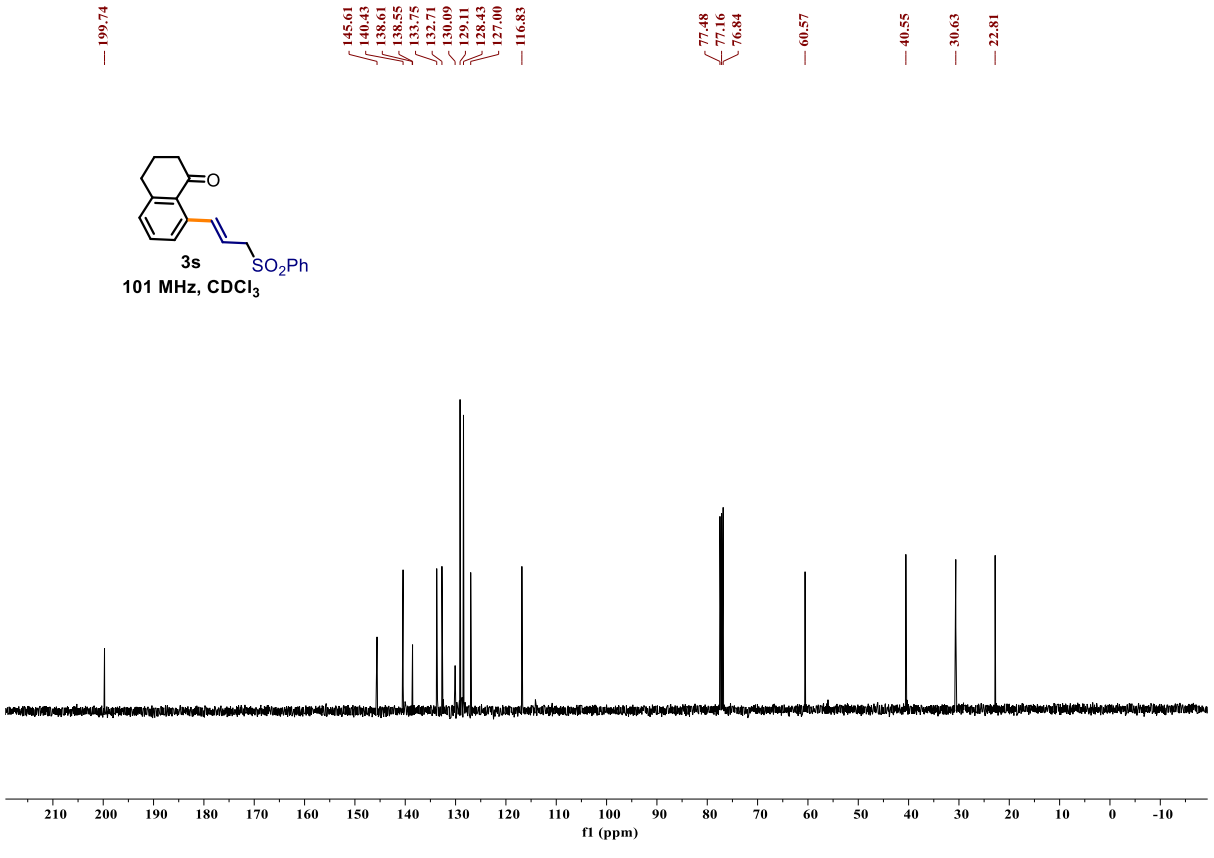


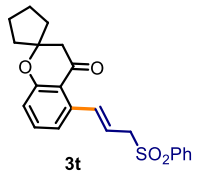
3r

101 MHz, $CDCl_3$



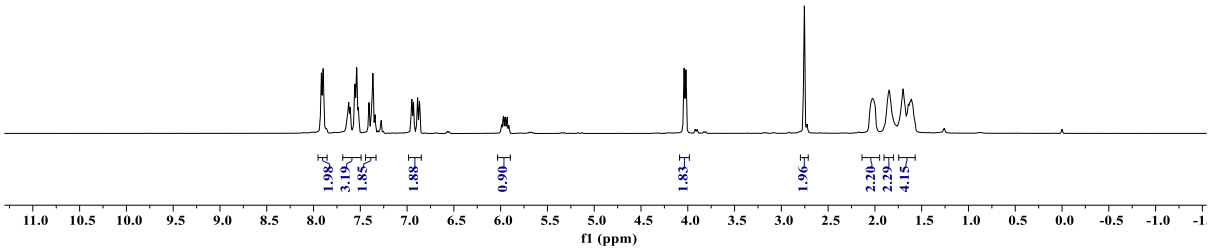

7.92
7.90
7.63
7.62
7.60
7.55
7.53
7.51
7.41
7.39
7.37
7.30
7.28
7.26
7.23
7.21
7.19
5.92
5.90
5.88
5.86
5.84
4.04
4.02
2.94
2.93
2.91
2.60
2.59
2.57
2.07
2.05
2.04
O
SO2Ph
3s
400 MHz, CDCl3
1.98
1.12
2.15
1.07
3.38
1.00
2.03
2.16
2.17
2.26
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

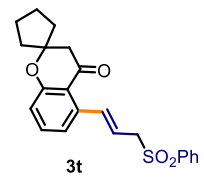

199.74
145.61
140.43
138.61
138.55
133.75
132.71
130.09
129.11
128.43
127.00
116.83
77.48
77.16
76.84
60.57
40.55
30.63
22.81
O
SO2Ph
3s
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



