Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Bi-Directional Alkyne Tandem Isomerization *via* Pd(0)/Carboxylic Acid Joint Catalysis: Expedient Access to 1,3-Dienes

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General Remarks

All chemicals those syntheses are not reported hereafter were purchased from commercial sources and used as received. Solvents were dried and stored over molecular sieves previously activated in an oven (450 °C overnight). Catalytic reactions required the use of dry solvents. Chromatographic purifications were performed under gradient using a Combiflash® system and prepacked disposable silica cartridges. ^{1}H and ^{13}C-NMR spectra were recorded at 300 K on a Bruker 400 MHz or Bruker 300 MHz spectrometer using solvent residual signals as internal standards (7.26 ppm for ^{1}H NMR and 77.00 ppm for ^{13}C NMR for $CDCl_3$, 2.05 ppm for ^{1}H-NMR and 29.84 ppm for ^{13}C-NMR for Acetone-*d*$_6$, 7.16 ppm for ^{1} H NMR and 128.06 for ^{13}C NMR for Benzene-*d*$_6$). ^{19}F NMR spectra were recorded in $CDCl_3$ at 298 K on a Bruker 400 spectrometer fitted with a BBFO probe head at 263 MHz. The terms m, s, d, t, q and quint represent multiplet, singlet, doublet, triplet, quadruplet and quintuplet respectively, and the term br means a broad signal. Exact masses were recorded on a LTQ ORBITRAP XL Thermo Mass Spectrometer (ESI source).

Materials

Targeted Sulfonamides were synthesized in variable yields (70-88%) from commercial benzylamines following typical protocols. Benzylamine/TsCl/TEA (1.0/1.2/2 equiv), CH_2Cl_2 (0.2 M), r.t., 4 hours.[1] Propargylic alcohols were purchased from commercial available sources or synthesized according to known procedures,[2] as well as propargylamides **1a**, **1f**, **1g**, **1h** and allenamide **1'h**.[3,4] Crystalline $Pd(PPh_3)_4$ has been synthesized from polymeric $PdCl_2$ following the conventional route.[5]

Calculations

Calculations were performed with Gaussian 09 at DFT level.[6] The geometries of all complexes were optimized without any constraints at the generalized gradient approximation using the M06 hybrid functional defined by Zhao and Truhlar.[7] Optimizations were carried out using both the LACVP(d) basis set,[8] which consists of the standard 6-31G(d) basis set for lighter atoms (H, C, N, O, S and P) and the LANL2DZ basis set for Pd, and using the Def2-SVP(d) set defined by Weigand and Ahlrichs,[9] to exclude bias due to basis sets effects. On Def2-SVP(d) optimized geometries, complete re-optimization was performed employing toluene as an implicit solvent as implemented in Gaussian 09 through the CPCM approach.[10] Key intermediates and products were modeled at the B3LYP and at the M11 level too to exclude significant dependencies of calculated results from functionals. No significant dependence on the general trend presented in the main article has been observed neither with different functionals nor with distinct basis sets. The starting approximate geometries for transition states (TS) were obtained through scans of the relative reaction coordinate starting from the corresponding reagents. Transition states were identified by the presence of one imaginary frequency in the Hessian matrix connecting the reagent with the product.

Calculated energetic profiles

Figure S1. Modelled competing pathways, ΔG values in kcal/mol at 298.15 K

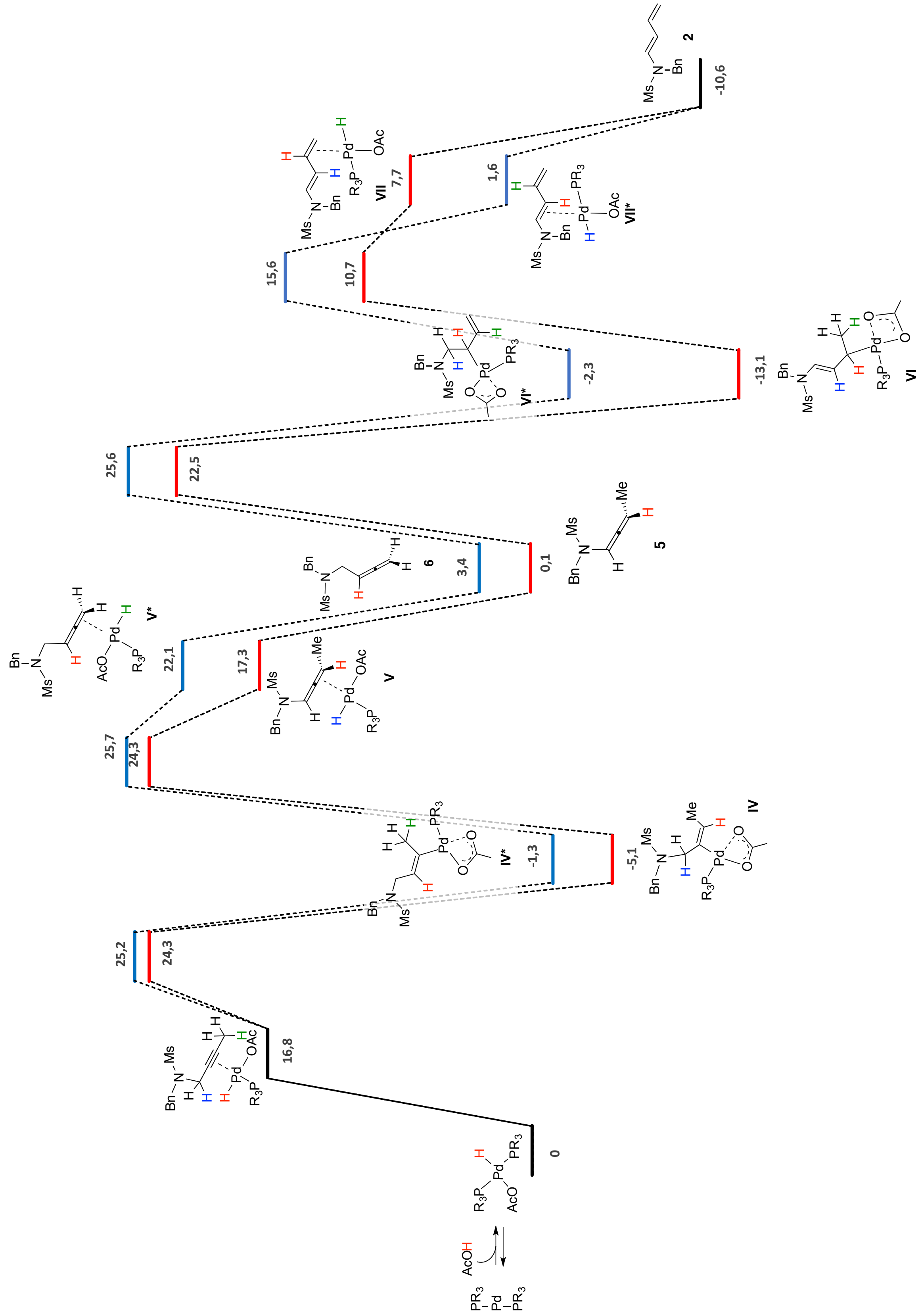
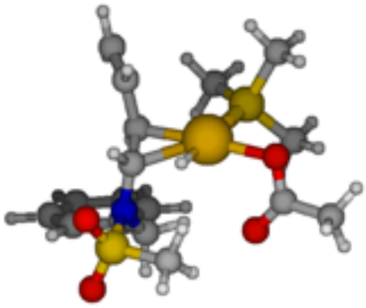
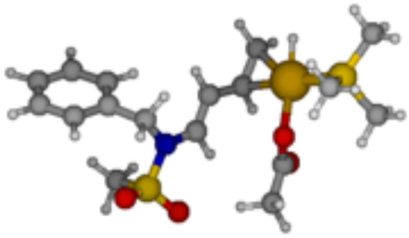


Figure S2. Structures of transition states



TS (VI-VII)*



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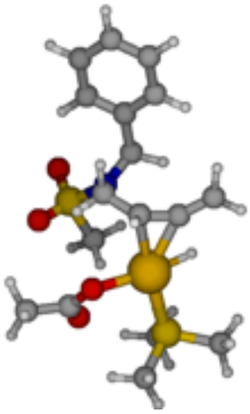

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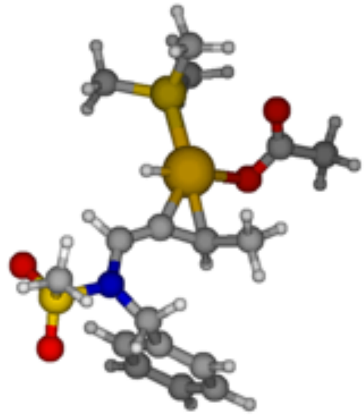

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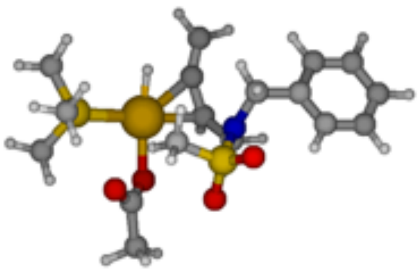

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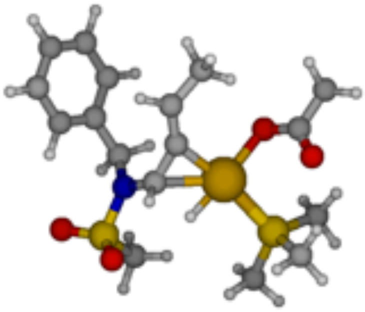
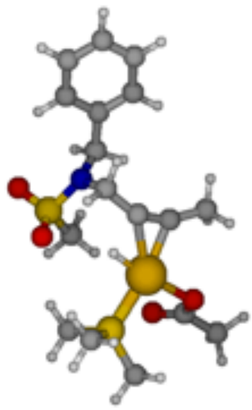


TS (IV-V)



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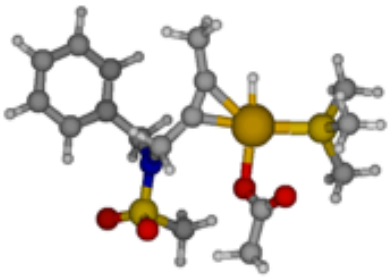
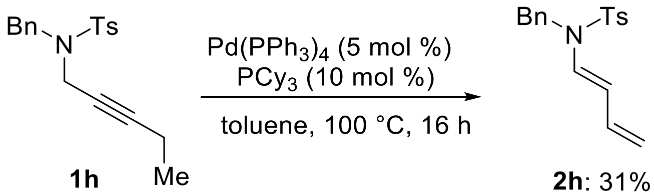
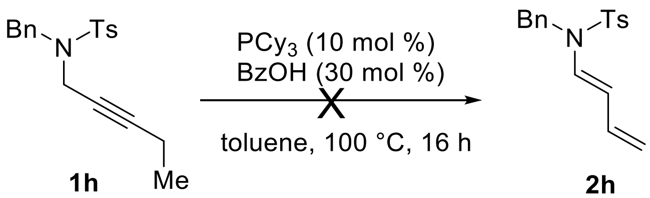


TS (III-IV)

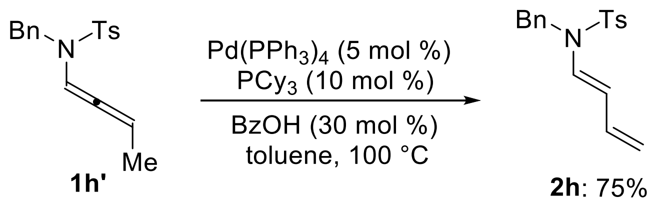
Control Experiments



In an oven dried tube, **1h** (0.10 mmol), $Pd(PPh_3)_4$ (0.005 mmol) and PCy_3 (0.01 mmol) were added sequentially and purged with nitrogen three times. Subsequently, toluene (1.0 ml, 0.1 M) was added under N_2 atmosphere and the tube placed in a pre-heated oil bath at 100 °C. After completion (16 hs), the reaction mixture was cooled down at room temperature and CH_2Cl_2 (10 ml) was added. The mixture was concentrated under reduced pressure and yields evaluated by ^{1}H-NMR analysis using 1,4-Dimethoxybenzene as the internal standard.

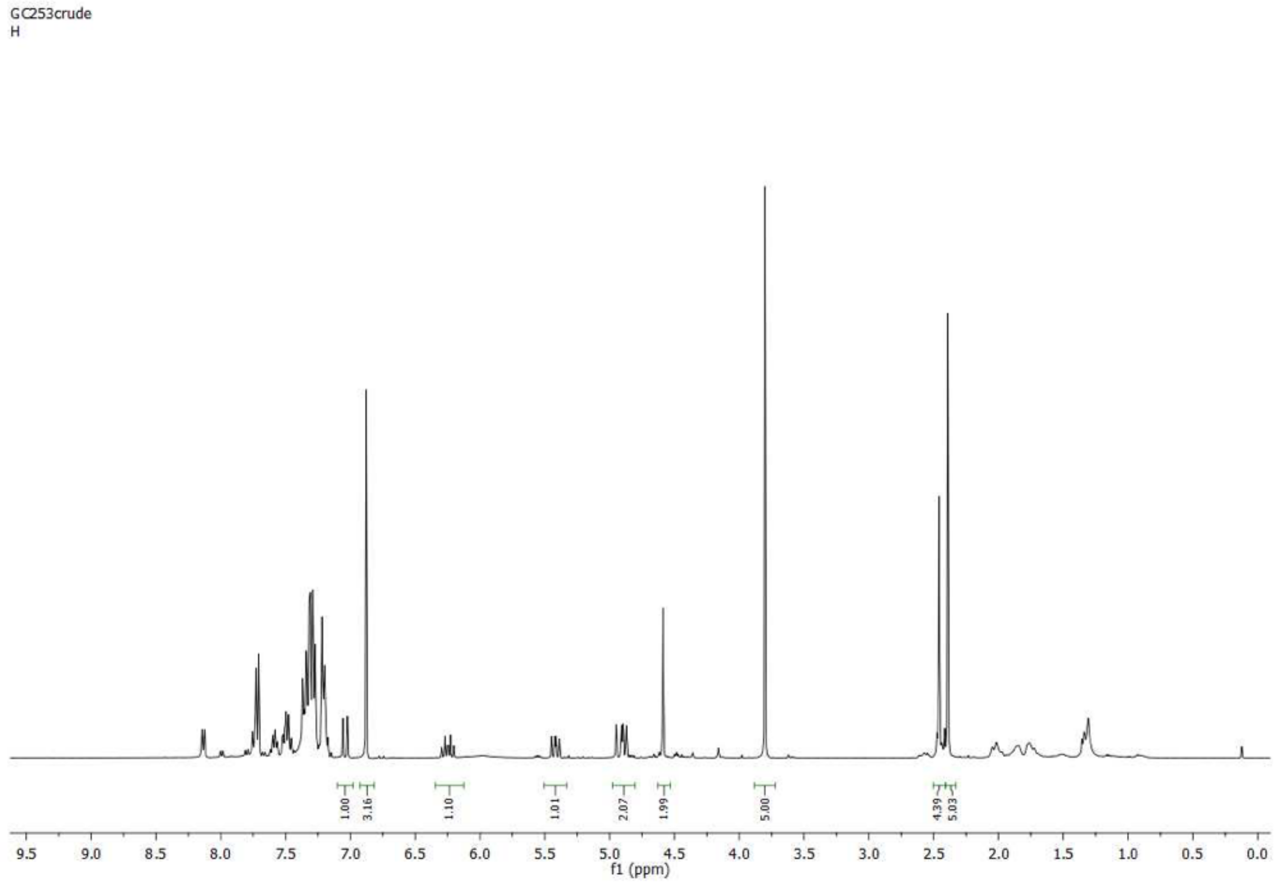


In an oven dried tube, **1h** (0.10 mmol), PCy_3 (0.01 mmol) and BzOH (0.03 mmol) were added sequentially and purged with nitrogen three times. Subsequently, toluene (1.0 ml, 0.1 M) was added under N_2 atmosphere and the tube placed in a pre-heated oil bath at 100 °C. After completion (16 hs), the reaction mixture was cooled down at room temperature and CH_2Cl_2 (10 ml) was added. The mixture was concentrated under reduced pressure. ^{1}H-NMR analysis showed no conversion of starting material with **1h** recovered in nearly quantitative yields (29.9 mg, >95%). The same outcome has been observed repeating the experiment without BzOH.



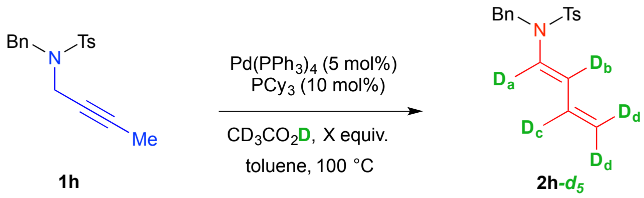
1h' **2h**: 75%

In an oven dried tube, **1h'** (0.18 mmol, 56.3 mg), $Pd(PPh_3)_4$ (0.009 mmol), PCy_3 (0.018 mmol) and BzOH (0.054 mmol) were added sequentially and purged with nitrogen three times. Subsequently, toluene (2.0 ml, 0.09 M) was added under N_2 atmosphere and the tube placed in a pre-heated oil bath at 100 °C. After completion (16 hs), the reaction mixture was cooled down at room temperature and CH_2Cl_2 (10 ml) was added. The mixture was concentrated under reduced pressure and yields evaluated by ^{1}H-NMR analysis (400 MHz, $CDCl_3$) using 1,4-Dimethoxybenzene (14.8 mg, 0.107 mmol) as the internal standard (spectrum copied hereafter). On the contrary, no formation of **2h** is observed treating **1h'** in the presence of PCy_3 under otherwise identical conditions.



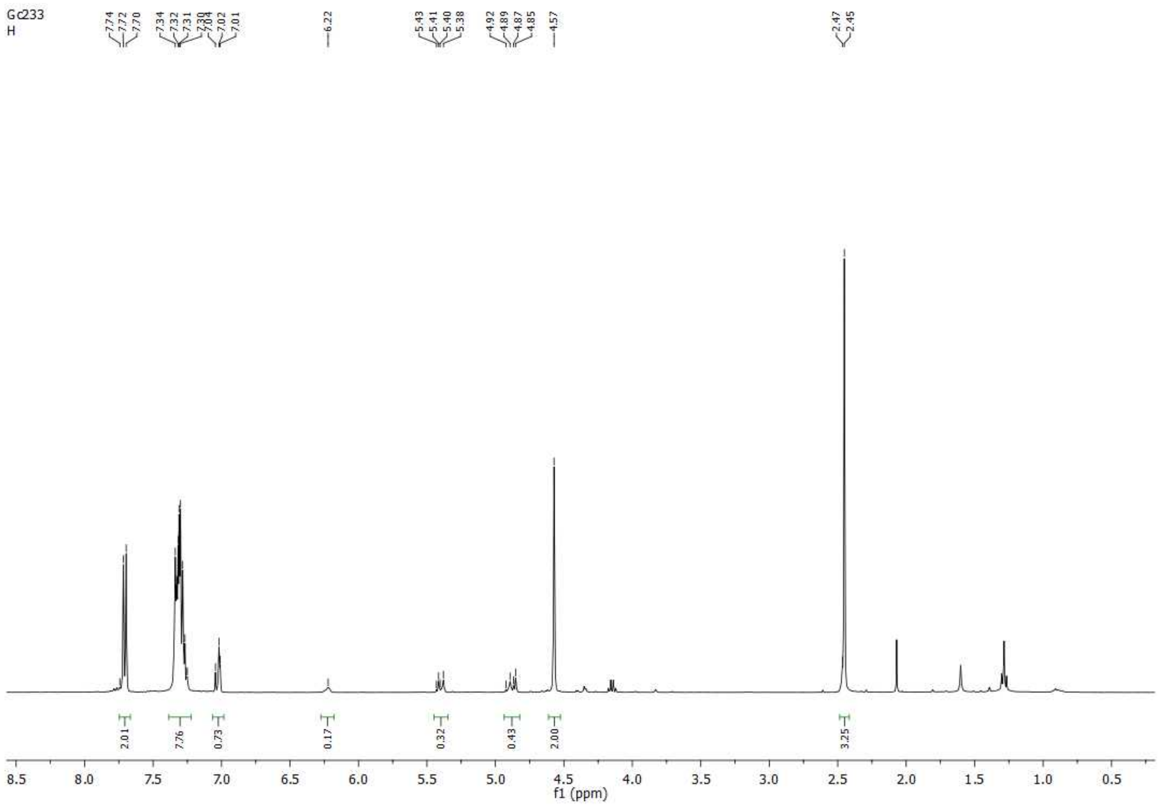
Deuterium labelling experiments

Representative Catalytic Procedure for Isomerization/Deuterium Incorporation (D)



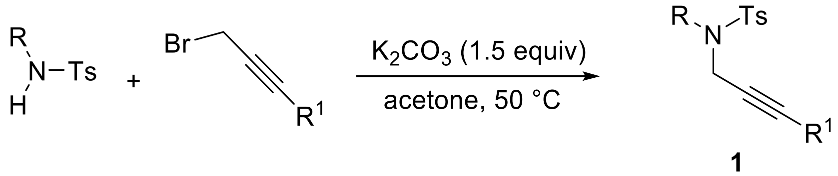
In an oven dried tube, **1h** (62.6 mg, 0.20 mmol), $Pd(PPh_3)_4$ (11.5 mg, 0.01 mmol) and PCy_3 (5.6 mg, 0.02 mmol) were added sequentially and purged with nitrogen three times. Subsequently, d_4-AcOD (X equiv) and toluene (2.0 ml, 0.1 M) was added under N_2 atmosphere and the tube placed in a pre-heated oil bath at 100 °C. After completion (16 hs), the reaction mixture was cooled down at room temperature and CH_2Cl_2 (10 ml) was added. The mixture was concentrated under reduced pressure and the crude purified by chromatography on silica gel.

Entry	d_4-AcOD (X equiv)	Yield [D]-2h [%]	D_a [%]	D_b [%]	D_c [%]	D_d [%]
1	5.0	78 (49.4 mg)	34	42	58	50
2	10.0	72 (46.0 mg)	32	43	64	50
3	20.0	66 (41.7 mg)	27	68	83	79



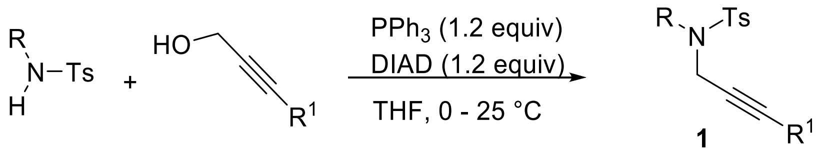
Synthesis of reagents

Representative Procedure A



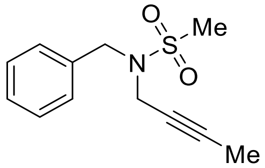
In a Schlenk flask, 1-Bromo-2-butyne (1.5 equiv) was added dropwise to a solution of the corresponding *N*-substituted-Tosylamide (1.0 equiv) and K_2CO_3 (1.5 equiv) in acetone (10 ml). Subsequently, the mixture was placed in a pre-heated oil bath at 50 °C and stirred overnight. After completion, the reaction mixture was cooled down to room temperature and sat. NH_4Cl (15 ml) was added. The mixture was extracted with EtOAc (3 x 15 ml), the organic layers separated and dried over Na_2SO_4. The combined fractions were concentrated under reduced pressure and the crude purified by chromatography on silica gel.

Representative Procedure B



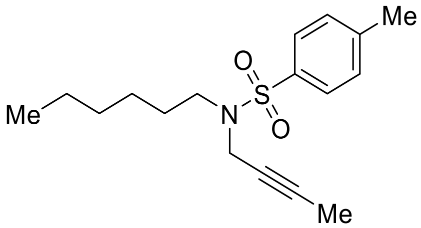
In an oven-dried two-necked round-bottomed flask, the corresponding propargylic alcohol derivative (1.2 equiv) was added to a 1.0 M solution in THF of the corresponding *N*-substituted-Tosylamide (1.0 equiv) and PPh_3 (1.2 equiv) under N_2 atmosphere. Subsequently, the mixture was placed at 0°C and DIAD (1.2 equiv) was carefully added dropwise over 10 min. The mixture was stirred until complete conversion (2-8 hs). Subsequently, a solution of HCl (0.1 M, 10 ml) was added, the mixture extracted with EtOAc (3 x 15 ml), the organic layers separated and dried over Na_2SO_4. The combined fractions were concentrated under reduced pressure and the crude purified by chromatography on silica gel.

_N_-Benzyl-_N_-(but-2-yn-1-yl)methanesulfonamide (1b)



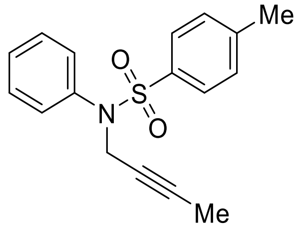
Representative procedure **A** was followed using *N*-Benzylmethanesulfonamide (185 mg, 1.0 mmol) and 1-Bromo-2-butyne (198 mg, 1.5 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1b** (207 mg, 87 %) as a white solid. **M. p.** = 60.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.41 – 7.31 (5H), 4.41 (s, 2H), 3.86 (q, *J* = 2.4 Hz, 2H), 3.00 (s, 3H), 1.88 (t, *J* = 2.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 135.1 (C_q), 128.7 (CH), 128.7 (CH), 128.1 (CH), 82.4 (C_q), 72.2 (C_q), 49.8 (CH_2), 38.2 (CH_2), 35.9 (CH_3), 3.5 (CH_3). **(ESI)-MS** calcd for $C_{14}H_{19}N_2O_2S$ $[M+CH_3CN+H]^+$ 279.12 found 279.24.

_N_-(But-2-yn-1-yl)-_N_-hexyl-4-methylbenzenesulfonamide (1c)



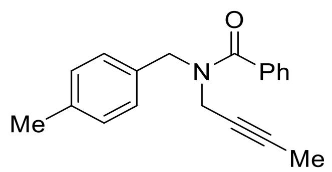
Representative procedure **A** was followed using *N*-Hexyl-4-methylbenzenesulfonamide (510 mg, 2.0 mmol) and 1-Bromo-2-butyne (396 mg, 3.0 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1c** (462 mg, 75%) as an oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.74 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.06 (q, *J* = 2.3 Hz, 2H), 3.23 – 3.04 (m, 2H), 2.42 (s, 3H), 1.62 – 1.45 (m, 5H), 1.35-1-20 (m, 6H), 0.89 (t, *J* = 6.7 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 143.0 (C_q), 136.2 (C_q), 129.2 (CH), 127.8 (CH), 81.3 (C_q), 71.8 (C_q), 46.2 (CH_2), 36.6 (CH_2), 31.4 (CH_2), 27.5 (CH_2), 26.2 (CH_2), 22.5 (CH_2), 21.5 (CH_3), 14.0 (CH_3), 3.2 (CH_3). **(ESI)-MS** calcd for $C_{17}H_{26}NO_2S$ $[M+H]^+$ 308.17 found 308.20.

_N_-(But-2-yn-1-yl)-4-methyl-_N_-phenylbenzenesulfonamide (1d)



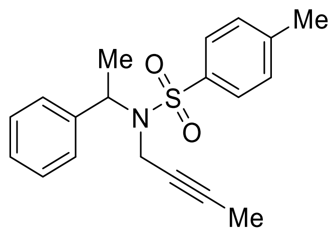
Representative procedure **A** was followed using 4-Methyl-*N*-phenylbenzenesulfonamide (494 mg, 2.0 mmol) and 1-Bromo-2-butyne (396 mg, 3.0 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1d** (523 mg, 87%) as a white solid. **M. p.** = 84.8 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.55 (d, *J* = 8.3 Hz, 2H), 7.46 – 7.09 (m, 7H), 4.40 (q, *J* = 2.3 Hz, 2H), 2.43 (s, 3H), 1.68 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 143.4 (C_q), 139.9 (C_q), 135.9 (C_q), 129.1 (CH), 128.9 (CH), 128.3 (CH), 128.1 (CH), 127.9 (CH), 81.7 (C_q), 73.4 (C_q), 41.7 (CH_2), 21.6 (CH_3), 3.5 (CH_3). **(ESI)-MS** calcd for $C_{17}H_{18}NO_2S$ $[M+H]^+$ 300.11 found 300.17.

_N_-(But-2-yn-1-yl)-N-(4-methylbenzyl)benzamide (1e)



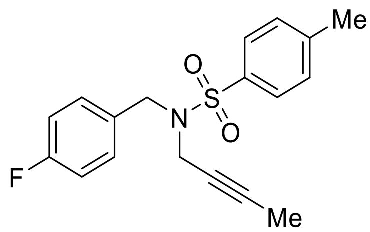
To a solution of *N*-(4-methylbenzyl)benzamide (500 mg, 2.2 mmol) in THF (10 ml), NaH (60% in mineral oil) (132 mg, 3.3 mmol) was added at 0°C and the mixture stirred at the same temperature for 30 min. Subsequently, 1-Bromo-2-butyne (435 mg, 3.3 mmol) was added and the reaction mixture stirred overnight. A solution of HCl (0.1 M, 10 ml) was added, the mixture extracted with EtOAc (3 x 15 ml) and the organic layers separated and dried over Na_2SO_4. The combined fractions were concentrated under reduced pressure and the crude purified by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielding **1e** (472 mg, 77%) as an orange solid. **M. p** = 65.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.62-7.49 (m, 3H), 7.48-7-29 (m, 3H), 7.17 (d, *J* = 7.2 Hz, 2H), 7.14-7.08 (m, 1H), 4.87 – 4.80 (m, 1H), 4.68 – 4.57 (m, 1H), 4.34 – 4.14 (m, 1H), 3.83 (s, 1H), 2.37 (s, 3H), 1.89 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ= 171.4 (C_q, rotA), 163.7 (C_q, rotB), 137.3 (C_q), 136.7 (CH), 129.9 (C_q), 129.4 (CH), 129.0 (CH), 128.8 (C_q), 128.5 (CH), 127.01 (CH), 77.2 (C_q), 73.76 (C_q), 51.4 (CH_2, rotA), 47.10 (CH_2, rotA), 38.5 (CH_2, rotA), 33.7 (CH_2, rotB), 21.1 (CH_3), 3.6 (CH_3). **(ESI)-MS** calcd for $C_{19}H_{20}NO$ $[M+H]^+$ 278.15 found 278.11.

N-(But-2-yn-1-yl)-4-methyl-N-(1-phenylethyl)benzenesulfonamide (1i)



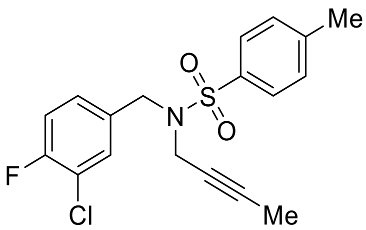
Representative procedure **A** was followed using 4-Methyl-*N*-(1-phenylethyl)benzenesulfonamide (495 mg, 1.8 mmol) and 1-Bromo-2-butyne (359 mg, 2.7 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1i** (502 mg, 85%) as a whitish oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.89 – 7.87 (m, 2H), 7.38 – 7.26 (m, 7H), 5.25 (q, *J* = 7.2 Hz, 1H), 4.13 (dd, *J* = 18.4, 2.7 Hz, 1H), 3.74 – 3.38 (m, 1H), 2.46 (s, 3H), 1.64 (s, 3H), 1.50 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 143.0 (C_q), 139.7 (C_q), 138.2 (C_q), 129.2 (CH), 128.3 (CH), 127.6 (CH), 127.6 (CH), 127.5 (CH), 80.3 (C_q), 75.1 (C_q), 55.7 (CH), 33.0 (CH_2), 21.5 (CH_3), 16.8 (CH_3), 3.3 (CH_3). **(ESI)-MS** calcd for $C_{19}H_{21}NNaO_2S$ $[M+Na]^+$ 350.12 found 350.19.

N-(But-2-yn-1-yl)-N-(4-fluorobenzyl)-4-methylbenzenesulfonamide (1j)



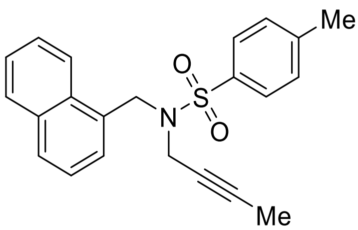
Representative procedure **B** was followed using *N*-(4-Fluorobenzyl)-4-methylbenzenesulfonamide (350 mg, 1.25 mmol) and But-2-yn-1-ol (91 mg, 1.3 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1j** (274 mg, 66%) as a white sticky oil. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 7.79 (d, *J* = 8.3 Hz, 2H), 7.34 – 7.31 (m, 4H), 7.01 (dd, *J* = 9.7, 7.7 Hz, 2H), 4.28 (s, 2H), 3.86 (q, *J* = 2.2 Hz, 2H), 2.44 (s, 3H), 1.54 (t, *J* = 2.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$): δ = 162.71 (d, $^{1}J_{C\text{-}F}$ = 246.5 Hz, C_q), 143.6 (C_q), 136.3 (C_q), 131.3 (d, $^{4}J_{C\text{-}F}$ = 3.2 Hz, C_q), 130.6 (d, $^{3}J_{C\text{-}F}$ = 8.2 Hz, CH), 129.5 (CH), 128.1 (CH), 115.69 (d, $^{2}J_{C\text{-}F}$ = 21.5 Hz, CH), 82.2 (C_q), 71.5 (C_q), 49.3 (CH_2), 36.3 (CH_2), 21.7 (CH_3), 3.4 (CH_3). **^{19}F NMR** (376 MHz, $CDCl_3$) δ = -114.27. **(ESI)-MS** calcd for $C_{18}H_{19}FNO_2S$ $[M+H]^+$ 332.11 found 332.15.