3t

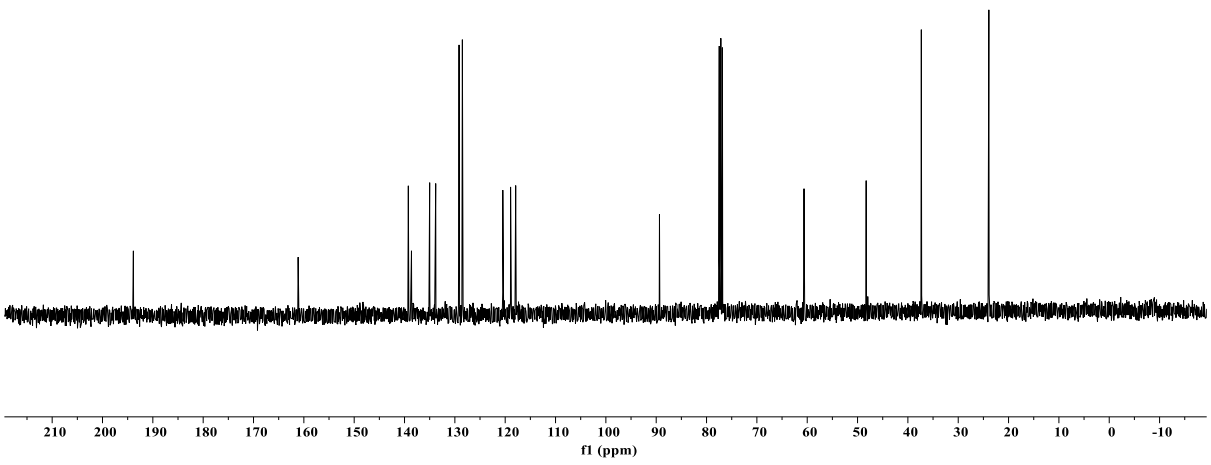
400 MHz, $CDCl_3$

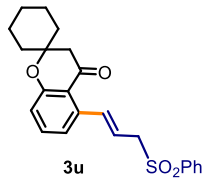




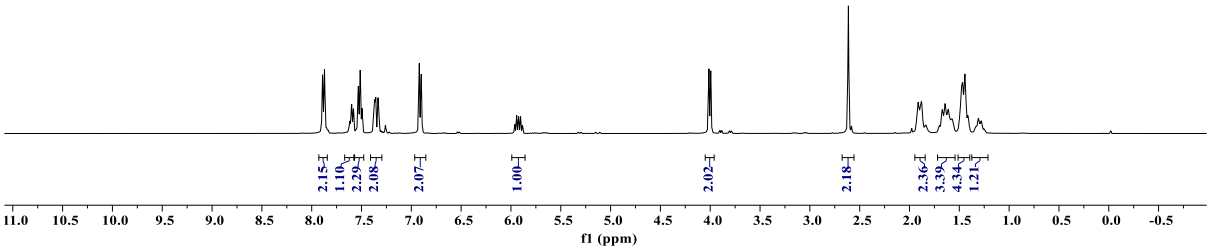
3t

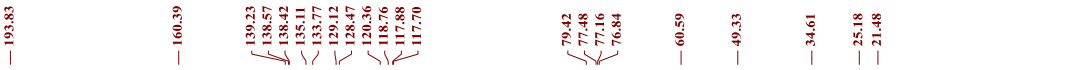
101 MHz, $CDCl_3$

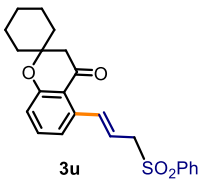




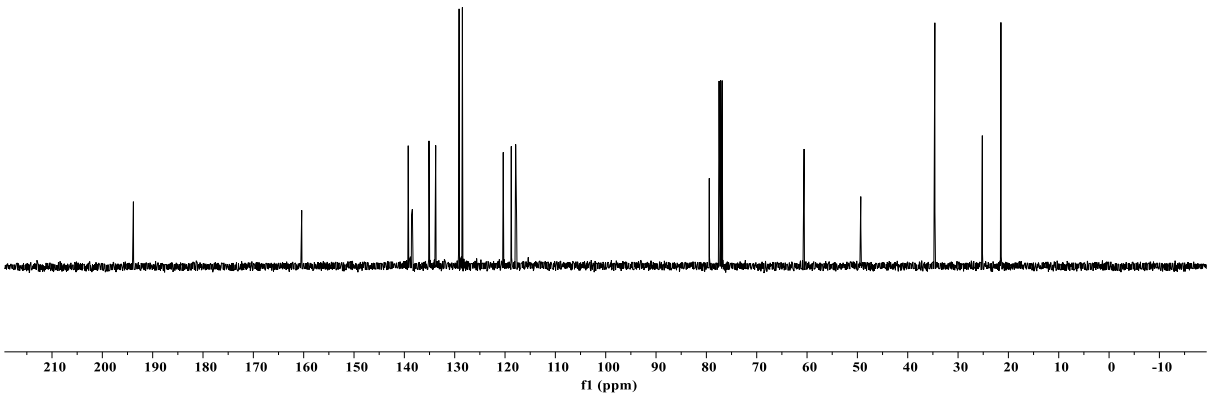
3u
400 MHz, $CDCl_3$

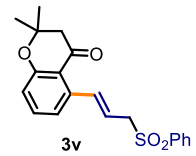




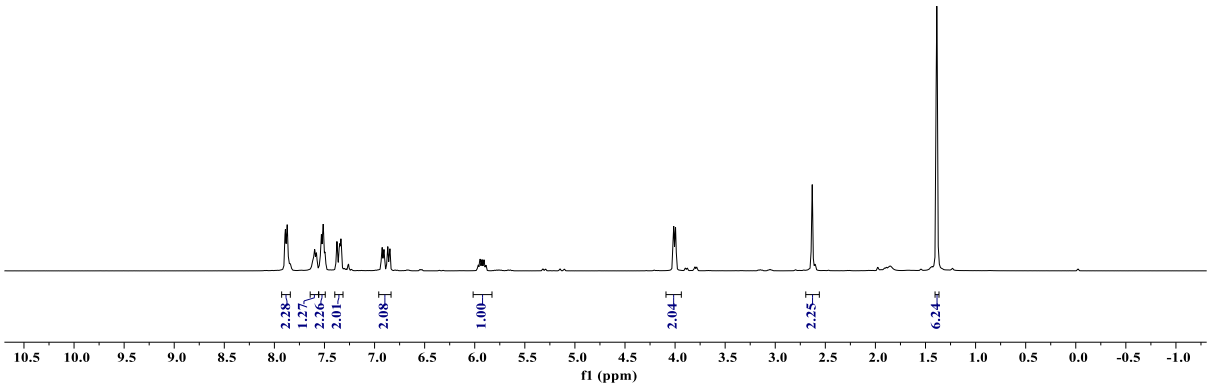


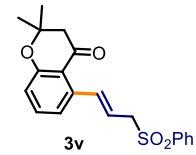
3u
101 MHz, $CDCl_3$



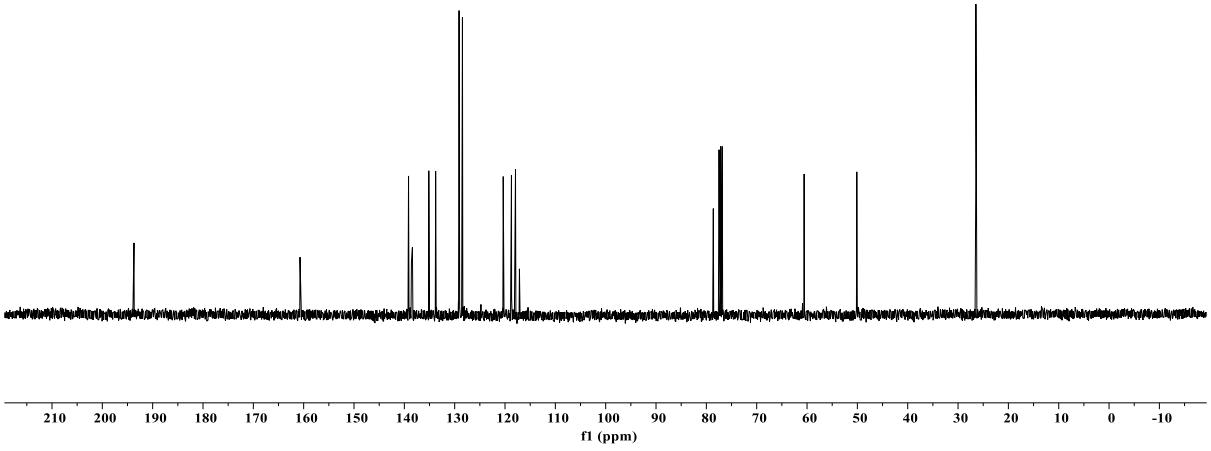


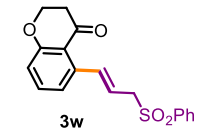
3v
400 MHz, $CDCl_3$



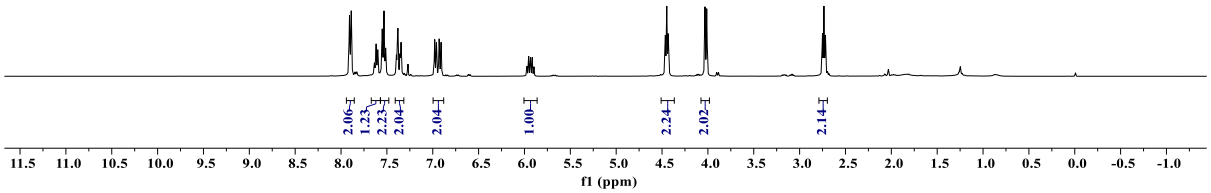


3v
101 MHz, $CDCl_3$

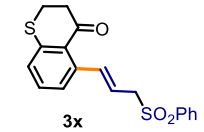




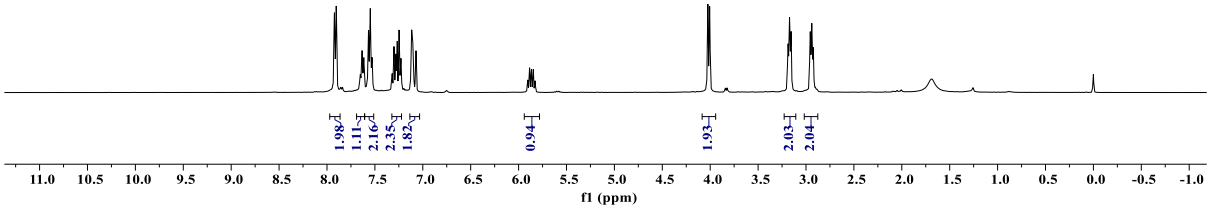
3w
400 MHz, $CDCl_3$

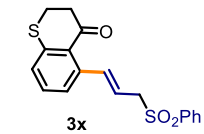


3w
101 MHz, $CDCl_3$

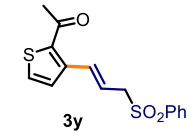


3x
400 MHz, $CDCl_3$



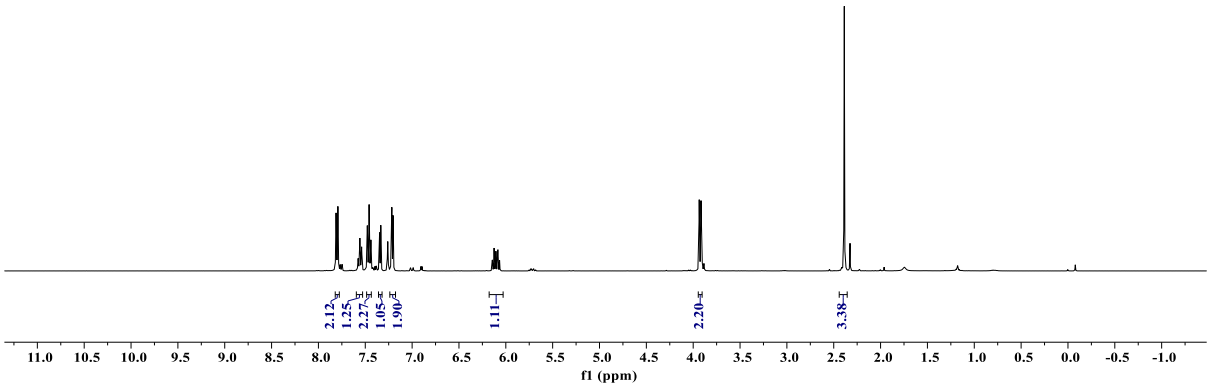


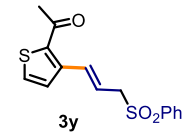
3x
101 MHz, $CDCl_3$



3y

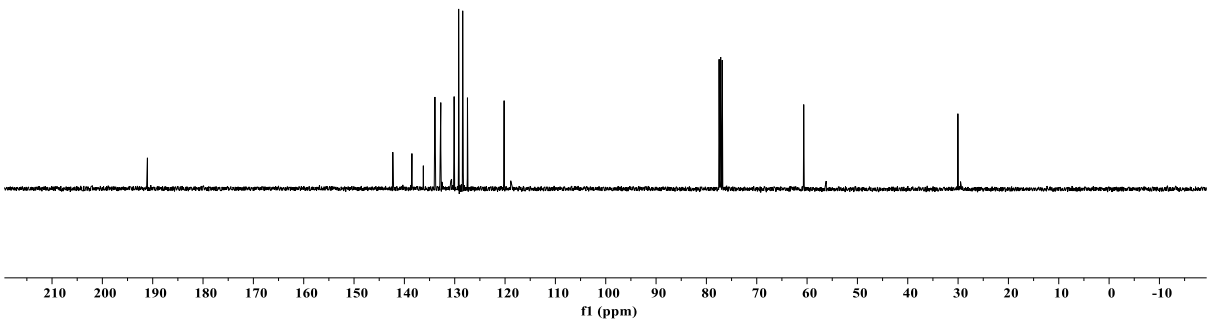
400 MHz, $CDCl_3$