_N_-(But-2-yn-1-yl)-_N_-(3-chloro-4-fluorobenzyl)-4-methylbenzenesulfonamide (1k)



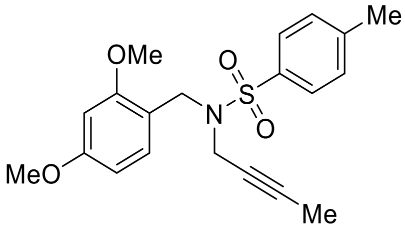
Representative procedure **A** was followed using *N*-(3-Chloro-4-fluorobenzyl)-4-methylbenzenesulfonamide (563 mg, 1.8 mmol) and 1-Bromo-2-butyne (356 mg, 2.7 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1k** (544 mg, 83%) as a white solid. **M. p.** = 90.4 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.76 (d, *J* = 8.3 Hz, 2H), 7.38 (dt, *J* = 6.7, 3.4 Hz, 1H), 7.32 (d, *J* = 8.3 Hz, 2H), 7.27 – 7.18 (m, 1H), 7.09 (t, *J* = 8.6 Hz, 1H), 4.26 (s, 2H), 3.88 (q, *J* = 2.2 Hz, 2H), 2.45 (s, 3H), 1.54 (t, *J* = 2.4 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 157.8 (d, $^{1}J_{C\text{-}F}$ = 249 Hz, C_q), 143.6 (C_q), 135.9 (C_q), 132.6 (d, $^{5}J_{C\text{-}F}$ = 4 Hz, C_q), 130.8 (CH), 129.6 (CH), 128.4 (d, $^{4}J_{C\text{-}F}$ = 7 Hz, CH), 128.1 (CH), 121.1 (d, $^{3}J_{C\text{-}F}$ = 18 Hz, C_q), 116.7 (d, $^{2}J_{C\text{-}F}$ = 21 Hz, CH), 82.3 (C_q), 71.2 (C_q), 48.9 (CH_2), 36.5 (CH_2), 21.5 (CH_3), 3.2 (CH_3). **^{19}F NMR** (376 MHz, $CDCl_3$) δ = -116.41. **(ESI)-MS** calcd for $C_{18}H_{17}ClFKNO_2S$ $[M+K]^+$ 404.03 found 404.11.

_N_-(But-2-yn-1-yl)-4-methyl-_N_-(naphthalen-1-ylmethyl)benzenesulfonamide (1l)



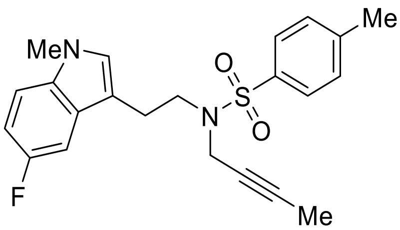
Representative procedure **A** was followed using 4-Methyl-*N*-(naphthalen-1-ylmethyl)benzenesulfonamide (555 mg, 1.8 mmol) and 1-Bromo-2-butyne (356 mg, 2.7 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1l** (544 mg, 83%) as a white solid. **M. p.** = 154.5 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 8.48 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.2 Hz, 2H), 7.88 – 7.83 (m, 2H), 7.65 – 7.50 (m, 2H), 7.50 – 7.43 (m, 2H), 7.42 – 7.37 (m, 2H), 4.79 (s, 2H), 3.80 (q, *J* = 2.2 Hz, 2H), 2.50 (s, 3H), 1.55 (t, *J* = 2.4 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ =143.4 (C_q), 135.5 (C_q), 133.9 (C_q), 132.1 (C_q), 130.1 (C_q), 129.3 (CH), 129.2 (CH), 128.5 (CH), 128.4 (CH), 128.3 (CH), 126.7 (CH), 126.1 (CH), 125.0 (CH), 124.4 (CH), 82.3 (C_q), 71.3 (C_q), 48.4 (CH_2), 36.1 (CH_2), 21.6 (CH_3), 3.3 (CH_3). **(ESI)-MS** calcd for $C_{22}H_{22}NO_2S$ $[M+H]^+$ 364.14 found 364.18.

N-(But-2-yn-1-yl)-N-(2,4-dimethoxybenzyl)-4-methylbenzenesulfonamide (1m)



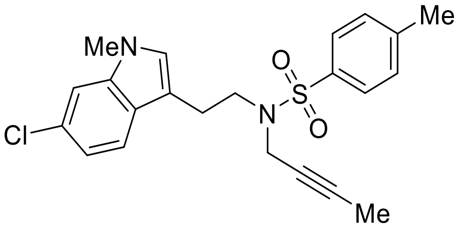
Representative procedure **A** was followed using *N*-(2,4-dimethoxybenzyl)-4-methylbenzenesulfonamide (481 mg, 1.5 mmol) and 1-Bromo-2-butyne (290 mg, 2.2 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1m** (448 mg, 80%) as a white solid. **M. p.** = 96.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.80 (d, *J* = 8.2 Hz, 2H), 7.34-7.28 (m, 3H), 6.48 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.44 (d, *J* = 2.2 Hz, 1H), 4.34 (s, 2H), 3.93 (d, *J* = 2.2 Hz, 2H), 3.79 (s, 3H), 3.77 (s, 3H), 2.44 (s, 3H), 1.57 (t, *J* = 2.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 160.7 (C_q), 158.8 (C_q), 143.0 (C_q), 136.6 (C_q), 130.9 (CH), 129.1 (CH), 128.0 (CH), 116.0 (C_q), 104.2 (CH), 98.5 (CH), 81.3 (C_q), 72.2 (C_q), 55.4 (CH_3), 55.3 (CH_3), 44.3 (CH_2), 36.6 (CH_2), 21.5 (CH_3), 3.3 (CH_3). **(ESI)-MS** calcd for $C_{20}H_{23}NaNO_4S$ $[M+Na]^+$ 396.12 found 396.18.

N-(But-2-yn-1-yl)-N-[2-(5-fluoro-1-methyl-1H-indol-3-yl)ethyl]-4-methylbenzenesulfonamide (1n)



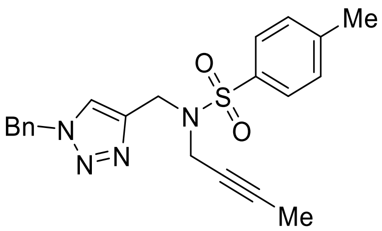
Representative procedure **A** was followed using *N*-[2-(5-fluoro-1-methyl-1*H*-indol-3-yl)ethyl]-4-methylbenzenesulfonamide (346 mg, 1.0 mmol) and 1-Bromo-2-butyne (198 mg, 1.5 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1n** (302 mg, 76%) as a white solid. **M. p.** = 114.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.74 (d, *J* = 8.3 Hz, 2H), 7.32 – 7.23 (m, 2H), 7.23 – 7.13 (m, 2H), 7.00 (s, 1H), 6.99-6.94 (m, 1H), 4.15 (d, *J* = 2.3 Hz, 2H), 3.75 (s, 3H), 3.45 (dd, *J* = 8.9, 6.9 Hz, 2H), 3.02 (dd, *J* = 17.7, 9.6 Hz, 2H), 2.42 (s, 3H), 1.63 (t, *J* = 2.3 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 157.6 (d, $^1J_{C-F}$ = 235 Hz, C_q), 143.2 (C_q), 136.0 (C_q), 133.6 (C_q), 129.3 (CH), 128.7 (CH), 128.0 (d, $^4J_{C-F}$ = 9 Hz, C_q), 127.8 (CH), 110.8 (d, $^6J_{C-F}$ = 5Hz, C_q), 110.0 (d, $^3J_{C-F}$ = 10 Hz, CH), 109.9 (d, $^5J_{C-F}$ = 6 Hz, CH), 103.6 (d, $^2J_{C-F}$ = 23 Hz, CH), 81.8 (C_q), 71.9 (C_q), 46.8 (CH_2), 37.2 (CH_3), 32.9 (CH_2), 24.0 (CH_2), 21.5 (CH_3), 3.2 (CH_3). **^{19}F NMR** (376 MHz, $CDCl_3$) δ = -116.9. . **(ESI)-MS** calcd for $C_{22}H_{23}KFN_2O_2S$ $[M+K]^+$ 437.11 found 437.15.

N-(But-2-yn-1-yl)-N-[2-(6-chloro-1-methyl-1H-indol-3-yl)ethyl]-4-methylbenzenesulfonamide (1o)



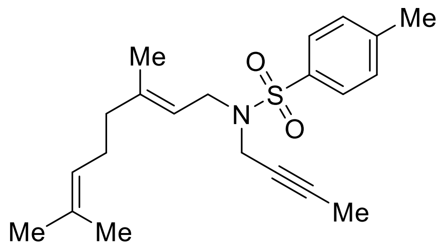
Representative procedure **A** was followed using *N*-[2-(6-chloro-1-methyl-1*H*-indol-3-yl)ethyl]-4-methylbenzenesulfonamide (207 mg, 0.5 mmol) and 1-Bromo-2-butyne (100 mg, 0.75 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1o** (156 mg, 75%) as a yellow viscous oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.70 (d, *J* = 8.3 Hz, 2H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.31 – 7.13 (m, 3H), 7.11 – 6.99 (m, 1H), 6.92 (s, 1H), 4.16 – 4.01 (m, 2H), 3.69 (s, 3H), 3.52 – 3.33 (m, 2H), 3.09 – 2.91 (m, 2H), 2.42 (s, 3H), 1.58 (t, *J* = 2.4 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 143.2 (C_q), 137.4 (C_q), 136.0 (C_q), 129.3 (CH), 127.8 (CH), 128.7 (C_q), 127.6 (CH), 126.3 (C_q), 119.7 (CH), 119.5 (CH), 111.3 (C_q), 109.3 (CH), 81.6 (C_q), 72.0 (C_q), 47.0 (CH_2), 37.3 (CH_3), 32.7 (CH_2), 24.1 (CH_2), 21.5 (CH_3), 3.3 (CH_3). **(ESI)-MS** calcd for $C_{22}H_{23}ClKN_2O_2S$ $[M+K]^+$ 453.08 found 453.16.

N-[(1-Benzyl-1H-1,2,3-triazol-4-yl)methyl]-N-(but-2-yn-1-yl)-4-methylbenzenesulfonamide (1p)



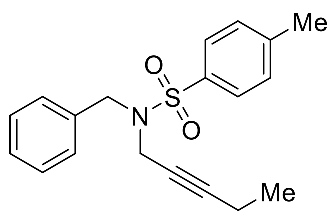
Representative procedure **A** was followed using *N*-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl]methyl)-*N*,4-dimethylbenzenesulfonamide (200 mg, 0.6 mmol) and 1-Bromo-2-butyne (119 mg, 0.9 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1p** (204 mg, 86%) as a white solid. **M. p.** = 107.1 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.74 (d, *J* = 8.6 Hz, 2H), 7.52 (s, 1H), 7.39 – 7.36 (m, 3H), 7.29 – 7.27 (m, 4H), 5.50 (s, 2H), 4.47 (s, 2H), 3.99 (d, *J* = 2.6 Hz, 2H), 2.43 (s, 3H), 1.54 (t, *J* = 2.4 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ = 144.2 (C_q), 143.5 (C_q), 136.1 (C_q), 134.4 (C_q), 129.4 (CH), 129.2 (CH), 128.8 (CH), 128.1 (CH), 127.8 (CH), 122.9 (CH), 82.0 (C_q), 71.6 (C_q), 54.3 (CH_2), 41.9 (CH_2), 37.3 (CH_2), 21.5 (CH_3), 3.3 (CH_3). (**ESI)-MS** calcd for $C_{21}H_{23}N_4O_2S$ $[M+H]^+$ 395.15 found 395.19.

(*E*)-*N*-(But-2-yn-1-yl)-*N*-(3,7-dimethylocta-2,6-dien-1-yl)-4-methylbenzenesulfonamide (1q)



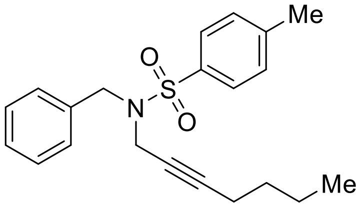
Representative procedure **A** was followed using (*E*)-*N*-(3,7-Dimethylocta-2,6-dien-1-yl)-4-methylbenzenesulfonamide (465 mg, 1.6 mmol) and 1-Bromo-2-butyne (317 mg, 2.4 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1q** (443 mg, 77%) as a yellow oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.1 Hz, 2H), 7.48 – 7.17 (m, 2H), 5.10 (t, *J* = 7.3 Hz, 1H), 5.05 (t, *J* = 6.3 Hz, 1H), 4.00 (d, *J* = 2.1 Hz, 2H), 3.80 (t, *J* = 8.5 Hz, 2H), 2.44 (s, 3H), 2.16 – 1.88 (m, 4H), 1.68 (s, 3H), 1.66 (s, 3H), 1.60 (s, 3H), 1.54 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 143.0 (C_q), 142.1 (C_q), 136.3 (C_q), 131.8 (C_q), 129.2 (CH), 127.9 (CH), 123.8 (CH), 118.1 (CH), 81.2 (C_q), 72.1 (C_q), 43.8 (CH_2), 39.6 (CH_2), 35.8 (CH_2), 26.2 (CH_3), 25.7 (CH_2), 21.5 (CH_3), 17.7 (CH_3), 16.1 (CH_3), 3.2 (CH_3). **(ESI)-MS** calcd for $C_{21}H_{29}KNO_2S$ $[M+K]^+$ 398.16 found 398.22.

***N*-Benzyl-4-methyl-*N*-(pent-2-yn-1-yl)benzenesulfonamide (1r)**



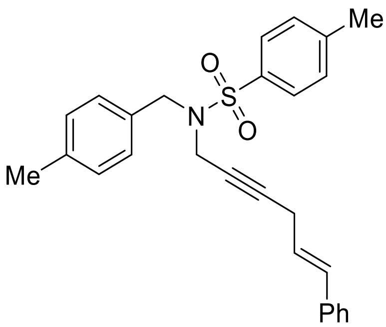
Representative procedure **A** was followed using *N*-Benzyl-4-methylbenzenesulfonamide (523 mg, 2.0 mmol) and 1-Bromo-2-pentyne (441 mg, 3.0 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1r** (568 mg, 87%) as a white solid. **M. p.** = 60.9 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.91 – 7.73 (m, 2H), 7.43 – 7.24 (m, 7H), 4.36 (s, 2H), 3.93 (t, *J* = 2.2 Hz, 2H), 2.46 (s, 3H), 1.94 (qt, *J* = 7.5, 2.2 Hz, 2H), 0.93 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ =143.3 (C_q), 136.2 (C_q), 135.3 (C_q), 129.4 (CH), 128.8 (CH), 128.6 (CH), 128.0 (CH), 127.9 (CH), 87.9 (C_q), 71.5 (C_q), 49.8 (CH_2), 36.1 (CH_2), 21.5 (CH_3), 13.5 (CH_3), 12.1 (CH_2). **(ESI)-MS** calcd for $C_{19}H_{21}KNO_2S$ $[M+K]^+$ 366.09 found 366.13.

N-Benzyl-N-(hept-2-yn-1-yl)-4-methylbenzenesulfonamide (1s)



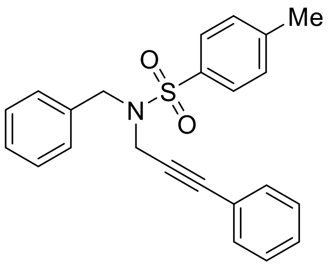
Representative procedure **B** was followed using *N*-Benzyl-4-methylbenzenesulfonamide (391 mg, 1.5 mmol) and Hept-2-yn-1-ol (202 mg, 1.8 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1s** (378 mg, 71%) as a white oil. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.80 (d, *J* = 8.2 Hz, 2H), 7.44 – 7.19 (m, 7H), 4.33 (s, 2H), 3.91 (s, 2H), 2.44 (s, 3H), 1.91 (s, 2H), 1.32 – 1.08 (m, 4H), 0.85 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 143.3 (C_q), 136.3 (C_q), 135.3 (C_q), 129.4 (CH), 128.8 (CH), 128.6 (CH), 128.0 (CH), 127.9 (CH), 86.6 (C_q), 72.1 (C_q), 49.8 (CH_2), 36.1 (CH_2), 30.5 (CH_2), 21.9 (CH_2), 21.5 (CH_3), 18.1, 13.6 (CH_3). **(ESI)-MS** calcd for $C_{21}H_{26}NO_2S$ $[M+H]^+$ 356.17 found 356.21.

(E)-4-Methyl-N-(4-methylbenzyl)-N-(6-phenylhex-5-en-2-yn-1-yl)benzenesulfonamide (1t)



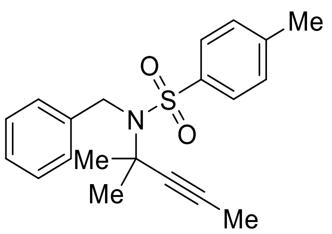
Representative procedure **B** was followed using 4-Methyl-*N*-(4-methylbenzyl)benzenesulfonamide (412 mg, 1.5 mmol) and (*E*)-6-Phenylhex-5-en-2-yn-1-ol (328 mg, 1.8 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1t** (380 mg, 59%) as a white oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.88 – 7.76 (m, 2H), 7.43 – 7.21 (m, 8H), 7.20 – 7.07 (m, 3H), 6.51 – 6.32 (m, 1H), 6.07 – 5.87 (m, 1H), 4.46 – 4.25 (m, 2H), 4.10 – 3.94 (m, 2H), 3.01 – 2.80 (m, 2H), 2.36 (s, 3H), 2.43 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 143.4 (C_q), 137.8 (C_q), 136.9 (C_q), 136.2 (C_q), 132.0 (C_q), 131.3 (CH), 129.4 (CH), 129.3 (CH), 128.8 (CH), 128.6 (CH), 127.9 (CH), 127.5 (CH), 126.2 (CH), 123.6 (CH), 83.0 (C_q), 74.9 (C_q), 49.7 (CH_2), 36.0 (CH_2), 22.1 (CH_2), 21.4 (CH_3), 21.2 (CH_3). **(ESI)-MS** calcd for $C_{27}H_{28}NO_2S$ $[M+H]^+$ 430.18 found 430.22.

***N*-Benzyl-4-methyl-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (1u)**



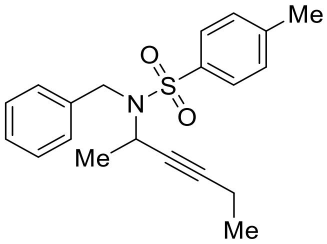
Representative procedure **B** was followed using *N*-Benzyl-4-methylbenzenesulfonamide (522 mg, 2.0 mmol) and 3-Phenylprop-2-yn-1-ol (317 mg, 2.4 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1u** (475 mg, 66%) as a white solid. **M. p.** = 96.6 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.87 (d, *J* = 8.3 Hz, 2H), 7.53 – 7.22 (m, 10H), 7.17 – 6.95 (m, 2H), 4.45 (s, 2H), 4.18 (s, 2H), 2.38 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 143.6 (C_q), 136.0 (C_q), 135.1 (C_q), 131.5 (CH), 129.6 (CH), 128.9 (CH), 128.8 (CH), 128.7 (CH), 128.4 (CH), 128.2 (CH), 127.9 (CH), 122.2 (C_q), 86.1 (C_q), 81.5 (C_q), 50.2 (CH_2), 36.5 (CH_2), 21.5 (CH_3). **(ESI)-MS** calcd for $C_{23}H_{22}NO_2S$ $[M+H]^+$ 376.14 found 376.18.

***N*-Benzyl-4-methyl-*N*-(2-methylpent-3-yn-2-yl)benzenesulfonamide (1v)**



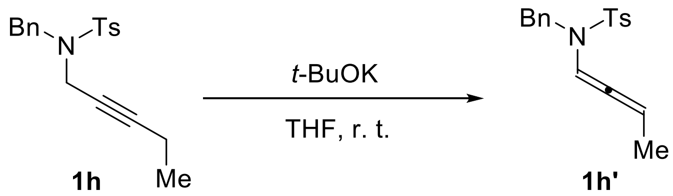
4-Methyl-*N*-(2-methylbut-3-yn-2-yl)benzenesulfonamide (560 mg, 2.3 mmol) and Benzylbromide (600 mg, 3.5 mmol) were stirred in a solution of K_2CO_3 (480 mg, 3.5 mmol) and acetone (10 ml) at 55 °C for 16 hs. The crude was purified by column chromatography (*n*-hexanes/EtOAc 80:20) yielding *N*-Benzyl-4-methyl-*N*-(2-methylbut-3-yn-2-yl)benzenesulfonamide **1v'** (576 mg, 50 %) as a yellow solid. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.69 (d, *J* = 8.3 Hz, 2H), 7.50 (d, *J* = 7.3 Hz, 2H), 7.35 (t, *J* = 7.3 Hz, 2H), 7.28 (dd, *J* = 8.3, 5.9 Hz, 4H), 4.85 (s, 2H), 2.43 (s, 3H), 2.29 (s, 1H), 1.63 (s, 6H). **1v'** (576 mg, 1.75 mmol) was dissolved in dry THF (10 ml) under inert atmosphere and the solution cooled down at -78 °C. Subsequently, *n*-BuLi (1.6 M, 1.64 ml, 2.6 mmol) was added dropwise over 30 min and mixture stirred for additional 30 min at the same temperature. Hence, MeI (369 mg, 2.6 mmol) was added in one pot and the reaction mixture stirred overnight. After completion, a solution of HCl (0.1 M, 10 ml) was added, the mixture extracted with EtOAc (3 x 15 ml), the organic layers separated and dried over Na_2SO_4. The combined fractions were concentrated under reduced pressure and the crude purified by chromatography on silica gel yielding **1v** (485 mg, 72 %) as a yellow solid. **M. p. =** 67.8 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.66 (t, *J* = 7.8 Hz, 2H), 7.49 (d, *J* = 7.6 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.29 – 7.21 (m, 3H), 4.80 (s, 2H), 2.43 (s, 3H), 1.61 (s, 3H), 1.58 (s, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 142.7 (C_q), 139.9 (C_q), 139.5 (C_q), 129.1 (CH), 128.2 (CH), 127.5 (CH), 127.5 (CH), 126.9 (CH), 81.7 (C_q), 80.0 (C_q), 57.4 (C_q), 52.0 (CH_2), 31.2 (CH_3), 21.5 (CH_3), 3.4 (CH_3). **(ESI)-MS** calcd for $C_{20}H_{24}NO_2S$ $[M+H]^+$ 342.15 found 342.28.

_N_-Benzyl-_N_-(hex-3-yn-2-yl)-4-methylbenzenesulfonamide (1w)



Representative procedure **B** was followed using *N*-Benzyl-4-methylbenzenesulfonamide (522 mg, 2.0 mmol) and Hex-3-yn-2-ol (216 mg, 2.2 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **1w** (402 mg, 56%) as a yellowish oil. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.77 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 7.4 Hz, 2H), 7.37 – 7.21 (m, 5H), 4.93 (dtd, *J* = 7.1, 5.3, 2.0 Hz, 1H), 4.64 (d, *J* = 16.0 Hz, 1H), 4.21 (d, *J* = 16.0 Hz, 1H), 2.45 (s, 3H), 1.99 (qd, *J* = 7.5, 2.1 Hz, 2H), 1.13 (d, *J* = 7.1 Hz, 3H), 0.94 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 143.2 (C_q), 138.7 (C_q), 136.4 (C_q), 129.4 (CH), 128.3 (CH), 127.9 (CH), 127.7 (CH), 127.2 (CH), 87.5 (C_q), 76.6 (C_q), 48.3 (CH_2), 47.2 (CH), 23.3(CH_3), 21.5 (CH_3), 13.6 (CH_3), 12.1 (CH_2). **(ESI)-MS** calcd for $C_{20}H_{24}NO_2S$ $[M+H]^+$ 342.15 found 342.18.

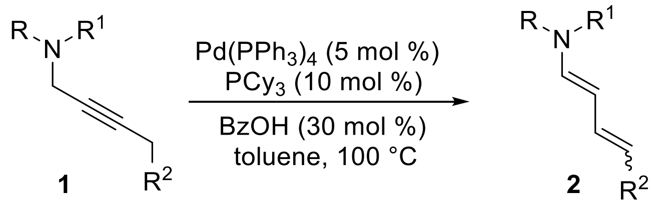
_N_-Benzyl-_N_-(buta-1,2-dien-1-yl)-4-methylbenzenesulfonamide (1h’)



1h’ was synthesized according to known procedure,[4] using **1h** (176 mg, 0.56 mmol) and *t*-BuOK (12.6 mg, 20 mol %) in THF (2.0 ml). After completion (4 hs), the reaction mixture was concentrated in vacuo and the residue purified by flash column chromatography (*n*-hexanes/EtOAc 95:5) to give the corresponding allenamide **1h’** as a whitish solid (68.7 mg, 39%). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.75 (d, *J* = 8.2 Hz, 2H), 7.43-7.15 (m, 7H), 6.74 (dq, *J* = 5.7, 2.8 Hz, 1H), 5.59 – 5.39 (m, 1H), 4.49 (d, *J* = 14.9 Hz, 1H), 4.12 (d, *J* = 14.9 Hz, 1H), 1.35 (dd, *J* = 7.0, 2.7 Hz, 3H).

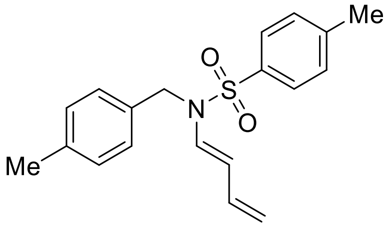
Synthesis of dienes

Representative Catalytic Procedure (C)



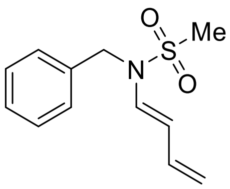
In an oven dried tube, **1** (0.20 mmol), $Pd(PPh_3)_4$ (0.01 mmol), PCy_3 (0.02 mmol) and BzOH (0.06 mmol) were added sequentially and purged with nitrogen three times. Subsequently, toluene (2.0 ml, 0.1 M) was added under N_2 atmosphere and the tube placed in a pre-heated oil bath at 100 °C overnight (16 hs). The reaction mixture was then cooled down at room temperature and CH_2Cl_2 (10 ml) was added. The mixture was concentrated under reduced pressure and the crude purified by chromatography on silica gel.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-4-methyl-*N*-(4-methylbenzyl)benzenesulfonamide (2a)



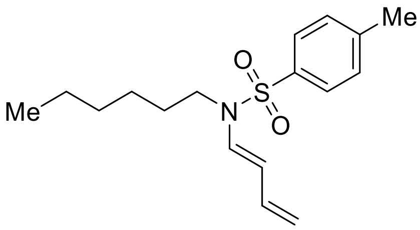
Representative procedure **C** was followed using **1a** (65.4 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2a** (56.8 mg, 87%) as a yellow solid. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.58. **M. p.** = 83.6 °C. ^{1}**H NMR** (400 MHz, $CDCl_3$) δ = 7.70 (t, *J* = 7.9 Hz, 2H), 7.33 (d, *J* = 8.1 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.01 (d, *J* = 14.0 Hz, 1H), 6.24 (dt, *J* = 16.9, 10.3 Hz, 1H), 5.42 (dd, *J* = 14.0, 10.5 Hz, 1H), 4.92 (d, *J* = 16.9 Hz, 1H), 4.87 (d, *J* = 10.5 Hz, 1H), 4.53 (s, 2H), 2.44 (s, 3H), 2.34 (s, 3H). ^{13}**C NMR** (101 MHz, $CDCl_3$) δ = 144.0 (C_q), 137.2 (C_q) , 136.0 (C_q), 134.7 (CH), 132.2 (C_q), 130.0 (CH), 129.9 (CH), 129.3 (CH), 127.0 (CH), 126.8 (CH), 113.8 (CH), 113.0 (CH_2), 49.3 (CH_2), 21.6 (CH_3), 21.1 (CH_3). **(ESI)-MS** calcd for $C_{19}H_{21}NNaO_2S$ $[M+Na]^+$ 350.12 found 350.03.

(*E*)-*N*-Benzyl-*N*-(buta-1,3-dien-1-yl)methanesulfonamide (2b)



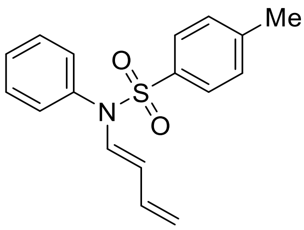
Representative procedure **C** was followed using **1b** (44.6 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2b** (32.6 mg, 73%) as a yellow oil. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.35. ^{1}**H NMR** (400 MHz, $CDCl_3$) δ = 7.52 – 7.13 (m, 5H), 6.88 (d, *J* = 14.0 Hz, 1H), 6.25 (dt, *J* = 16.9, 10.3 Hz, 1H), 5.58 (dd, *J* = 14.0, 10.4 Hz, 1H), 4.99 (t, *J* = 13.8 Hz, 1H), 4.93 (d, *J* = 10.3 Hz, 1H), 4.76 (s, 2H), 2.92 (s, 3H). ^{13}**C NMR** (101 MHz, $CDCl_3$) δ = 135.4 (C_q), 134.4 (CH), 129.5 (CH), 128.8 (CH), 127.8 (CH), 127.0 (CH), 114.3 (CH), 112.8 (CH_2), 49.4 (CH_2), 39.8 (CH_3). **(ESI)-MS** calcd for $C_{14}H_{19}N_2O_2S$ $[M+CH_3CN+H]^+$ 279.12 found 279.37.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-*N*-hexyl-4-methylbenzenesulfonamide (2c)



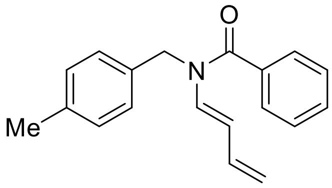
Representative procedure **C** was followed using **1c** (76.8 mg, 0.25 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2c** (58.8 mg, 78%) as a yellow oil. **R_f** *n*-hexanes/EtOAc 8:2 = 0.58. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.67 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 2H), 6.94 (d, *J* = 14.1 Hz, 1H), 6.33 (dt, *J* = 16.9, 10.3 Hz, 1H), 5.48 (dd, *J* = 14.1, 10.5 Hz, 1H), 5.06 (d, *J* = 17.1 Hz, 1H), 4.95 (d, *J* = 10.3 Hz, 1H), 3.36 – 3.25 (m, 2H), 2.44 (s, 3H), 1.59 (dd, *J* = 14.0, 6.6 Hz, 2H), 1.34 – 1.26 (m, 6H), 0.99 – 0.80 (m, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 143.8 (C_q), 136.2 (C_q), 135.0 (CH), 130.0 (CH), 129.8 (CH), 126.9 (CH), 113.4 (CH), 111.5 (CH_2), 45.7 (CH_2), 31.3 (CH_2), 27.0 (CH_2), 26.4 (CH_2), 22.5 (CH_2), 21.5 (CH_3), 14.0 (CH_3). **(ESI)-MS** calcd for $C_{17}H_{26}NO_2S$ $[M+H]^+$ 308.17 found 308.25.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide (2d)



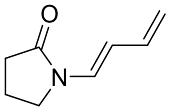
Representative procedure **C** was followed using **1d** (59.2 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2d** (20.4 mg, 34%) as a yellow solid. **R_f** *n*-hexanes/EtOAc 8:2 = 0.62. **M. p.** = 97.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.57 (d, *J* = 7.6 Hz, 2H), 7.43 – 7.37 (m, 3H), 7.32-7.26 (m, 3H), 7.01-6.99 (m, 2H), 6.32 (dt, *J* = 16.8, 10.5 Hz, 1H), 5.03 (dd, *J* = 13.5, 11.1 Hz, 1H), 4.86 (dd, *J* = 13.5, 6.8 Hz, 2H), 2.46 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 144.1 (C_q), 136.1 (C_q), 135.6 (C_q), 134.4 (CH), 132.5 (CH), 130.2 (CH), 129.7 (CH), 129.5 (CH), 129.2 (CH), 127.5 (CH), 113.8 (CH), 112.8 (CH_2), 21.6 (CH_3). **(ESI)-MS** calcd for $C_{17}H_{18}NO_2S$ $[M+H]^+$ 300.11 found 300.20.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-*N*-(4-methylbenzyl)benzamide (2e)



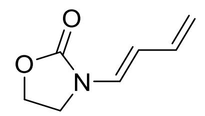
Representative procedure **C** was followed using **1e** (55.4 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2e** (43.4 mg, 78%) as an orange viscous oil. **R_f** *n*-hexanes/EtOAc 8:2 = 0.51. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.61-7.43 (m, 5H), 7.26-7.14 (m, 4H), 6.80 (bs, 1H), 6.09 (bs, 1H), 5.73 (dd, *J* = 13.5, 10.9 Hz, 1H), 5.03 (d, *J* = 16.8 Hz, 2H), 4.92 (d, *J* = 10.0 Hz, 2H), 2.37 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 170.7 (C_q), 136.9 (CH), 136.1 (C_q), 134.9 (C_q), 133.6 (C_q), 130.6 (CH), 129.5 (CH), 128.6 (CH), 128.1 (CH), 128.0 (CH), 126.7 (CH), 114.6 (CH), 112.9 (CH_2), 47.7 (CH_2), 21.1 (CH_3). **(ESI)-MS** calcd for $C_{19}H_{20}NO$ $[M+H]^+$ 278.15 found 278.06.