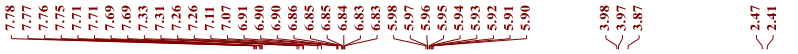


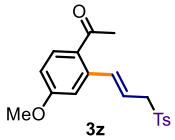


3y

101 MHz, $CDCl_3$

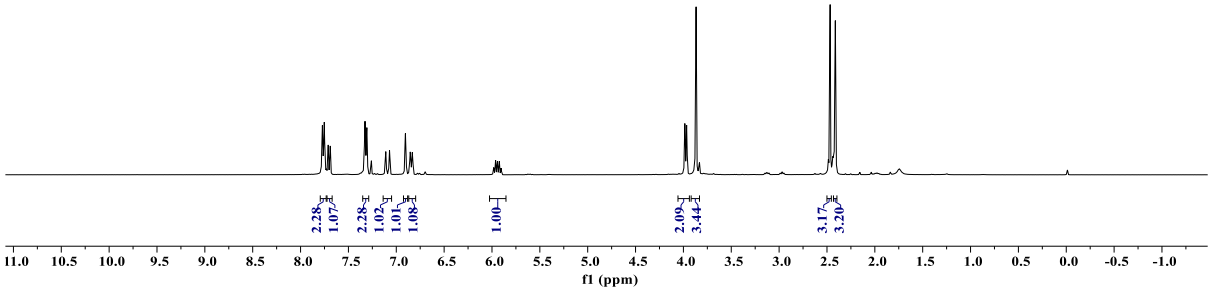


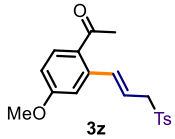




3z

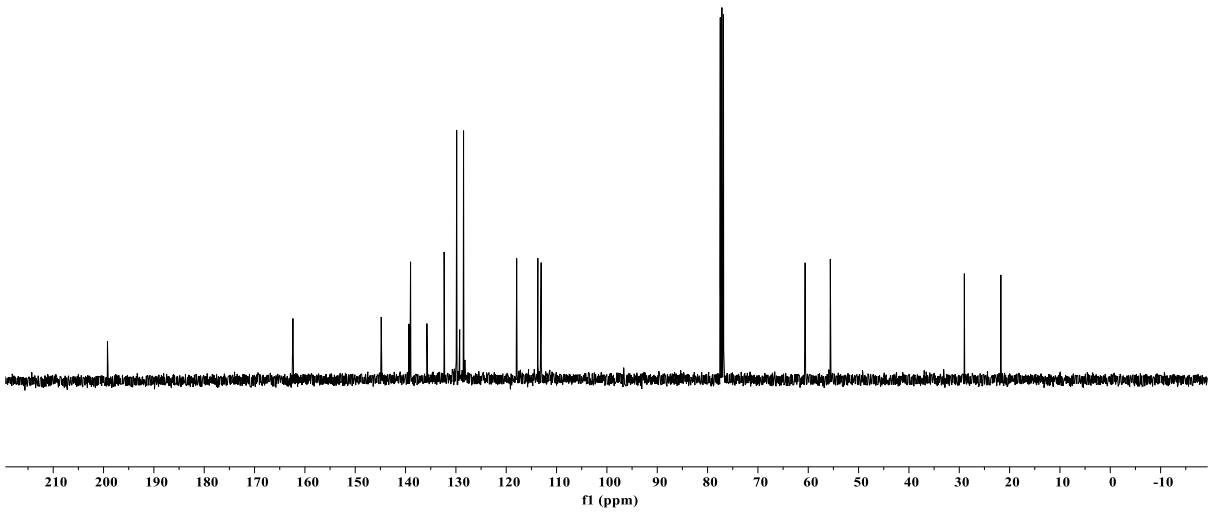
400 MHz, $CDCl_3$

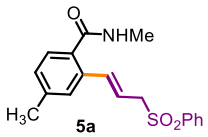




3z

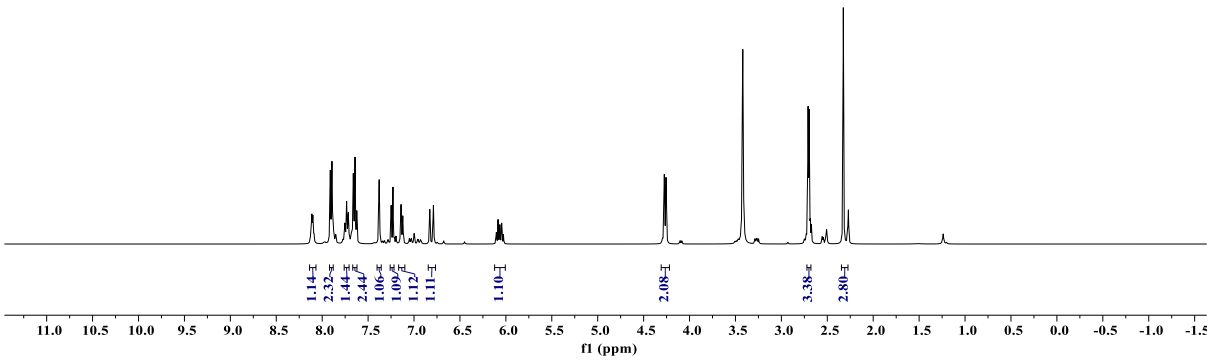
101 MHz, $CDCl_3$

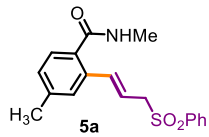




5a

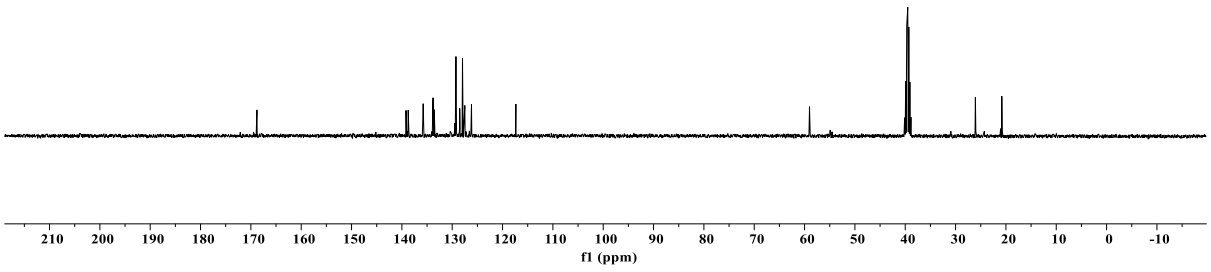
400 MHz, DMSO-d_6

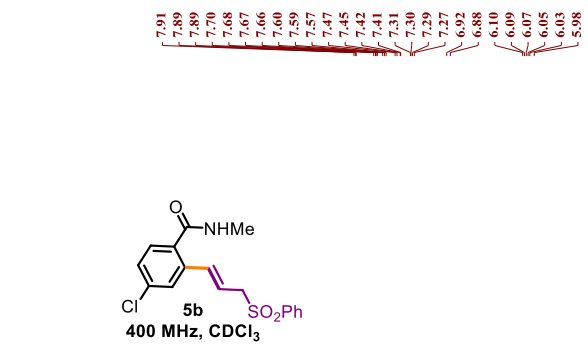


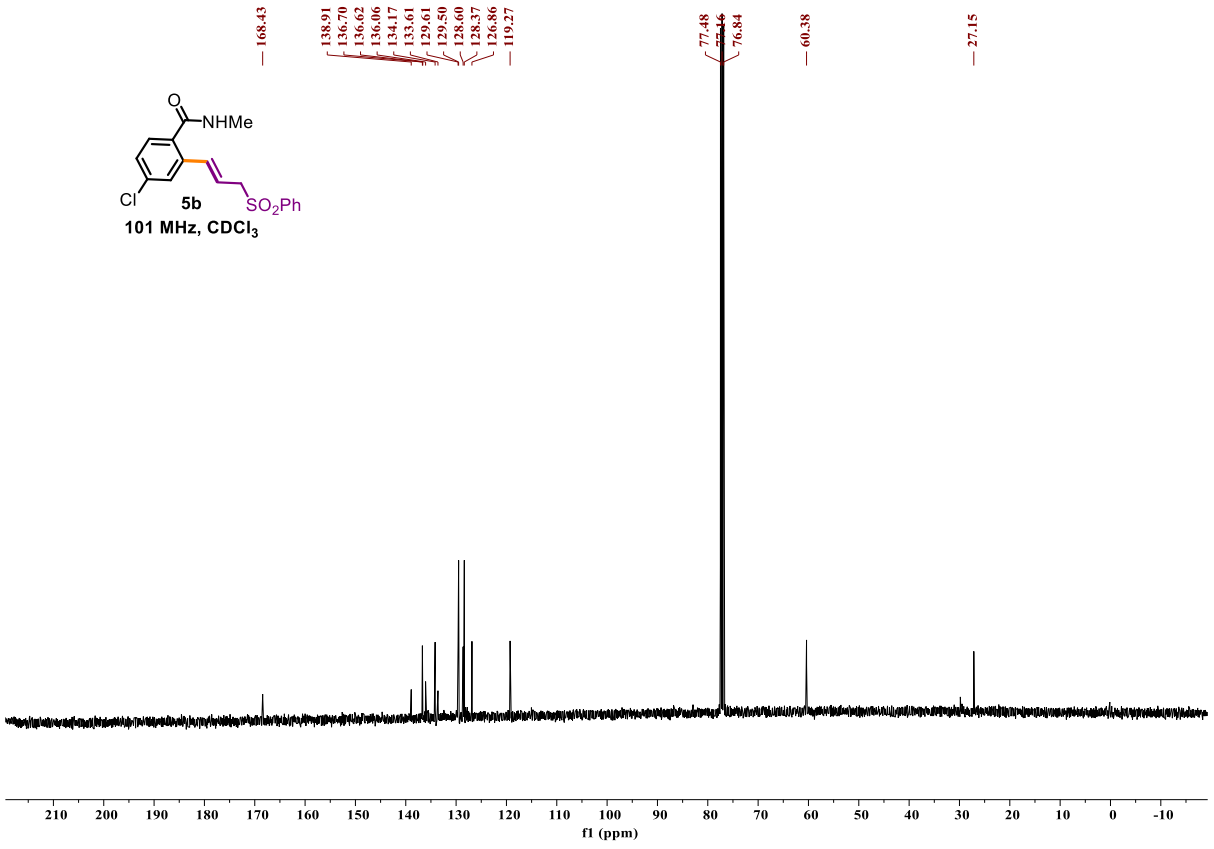


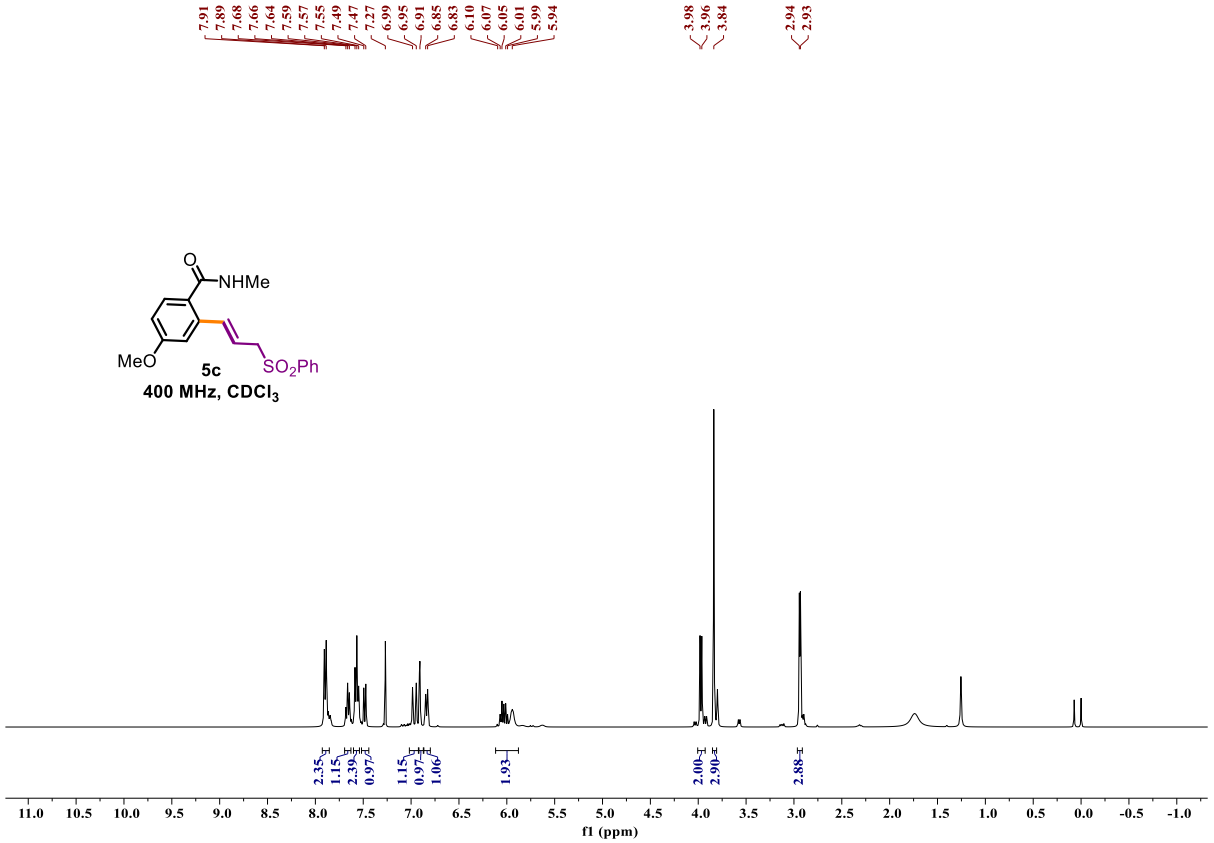
5a

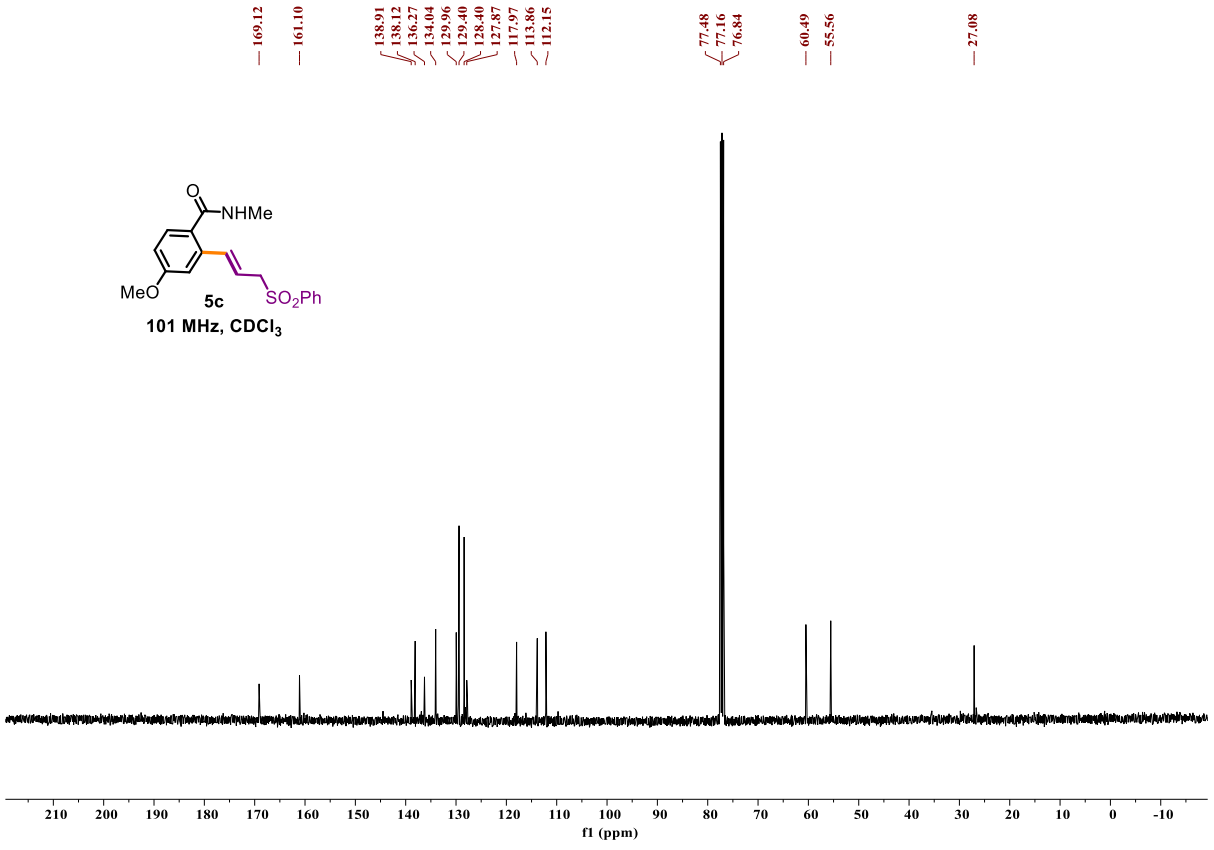
101 MHz, DMSO-d_6

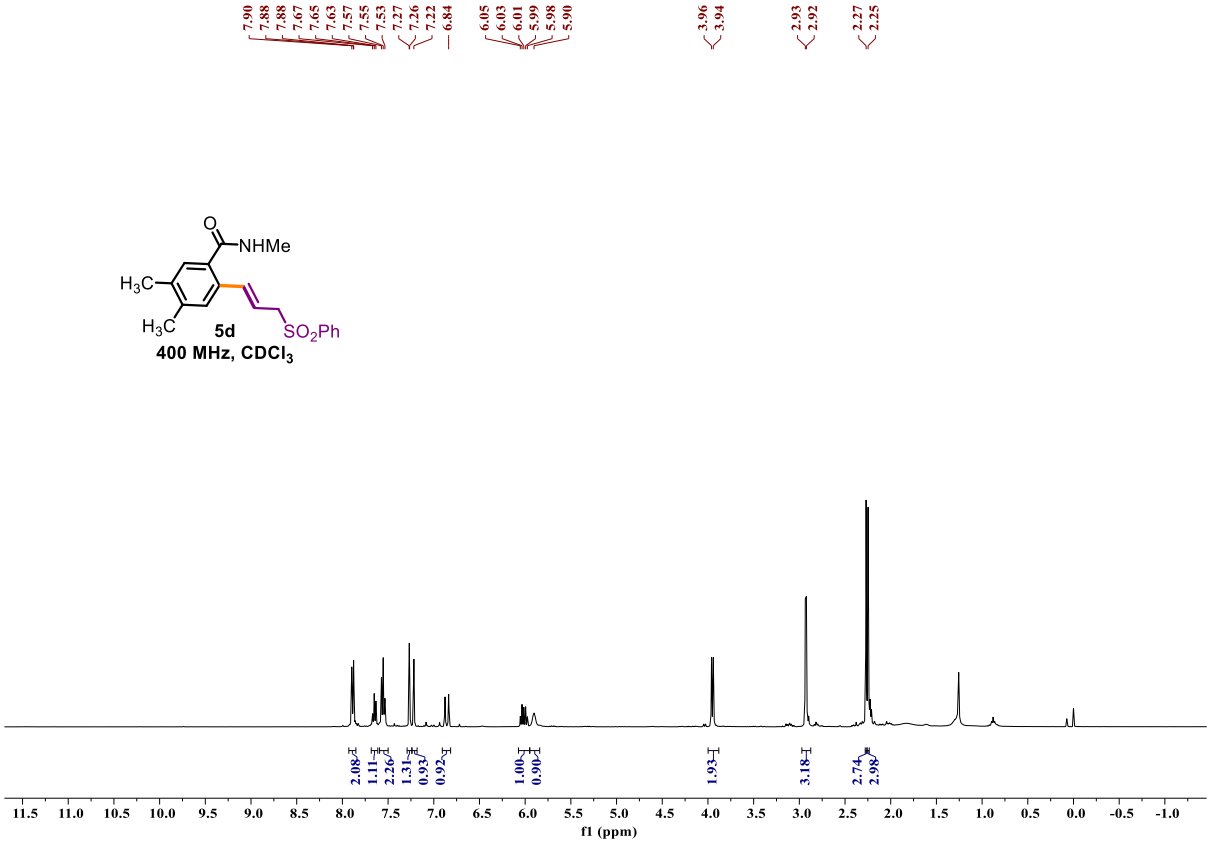


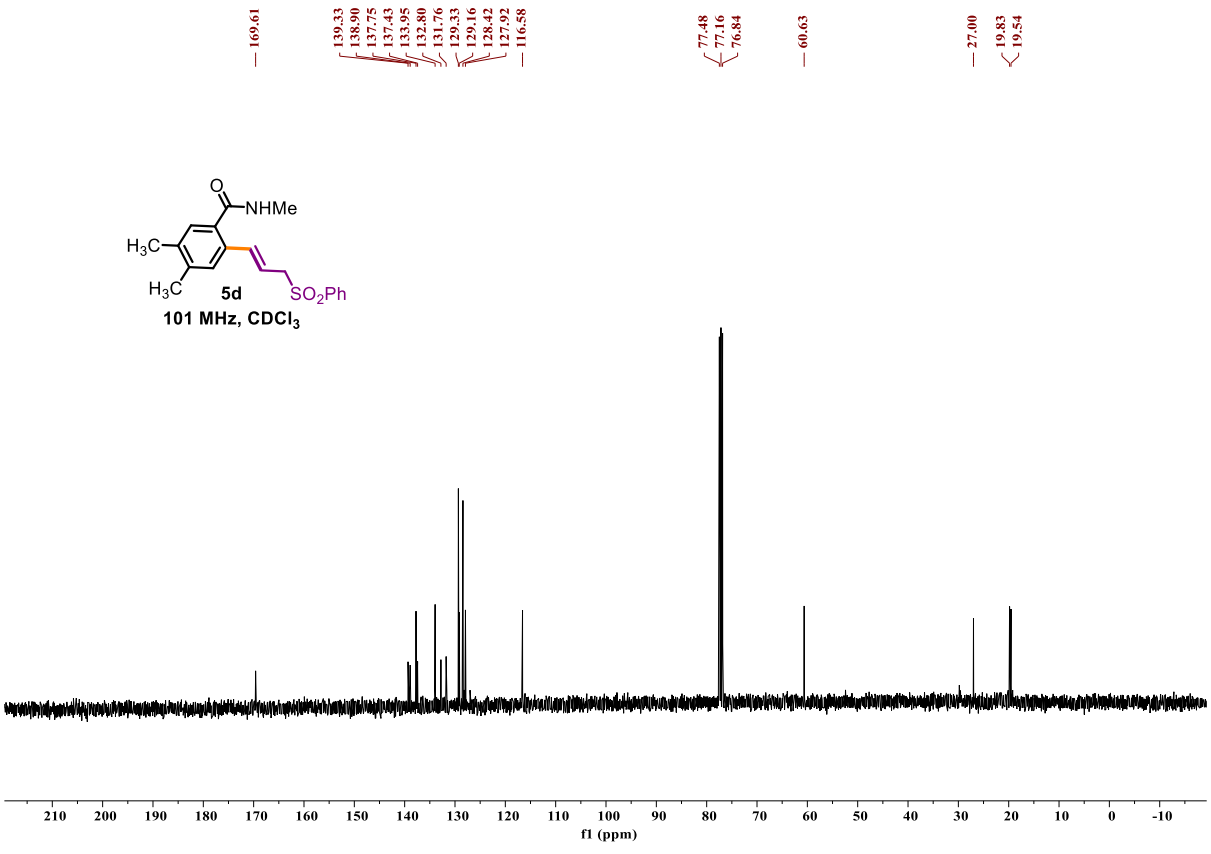

7.91
7.89
7.89
7.70
7.68
7.67
7.66
7.60
7.59
7.57
7.47
7.45
7.42
7.41
7.31
7.30
7.29
7.27
6.92
6.88
6.10
6.09
6.07
6.05
6.03
5.98
3.98
3.96
2.97
2.96
O
NHMe
Cl
5b
SO2Ph
400 MHz, CDCl3
2.07
1.22
2.29
1.07
0.95
1.01
1.00
2.04
2.14
3.18
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