(*E*)-1-(Buta-1,3-dien-1-yl)pyrrolidin-2-one (2f)



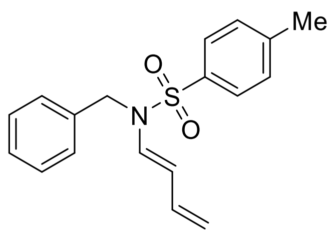
Representative procedure **C** was followed using **1f** (54.8 mg, 0.40 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 70:30) yielded **2f** (33.4 mg, 61%) as a yellow solid. **R_f** *n*-hexanes/EtOAc 8:2 = 0.16. **M. p.** = 59.8 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.11 (d, *J* = 14.1 Hz, 1H), 6.35 (dt, *J* = 17.0, 10.4 Hz, 1H), 5.63 (dd, *J* = 14.2, 10.7 Hz, 1H), 5.14 (dd, *J* = 17.0, 1.8 Hz, 1H), 4.99 (dd, *J* = 10.2, 1.6 Hz, 1H), 3.64 – 3.48 (m, 2H), 2.61 – 2.41 (m, 2H), 2.23 – 2.03 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 172.96 (C_q), 134.9 (CH), 126.7 (CH), 114.7 (CH), 112.9 (CH_2), 45.1 (CH_2), 31.2 (CH_2), 17.4 (CH_2). **(ESI)-MS** calcd for $C_8H_{12}NO$ $[M+H]^+$ 138.09 found 138.18.

(*E*)-3-(Buta-1,3-dien-1-yl)oxazolidin-2-one (2g)



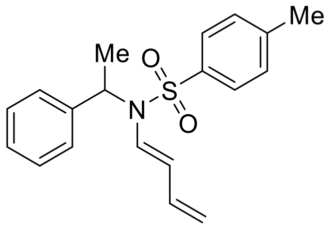
Representative procedure **C** was followed using **1g** (27.8 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **2g** (22.8 mg, 82%) as a yellow oil. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.15. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 6.87 (d, *J* = 14.1 Hz, 1H), 6.31 (dt, *J* = 17.0, 10.4 Hz, 1H), 5.51 (dd, *J* = 14.0, 10.6 Hz, 1H), 5.11 (d, *J* = 16.9 Hz, 1H), 4.97 (d, *J* = 10.2 Hz, 1H), 4.54 – 4.30 (m, 2H), 3.83 – 3.59 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 155.4 (C_q), 134.3 (CH), 127.0 (CH), 114.8 (CH), 112.3 (CH_2), 62.4 (CH_2), 42.6 (CH_2). **(ESI)-MS** calcd for $C_7H_9NNaO_2$ $[M+Na]^+$ 162.05 found 162.18.

(*E*)-*N*-Benzyl-*N*-(buta-1,3-dien-1-yl)-4-methylbenzenesulfonamide (2h)



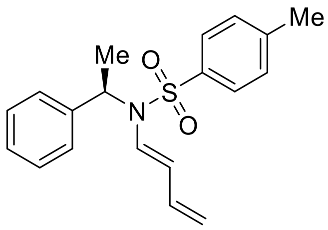
Representative procedure **C** was followed using **1h** (939 mg, 3.0 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2h** (710 mg, 76%) as a tan orange solid. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.52. **M. p.** = 83.0 °C. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ = 7.79 – 7.54 (m, 2H), 7.45 – 7.23 (m, 7H), 7.05 (d, *J* = 14.1 Hz, 1H), 6.28 (dt, *J* = 16.9, 10.4, 1H), 5.43 (dd, *J* = 14.0, 10.5 Hz, 1H), 4.94 (d, *J* = 16.9 Hz, 1H), 4.89 (d, *J* = 10.4 Hz, 1H), 4.60 (s, 2H), 2.49 (s, 3H). **^{13}C NMR** (101 MHz, CD_2Cl_2) δ = 144.4 (C_q), 135.8 (C_q), 135.6 (C_q), 134.6 (CH), 130.0 (CH), 129.9 (CH), 128.6 (CH), 127.5 (CH), 126.9 (CH), 126.8 (CH), 113.6 (CH), 112.9 (CH_2), 49.3 (CH_2), 21.3 (CH_3). **(ESI)-MS** calcd for $C_{18}H_{20}NO_2S$ $[M+H]^+$ 314.12 found 314.27.

(*E*)-*N*-(buta-1,3-dien-1-yl)-4-methyl-*N*-(1-phenylethyl)benzenesulfonamide (2i)



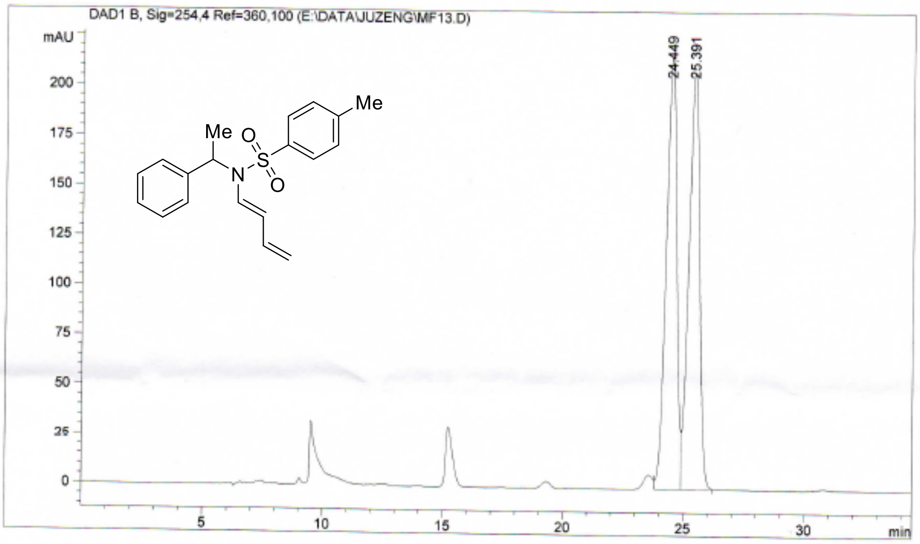
Representative procedure **C** was followed using **1i** (65.5 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 90:10) yielded **2i** (44.0 mg, 67%) as a yellow viscous oil. **R_f** *n*-hexanes/EtOAc 8:2 = 0.58. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.73 (d, *J* = 7.8 Hz, 2H), 7.39 – 7.16 (m, 7H), 6.52 (d, *J* = 14.3 Hz, 1H), 6.14 (dt, *J* = 16.9, 10.3 Hz, 1H), 5.53 (dt, *J* = 14.0, 9.1 Hz, 2H), 4.98 – 4.75 (m, 2H), 2.47 (d, *J* = 7.8 Hz, 3H), 1.51 (t, *J* = 6.1 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 143.9 (C_q), 139.2 (C_q), 137.0 (C_q), 135.1 (CH), 129.8 (CH), 128.5 (CH), 127.4 (CH), 127.2 (CH), 126.8 (CH), 126.7 (CH), 117.5 (CH), 114.1 (CH_2), 55.6 (CH), 21.6 (CH_3), 16.1 (CH_3). **(ESI)-MS** calcd for $C_{19}H_{21}NNaO_2S$ $[M+Na]^+$ 350.12 found 350.31.

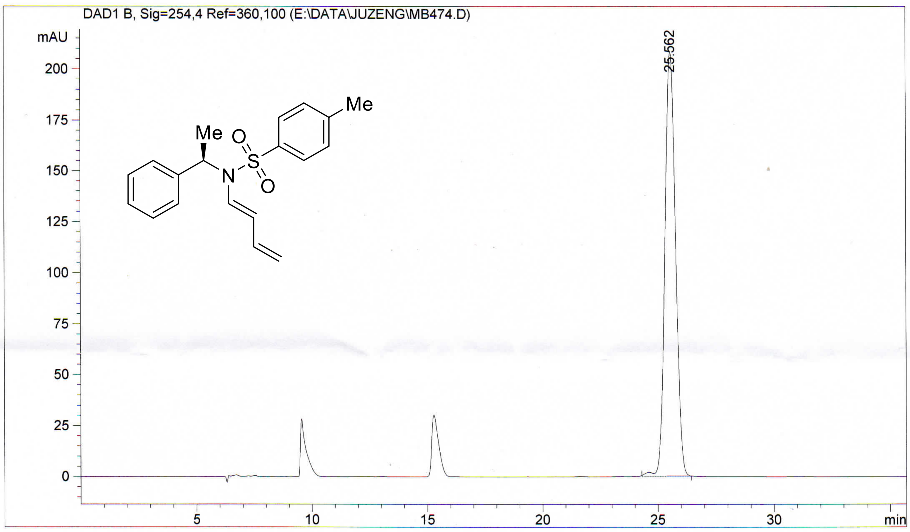
(*R*)-(*E*)-*N*-(buta-1,3-dien-1-yl)-4-methyl-*N*-(1-phenylethyl)benzenesulfonamide (2i)

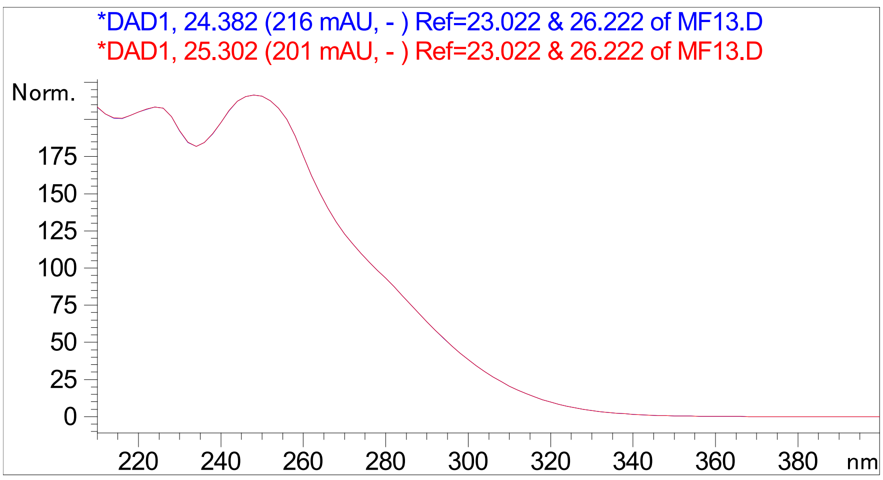


Representative procedure **C** was followed using **(*R*)-1i** (65.5 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 9:1) yielded **(*R*)-2i** (48.2 mg, 74%, *ee* > 99%) as a yellow viscous oil.

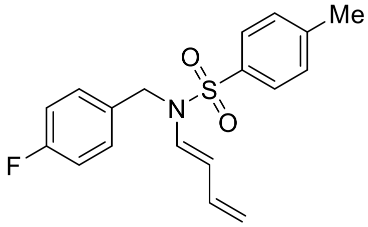
IA-Chiralpack 95:5 *n*-Hexanes:EtOAc 95:5, 30 °C





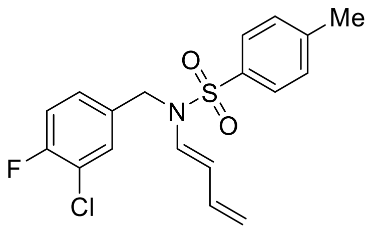


(*E*)-*N*-(Buta-1,3-dien-1-yl)-N-(4-fluorobenzyl)-4-methylbenzenesulfonamide (2j)



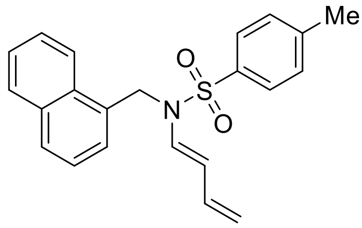
Representative procedure **C** was followed using **1j** (66.3 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2j** (57.1 mg, 86%) as a viscous orange oil. **R$_f$** *n*-hexanes/EtOAc 8:2 = 0.55. **^{1}H NMR** (400 MHz, Acetone-*d$_6$*) δ = 7.79 (t, *J* = 7.9 Hz, 2H), 7.51 – 7.36 (m, 4H), 7.15 – 7.09 (m, 2H), 7.06 (d, *J* = 14.0 Hz, 1H), 6.32 (dt, *J* = 17.0, 10.3 Hz, 1H), 5.54 (dd, *J* = 14.0, 10.5 Hz, 1H), 4.90 (d, *J* = 17.0 Hz, 1H), 4.82 (d, *J* = 10.2 Hz, 1H), 4.65 (s, 2H), 2.46 (s, 3H). **^{13}C NMR** (101 MHz, Acetone-*d$_6$*) δ = 162.1 (d, $^1J_{C\text{-}F}$ = 246 Hz, C$_q$), 144.4 (C$_q$), 136.1 (C$_q$), 134.9 (CH), 132.2 (d, $^4J_{C\text{-}F}$ = 3 Hz, C$_q$), 130.0 (CH), 129.8 (CH), 129.0 (d. $^3J_{C\text{-}F}$ = 8 Hz, CH), 127.0 (CH), 115.2 (d, $^2J_{C\text{-}F}$ = 22 Hz, CH), 113.3 (CH), 113.2 (CH$_2$), 48.3 (CH$_2$), 20.6 (CH$_3$). **^{19}F NMR** (376 MHz, Acetone-*d$_6$*) δ = -116.7. **(ESI)-MS** calcd for $C_{18}H_{19}FNO_2S$ [M+H]$^+$ 332.11 found 332.29.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-*N*-(3-chloro-4-fluorobenzyl)-4-methylbenzenesulfonamide (2k)



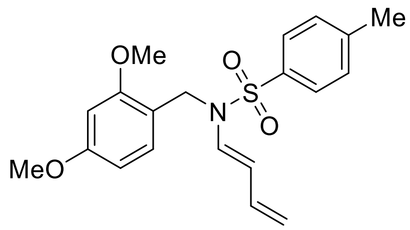
Representative procedure **C** was followed using **1k** (91.2 mg, 0.25 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2k** (59.1 mg, 65%) as a yellow solid. **R$_f$** *n*-hexanes/EtOAc 8:2 = 0.56. **M. p.** = 101.7 °C. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ = 7.71 (d, *J* = 8.3 Hz, 2H), 7.35 – 7.30 (m, 2H), 7.33 – 7.31 (m, 1H), 7.17 – 7.14 (m, 1H), 7.12 – 7.05 (m, 1H), 7.03 (d, *J* = 14.1 Hz, 1H), 6.29 (dt, *J* = 16.9, 10.3 Hz, 1H), 5.43 – 5.33 (m, 1H), 4.97 (d, *J* = 16.9 Hz, 1H), 4.89 (d, *J* = 10.3 Hz, 1H), 4.54 (s, 2H), 2.47 (s, 3H). **^{13}C NMR** (101 MHz, CD_2Cl_2) δ = 157.3 (d, $^1J_{C\text{-}F}$ = 254 Hz, C$_q$), 144.7 (C$_q$), 135.6 (C$_q$), 134.4 (CH), 132.8 (CH), 130.0 (CH), 129.5 (d, $^4J_{C\text{-}F}$ = 6 Hz, CH), 128.9 (CH), 126.8 (CH), 126.7 (d, $^5J_{C\text{-}F}$ = 5 Hz, C$_q$), 121.1 (d, $^3J_{C\text{-}F}$ = 18 Hz, C$_q$), 116.6 (d, $^2J_{C\text{-}F}$ = 21 Hz, CH), 114.1 (CH), 113.0 (CH$_2$), 48.2 (CH$_2$), 21.3 (CH$_3$). **^{19}F NMR** (376 MHz, CD_2Cl_2) δ = -118.0. **(ESI)-MS** calcd for $C_{18}H_{18}ClFNO_2S$ [M+H]$^+$ 366.07 found 366.21.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-4-methyl-N-(naphthalen-1-ylmethyl)benzenesulfonamide (2l)



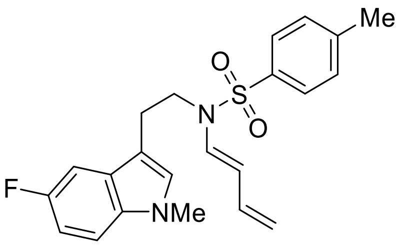
Representative procedure **C** was followed using **1l** (90.8 mg, 0.25 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2l** (68.6 mg, 76%) as a pale orange solid. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.60. **M. p.** = 127.9 °C. ^{1}**H NMR** (400 MHz, $CDCl_3$) δ = 7.96 – 7.87 (m, 2H), 7.81 – 7.72 (m, 2H), 7.59 – 7.50 (m, 2H), 7.44 – 7.32 (m, 5H), 7.14 (d, *J* = 14.0 Hz, 1H), 6.26 (dt, *J* = 16.8, 10.4 Hz, 1H), 5.31 (dd, *J* = 14.7, 9.8 Hz, 1H), 5.12 (s, 2H), 4.88 – 4.73 (m, 2H), 2.48 (s, 3H). ^{13}**C NMR** (101 MHz, $CDCl_3$) δ = 144.2 (C_q), 135.9 (C_q), 134.5 (CH), 133.7 (C_q), 130.3 (C_q), 130.0 (CH), 129.5 (CH), 129.1 (CH), 128.4 (C_q), 127.9 (CH), 127.1 (CH), 126.3 (CH), 125.7 (CH), 125.6 (CH), 124.1 (CH), 122.1 (CH) , 114.1 (CH), 113.2 (CH_2), 47.5 (CH_2), 21.6 (CH_3). **(ESI)-MS** calcd for $C_{22}H_{21}KNO_2S$ $[M+K]^+$ 402.09 found 402.06.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-*N*-(2,4-dimethoxybenzyl)-4-methylbenzenesulfonamide (2m)



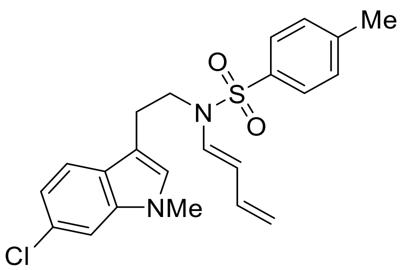
Representative procedure **C** was followed using **1m** (74.6 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2m** (60.6 mg, 81%) as a yellowish solid. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.42. **M. p.** = 93.7 °C. ^{1}**H NMR** (400 MHz, CD_2Cl_2) δ = 7.73 (d, *J* = 8.2 Hz, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.20 (dd, *J* = 13.8, 8.8 Hz, 1H), 7.03 (d, *J* = 14.0 Hz, 1H), 6.50 (dd, *J* = 5.3, 2.2 Hz, 2H), 6.30 (dt, *J* = 17.0, 10.4 Hz, 1H), 5.48 – 5.37 (m, 1H), 4.93 (d, *J* = 16.9 Hz, 1H), 4.88 (d, *J* = 10.3 Hz, 1H), 4.51 (s, 2H), 3.85 (s, 3H), 3.82 (s, 3H), 2.47 (s, 3H). ^{13}**C NMR** (101 MHz, CD_2Cl_2) δ = 160.4 (C_q), 157.5 (C_q), 144.2 (C_q), 136.0 (C_q), 134.9 (CH), 130.0 (CH), 129.9 (CH), 128.3 (CH), 126.8 (CH), 115.4 (C_q), 113.3 (CH), 112.4 (CH_2), 104.4 (CH), 98.1 (CH), 55.3 (CH_3), 55.3 (CH_3), 43.6 (CH_2), 21.3 (CH_3). **(ESI)-MS** calcd for $C_{20}H_{23}KNO_4S$ $[M+K]^+$ 412.10 found 412.22.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-*N*-[2-(5-fluoro-1-methyl-1*H*-indol-3-yl)ethyl]-4-methylbenzenesulfonamide (2n)



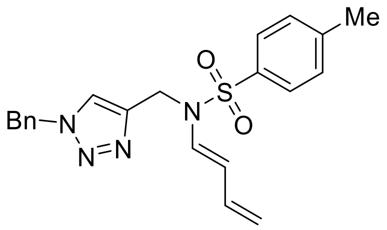
Representative procedure **C** was followed using **1n** (79.6 mg, 0.20 mmol) and PPh_3 (0.02 mmol, 5.2 mg). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **2n** (45.3 mg, 57%) as a yellowish oil. **R_f** *n*-hexanes/EtOAc 8:2 = 0.35. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ = 7.73 – 7.67 (m, 2H), 7.35 (d, *J* = 7.5 Hz, 2H), 7.29 – 7.23 (m, 2H), 7.03 (s, 1H), 7.02 – 6.95 (m, 2H), 6.48 – 6.32 (m, 1H), 5.70 – 5.58 (m, 1H), 5.15 – 5.06 (m, 1H), 5.02 – 4.94 (m, 1H), 3.76 (d, *J* = 3.5 Hz, 3H), 3.66 – 3.56 (m, 2H), 3.05 – 2.97 (m, 2H), 2.44 (s, 3H). **^{13}C NMR** (101 MHz, CD_2Cl_2) δ = 157.6 (d, $^1J_{C\text{-}F}$ = 234 Hz, C_q), 141.2 (C_q), 136.1 (C_q), 134.8 (CH), 133.7 (C_q), 129.9 (CH), 129.7 (CH), 128.7 (CH), 127.9 (d, $^5J_{C\text{-}F}$ = 9Hz, C_q), 126.8 (CH), 113.3 (CH), 111.7 (CH_2), 110.6 (d, $^6J_{C\text{-}F}$ = 5 Hz, C_q), 110.1 (d, $^4J_{C\text{-}F}$ = 10 Hz, CH), 109.7 (d, $^2J_{C\text{-}F}$ = 27 Hz, CH), 103.4 (d, $^3J_{C\text{-}F}$ = 24 Hz, CH), 46.2 (CH_2), 32.8 (CH_3), 23.4 (CH_2), 21.2 (CH_3). **^{19}F NMR** (376 MHz, CD_2Cl_2) δ = -126.1. **(ESI)-MS** calcd for $C_{22}H_{23}KFN_2O_2S$ $[M+K]^+$ 437.11 found 437.19.

(*E*)-*N*-(Buta-1,3-dien-1-yl)-*N*-[2-(6-chloro-1-methyl-1*H*-indol-3-yl)ethyl]-4-methylbenzenesulfonamide (2o)



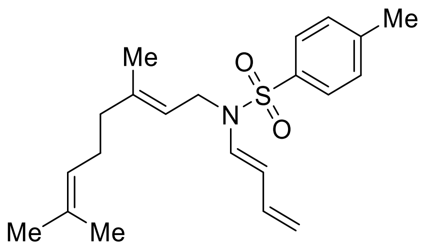
Representative **C** procedure was followed using **1o** (41.4 mg, 0.10 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **2o** (25.2 mg, 61%) as a sticky orange oil. **R_f** *n*-hexanes/EtOAc 8:2 = 0.36. **^{1}H NMR** (300 MHz, CD_2Cl_2) δ = 7.69 – 7.62 (m, 2H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.33-7.26 (m, 3H), 7.09 (dd, *J* = 8.5, 1.8 Hz, 1H), 6.98 (d, *J* = 14.0 Hz, 1H), 6.92 (s, 1H), 6.37 (dd, *J* = 16.8, 10.4 Hz, 1H), 5.77 – 5.47 (m, 1H), 5.06 (d, *J* = 16.8 Hz, 1H), 4.96 (d, *J* = 10.2 Hz, 1H), 3.71 (s, 3H), 3.59 (dt, *J* = 13.2, 6.8 Hz, 2H), 3.03 (dd, *J* = 9.2, 6.6 Hz, 2H), 2.46 – 2.35 (m, 3H). **^{13}C NMR** (75 MHz, CD_2Cl_2) δ = 144.2 (C_q), 137.4 (C_q), 136.1 (C_q), 134.8 (CH), 129.8 (CH), 129.7 (CH), 127.8 (C_q), 127.5 (CH), 126.7 (CH), 126.3 (C_q), 119.6 (CH), 119.4 (CH), 113.3 (CH), 111.6 (C_q), 111.0 (CH_2), 109.3 (CH), 46.3(CH_2), 32.6 (CH_3), 23.3 (CH_2), 21.2 (CH_3). **(ESI)-MS** calcd for $C_{22}H_{24}ClN_2O_2S$ $[M+H]^+$ 415.13 found 415.28.

(*E*)-*N*-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-*N*-(buta-1,3-dien-1-yl)-4-methylbenzenesulfonamide (2p)



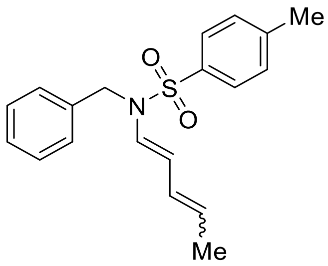
Representative **C** procedure was followed using **1p** (78.8 mg, 0.20 mmol) and PPh_3 (0.02 mmol). Purification by column cchromatography on silica gel (*n*-hexanes/EtOAc 80:20) yielded **2p** (40.5 mg, 51%) as a white solid. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.15. **M. p. =** 125.8 °C. **^{1}H NMR** (300 MHz, $CDCl_3$) δ = 7.65 (d, *J* = 7.8 Hz, 2H), 7.38 – 7.21 (m, 8H), 6.89 (d, *J* = 13.9 Hz, 1H), 6.20 (dd, *J* = 17.3, 10.1 Hz, 1H), 5.68 (dd, *J* = 14.1, 10.5 Hz, 1H), 5.46 (s, 2H), 4.98 (d, *J* = 17.2 Hz, 1H), 4.88 (d, *J* = 10.5 Hz, 1H), 4.65 (s, 2H), 2.40 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ = 144.2 (C_q), 143.7 (C_q), 135.5 (C_q), 134.4 (C_q), 134.3 (CH), 129.9 (CH), 129.0 (CH), 128.9 (CH), 128.7 (CH), 127.9 (CH), 126.8 (CH), 122.7 (CH), 114.5 (CH), 112.8 (CH_2), 54.1 (CH_2), 41.6 (CH_2), 21.5 (CH_3). (**ESI)-MS** calcd for $C_{21}H_{23}N_4O_2S$ $[M+H]^+$ 395.15 found 395.33.

***N*-[(*E*)-buta-1,3-dien-1-yl]-*N*-[(*E*)-3,7-dimethylocta-2,6-dien-1-yl]-4-methylbenzenesulfonamide (2q)**



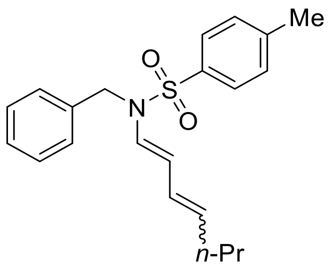
Representative **C** procedure was followed using **1q** (71.8 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 98:2) yielded **2q** (43.4 mg, 60%) as a yellow oil. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.71. **^{1}H NMR** (400 MHz, CD_2Cl_2) δ = 7.67 (t, *J* = 6.2 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 6.96 (dd, *J* = 14.0, 4.7 Hz, 1H), 6.34 (dt, *J* = 16.9, 10.4 Hz, 1H), 5.49 (dd, *J* = 14.0, 10.5 Hz, 1H), 5.09 – 4.99 (m, 2H), 4.93 (dd, *J* = 11.3, 5.2 Hz, 2H), 4.08 (t, *J* = 7.5 Hz, 2H), 2.45 (s, 3H), 1.95 (tt, *J* = 26.7, 13.5 Hz, 4H), 1.74 – 1.63 (m, 6H), 1.61 – 1.53 (m, 3H). **^{13}C NMR** (101 MHz, CD_2Cl_2) δ = 144.1 (C_q), 139.2 (C_q), 136.5 (C_q), 135.0 (CH), 131.6 (C_q), 130.0 (CH), 129.7 (CH), 126.9 (CH), 123.7 (CH), 118.2 (CH), 113.1 (CH), 112.0 (CH_2), 44.1 (CH_2), 39.2 (CH_2), 26.1 (CH_2), 25.3 (CH_3), 21.2 (CH_3), 17.3 (CH_3), 16.1 (CH_3). **(ESI)-MS** calcd for $C_{21}H_{29}KNO_2S$ $[M+K]^+$ 398.16 found 398.26.

***N*-Benzyl-4-methyl-*N*-[(*1E,3E*)-penta-1,3-dien-1-yl]benzenesulfonamide (2r)**



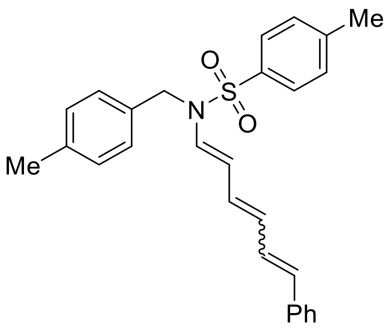
Representative procedure **C** was followed using **1r** (65.4 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2r** (41.3 mg, 63% as a mixture *E*,*E* :*E*,*Z* = 3.2:1) as a yellow oil. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.64. ^{1}**H NMR** (400 MHz, $CDCl_3$, major isomer) δ = 7.77 – 7.67 (m, 2H), 7.39 – 7.22 (m, 7H), 6.86 (d, *J* = 14.0 Hz, 1H), 6.01 – 5.83 (m, 1H), 5.47 – 5.32 (m, 2H), 4.52 (s, 2H), 2.46 (s, 3H), 1.69 (dd, *J* = 6.8, 1.3 Hz, 3H). ^{13}**C NMR** (101 MHz, $CDCl_3$, major isomer) δ = 143.9 (C_q), 136.0 (C_q), 135.6 (C_q), 129.9 (CH), 128.8 (CH), 128.6 (CH), 127.4 (CH), 127.1 (CH), 127.0 (CH), 126.8 (CH), 126.4 (CH), 113.4 (CH), 49.51 (CH_2), 21.6 (CH_3), 18.1 (CH_3). **(ESI)-MS** calcd for $C_{19}H_{21}KNO_2S$ $[M+K]^+$ 366.09 found 366.52.

***N*-Benzyl-*N*-[(*1E,3E*)-hepta-1,3-dien-1-yl]-4-methylbenzenesulfonamide (2s)**



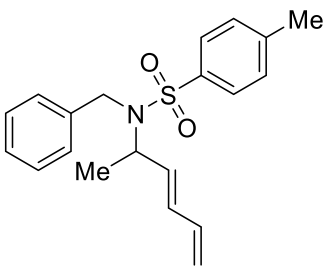
Representative procedure **C** was followed using **1s** (88.8 mg, 0.25 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2s** (48.0 mg, 54% as a mixture *E*,*E* :*E*,*Z* = 4.0:1) as a yellow oil. $\mathbf{R_f}$ *n*-hexanes/EtOAc 8:2 = 0.55. ^{1}**H NMR** (400 MHz, CD_2Cl_2, major isomer) δ = 7.74 – 7.70 (m, 2H), 7.41 – 7.29 (m, 7H), 6.87 (d, *J* = 14.0 Hz, 1H), 6.03 – 5.89 (m, 1H), 5.47 – 5.38 (m, 2H), 4.56 (s, 2H), 2.48 (s, 3H), 2.08 – 1.91 (m, 2H), 1.41 – 1.22 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H). ^{13}**C NMR** (101 MHz, CD_2Cl_2, major isomer) δ = 144.2 (C_q), 136.9 (C_q), 136.8 (C_q), 131.9 (CH), 129.9 (CH), 128.6 (CH), 127.5 (CH), 127.4 (CH), 127.2 (CH), 126.8 (CH), 113.3 (CH), 49.4 (CH_2), 34.7 (CH_2), 29.6 (CH_2), 22.6 (CH_2), 21.3 (CH_3), 13.4 (CH_3). **(ESI)-MS** calcd for $C_{21}H_{26}NO_2S$ $[M+H]^+$ 356.17 found 356.36.