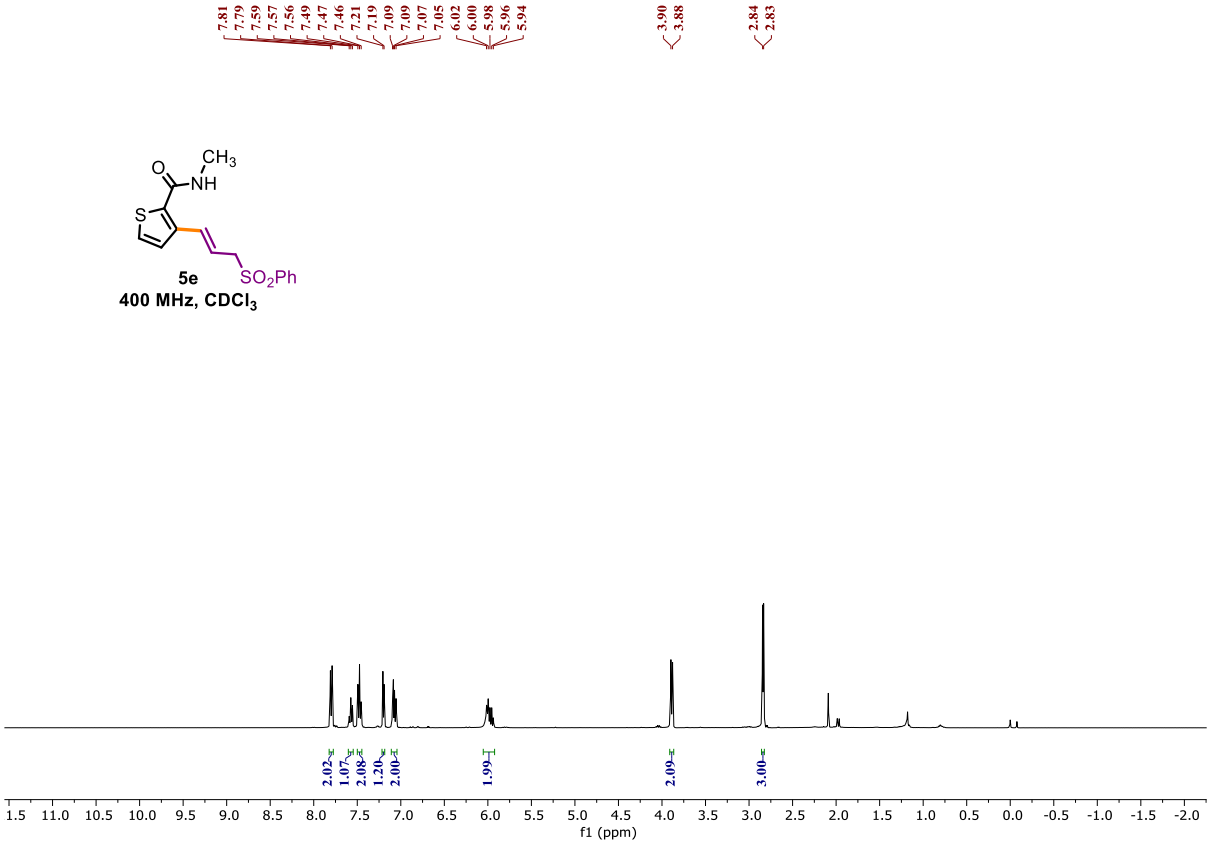

168.43
138.91
136.70
136.62
136.06
134.17
133.61
129.61
129.50
128.60
128.37
126.86
119.27
77.48
77.16
76.84
60.38
27.15
O
NHMe
Cl
5b
SO2Ph
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

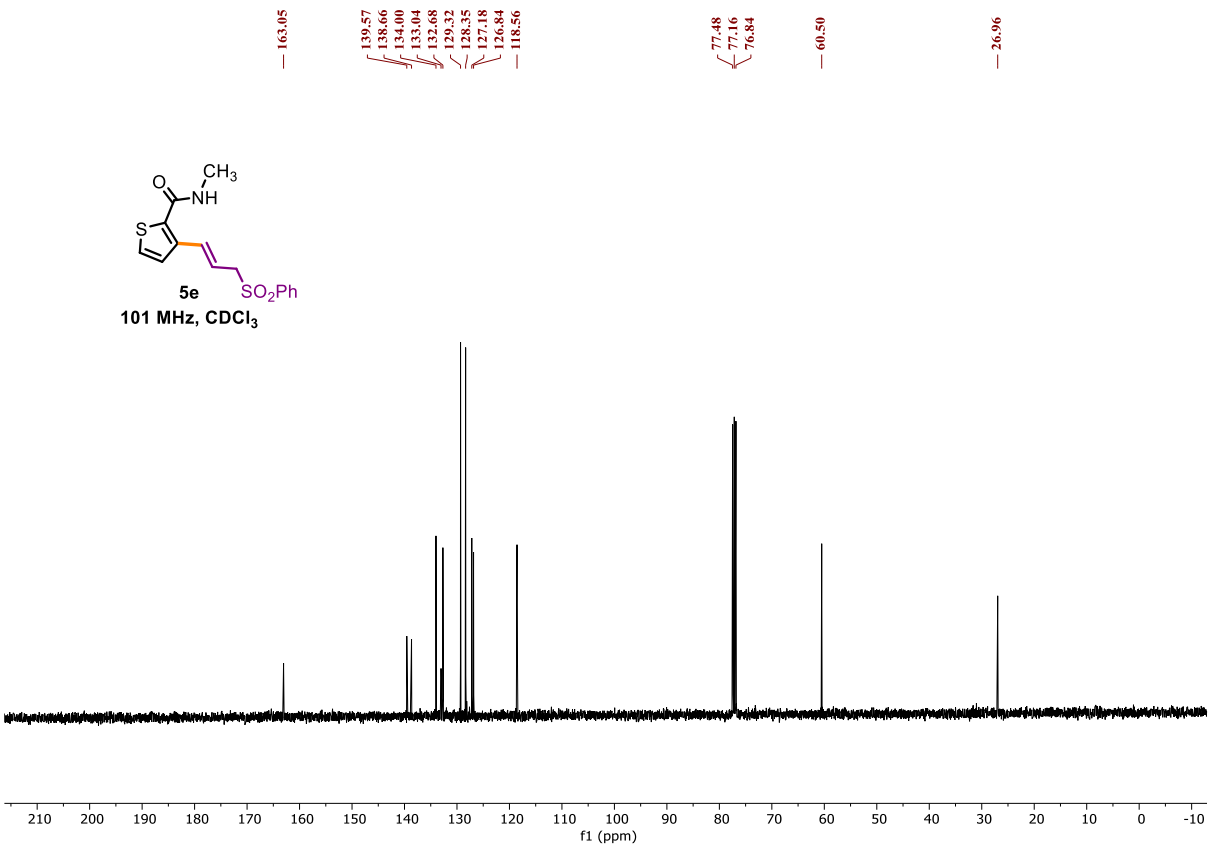

7.91
7.89
7.68
7.66
7.64
7.59
7.57
7.55
7.49
7.47
7.27
6.99
6.95
6.91
6.85
6.83
6.10
6.07
6.05
6.01
5.99
5.94
3.98
3.96
3.84
2.94
2.93
O
NHMe
MeO
SO2Ph
5c
400 MHz, CDCl3
2.35
1.15
2.39
0.97
1.15
0.97
1.06
1.93
2.00
2.90
2.88
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

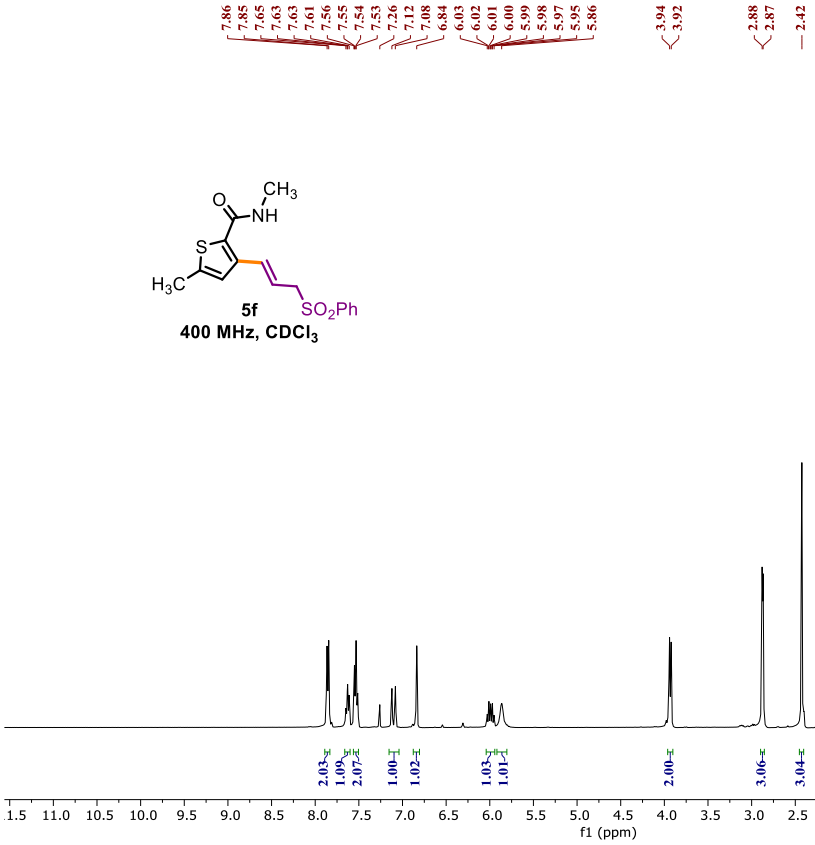

169.12
161.10
138.91
138.12
136.27
134.04
129.96
129.40
128.40
127.87
117.97
113.86
112.15
77.48
77.16
76.84
60.49
55.56
27.08
O
NHMe
MeO
SO2Ph
5c
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

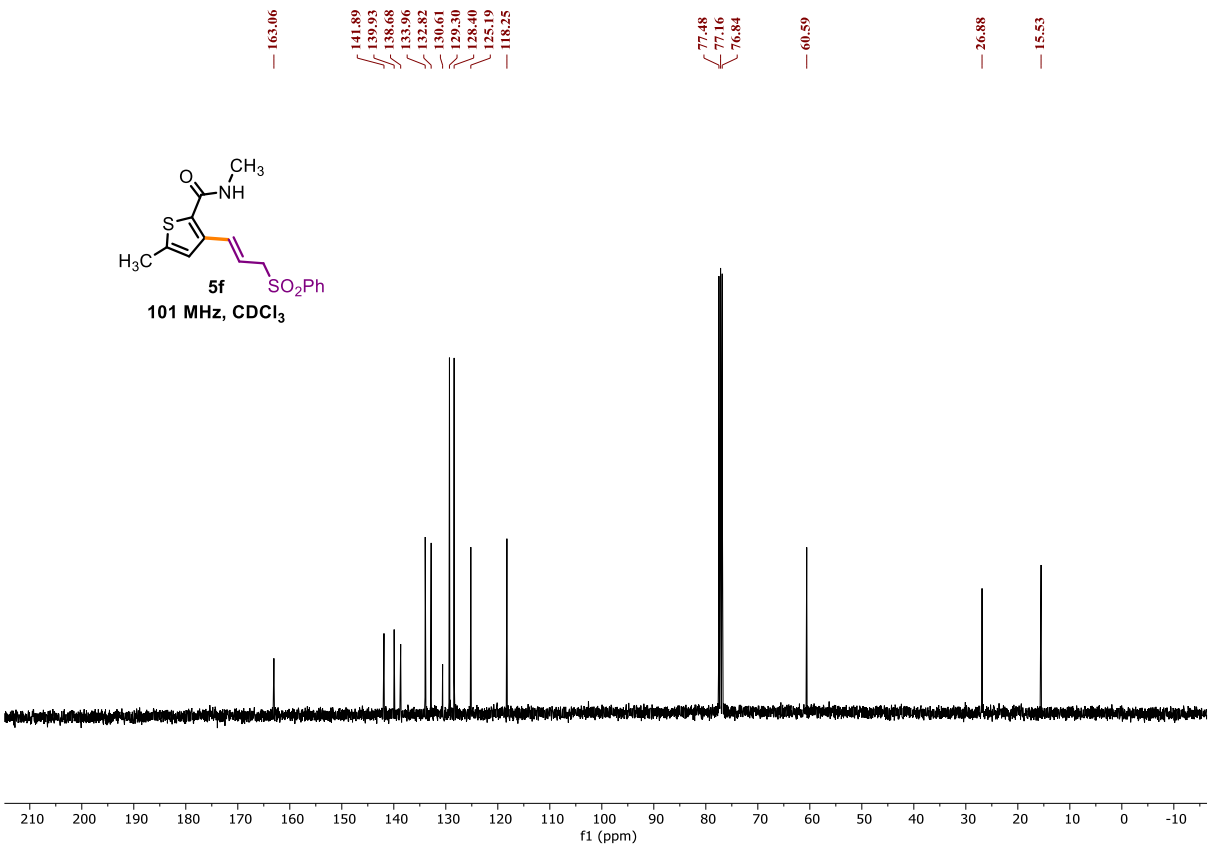

7.90
7.88
7.88
7.67
7.65
7.63
7.57
7.55
7.53
7.27
7.26
7.22
6.84
6.05
6.03
6.01
5.99
5.98
5.90
3.96
3.94
2.93
2.92
2.27
2.25
NHMe
H3C
H3C
5d
SO2Ph
400 MHz, CDCl3
2.08
1.11
2.26
1.31
0.93
0.92
1.00
0.90
1.93
3.18
2.74
2.98
f1 (ppm)

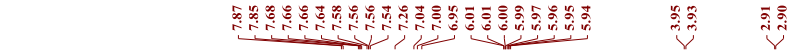

169.61
139.33
138.90
137.75
137.43
133.95
132.80
131.76
129.33
129.16
128.42
127.92
116.58
77.48
77.16
76.84
60.63
27.00
19.83
19.54
NHMe
H3C
H3C
5d
SO2Ph
101 MHz, CDCl3
f1 (ppm)

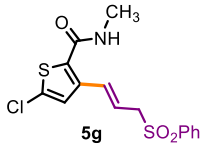

7.81
7.79
7.59
7.57
7.56
7.49
7.47
7.46
7.21
7.19
7.09
7.09
7.07
7.05
6.02
6.00
5.98
5.96
5.94
3.90
3.88
2.84
2.83
CH3
O
NH
S
5e
SO2Ph
400 MHz, CDCl3
2.02
1.07
2.08
1.20
2.00
1.99
2.09
3.00
f1 (ppm)


163.05
139.57
138.66
134.00
133.04
132.68
129.32
128.35
127.18
126.84
118.56
77.48
77.16
76.84
60.50
26.96
CH3
O
NH
S
5e
SO2Ph
101 MHz, CDCl3
f1 (ppm)

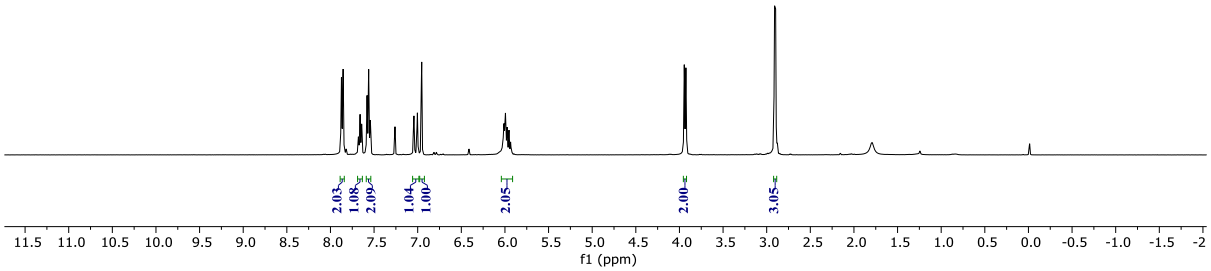

7.86
7.85
7.65
7.63
7.63
7.61
7.56
7.55
7.54
7.53
7.26
7.12
7.08
6.84
6.03
6.02
6.01
6.00
5.99
5.98
5.97
5.95
5.86
3.94
3.92
2.88
2.87
2.42
O
CH3
NH
S
H3C
5f
SO2Ph
400 MHz, CDCl3
2.03
1.09
2.07
1.00
1.02
1.03
1.01
2.00
3.06
3.04
f1 (ppm)

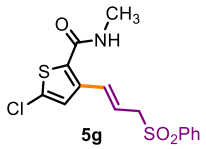

163.06
141.89
139.93
138.68
133.96
132.82
130.61
129.30
128.40
125.19
118.25
77.48
77.16
76.84
60.59
26.88
15.53
O
CH3
NH
S
H3C
5f
SO2Ph
101 MHz, CDCl3
f1 (ppm)