4-Methyl-*N*-(4-methylbenzyl)-*N*-[(*1E,3E,5E*)-6-phenylhexa-1,3,5-trien-1-yl]benzenesulfonamide (2t)



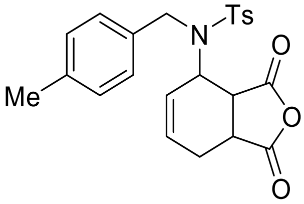
Representative procedure **C** was followed using **1t** (85.8 mg, 0.20 mmol). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 95:5) yielded **2t** (56.8 mg, 66% as a mixture *E*,*E,E* : *E*,*Z,E* = 6.6:1) as an orange viscous oil. **R$_f$** *n*-hexanes/EtOAc 8:2 = 0.48. **^{1}H NMR** (400 MHz, CD_2Cl_2, major isomer) δ = 7.79 – 7.70 (m, 2H), 7.42 – 7.37 (m, 4H), 7.35-7.30 (m, 3H), 7.25-7.17 (m, 4H), 7.08 (d, *J* = 14.8 Hz, 1H), 6.82 (dd, *J* = 15.5, 10.6 Hz, 1H), 6.45 (d, *J* = 15.5 Hz, 1H), 6.32 (dd, *J* = 14.8, 10.6 Hz, 1H), 6.16 (dd, *J* = 14.8, 10.6 Hz, 1H), 5.52 (dt, *J* = 18.4, 9.2 Hz, 1H), 4.56 (d, *J* = 7.2 Hz, 2H), 2.47 (s, 3H), 2.35 (s, 3H). **^{13}C NMR** (101 MHz, CD_2Cl_2, major isomer) δ = 144.4 (C_q), 137.6 (C_q), 137.4 (C_q), 135.8 (C_q), 132.4 (C_q), 131.3 (CH), 130.6 (CH), 130.0 (CH), 129.9 (CH), 129.8 (CH), 129.3 (CH), 129.1 (CH), 128.6 (CH), 127.2 (CH), 126.9 (CH), 126.8 (CH), 126.1 (CH), 112.7 (CH), 49.2 (CH_2), 21.3 (CH_3), 20.8 (CH_3). **(ESI)-MS** calcd for $C_{27}H_{27}KNO_2S$ $[M+K]^+$ 468.14 found 468.28.

(*E*)-*N*-Benzyl-*N*-(hexa-3,5-dien-2-yl)-4-methylbenzenesulfonamide (2w)



Representative procedure **C** was followed using **1w** (68.3 mg, 0.20 mmol), $Pd(PPh_3)_4$ (10 mol %) and PCy_3 (20 mol %). Purification by column chromatography on silica gel (*n*-hexanes/EtOAc 98:2) yielded **2w** (37.3 mg, 55%) as a yellow oil. **R$_f$** *n*-hexanes/EtOAc 8:2 = 0.63. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.78 – 7.68 (m, 2H), 7.45 – 7.12 (m, 7H), 6.13 (dt, *J* = 16.9, 10.2 Hz, 1H), 5.89 (dt, *J* = 10.4, 8.4 Hz, 1H), 5.38 (dd, *J* = 15.5, 5.8 Hz, 1H), 5.11 (t, *J* = 11.6 Hz, 1H), 5.06 (d, *J* = 10.1 Hz, 1H), 4.61 (p, *J* = 6.3 Hz, 1H), 4.50 (d, *J* = 15.8 Hz, 1H), 4.23 (d, *J* = 15.9 Hz, 1H), 2.61 – 2.33 (m, 3H), 1.14 (dd, *J* = 11.1, 8.2 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ = 143.1 (C_q), 138.4 (C_q), 138.1 (C_q), 136.0 (CH), 132.8 (CH), 132.8 (CH), 129.6 (CH), 128.3 (CH), 128.0 (CH), 127.3 (CH), 127.2 (CH), 117.9 (CH_2), 54.8 (CH_2), 47.8 (CH), 21.5 (CH_3), 18.8 (CH_3). **(ESI)-MS** calcd for $C_{20}H_{23}NNaO_2S$ $[M+Na]^+$ 364.13 found 364.02.

***N*-(1,3-dioxo-1,3,3*a*,4,7,7*a*-hexahydroisobenzofuran-4-yl)-4-methyl-*N*-(4-methylbenzyl)benzenesulfonamide (4aa)**

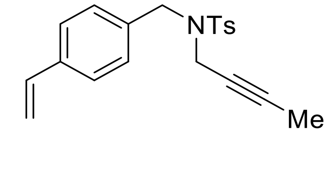
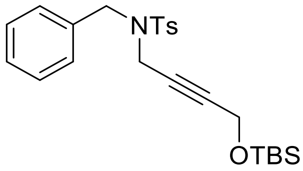
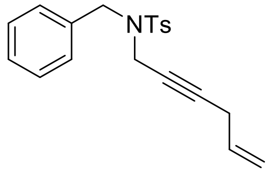
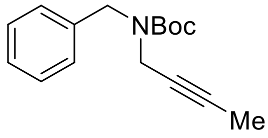
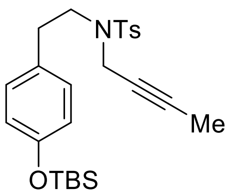
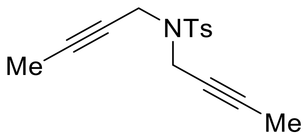
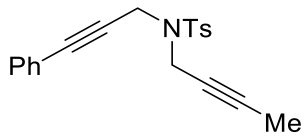
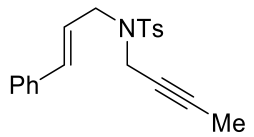
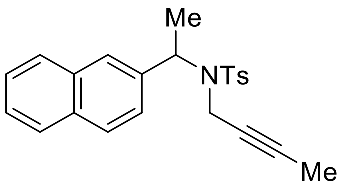
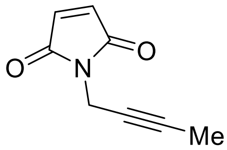
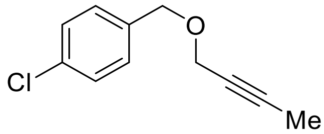
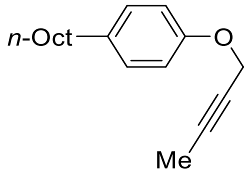
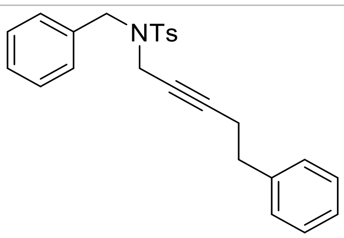


In an oven-dried tube, **2a** (98.1 mg, 0.30 mmol) and maleic anhydride (44.1 mg, 0.45 mmol) were added sequentially and purged with nitrogen three times. Subsequently, toluene (2.0 ml) was added and the tube placed in a pre-heated oil bath at 100 °C. After completion (16 hs), the reaction mixture was cooled down at room temperature and CH_2Cl_2 (10 ml) was added. The mixture was concentrated under reduced pressure and the crude purified by column chromatography on silica gel (*n*-hexanes/EtOAc 9:1 → 6:4) to deliver **4aa** (84.4 mg, 64%) as a yellow solid. **M. p.** = 194.1 °C. **^{1}H NMR** (400 MHz, DMSO-d_6) δ = 7.55 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.12 – 6.99 (m, 4H), 5.87 – 5.67 (m, 1H), 5.19 (d, *J* = 10.2 Hz, 1H), 4.93 (s, 1H), 4.51 (d, *J* = 16.6 Hz, 1H), 4.17 (d, *J* = 16.6 Hz, 1H), 3.39 (dd, *J* = 5.6, 4.0 Hz, 1H), 3.13 – 2.93 (m, 1H), 2.49 – 2.41 (m, 1H), 2.39 (d, *J* = 9.5 Hz, 3H), 2.27 (s, 3H), 2.14 (s, 1H). **^{13}C NMR** (101 MHz, DMSO) δ = 174.2 (C_q), 173.0 (C_q), 143.4 (C_q), 137.8 (C_q), 136.1 (CH), 136.0 (C_q), 130.7 (CH), 129.9 (CH), 128.9 (CH), 127.8 (CH), 127.4 (CH), 124.1 (C_q), 57.8 (CH_2), 49.5 (CH), 44.6 (CH), 41.0 (CH), 24.4 (CH_2), 21.4 (CH_3), 21.1 (CH_3). **(ESI)-MS** calcd for $C_{48}H_{53}N_4O_{10}S_2$ $[2M+NH_4+CH_3CN]^+$ 909.32 found 909.61.

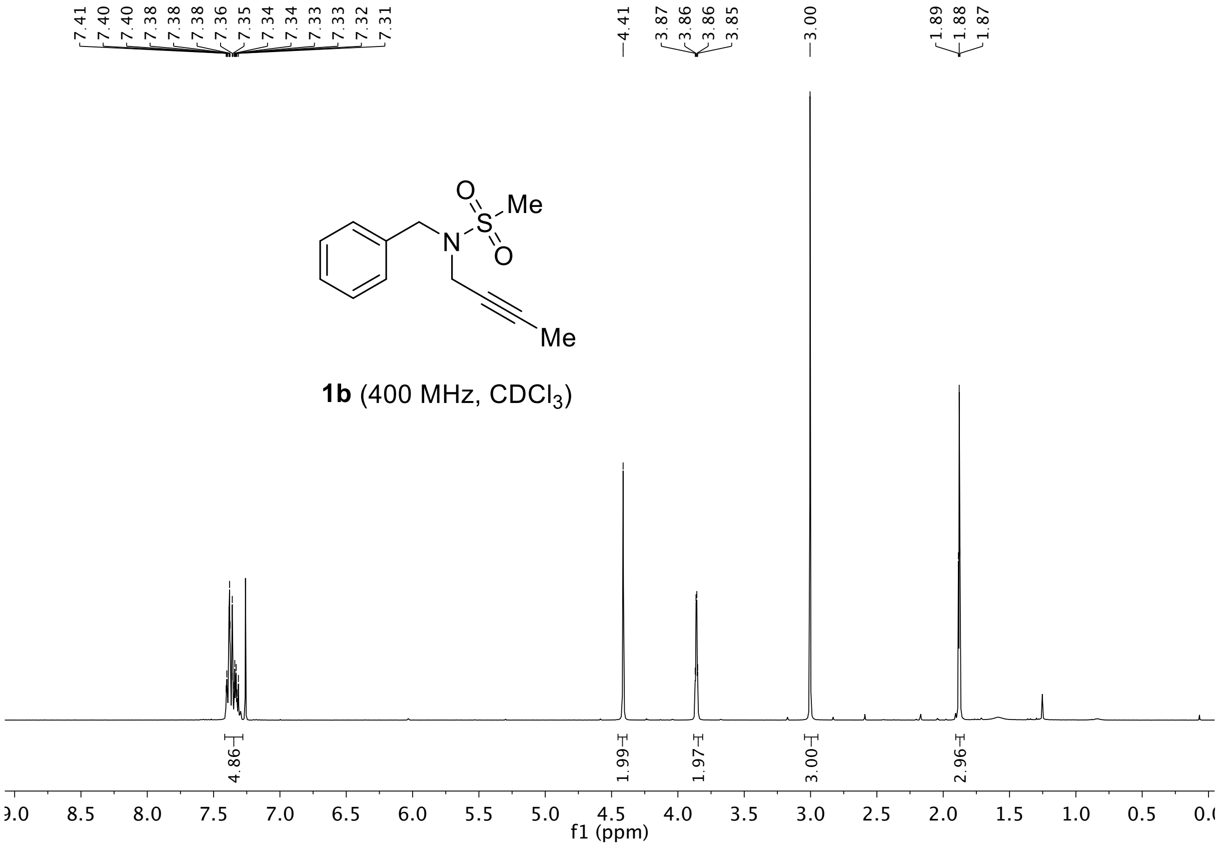
One pot procedure: In an oven dried tube, **1a** (98.1 mg, 0.30 mmol), $Pd(PPh_3)_4$ (0.015 mmol), PPh_3 (0.03 mmol) and BzOH (0.09 mmol) were added sequentially and purged with nitrogen three times. Subsequently, toluene (2.0 ml, 0.1 M) was added under N_2 atmosphere and the tube placed in a pre-heated oil bath at 100 °C. After 16 hs, maleic anhydride (44.1 mg, 0.45 mmol) was added and the reaction mixture further stirred for 24 hs. After completion, the tube was cooled down at room temperature and CH_2Cl_2 (10 ml) was added. The mixture was concentrated under reduced pressure and the crude purified by chromatography on silica gel (*n*-hexanes/EtOAc 9:1 → 6:4) to deliver **4aa** (75.2 mg, 57%) as a yellow solid.

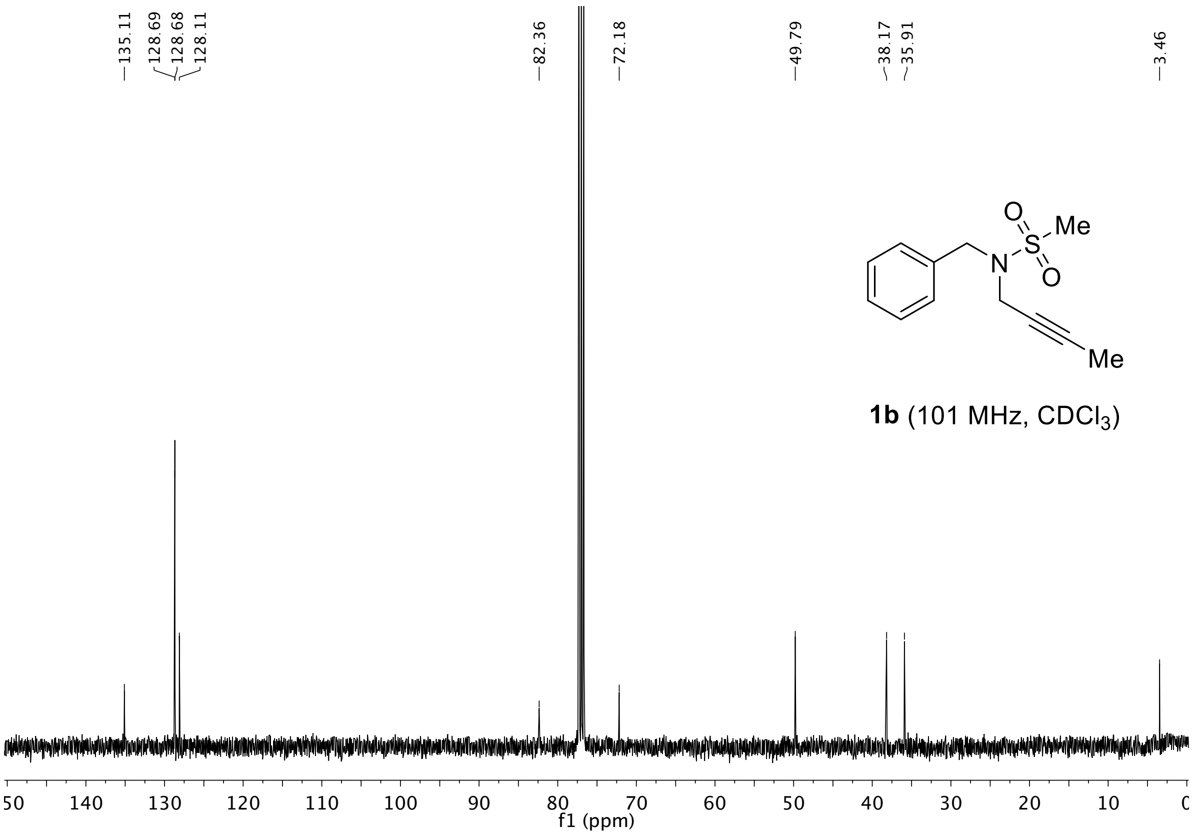
Scope limitations

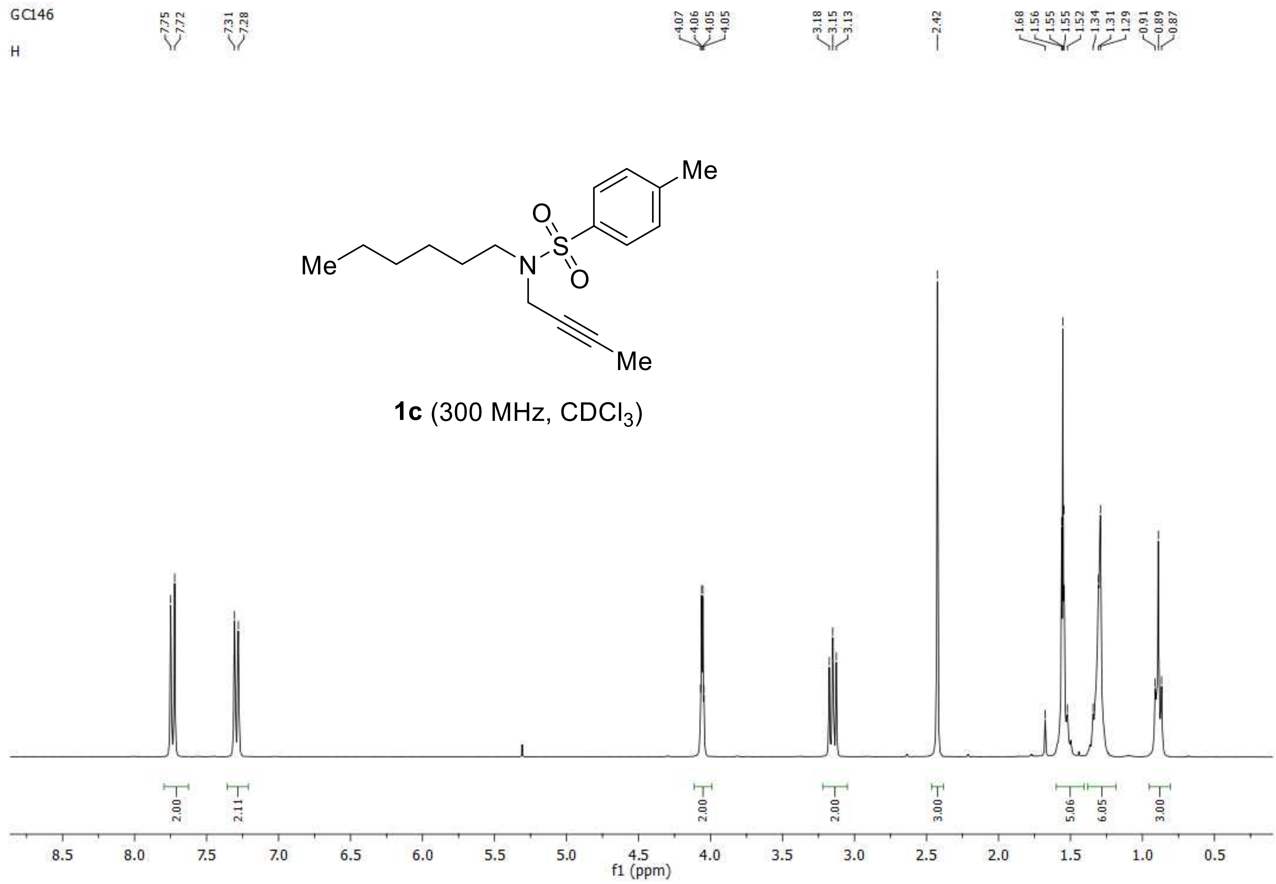
Figure S3. Unsuccessful Substrates

			
			
 28% conv by ^{1}H-NMR			
 54% conv by ^{1}H-NMR, mixture of products			

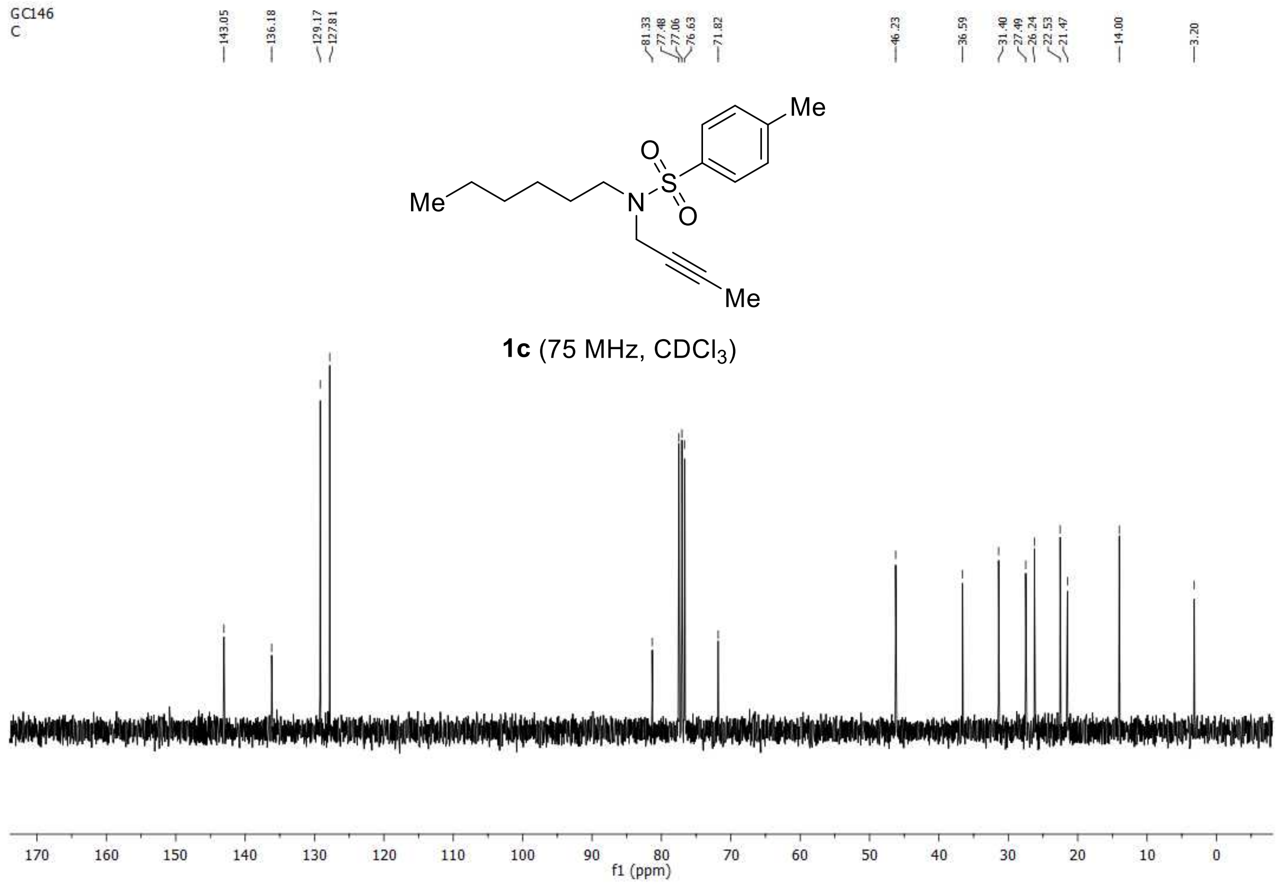
Copies of NMR spectra



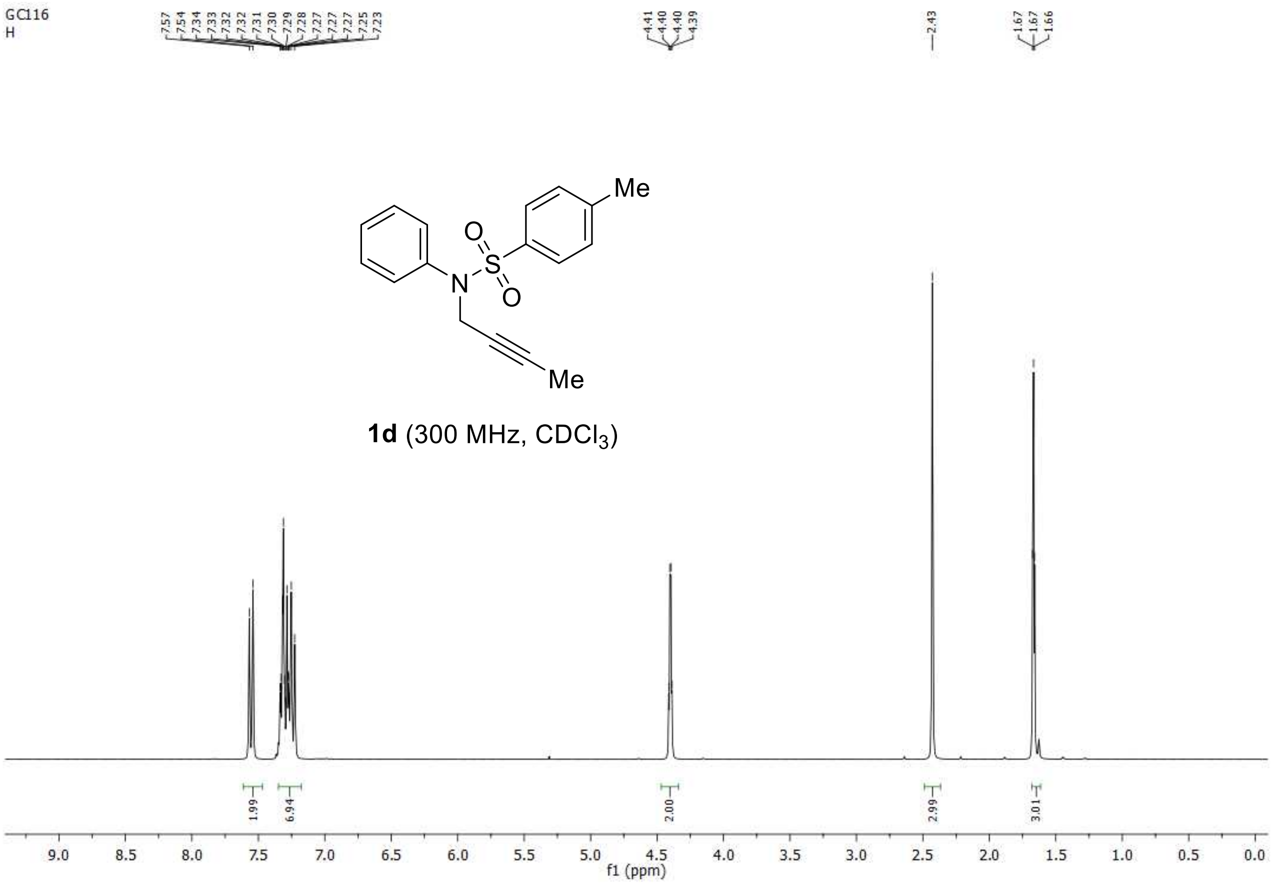


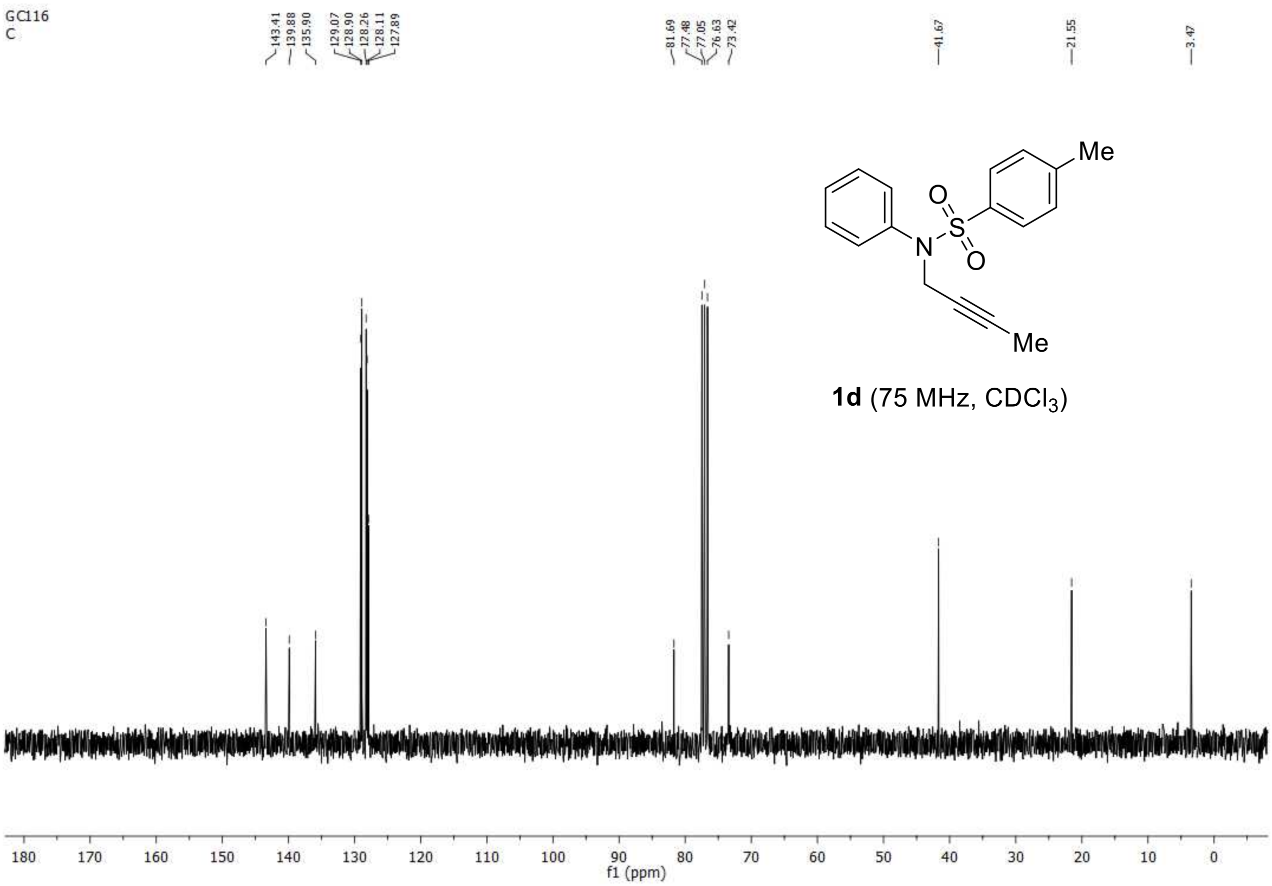


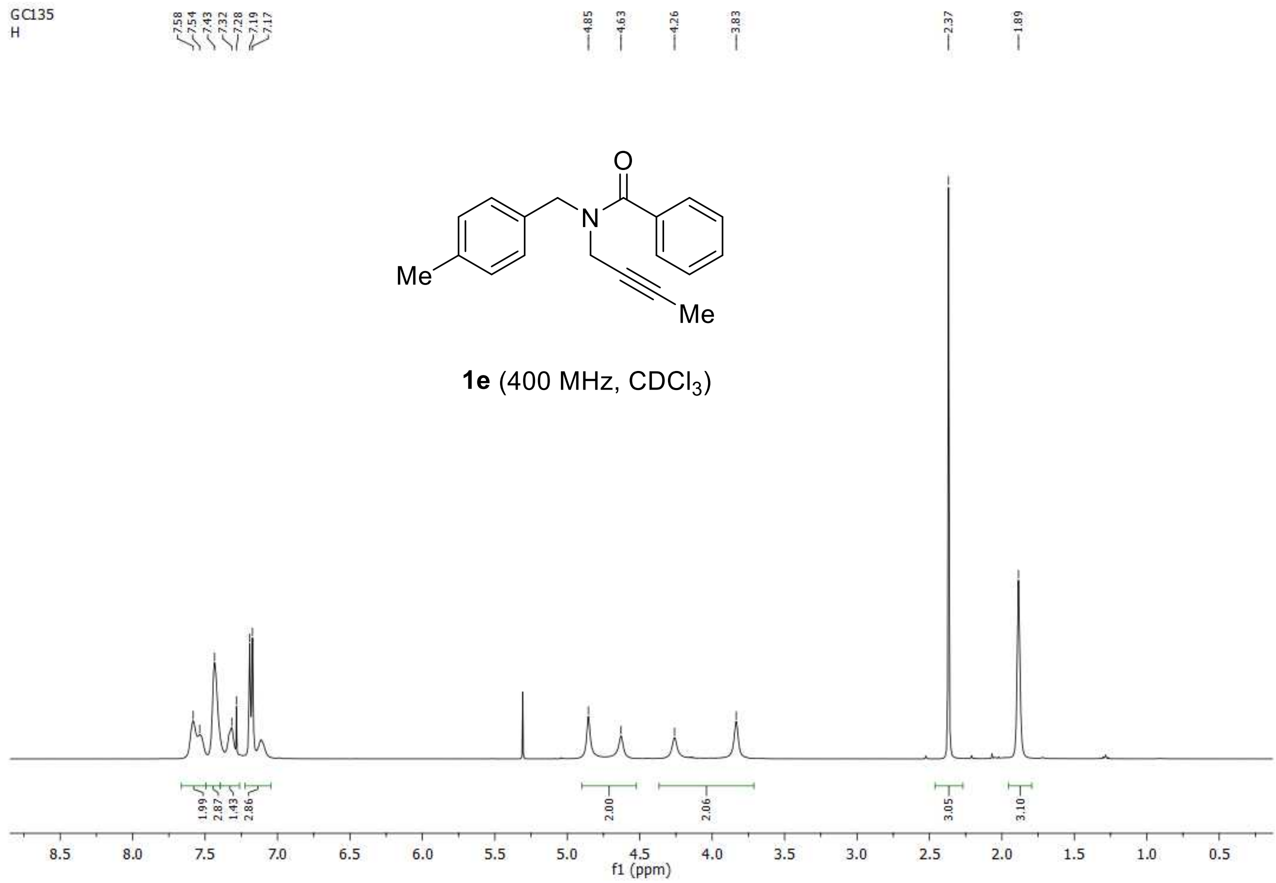
1c (300 MHz, $CDCl_3$)