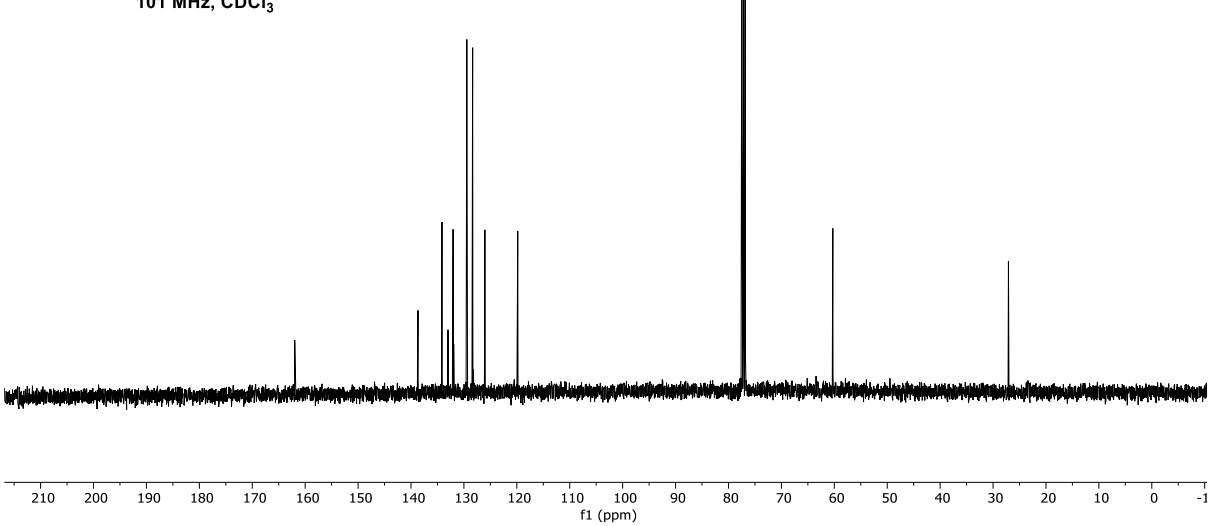


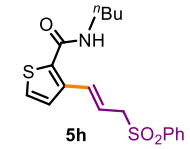
5g
400 MHz, $CDCl_3$



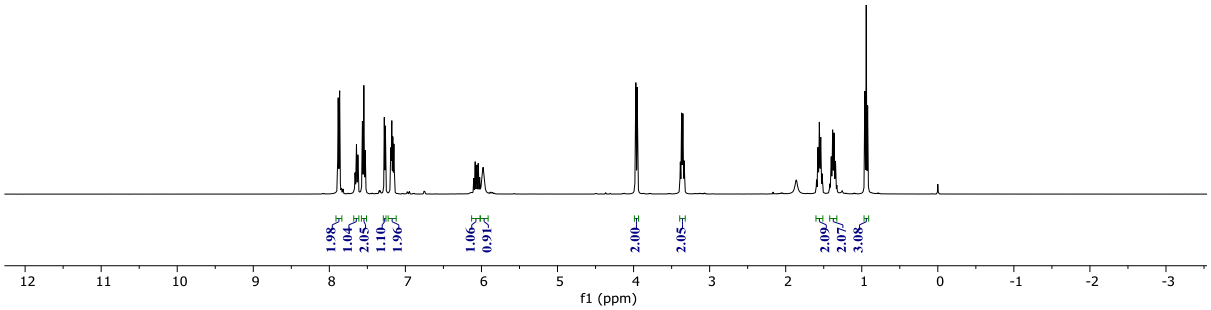


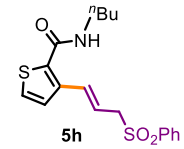
5g
101 MHz, $CDCl_3$



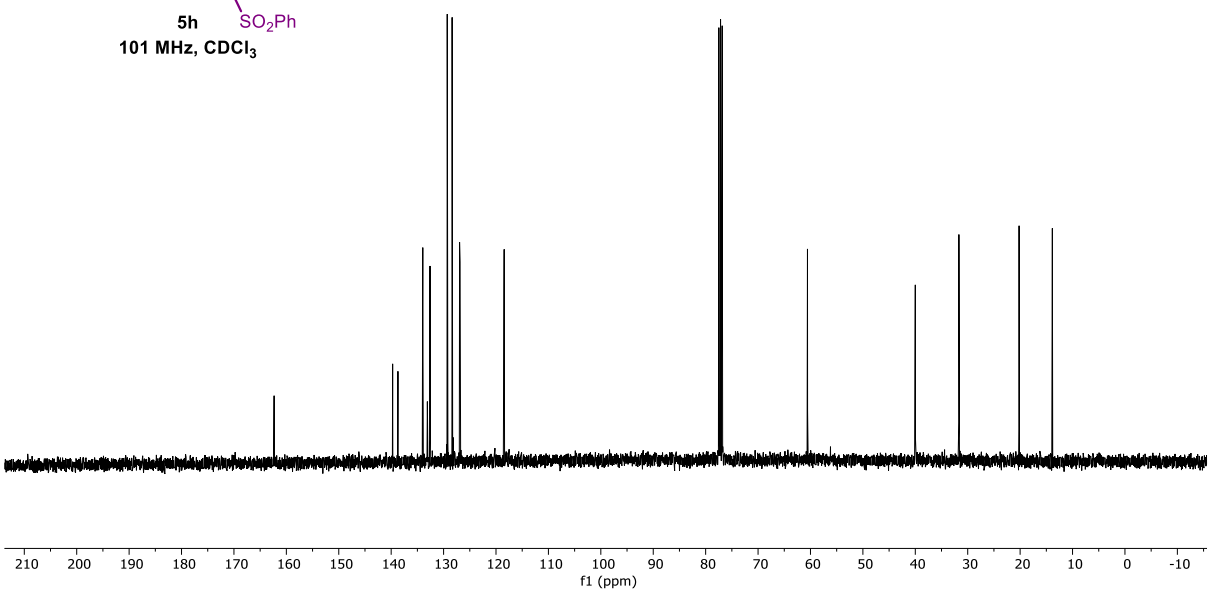


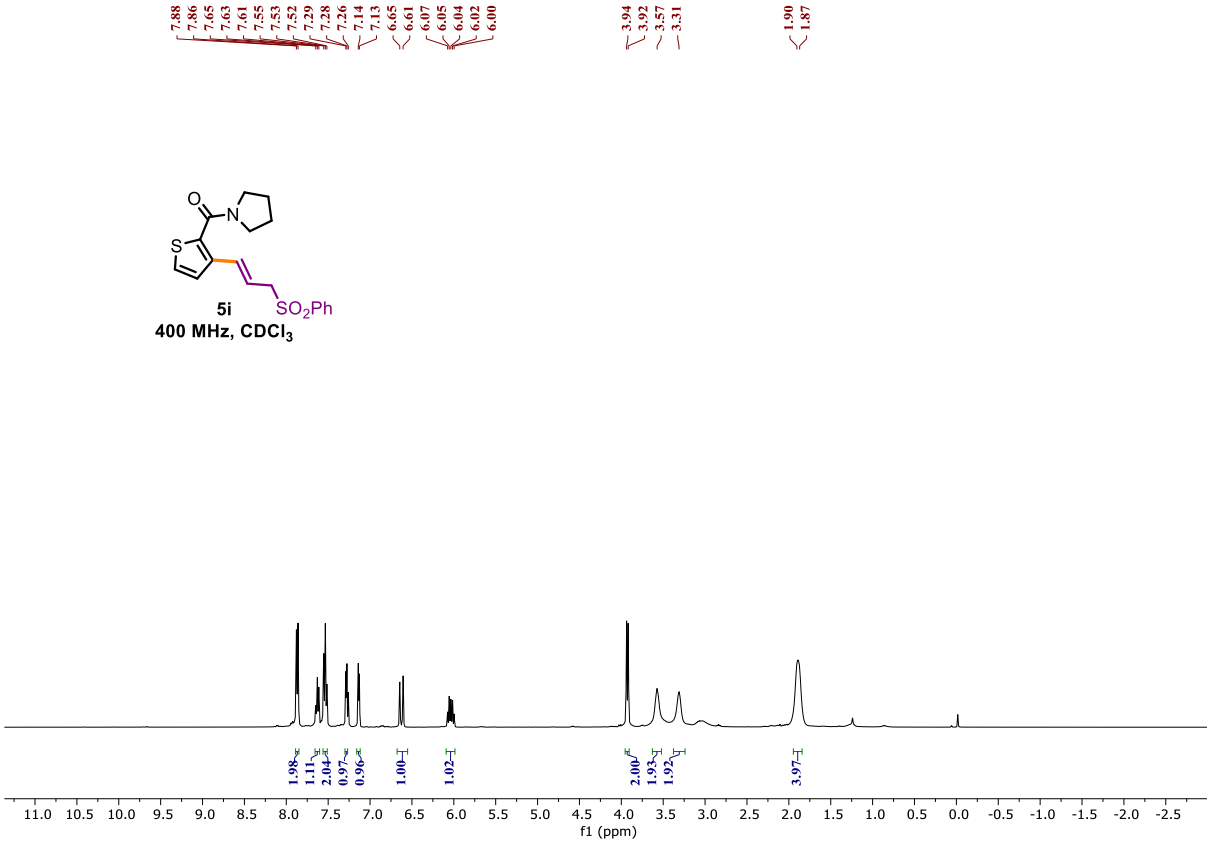
5h
400 MHz, $CDCl_3$

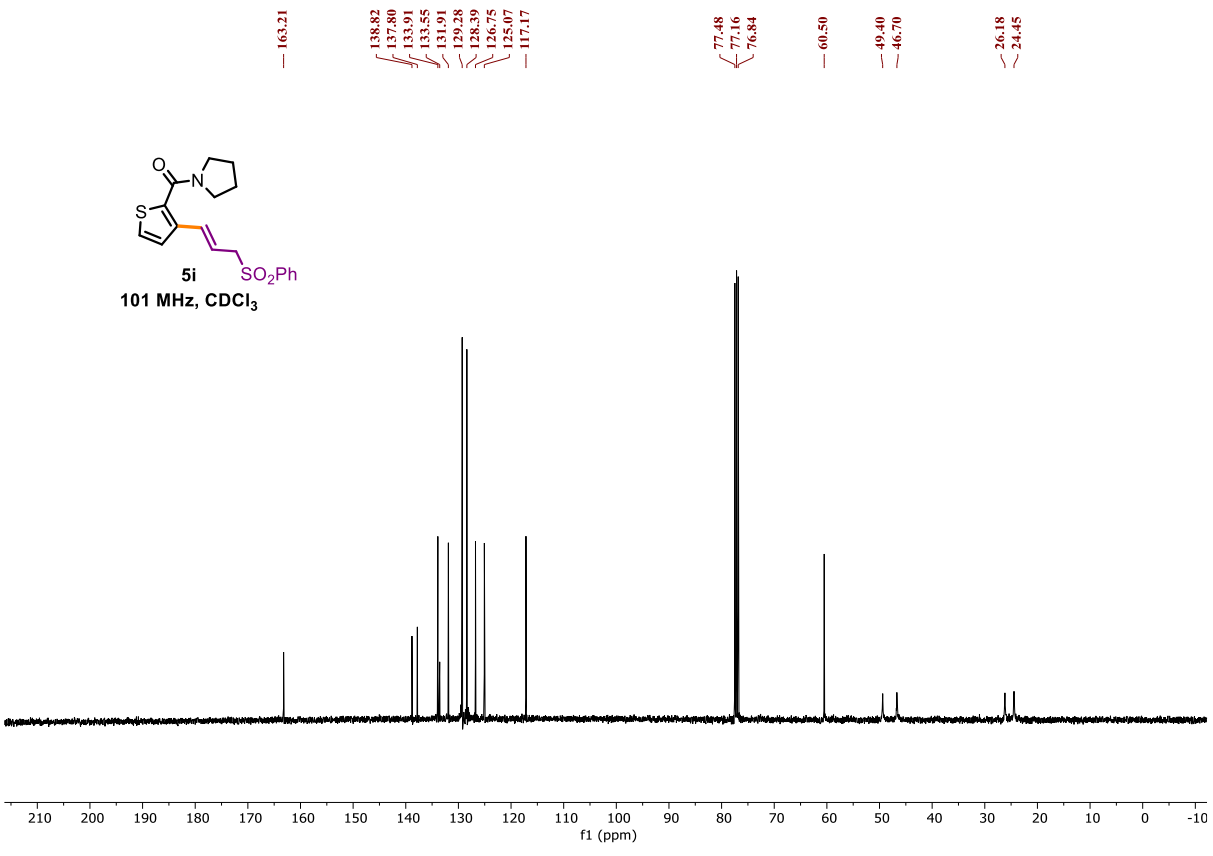


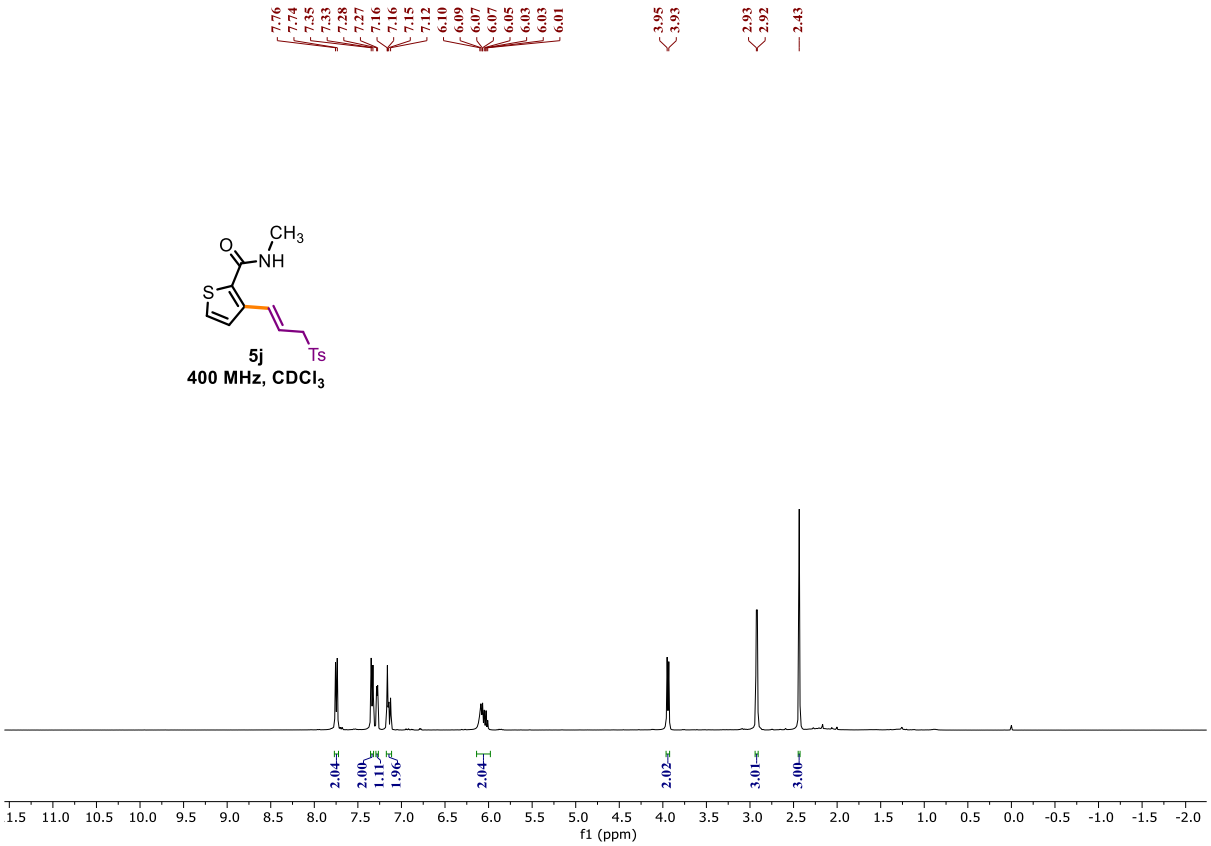


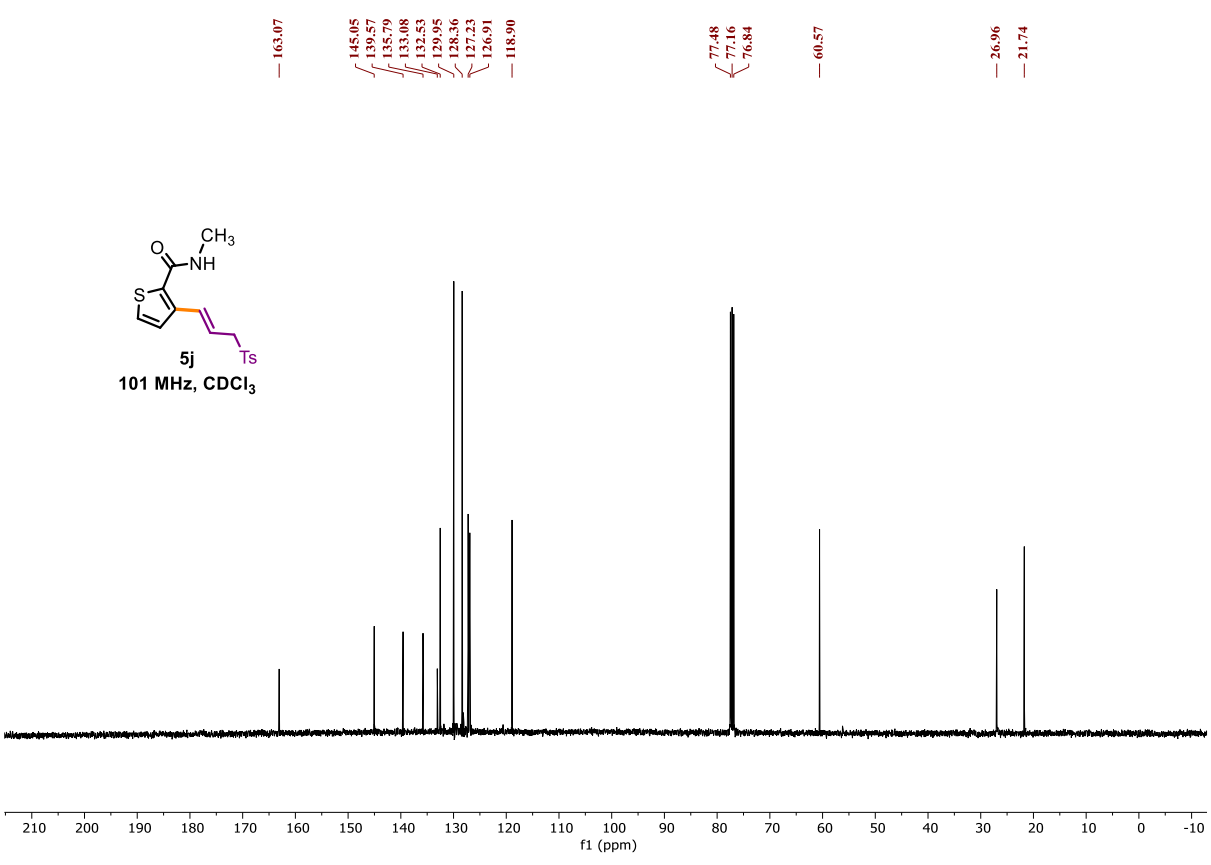
5h
101 MHz, $CDCl_3$

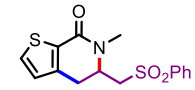



7.88
7.86
7.65
7.63
7.61
7.55
7.53
7.52
7.29
7.28
7.26
7.14
7.13
6.65
6.61
6.07
6.05
6.04
6.02
6.00
3.94
3.92
3.57
3.31
1.90
1.87
O
N
S
5i
SO2Ph
400 MHz, CDCl3
1.98
1.11
2.04
0.97
0.96
1.00
1.02
2.00
1.93
1.92
3.97
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

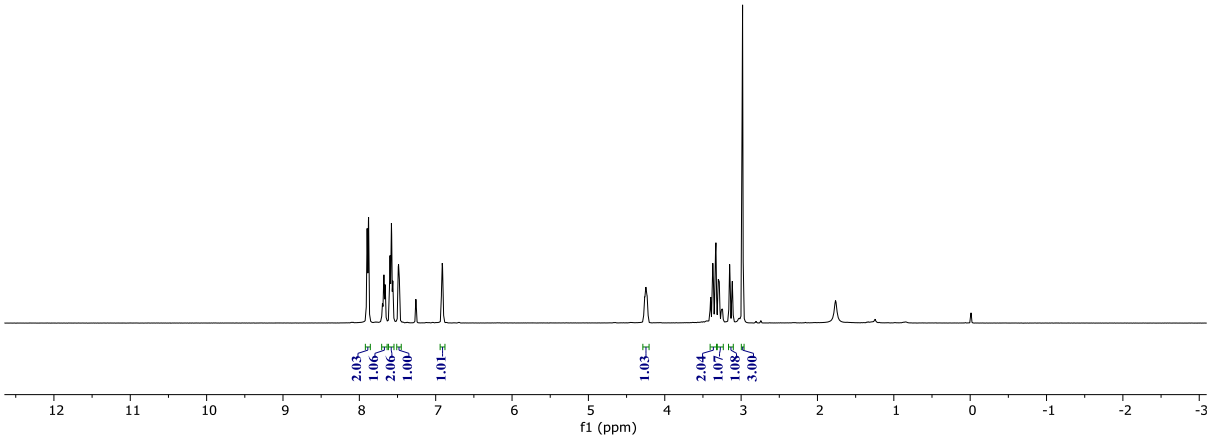

163.21
138.82
137.80
133.91
133.55
131.91
129.28
128.39
126.75
125.07
117.17
77.48
77.16
76.84
60.50
49.40
46.70
26.18
24.45
O
N
S
5i
SO2Ph
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.76
7.74
7.35
7.33
7.28
7.27
7.16
7.16
7.15
7.12
6.10
6.09
6.07
6.07
6.05
6.03
6.03
6.01
3.95
3.93
2.93
2.92
2.43
CH3
O
NH
S
Ts
5j
400 MHz, CDCl3
2.04
2.00
1.11
1.96
2.04
2.02
3.01
3.00
f1 (ppm)

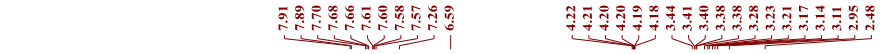

163.07
145.05
139.57
135.79
133.08
132.53
129.95
128.36
127.23
126.91
118.90
77.48
77.16
76.84
60.57
26.96
21.74
CH3
O
NH
S
Ts
5j
101 MHz, CDCl3
f1 (ppm)

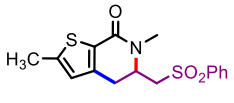


6a
400 MHz, $CDCl_3$

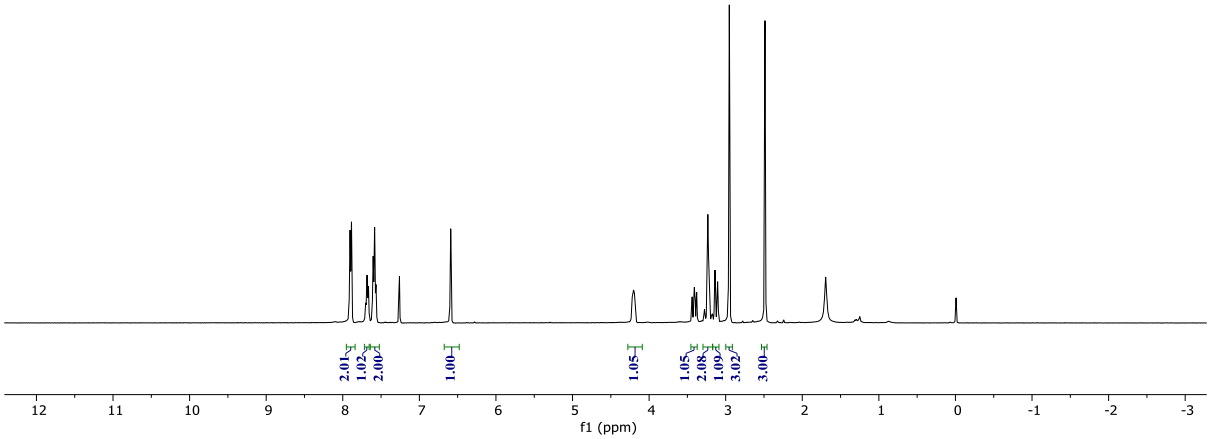


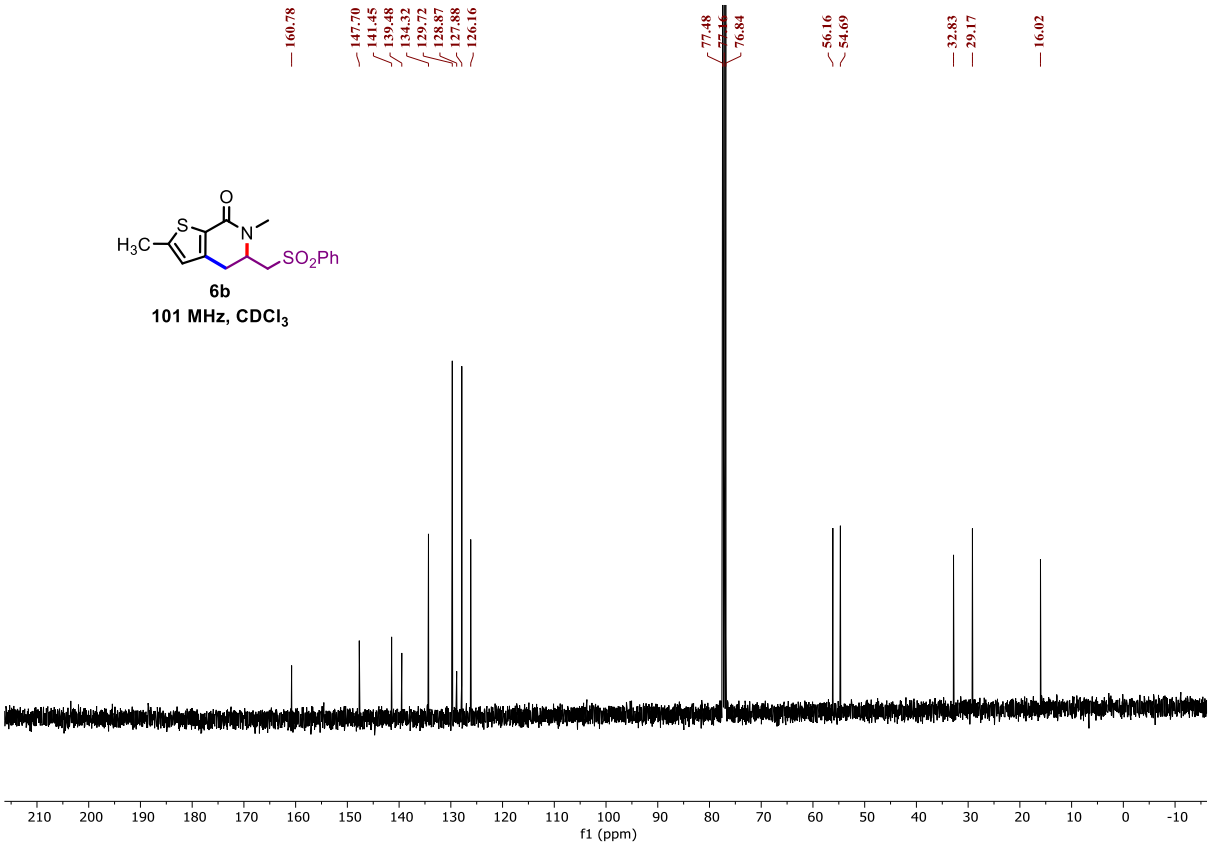
6a
101 MHz, $CDCl_3$



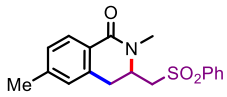


6b
400 MHz, $CDCl_3$



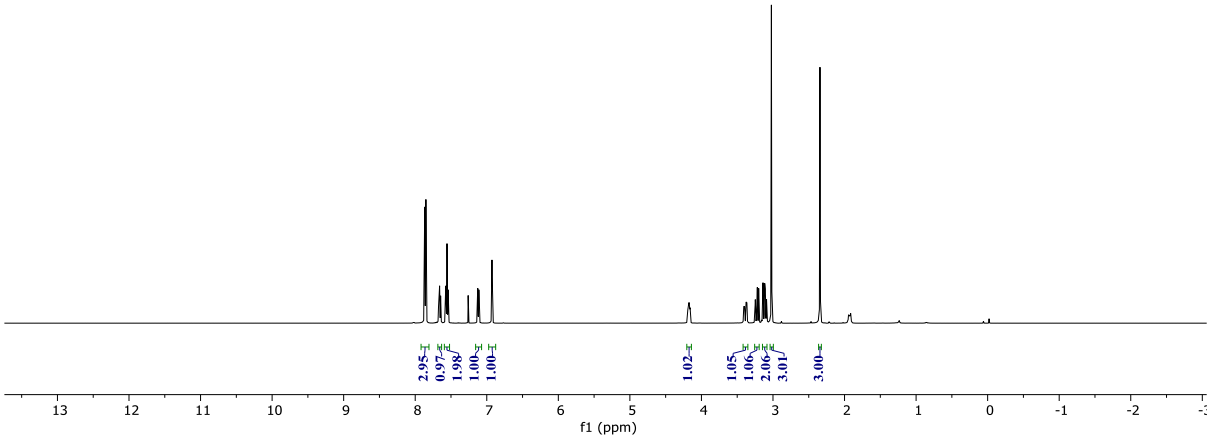


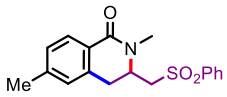
6b
101 MHz, $CDCl_3$



6c

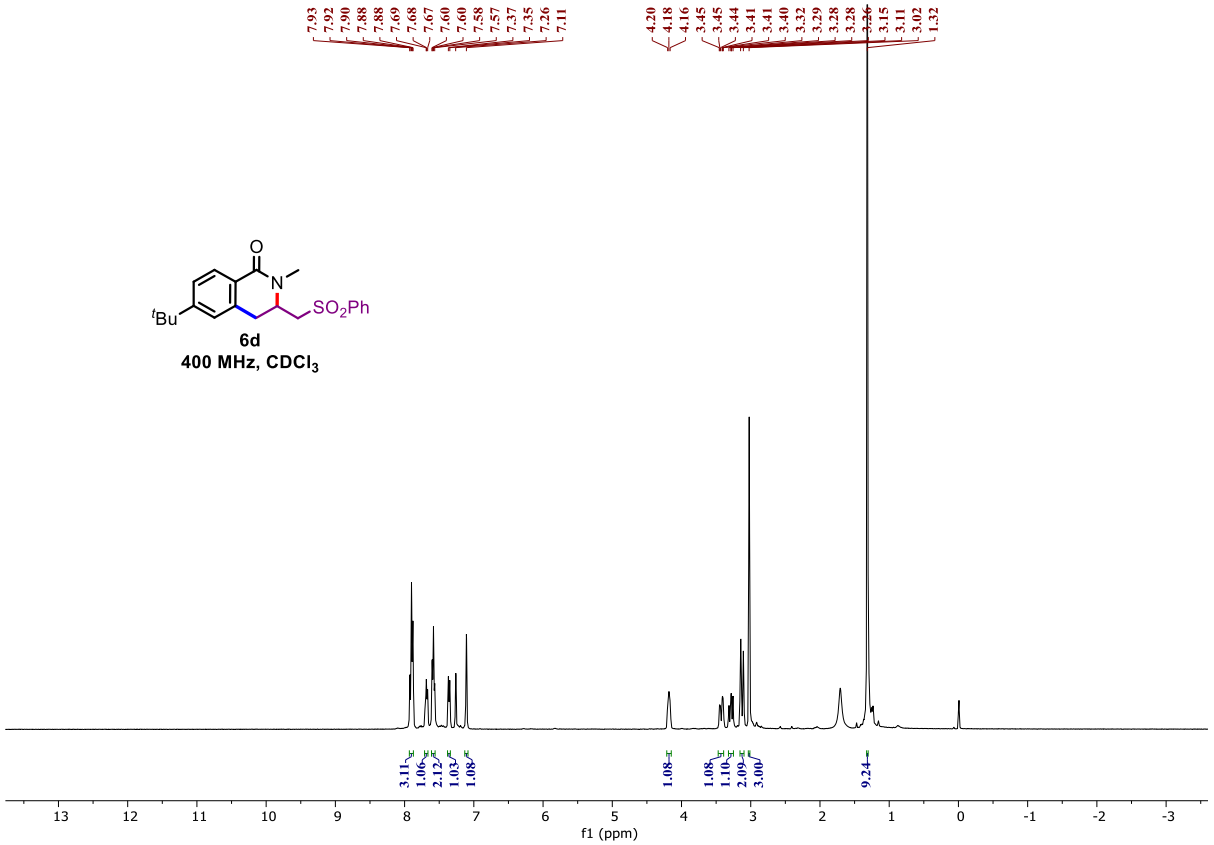
500 MHz, $CDCl_3$

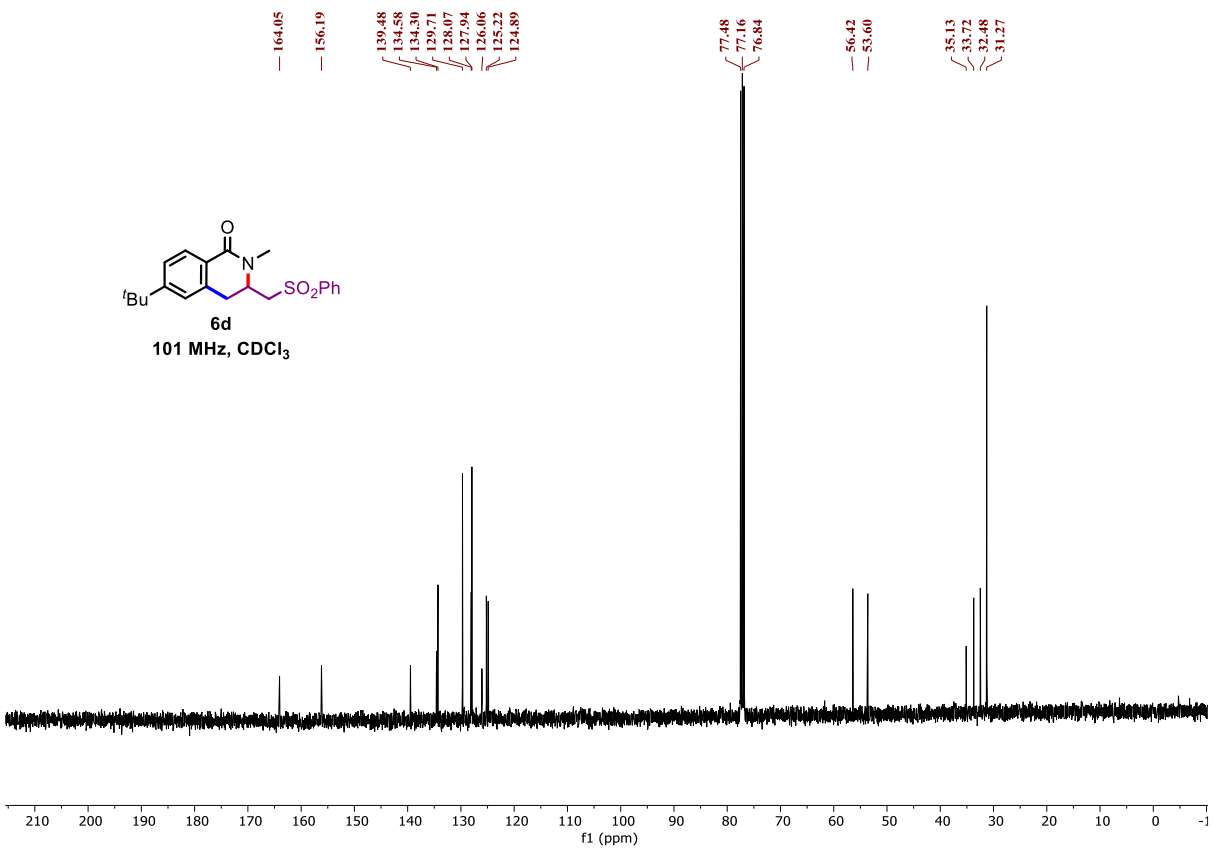


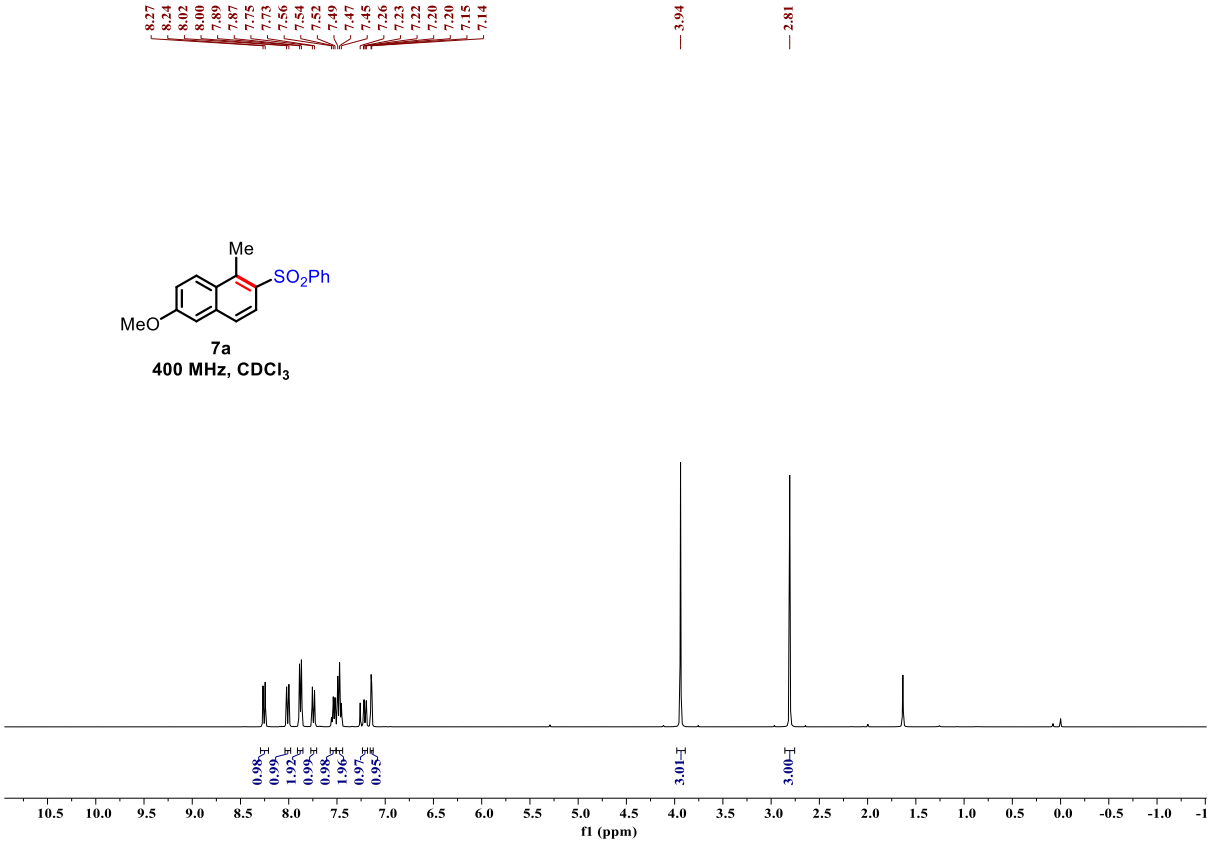


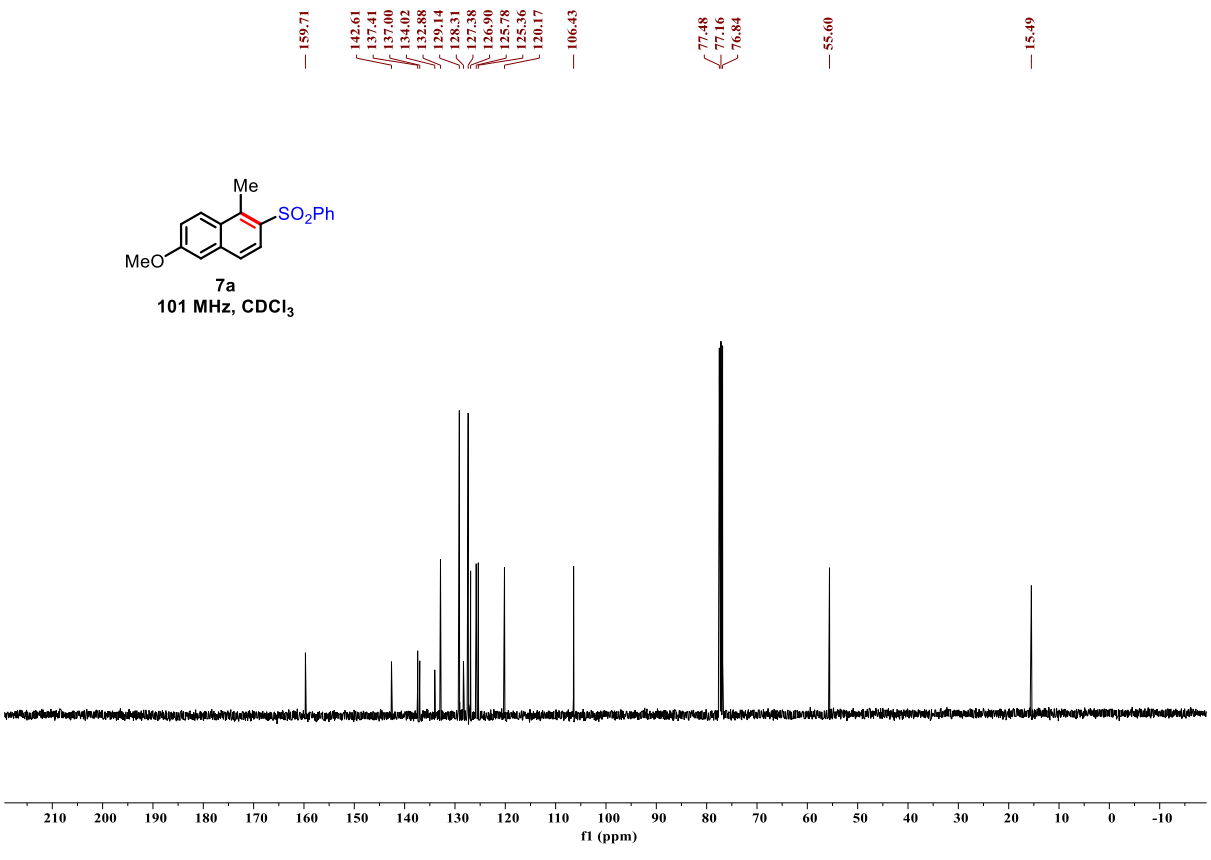
6c

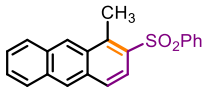
126 MHz, $CDCl_3$


7.93
7.92
7.90
7.88
7.88
7.69
7.68
7.67
7.60
7.60
7.58
7.57
7.37
7.35
7.26
7.11
4.20
4.18
4.16
3.45
3.45
3.44
3.41
3.41
3.40
3.32
3.29
3.28
3.28
3.26
3.15
3.11
3.02
1.32
O
N
SO2Ph
tBu
6d
400 MHz, CDCl3
3.11
1.06
2.12
1.03
1.08
1.08
1.08
1.10
2.09
3.00
9.24
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

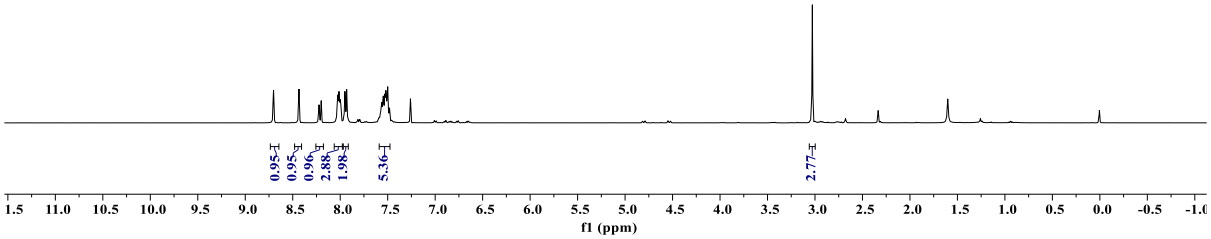

164.05
156.19
139.48
134.58
134.30
129.71
128.07
127.94
126.06
125.22
124.89
77.48
77.16
76.84
56.42