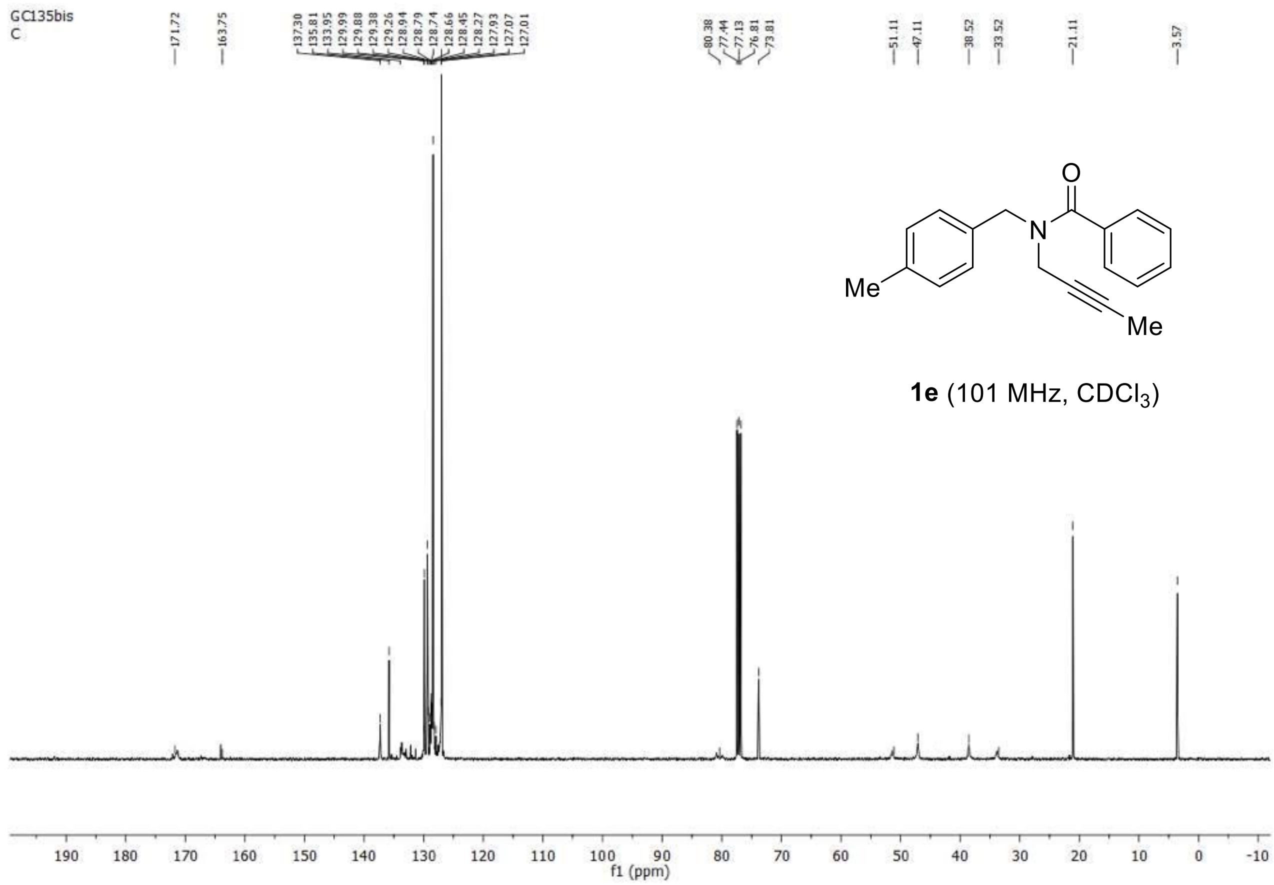


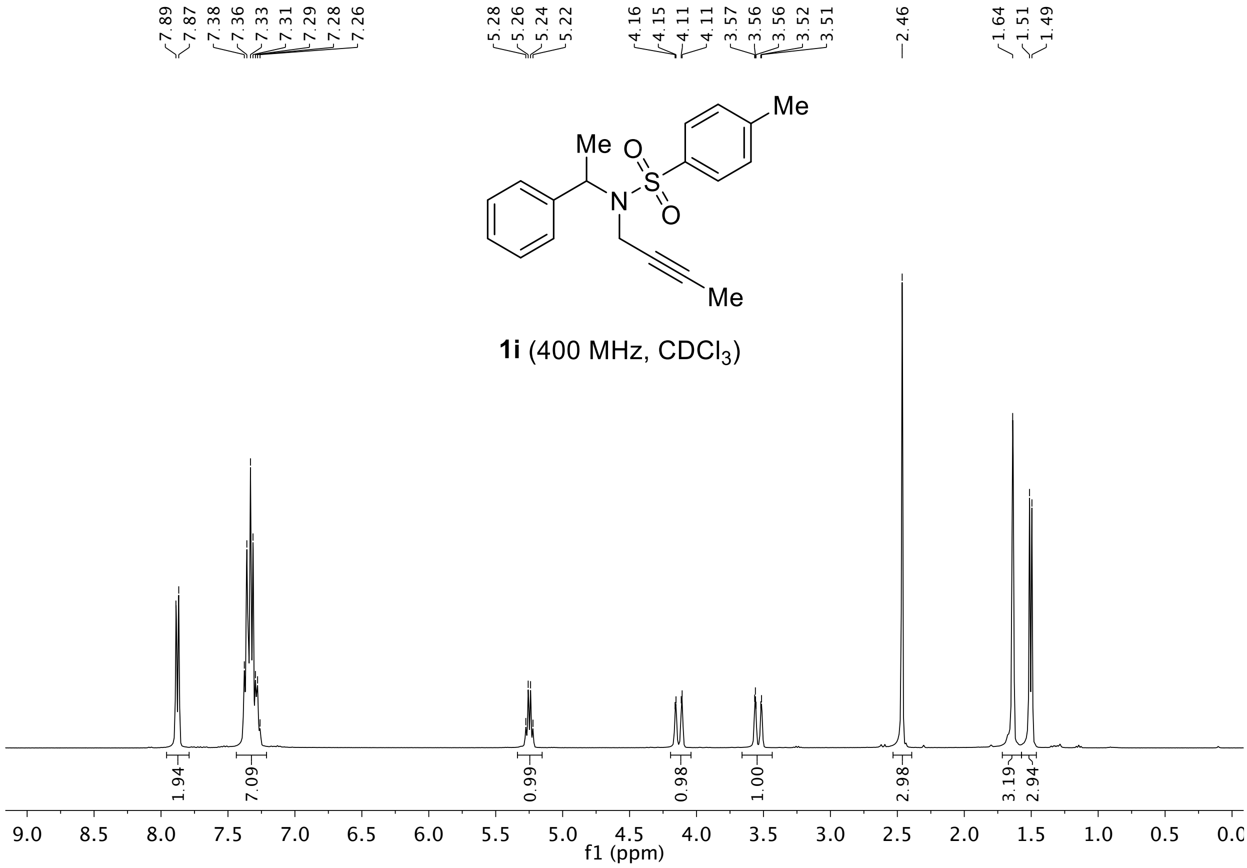
1c (75 MHz, $CDCl_3$)

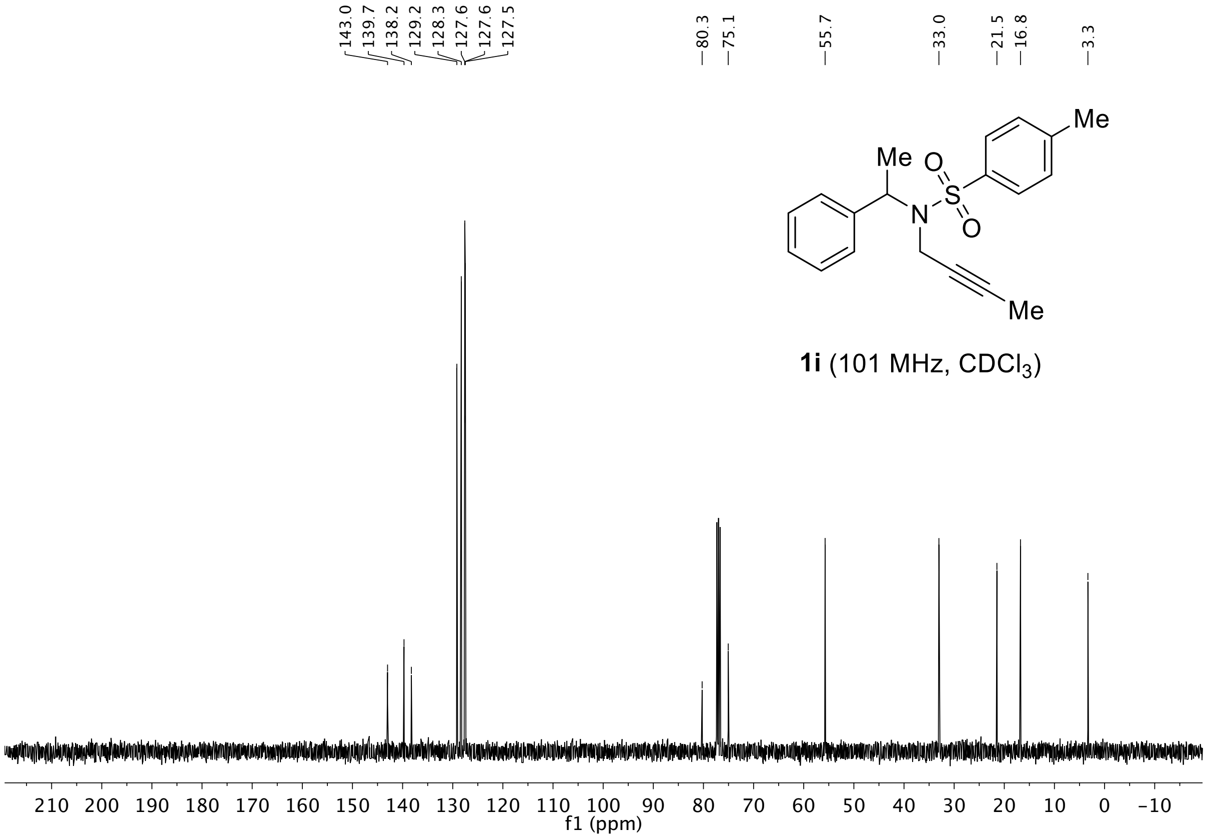

GC116
H
7.57 7.54 7.34 7.33 7.32 7.32 7.31 7.30 7.29 7.28 7.27 7.27 7.27 7.25 7.23
4.41 4.40 4.40 4.39
2.43
1.67 1.67 1.66
Me
O
S
N
O
Me
1d (300 MHz, CDCl3)
1.99
6.94
2.00
2.99
3.01
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

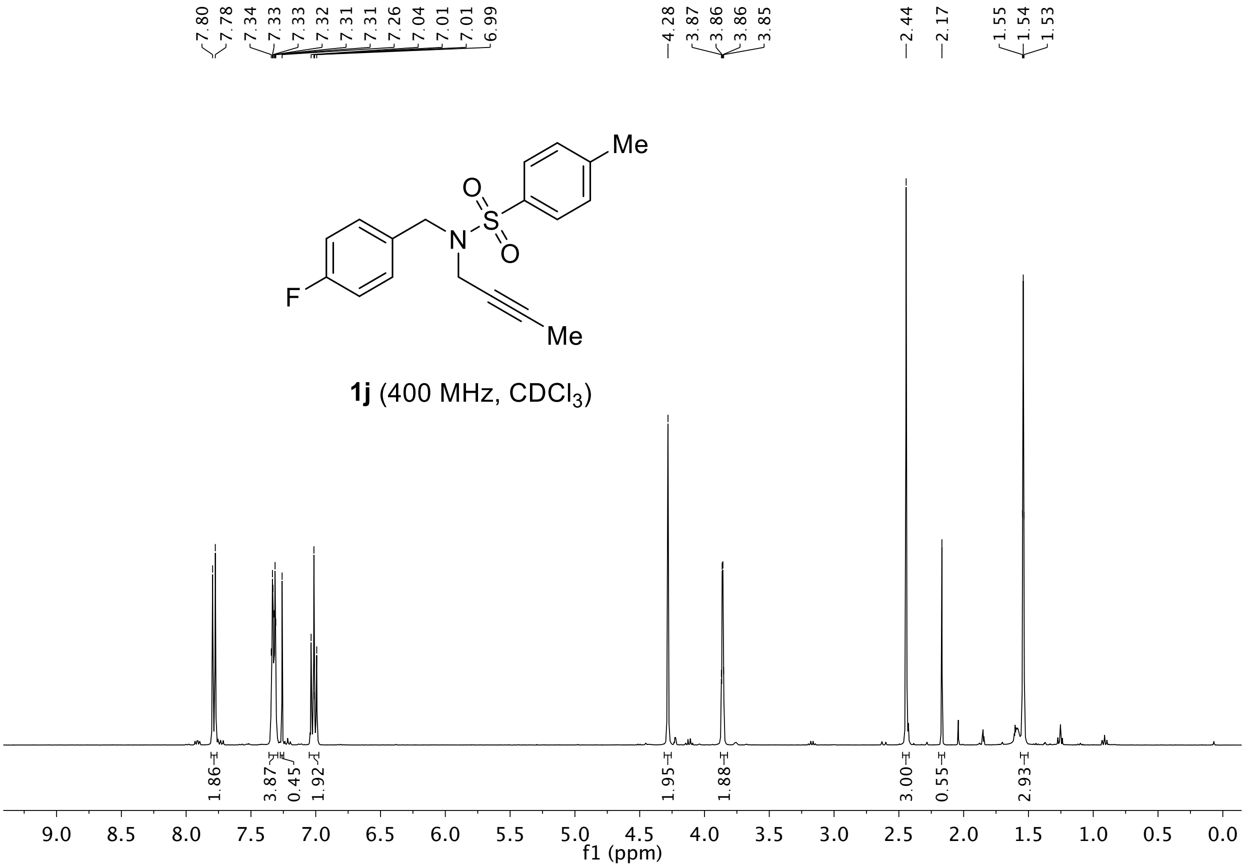

GC116
C
143.41 139.88 135.90
129.07 128.90 128.26 128.11 127.89
81.69 77.48 77.05 76.63 73.42
41.67
21.55
3.47
Me
O
S
N
O
Me
1d (75 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

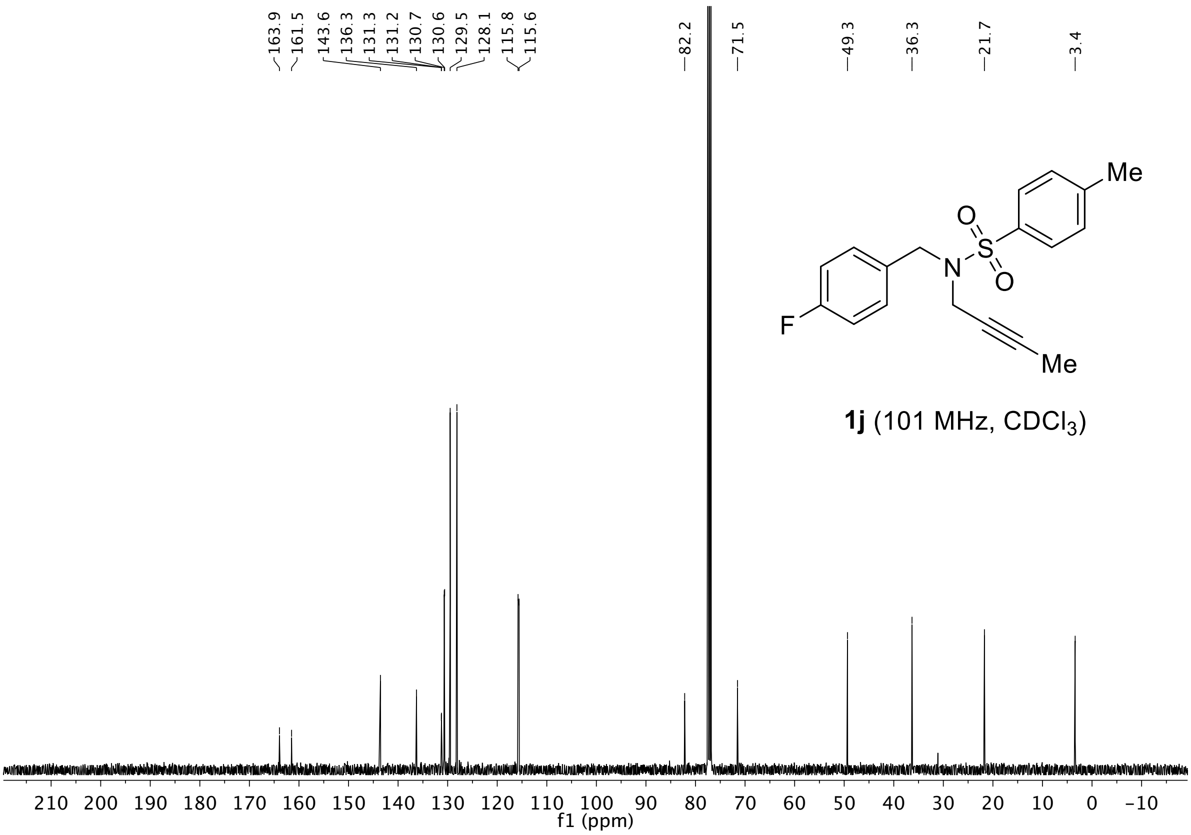

GC135
H
7.58 7.54 7.43 7.32 7.28 7.19 7.17
4.85 4.63 4.26 3.83
2.37 1.89
O
N
Me
Me
1e (400 MHz, $CDCl_3$)
1.99 2.87 1.43 2.86
2.00 2.06
3.05 3.10
f1 (ppm)

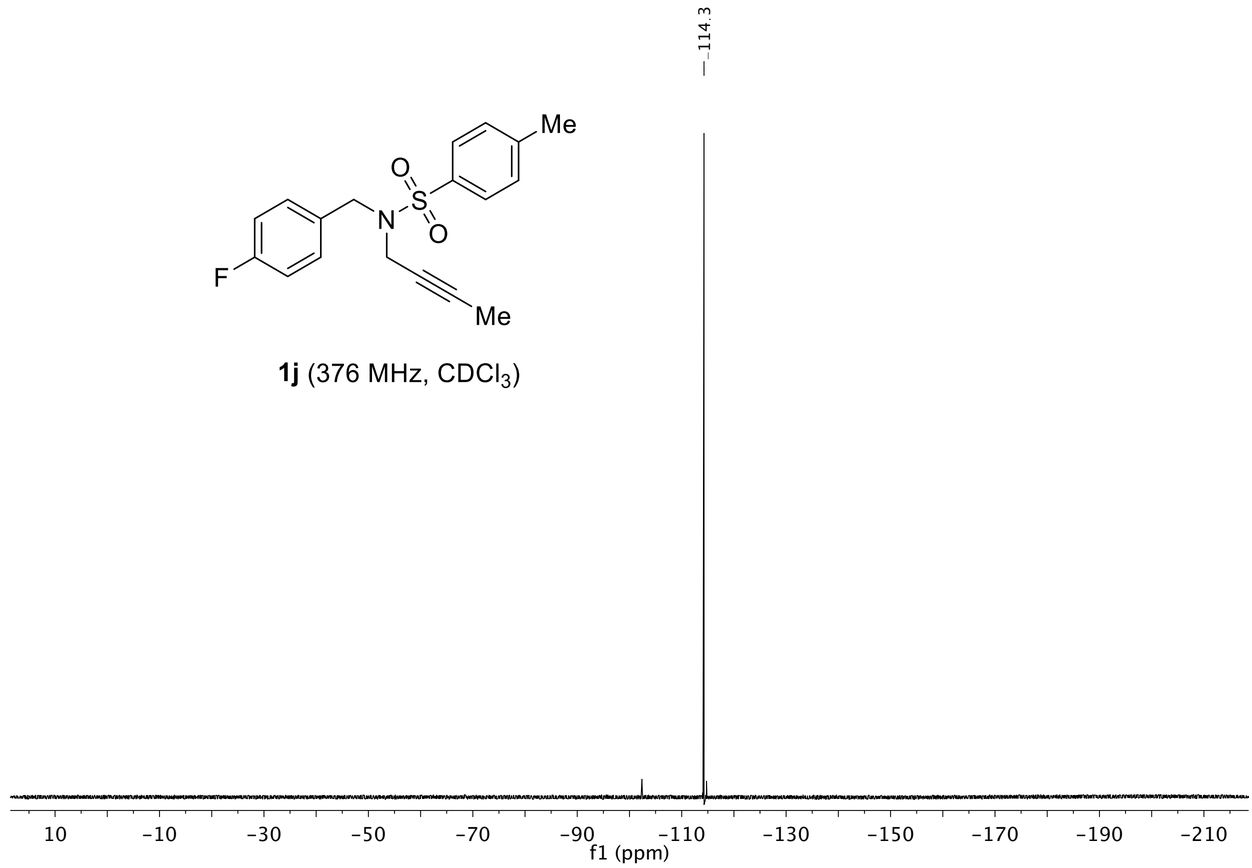

GC135bis
C
171.72 163.75
137.30 135.81 133.95 129.99 129.88 129.38 129.26 128.94 128.79 128.74 128.66 128.45 128.27 127.93 127.07 127.01
80.38 77.44 77.13 76.81 73.81
51.11 47.11 38.52 33.52 21.11 3.57
O
N
Me
Me
1e (101 MHz, $CDCl_3$)
f1 (ppm)

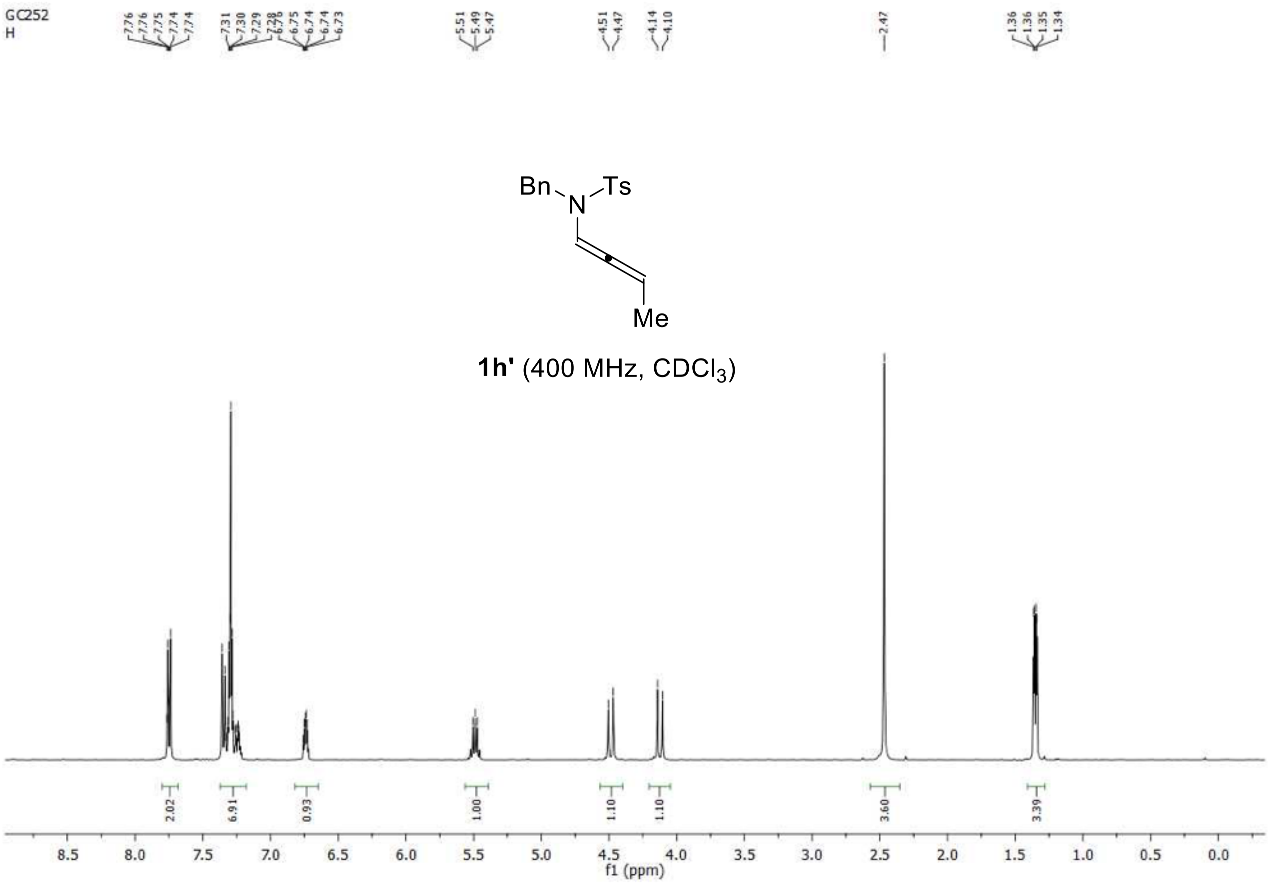

7.89
7.87
7.38
7.36
7.33
7.31
7.29
7.28
7.26
5.28
5.26
5.24
5.22
4.16
4.15
4.11
4.11
3.57
3.56
3.56
3.52
3.51
2.46
1.64
1.51
1.49
Me
Me
O
S
O
N
Me
1i (400 MHz, CDCl3)
1.94
7.09
0.99
0.98
1.00
2.98
3.19
2.94
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

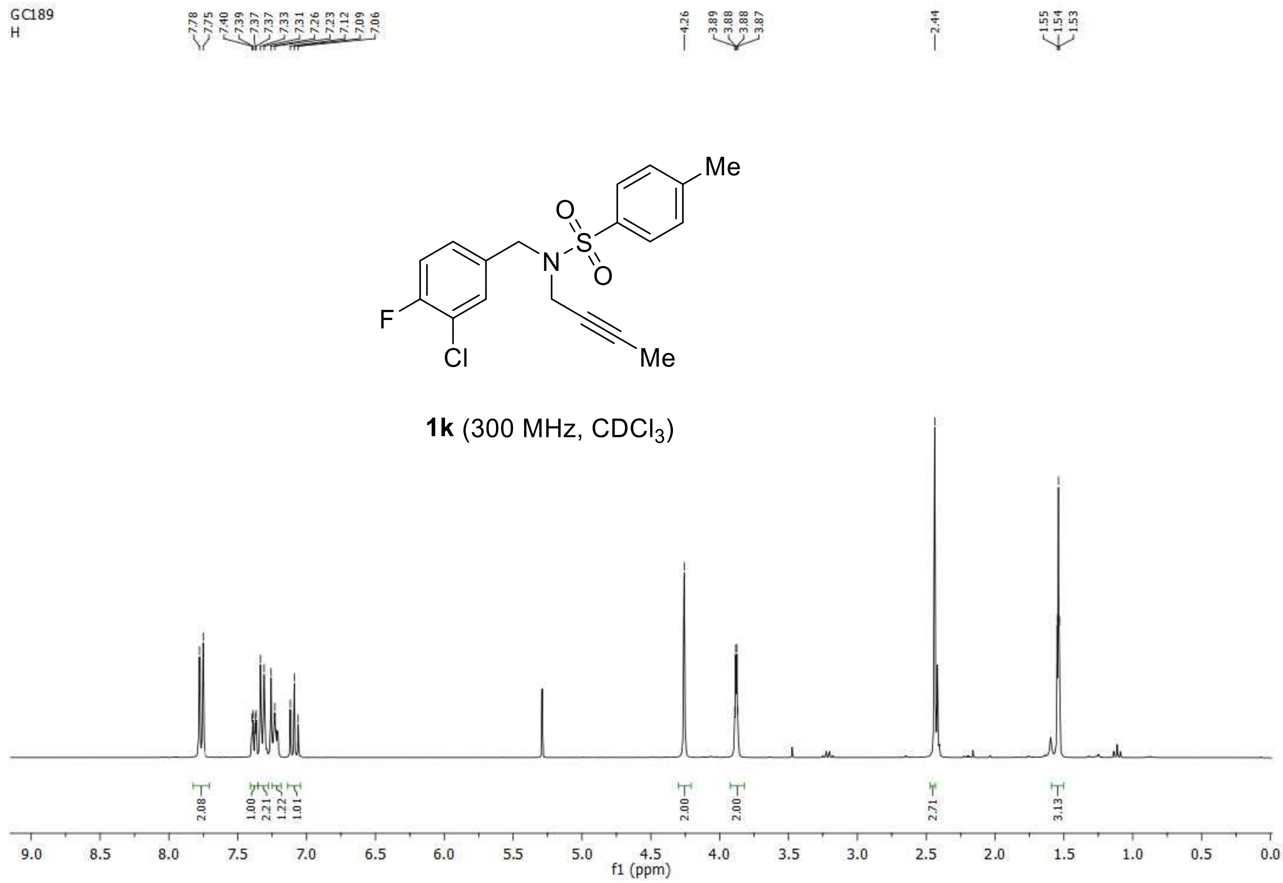

143.0
139.7
138.2
129.2
128.3
127.6
127.6
127.5
80.3
75.1
55.7
33.0
21.5
16.8
3.3
Me
Me
O
S
O
N
Me
1i (101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)


7.80
7.78
7.34
7.33
7.33
7.32
7.31
7.31
7.26
7.04
7.01
7.01
6.99
4.28
3.87
3.86
3.86
3.85
2.44
2.17
1.55
1.54
1.53
Me
O
S
O
N
F
Me
1j (400 MHz, CDCl3)
1.86
3.87
0.45
1.92
1.95
1.88
3.00
0.55
2.93
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
f1 (ppm)

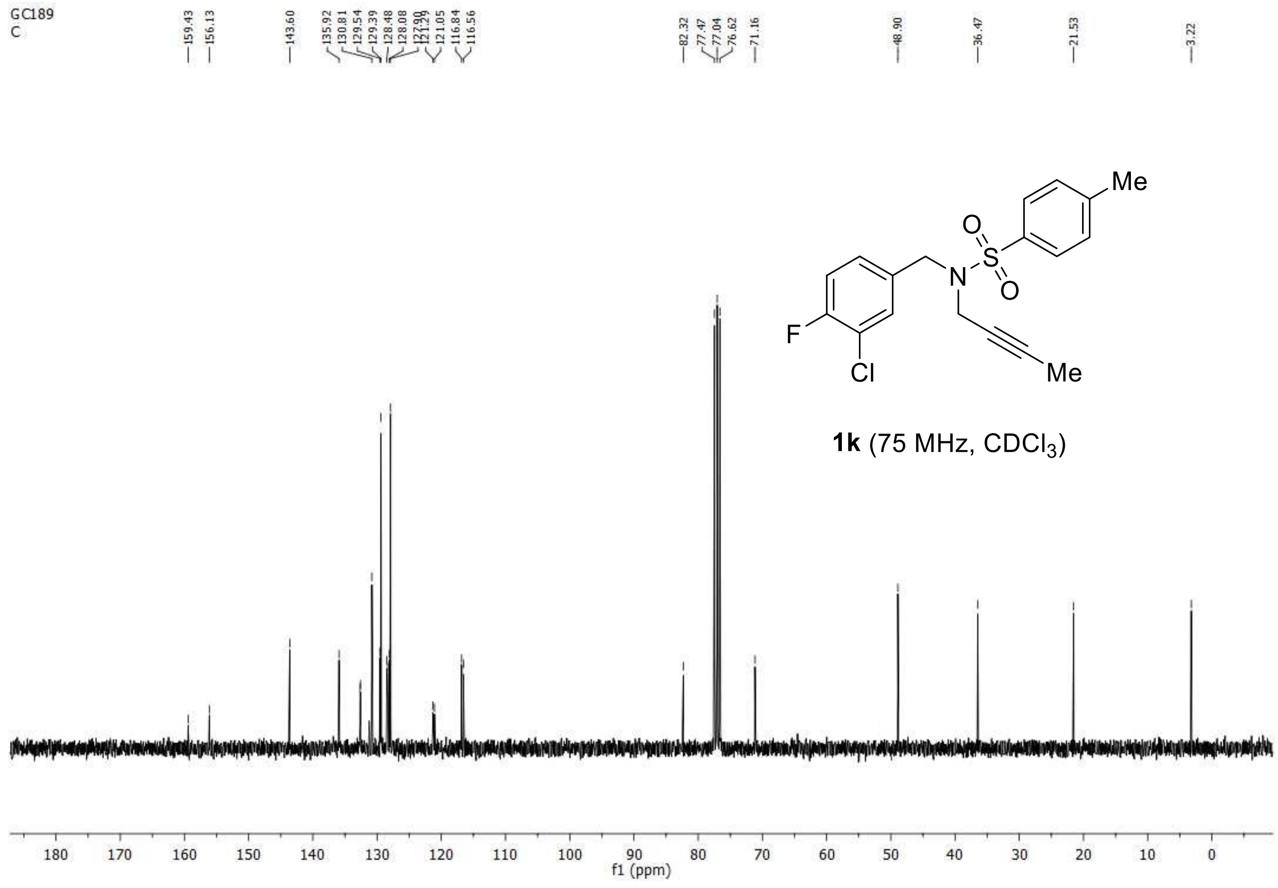

163.9
161.5
143.6
136.3
131.3
131.2
130.7
130.6
129.5
128.1
115.8
115.6
82.2
71.5
49.3
36.3
21.7
3.4
Me
O
S
O
N
F
Me
1j (101 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 –10
f1 (ppm)