53.60
35.13
33.72
32.48
31.27
O
N
SO2Ph
tBu
6d
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

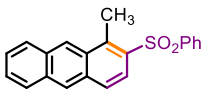

8.27
8.24
8.02
8.00
7.89
7.87
7.75
7.73
7.56
7.54
7.52
7.49
7.47
7.45
7.26
7.23
7.22
7.20
7.20
7.15
7.14
3.94
2.81
Me
SO2Ph
MeO
7a
400 MHz, CDCl3
0.98
0.99
1.92
0.99
0.98
1.96
0.97
0.95
3.01
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1
f1 (ppm)


159.71
142.61
137.41
137.00
134.02
132.88
129.14
128.31
127.38
126.90
125.78
125.36
120.17
106.43
77.48
77.16
76.84
55.60
15.49
Me
SO2Ph
MeO
7a
101 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

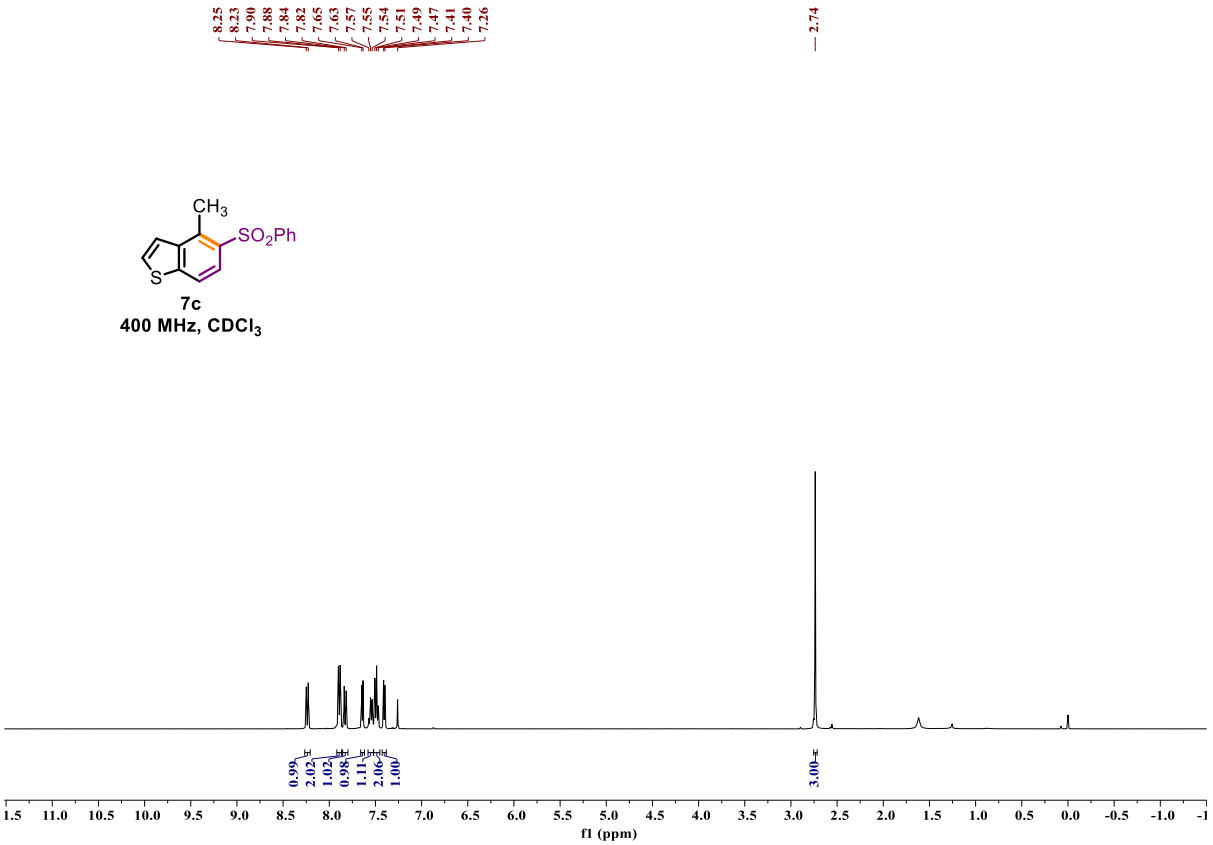


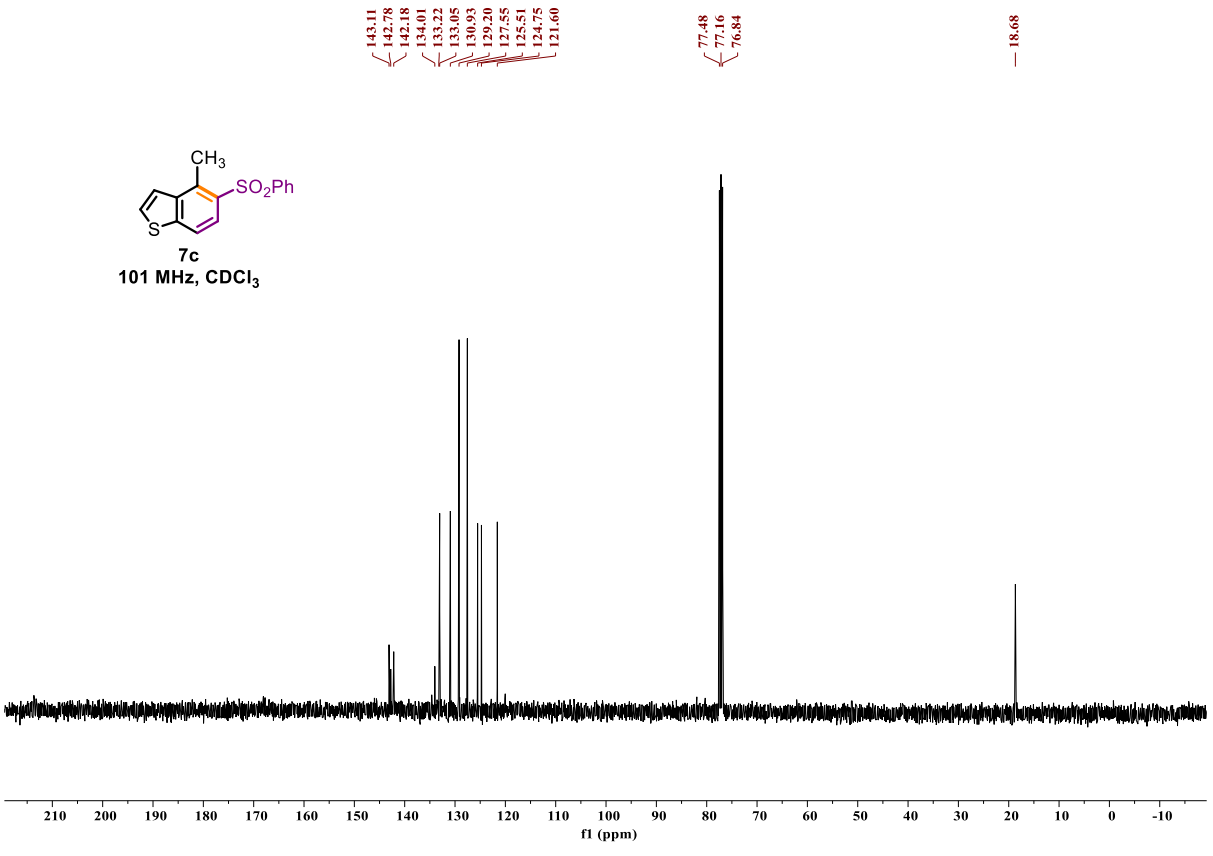
7b
400 MHz, $CDCl_3$





7b
101 MHz, $CDCl_3$


8.25
8.23
7.90
7.88
7.84
7.82
7.65
7.63
7.57
7.55
7.54
7.51
7.49
7.47
7.41
7.40
7.26
2.74
CH3
SO2Ph
S
7c
400 MHz, CDCl3
0.99
2.02
1.02
0.98
1.11
2.06
1.00
3.00
f1 (ppm)


143.11
142.78
142.18
134.01
133.22
133.05
130.93
129.20
127.55
125.51
124.75
121.60
77.48
77.16
76.84
18.68
CH3
SO2Ph
S
7c
101 MHz, CDCl3
f1 (ppm)