1j (376 MHz, $CDCl_3$)
−114.3
f1 (ppm)


GC252
H
1h' (400 MHz, $CDCl_3$)
f1 (ppm)

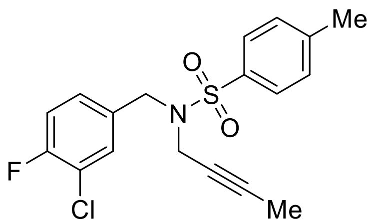


1k (300 MHz, $CDCl_3$)

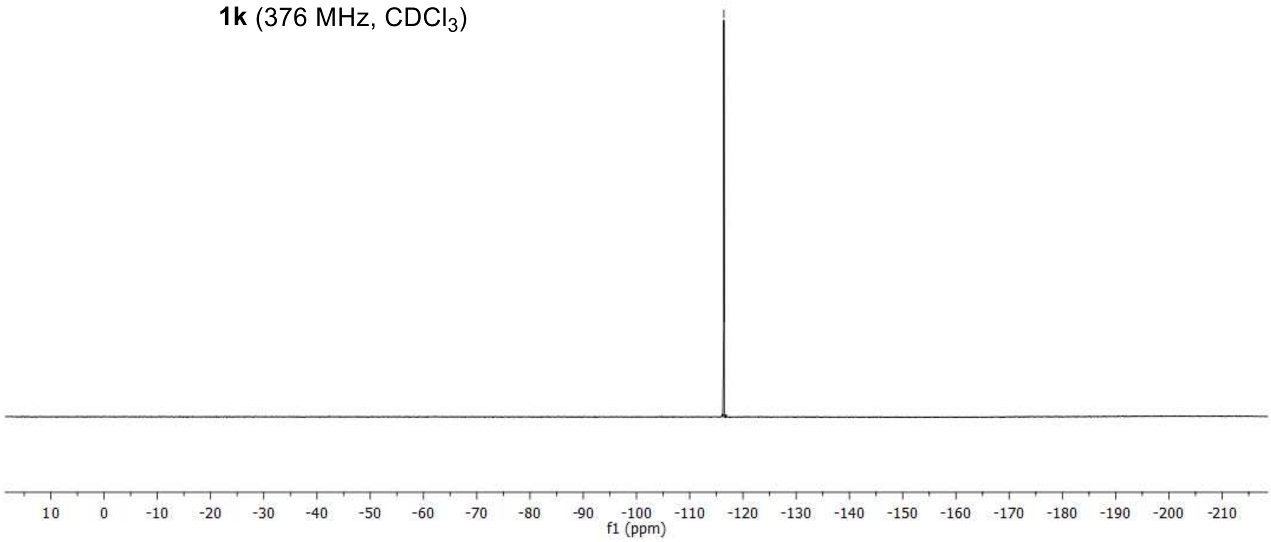


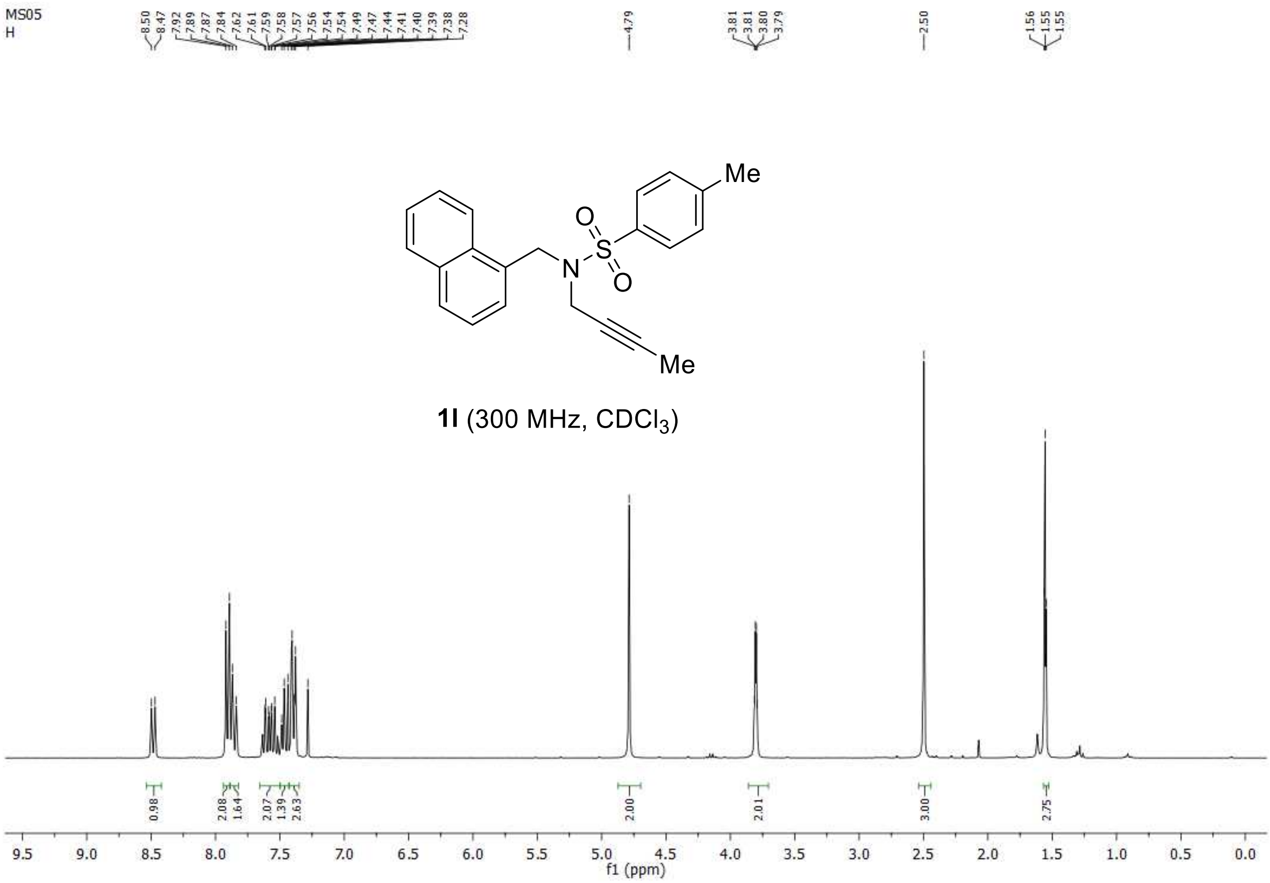
1k (75 MHz, $CDCl_3$)

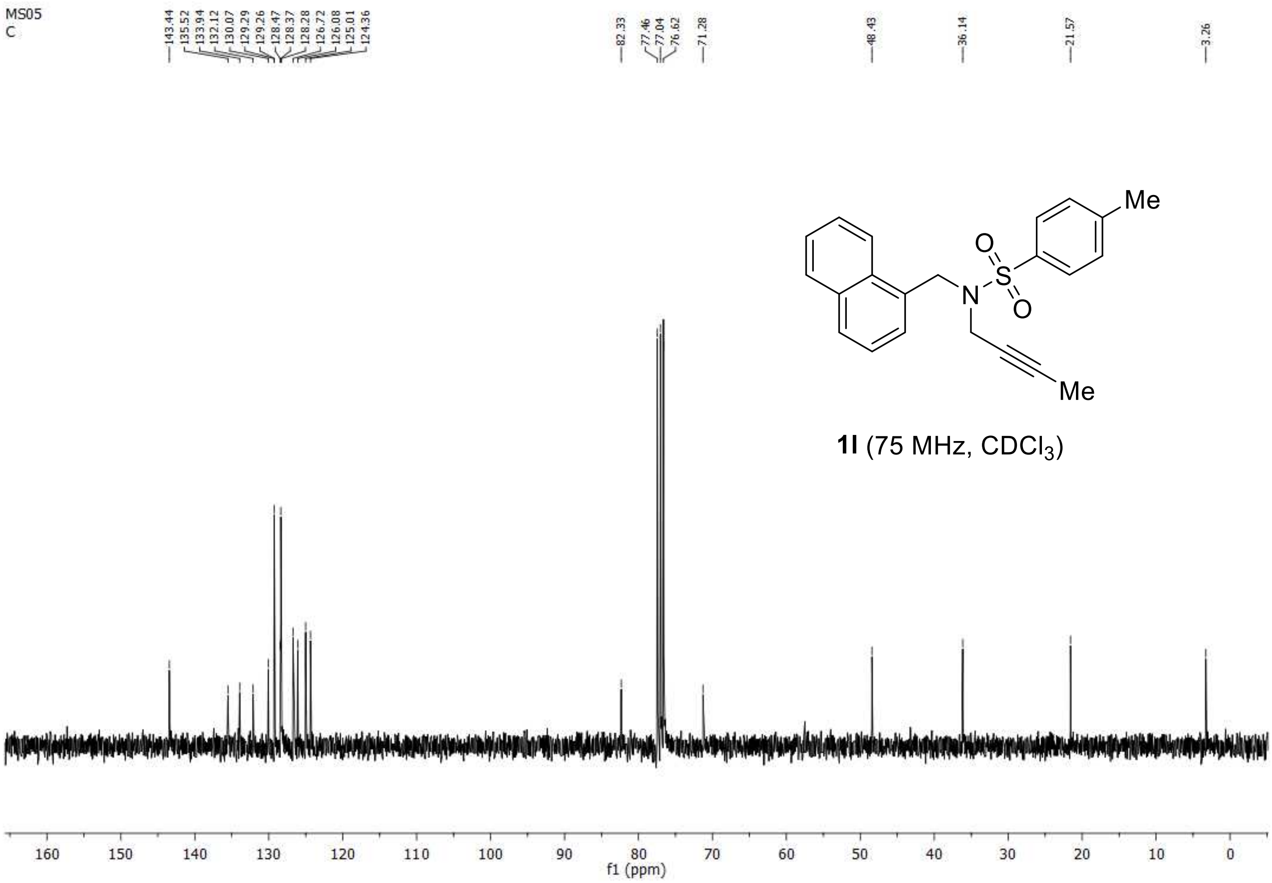
GC189A
F

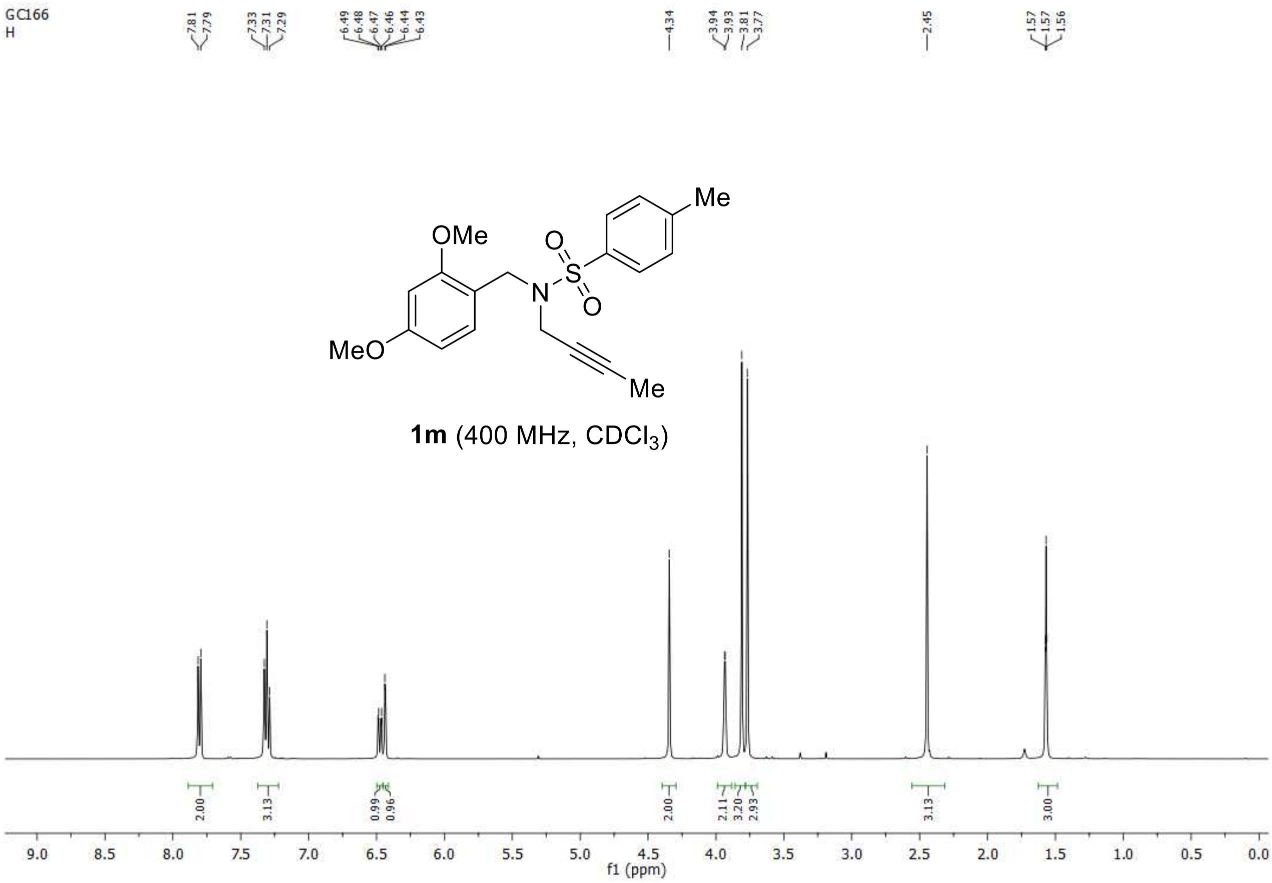


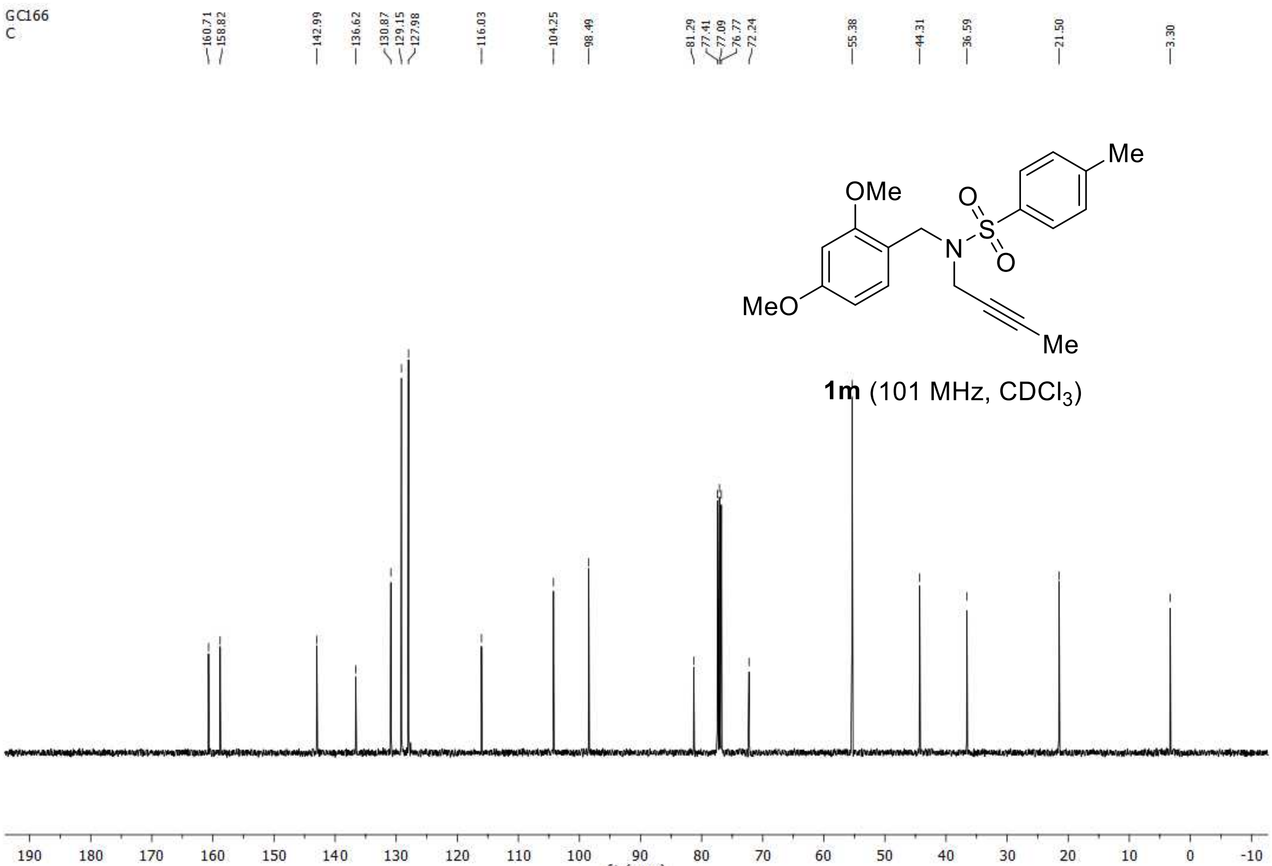
1k (376 MHz, $CDCl_3$)

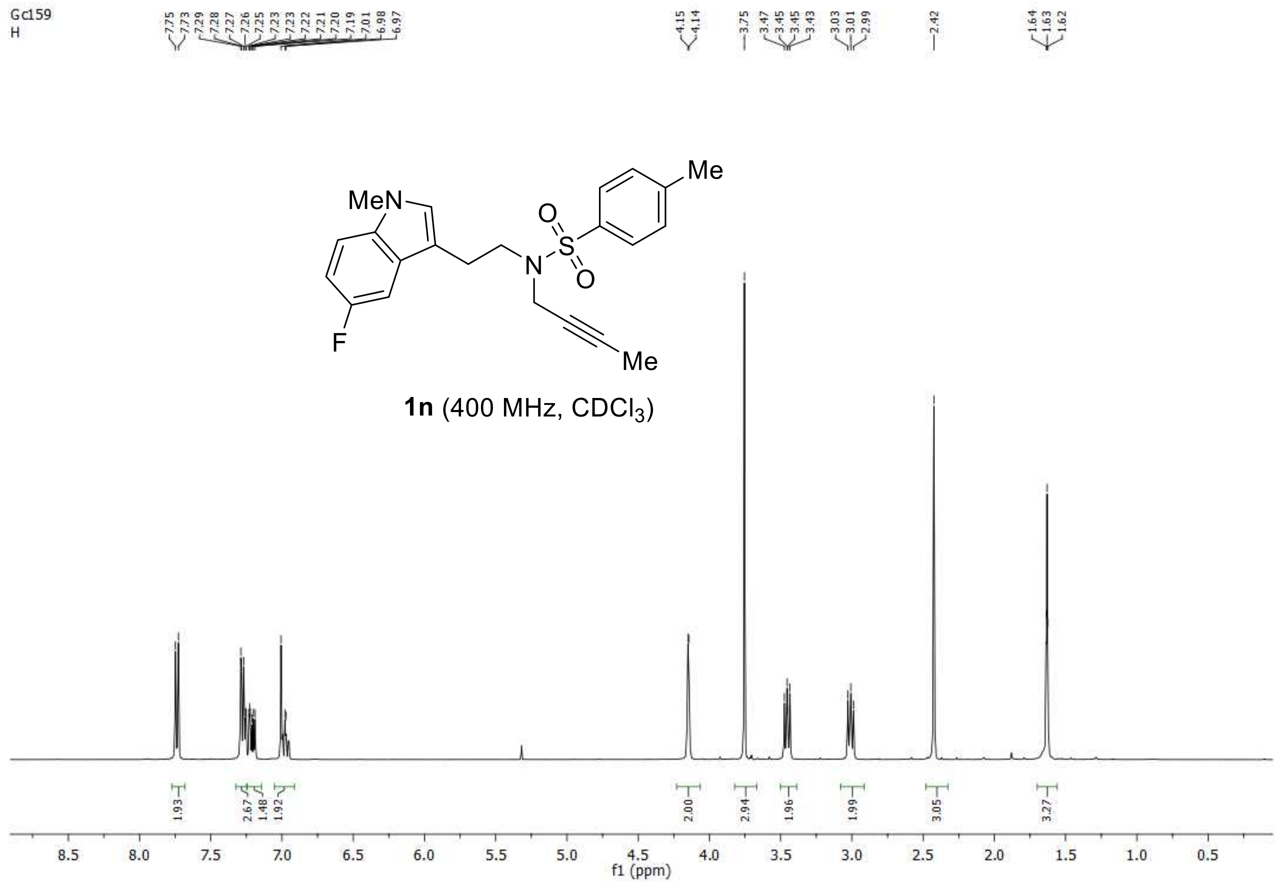


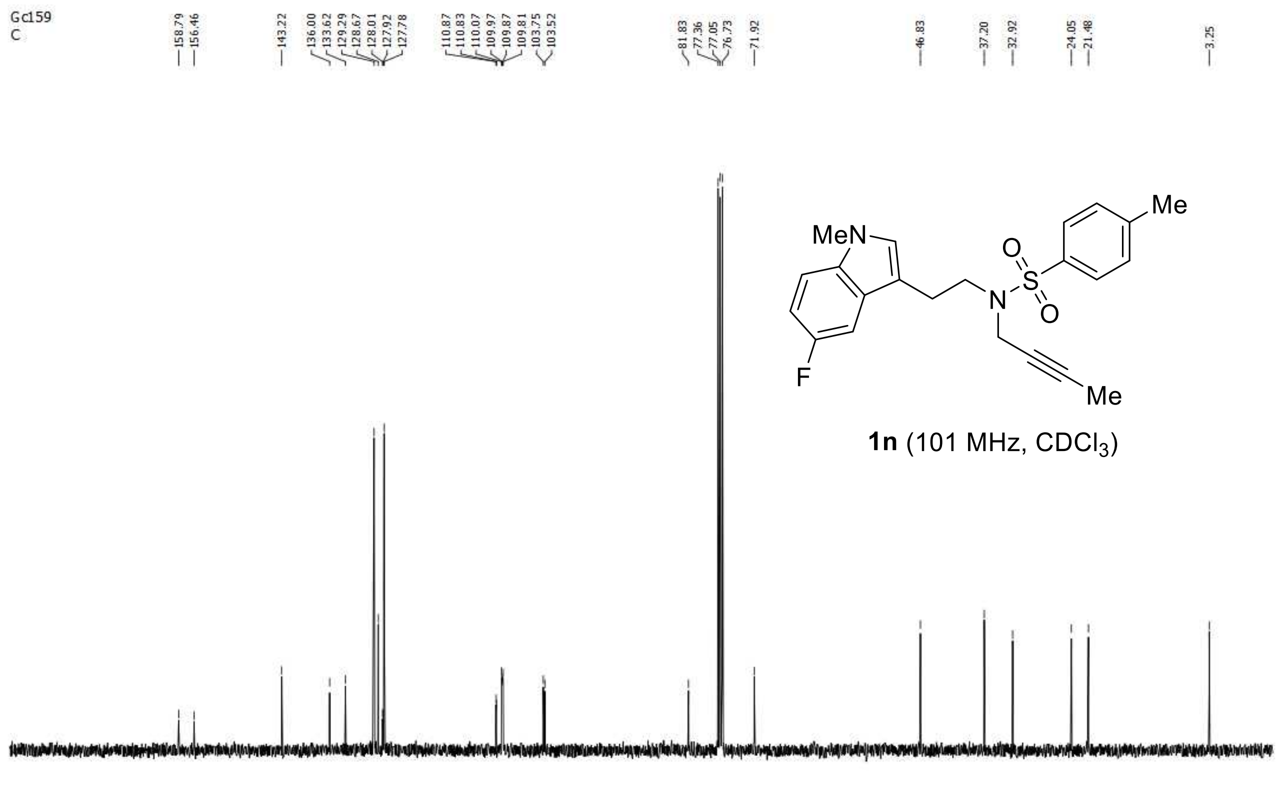

MS05
H
8.50
8.47
7.92
7.89
7.87
7.84
7.62
7.61
7.59
7.58
7.57
7.56
7.54
7.54
7.49
7.47
7.44
7.41
7.40
7.39
7.38
7.28
4.79
3.81
3.81
3.80
3.79
2.50
1.56
1.55
1.55
Me
O
S
N
O
Me
1l (300 MHz, CDCl$_3$)
0.98
2.08
1.64
2.07
1.39
2.63
2.00
2.01
3.00
2.75
f1 (ppm)

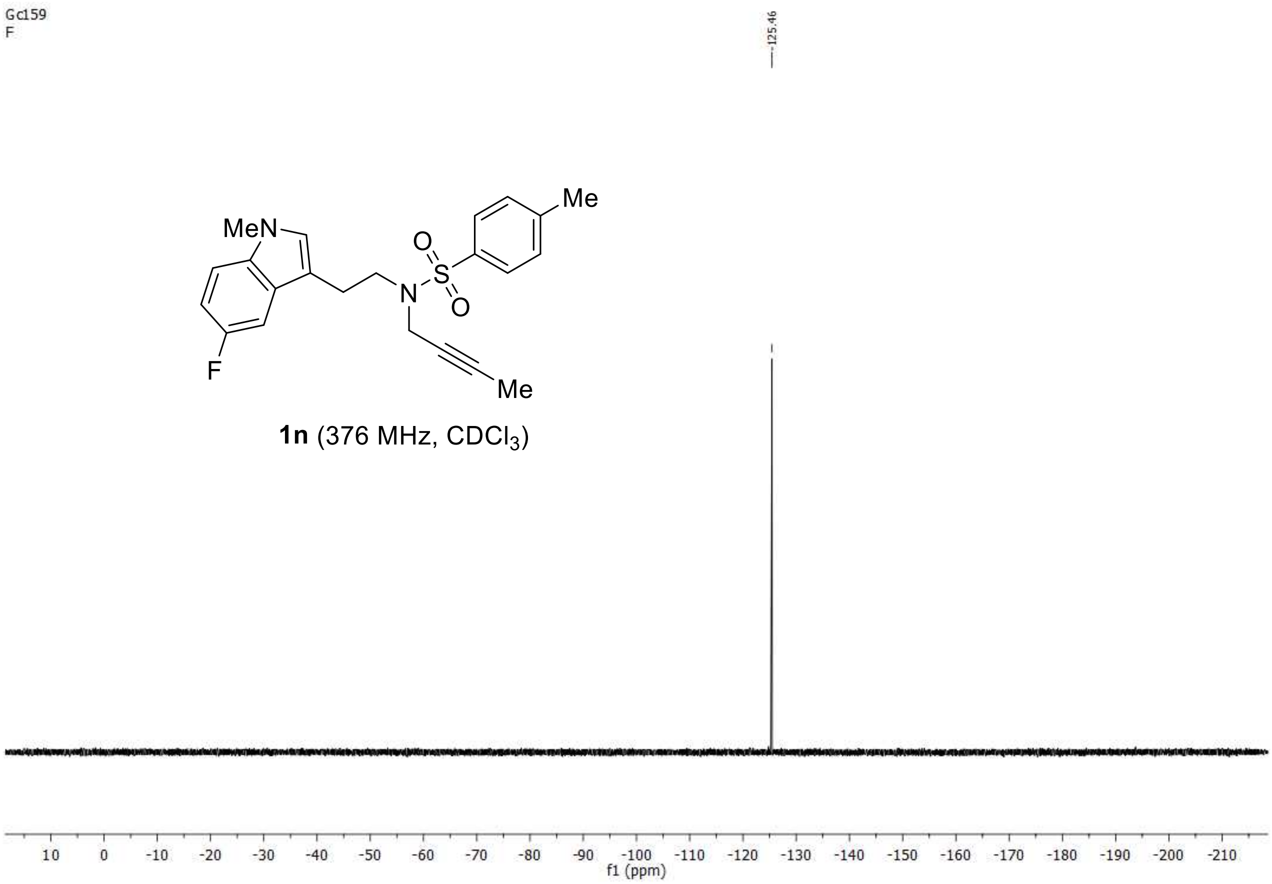

MS05
C
143.44
135.52
133.94
132.12
130.07
129.29
129.26
128.47
128.37
128.28
126.72
126.08
125.01
124.36
82.33
77.46
77.04
76.62
71.28
48.43
36.14
21.57
3.26
Me
O
S
N
O
Me
1l (75 MHz, CDCl$_3$)
f1 (ppm)


GC166
H
7.81
7.79
7.33
7.31
7.29
6.49
6.48
6.47
6.46
6.44
6.43
4.34
3.94
3.93
3.81
3.77
2.45
1.57
1.57
1.56
OMe
Me
MeO
N
S
O
O
Me
1m (400 MHz, CDCl3)
2.00
3.13
0.99
0.96
2.00
2.11
3.20
2.93
3.13
3.00
f1 (ppm)

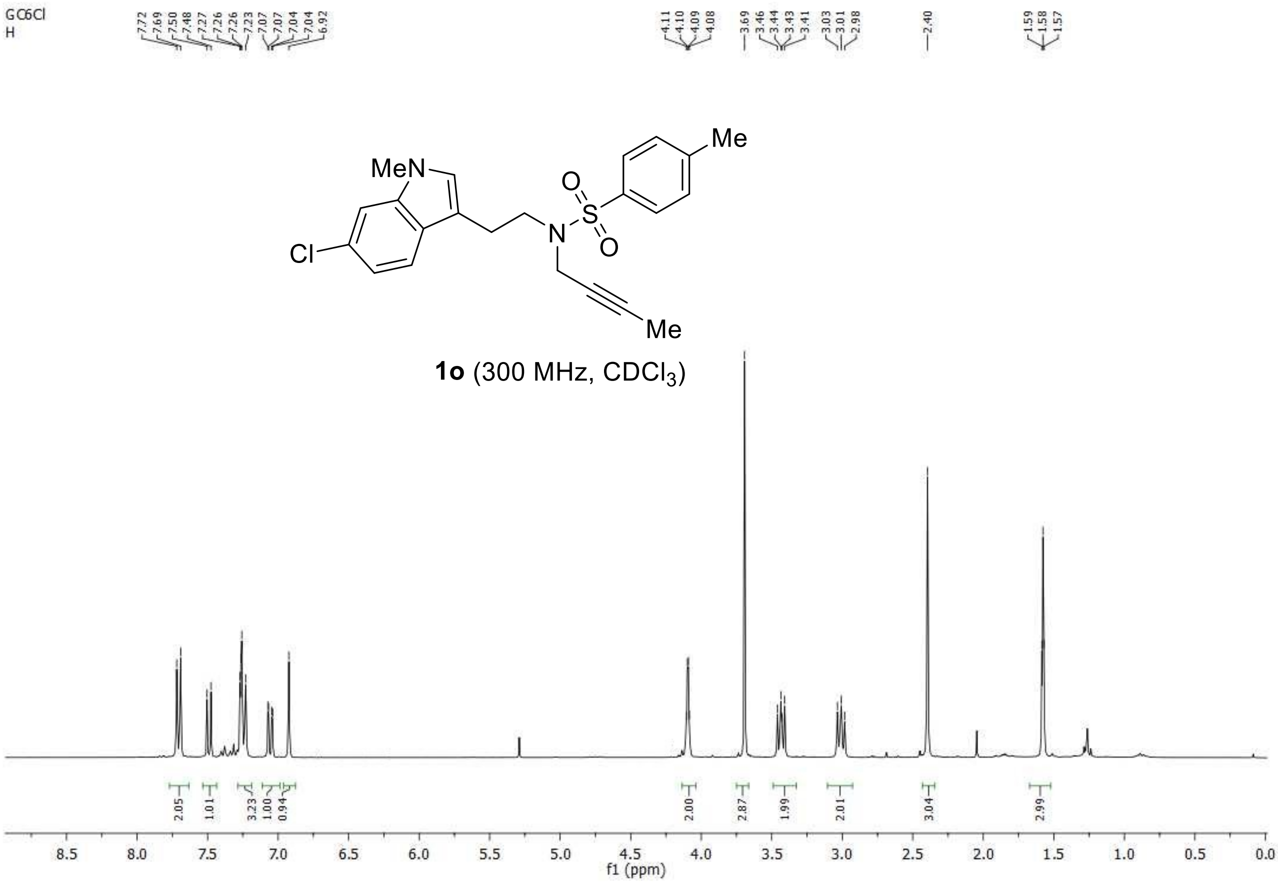

GC166
C
160.71
158.82
142.99
136.62
130.87
129.15
127.98
116.03
104.25
98.49
81.29
77.41
77.09
76.77
72.24
55.38
44.31
36.59
21.50
3.30
OMe
Me
MeO
N
S
O
O
Me
1m (101 MHz, CDCl3)
f1 (ppm)


Gc159
H
7.75 7.73 7.29 7.28 7.27 7.26 7.25 7.23 7.23 7.22 7.21 7.20 7.19 7.01 6.98 6.97
4.15 4.14
3.75 3.47 3.45 3.45 3.43 3.03 3.01 2.99
2.42
1.64 1.63 1.62
MeN
Me
O
S
N
O
F
Me
1n (400 MHz, CDCl3)
1.93 2.67 1.48 1.92 2.00 2.94 1.96 1.99 3.05 3.27
f1 (ppm)

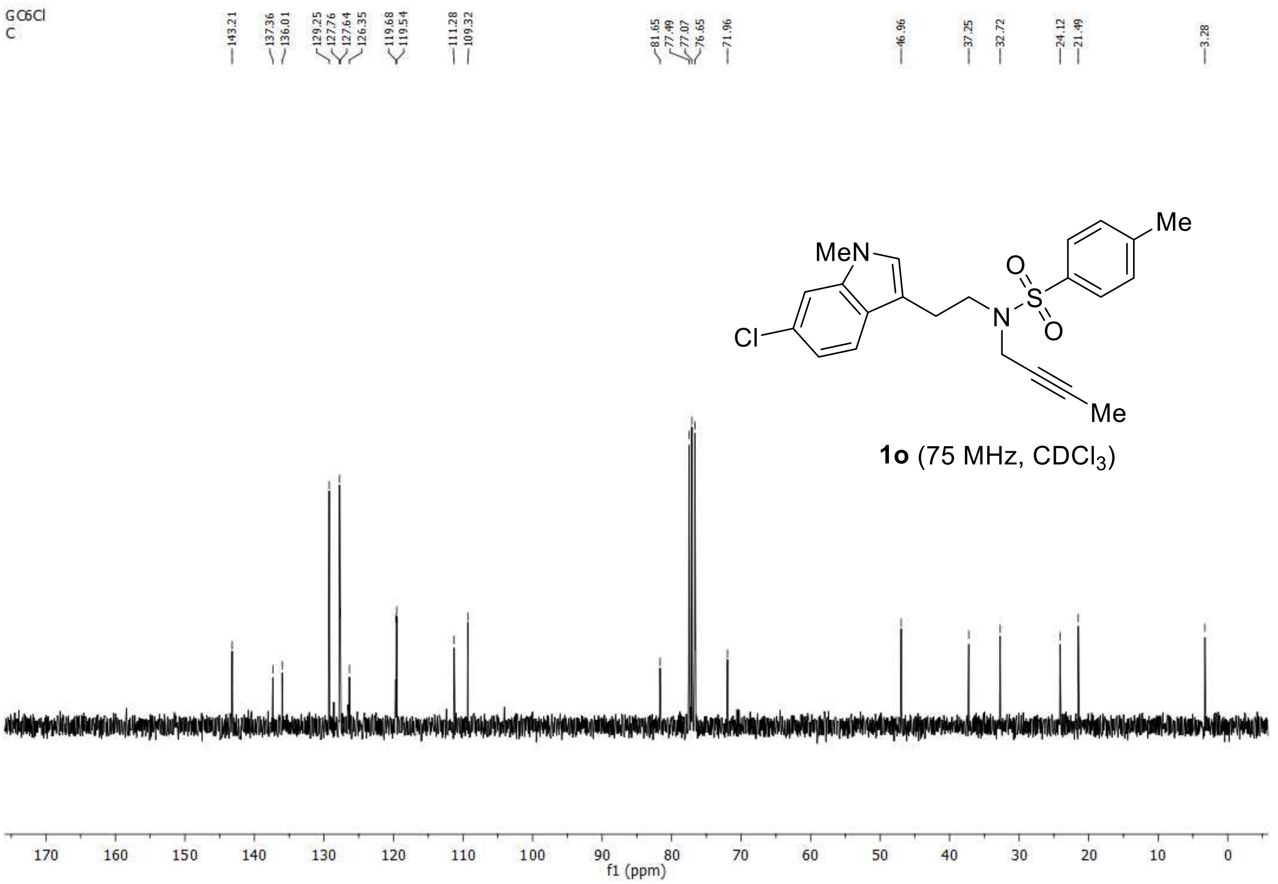

Gc159
C
158.79 156.46 143.22 136.00 133.62 129.29 128.67 128.01 127.92 127.78 110.87 110.83 110.07 109.97 109.87 109.81 103.75 103.52 81.83 77.36 77.05 76.73 71.92 46.83 37.20 32.92 24.05 21.48 3.25
MeN
Me
O
S
N
O
F
Me
1n (101 MHz, CDCl3)
f1 (ppm)



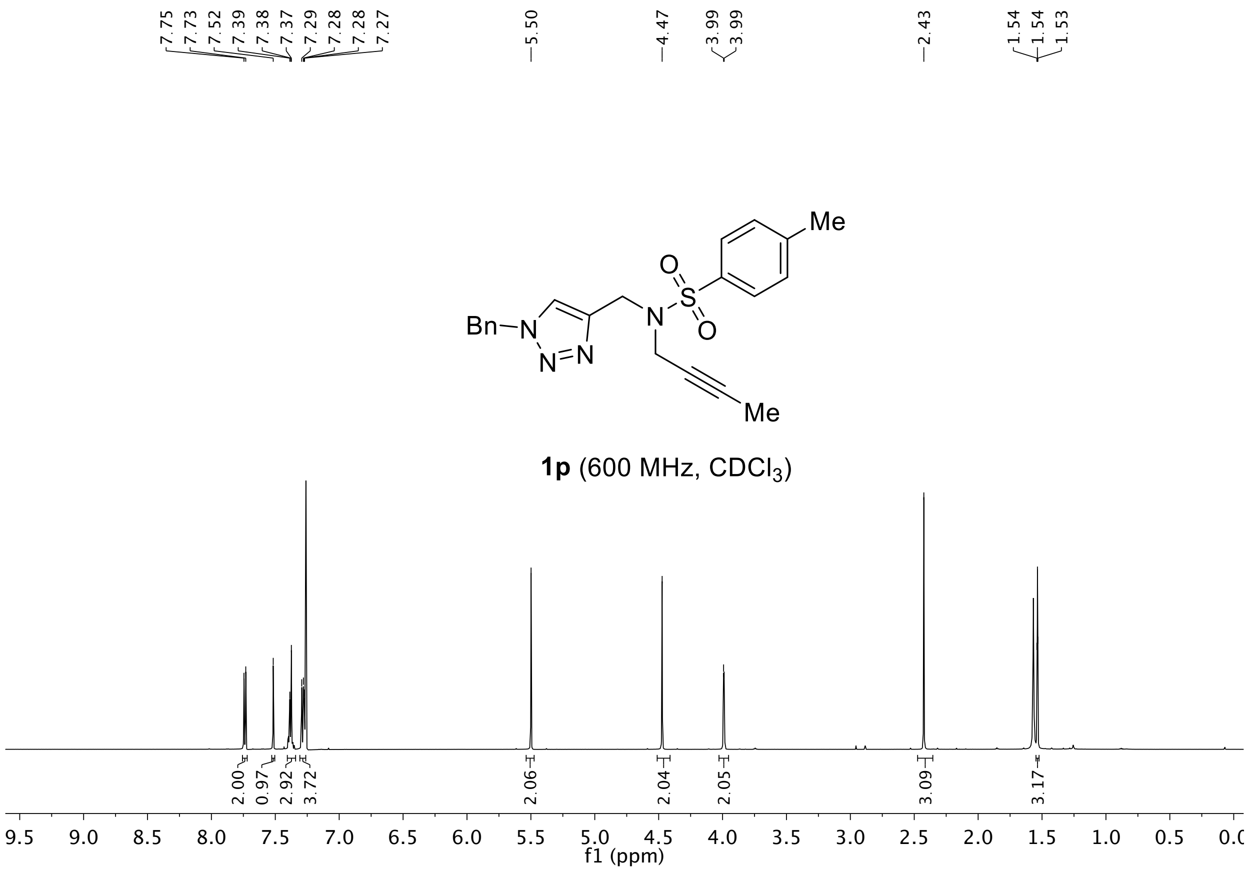
1n (376 MHz, $CDCl_3$)

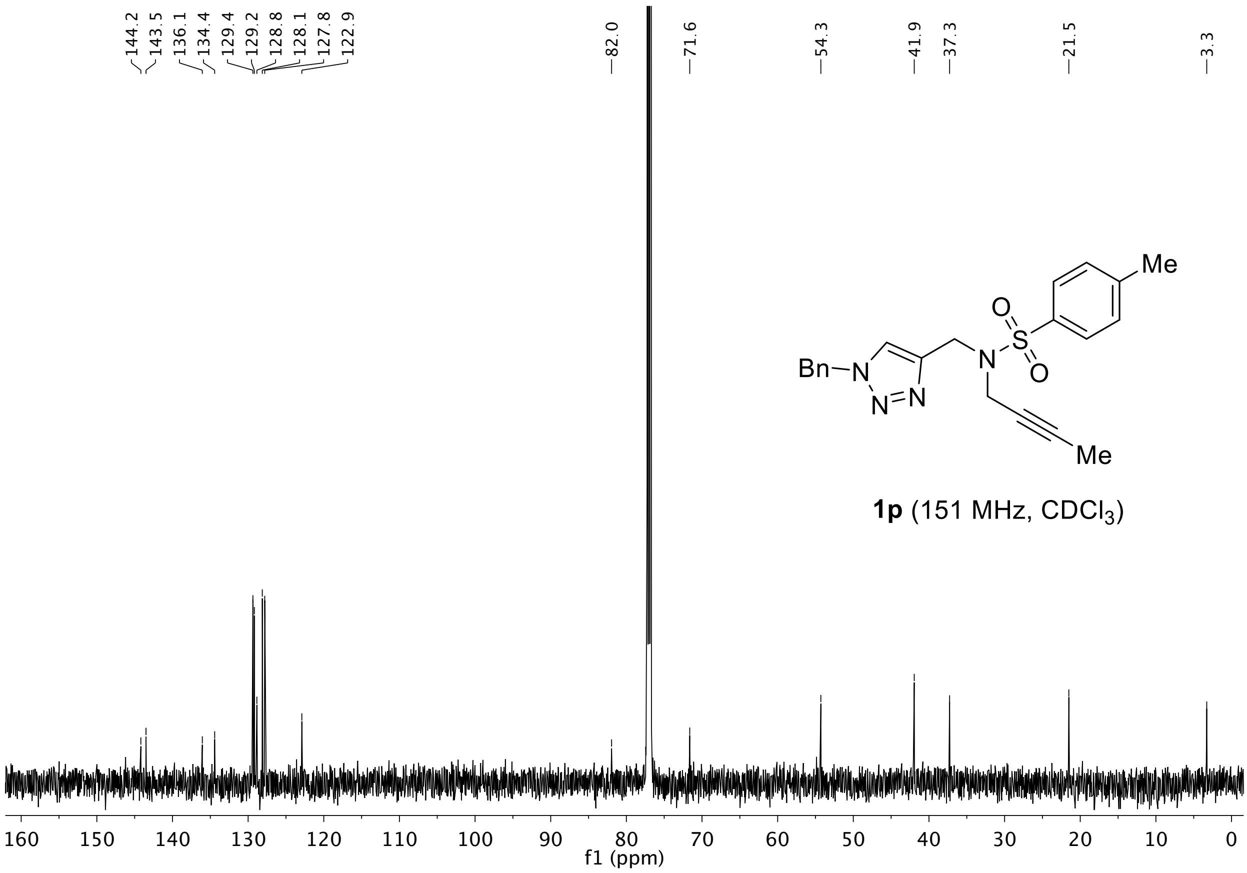


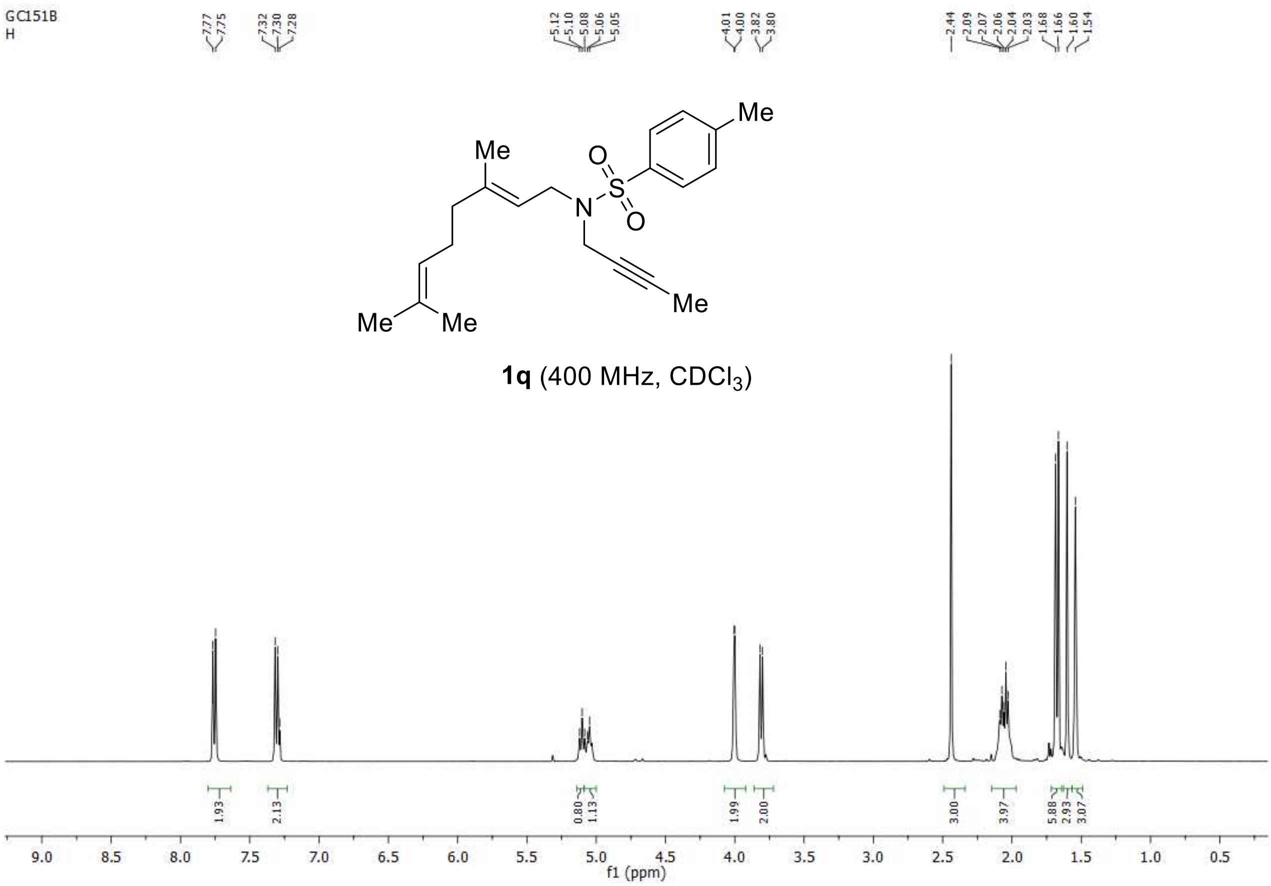
1o (300 MHz, $CDCl_3$)

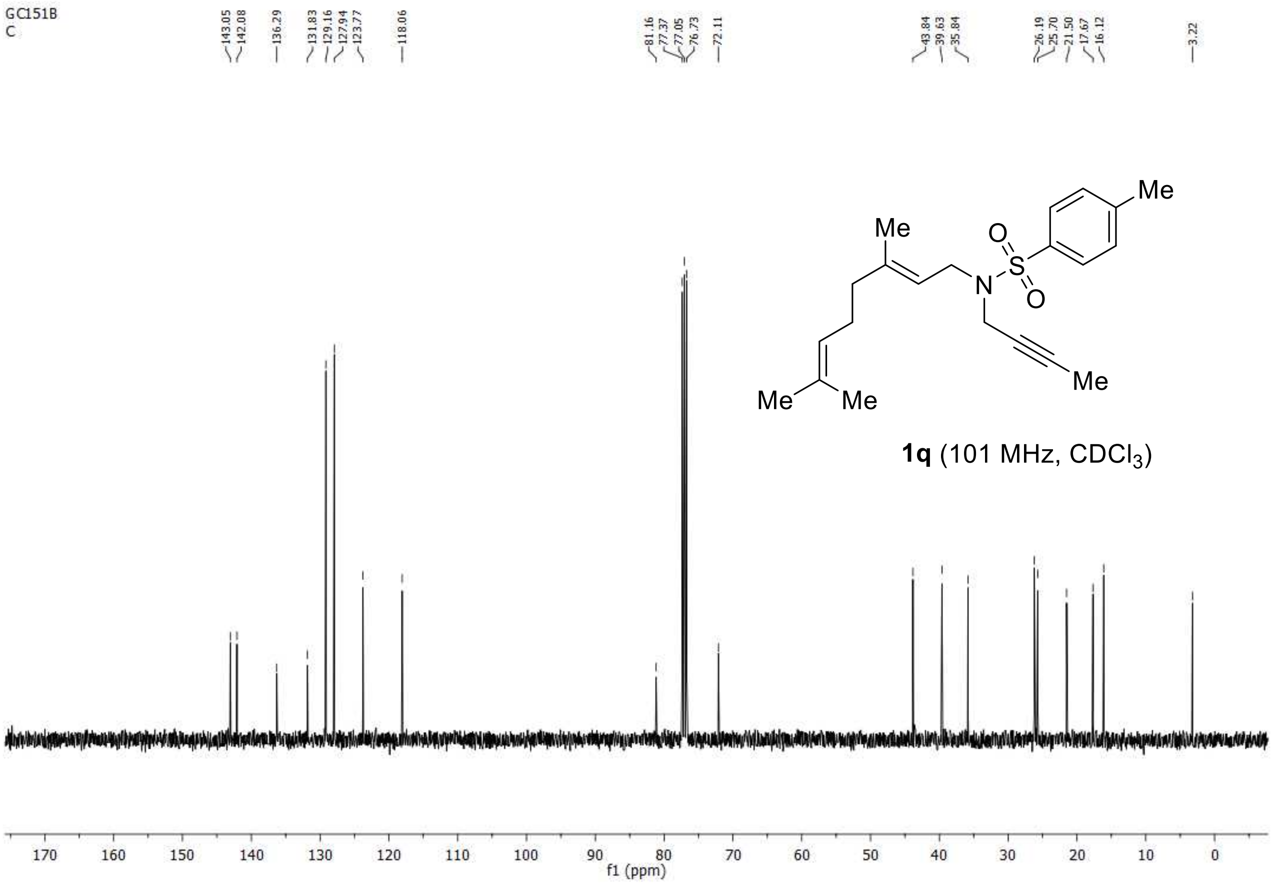


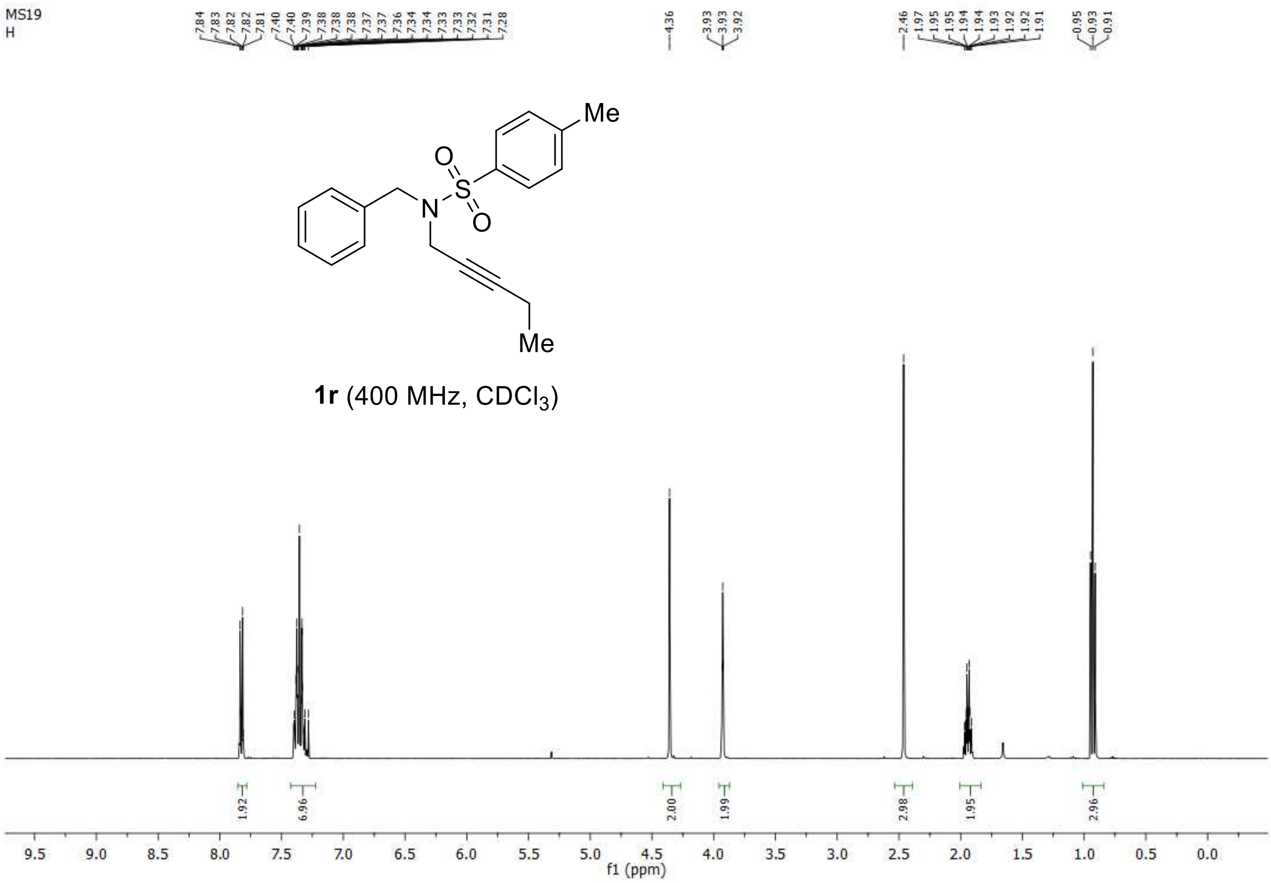
1o (75 MHz, $CDCl_3$)

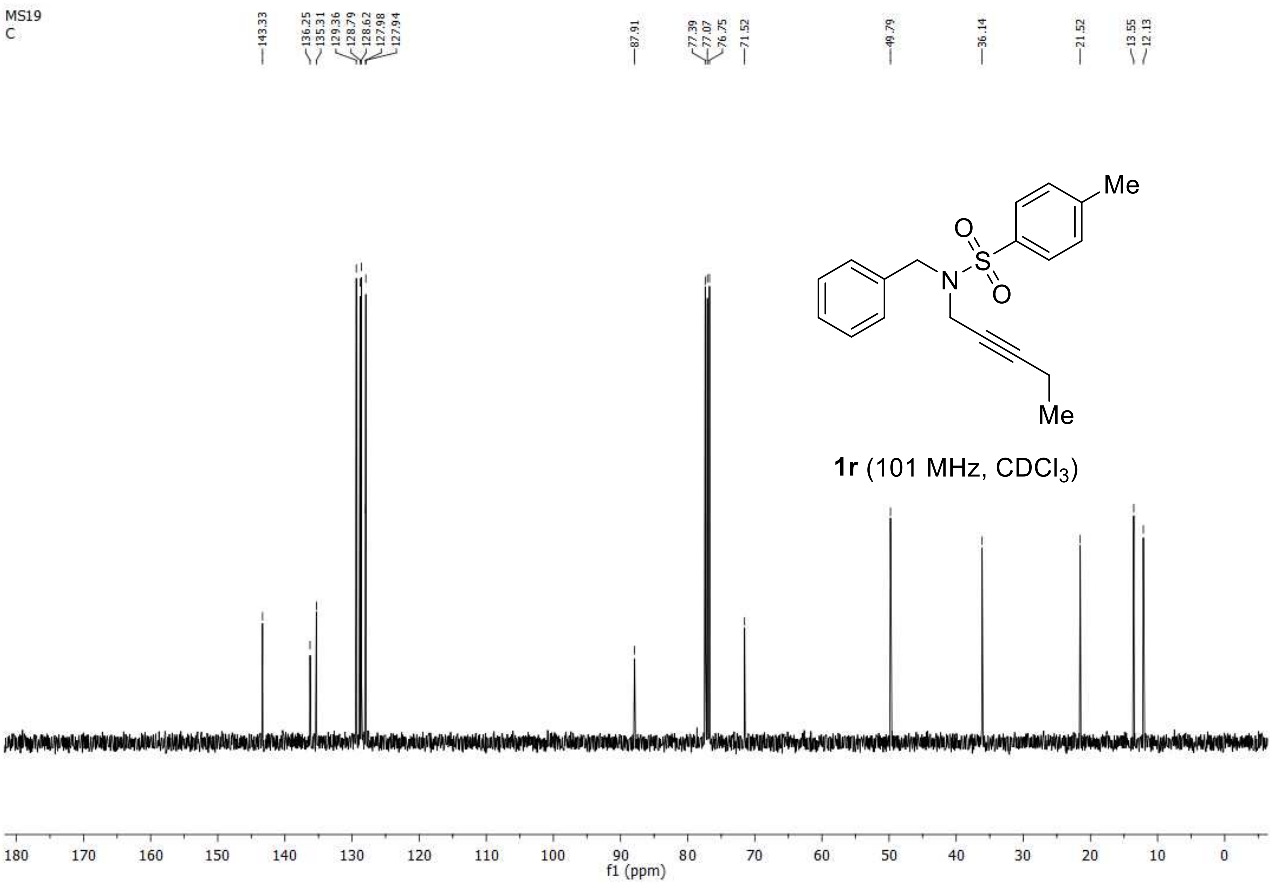

7.75
7.73
7.52
7.39
7.38
7.37
7.29
7.28
7.28
7.27
5.50
4.47
3.99
3.99
2.43
1.54
1.54
1.53
Me
O
S
O
Bn
N
N
N
N
Me
1p (600 MHz, CDCl3)
2.00
0.97
2.92
3.72
2.06
2.04
2.05
3.09
3.17
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

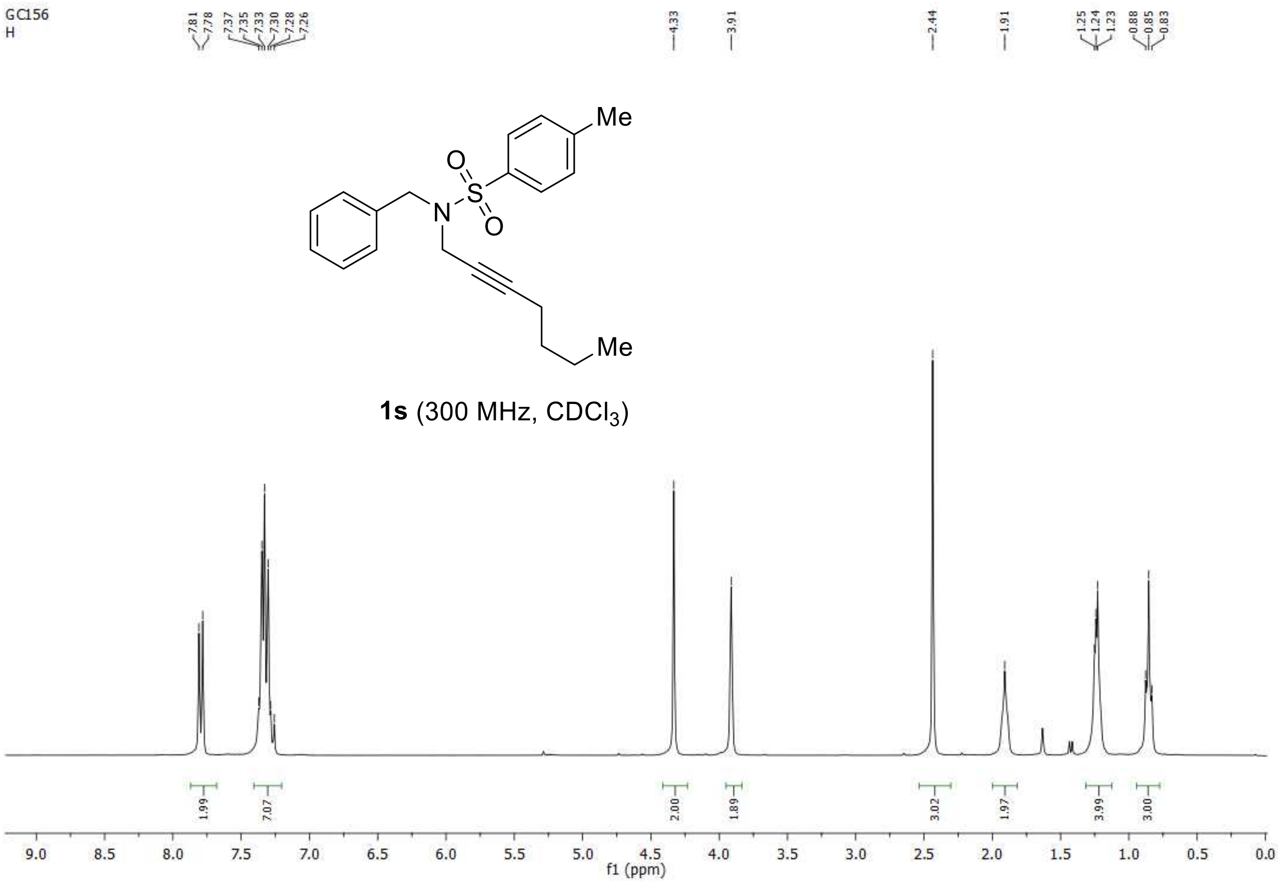

144.2
143.5
136.1
134.4
129.4
129.2
128.8
128.1
127.8
122.9
82.0
71.6
54.3
41.9
37.3
21.5
3.3
Me
O
S
O
Bn
N
N
N
N
Me
1p (151 MHz, CDCl3)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


GC151B
H
7.77 7.75 7.32 7.30 7.28
5.12 5.10 5.08 5.06 5.05
4.01 4.00 3.82 3.80
2.44 2.09 2.07 2.06 2.04 2.03 1.68 1.66 1.60 1.54
Me
Me
O
N
S
O
Me
Me
Me
1q (400 MHz, CDCl3)
1.93 2.13 0.80 1.13 1.99 2.00 3.00 3.97 5.88 2.93 3.07
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
f1 (ppm)

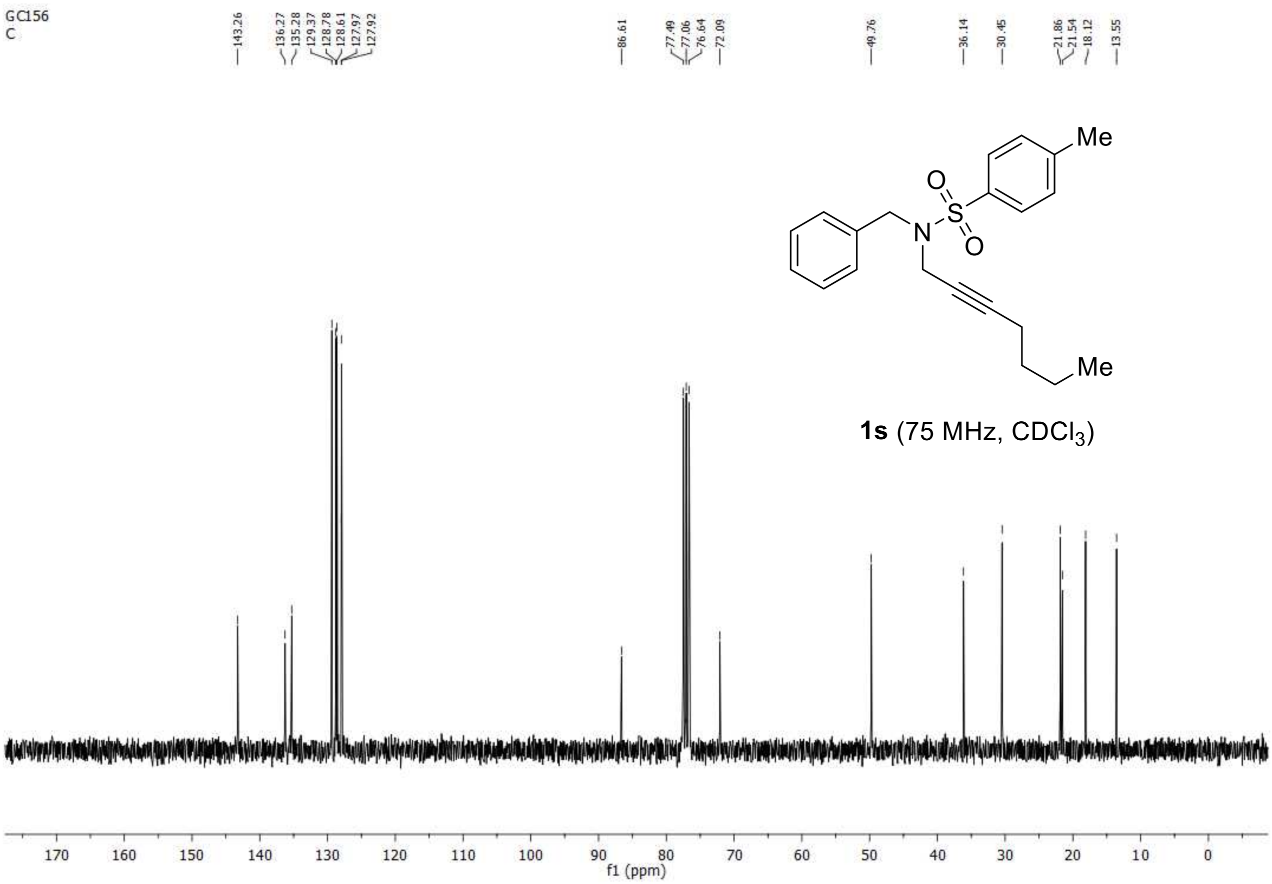

GC151B
C
143.05 142.08 136.29 131.83 129.16 127.94 123.77 118.06
81.16 77.37 77.05 76.73 72.11
43.84 39.63 35.84
26.19 25.70 21.50 17.67 16.12
3.22
Me
Me
O
N
S
O
Me
Me
Me
1q (101 MHz, CDCl3)
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MS19
H
1r (400 MHz, CDCl3)
f1 (ppm)

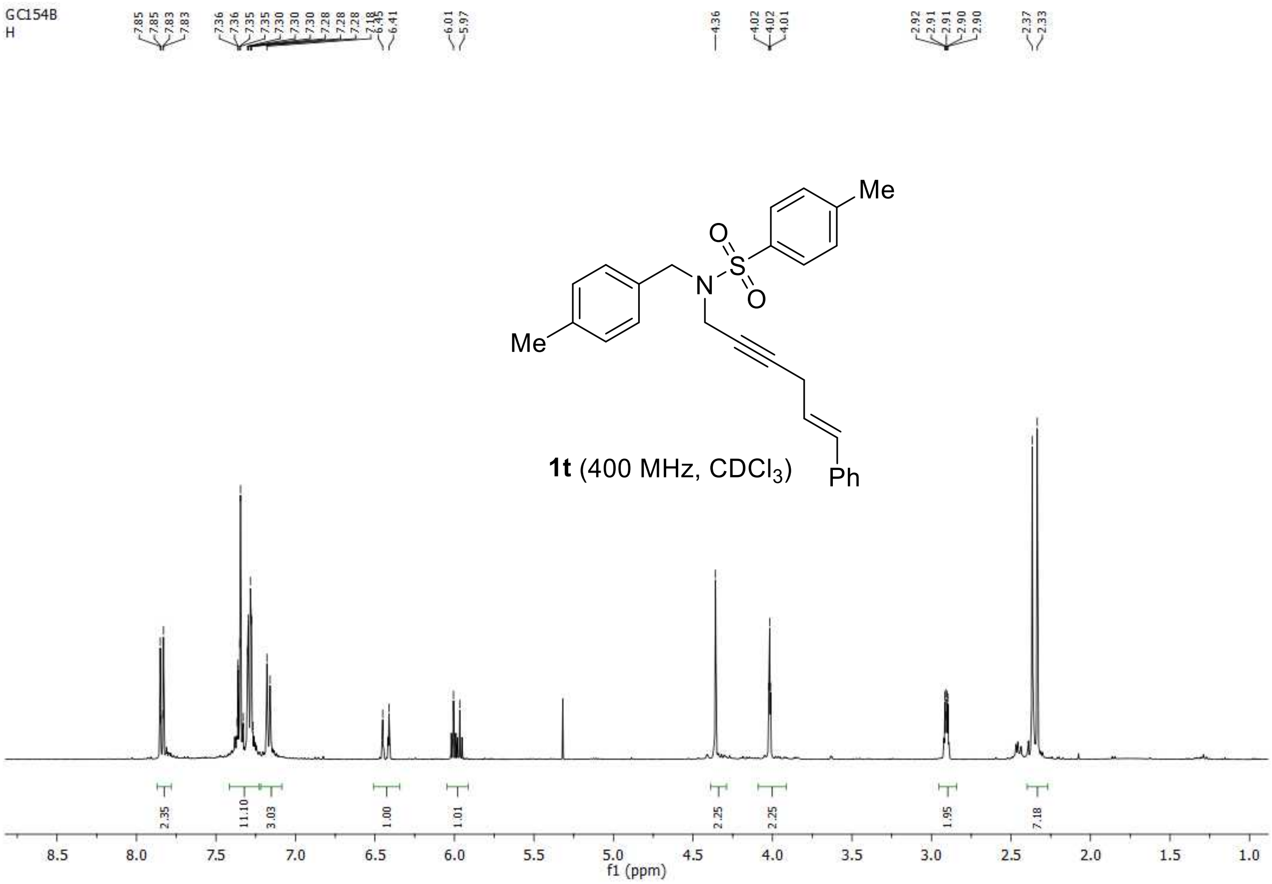

MS19
C
1r (101 MHz, CDCl3)
f1 (ppm)

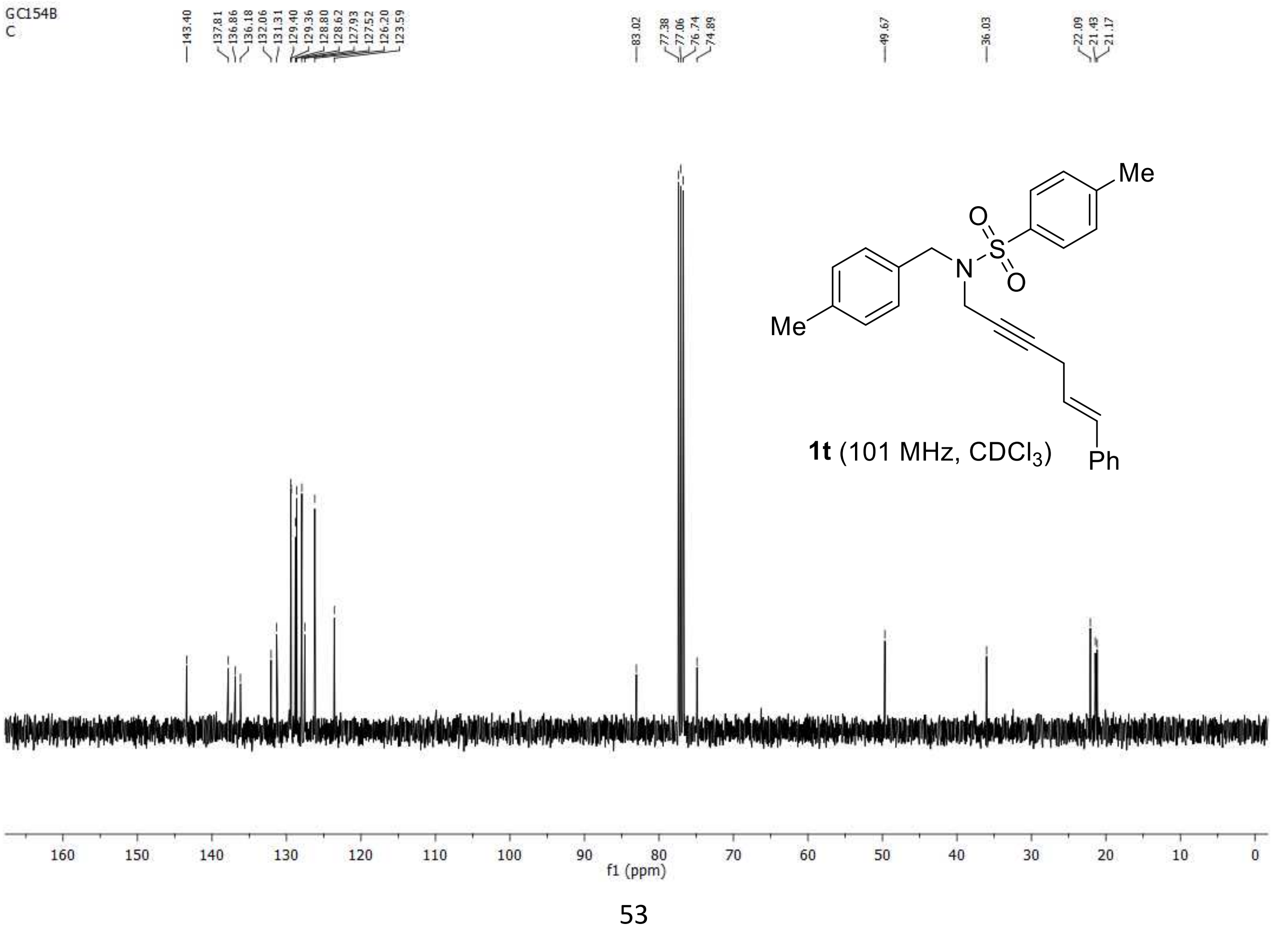


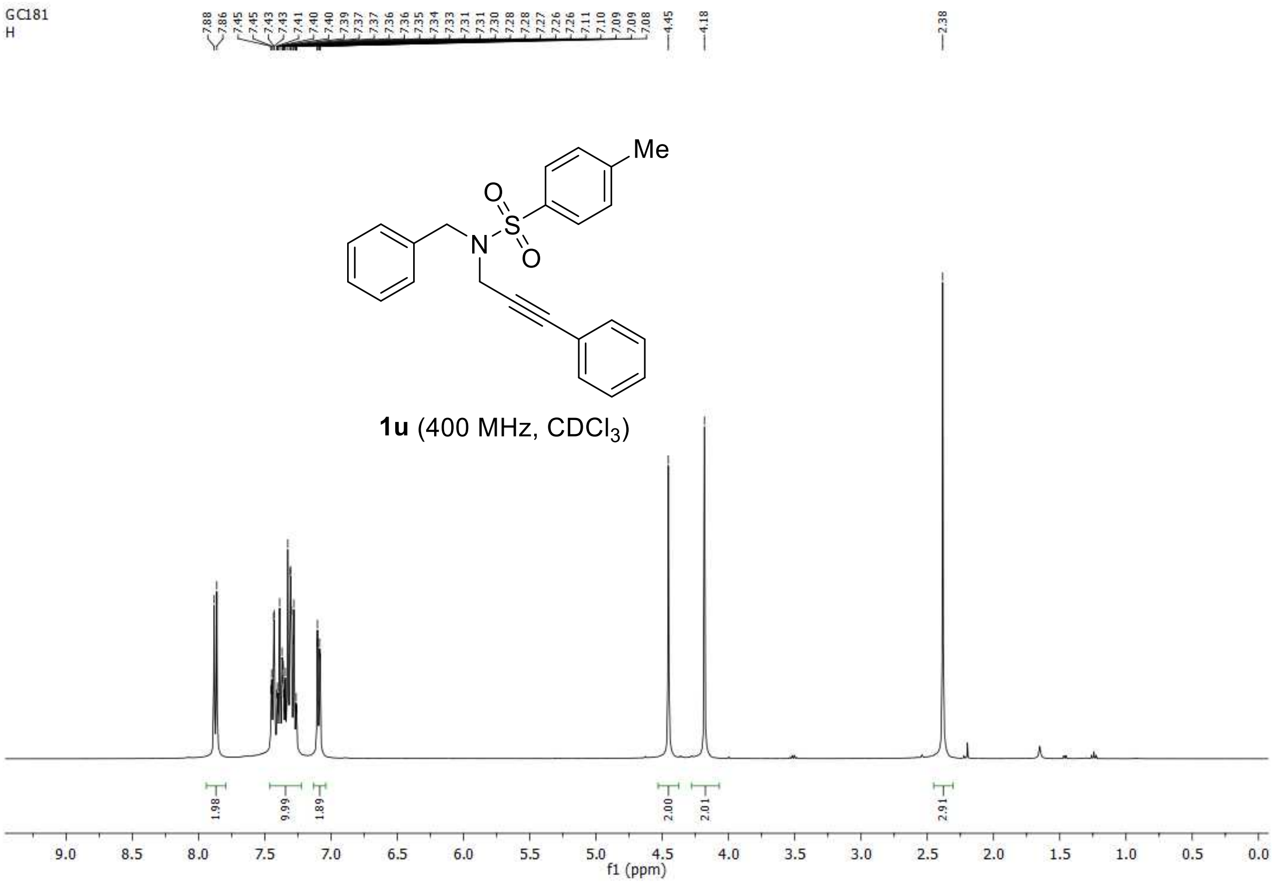
1s (300 MHz, $CDCl_3$)

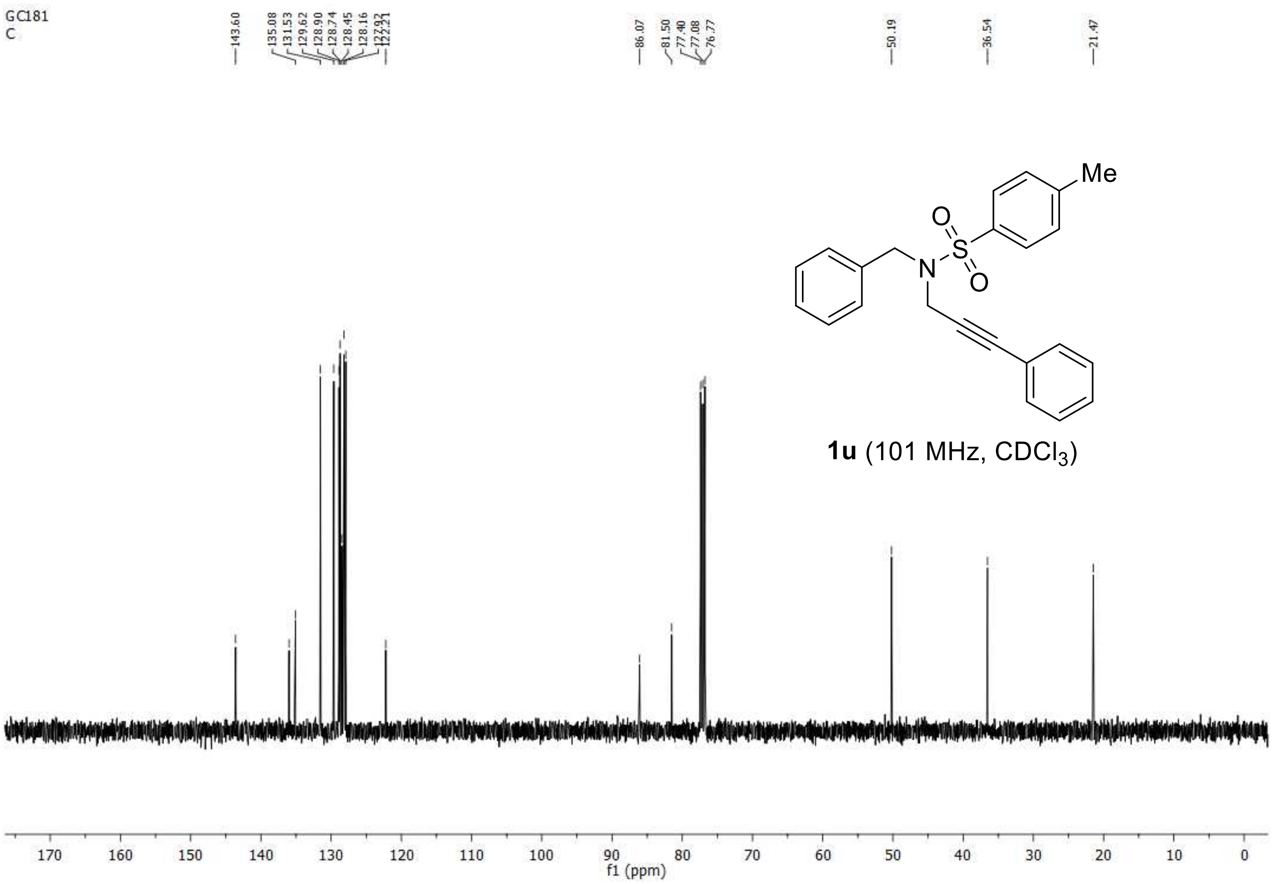


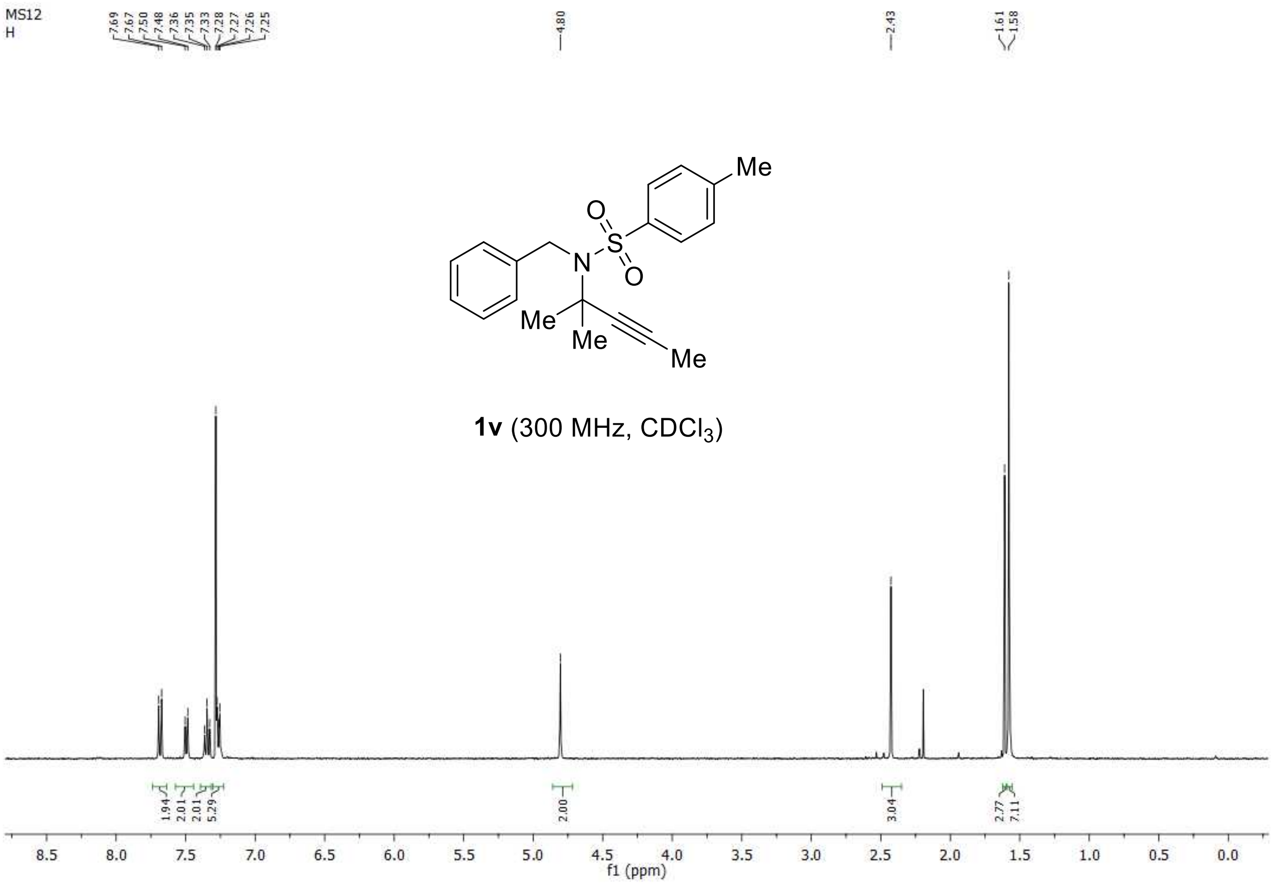
1s (75 MHz, $CDCl_3$)

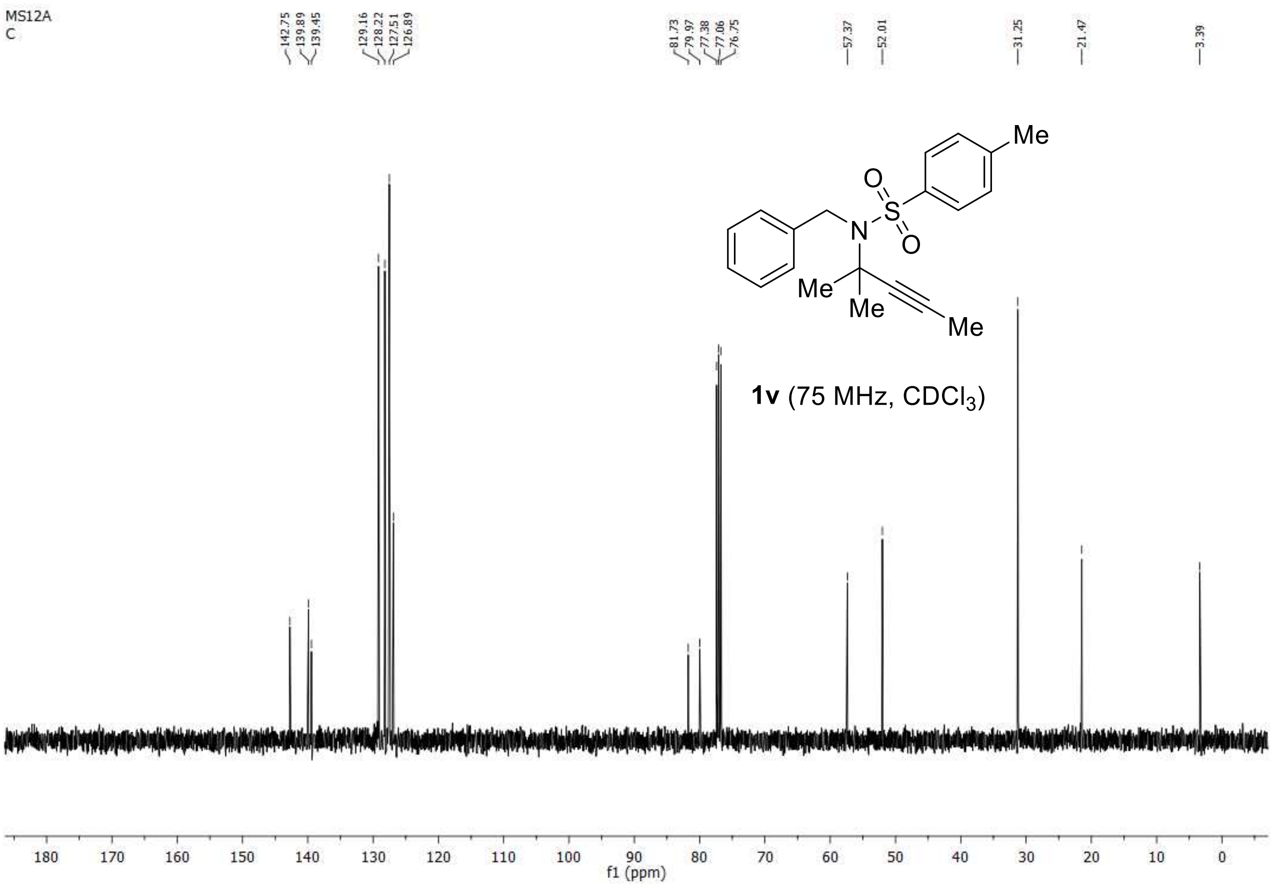

GC154B
H
7.85 7.85 7.83 7.83
7.36 7.36 7.35 7.35 7.30 7.30 7.30 7.28 7.28 7.28 7.18 6.45 6.41
6.01 5.97
4.36
4.02 4.02 4.01
2.92 2.91 2.91 2.90 2.90
2.37 2.33
Me
O
S
O
N
Me
Ph
1t (400 MHz, CDCl3)
2.35
11.10
3.03
1.00
1.01
2.25
2.25
1.95
7.18
f1 (ppm)

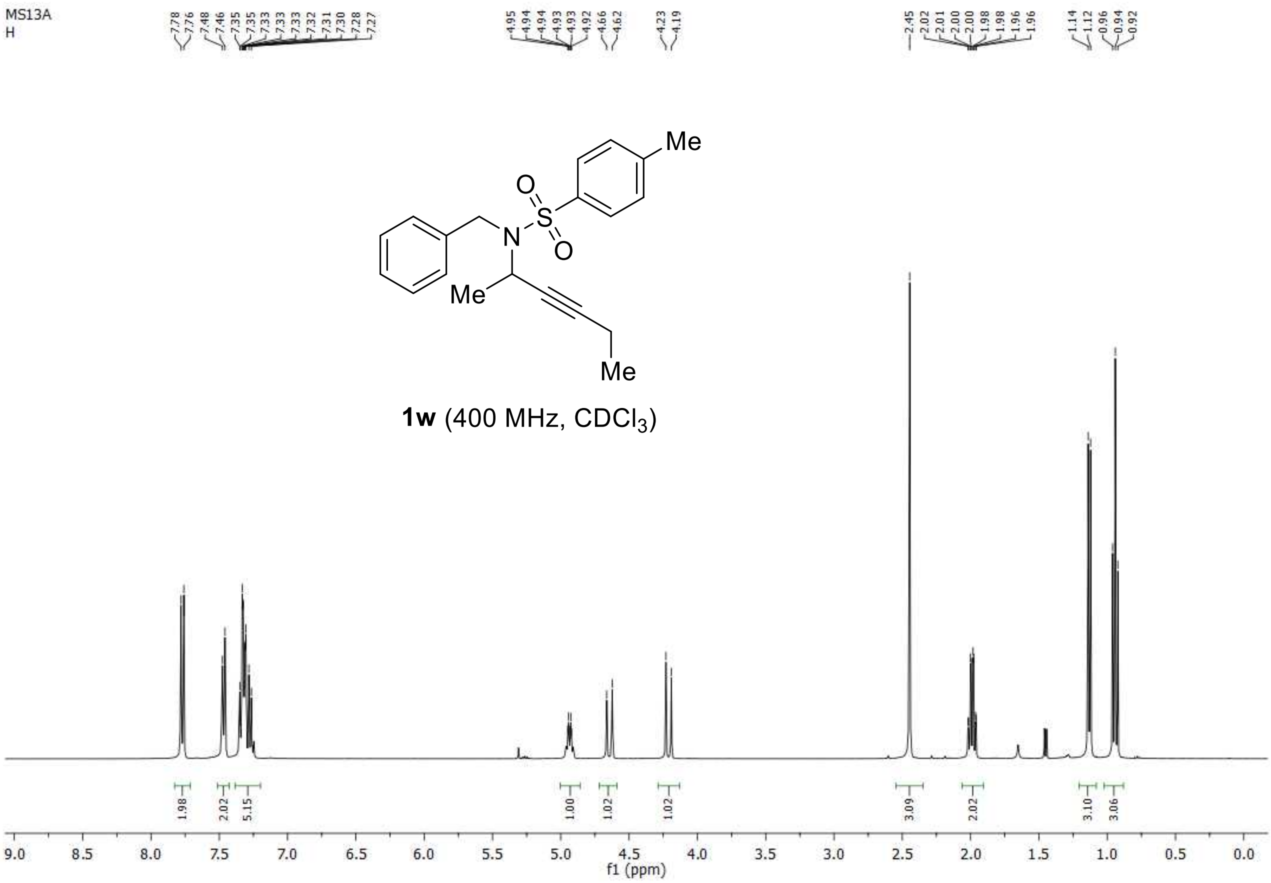

GC154B
C
143.40
137.81 136.86 136.18 132.06 131.31 129.40 129.36 128.80 128.62 127.93 127.52 126.20 123.59
83.02
77.38 77.06 76.74 74.89
49.67
36.03
22.09 21.43 21.17
Me
O
S
O
N
Me
Ph
1t (101 MHz, CDCl3)
f1 (ppm)

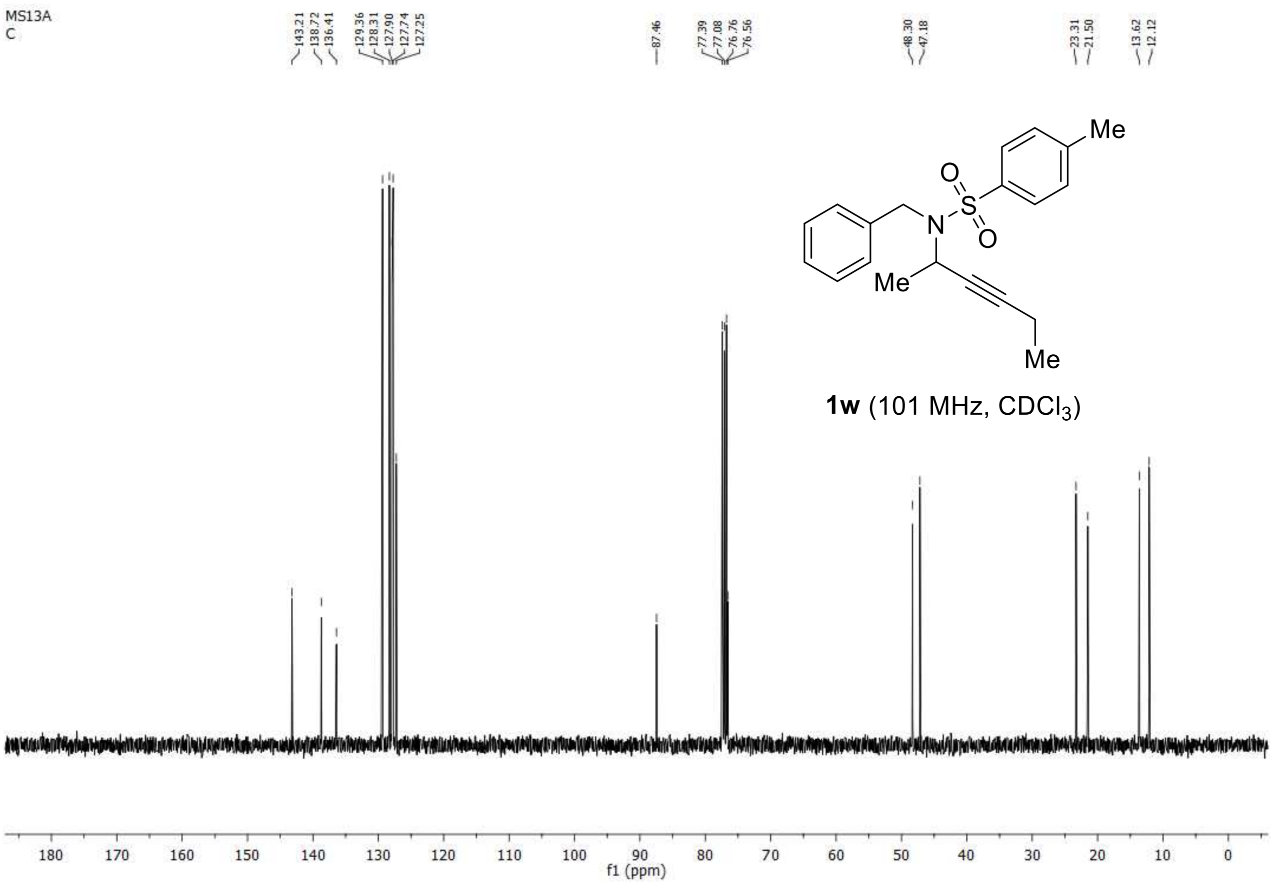

GC181
H
7.88
7.86
7.45
7.43
7.43
7.41
7.40
7.39
7.37
7.37
7.36
7.36
7.35
7.34
7.33
7.31
7.31
7.30
7.28
7.28
7.27
7.26
7.26
7.11
7.10
7.09
7.09
7.08
4.45
4.18
2.38
Me
O
S
O
N
1u (400 MHz, CDCl3)
1.98
9.99
1.89
2.00
2.01
2.91
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

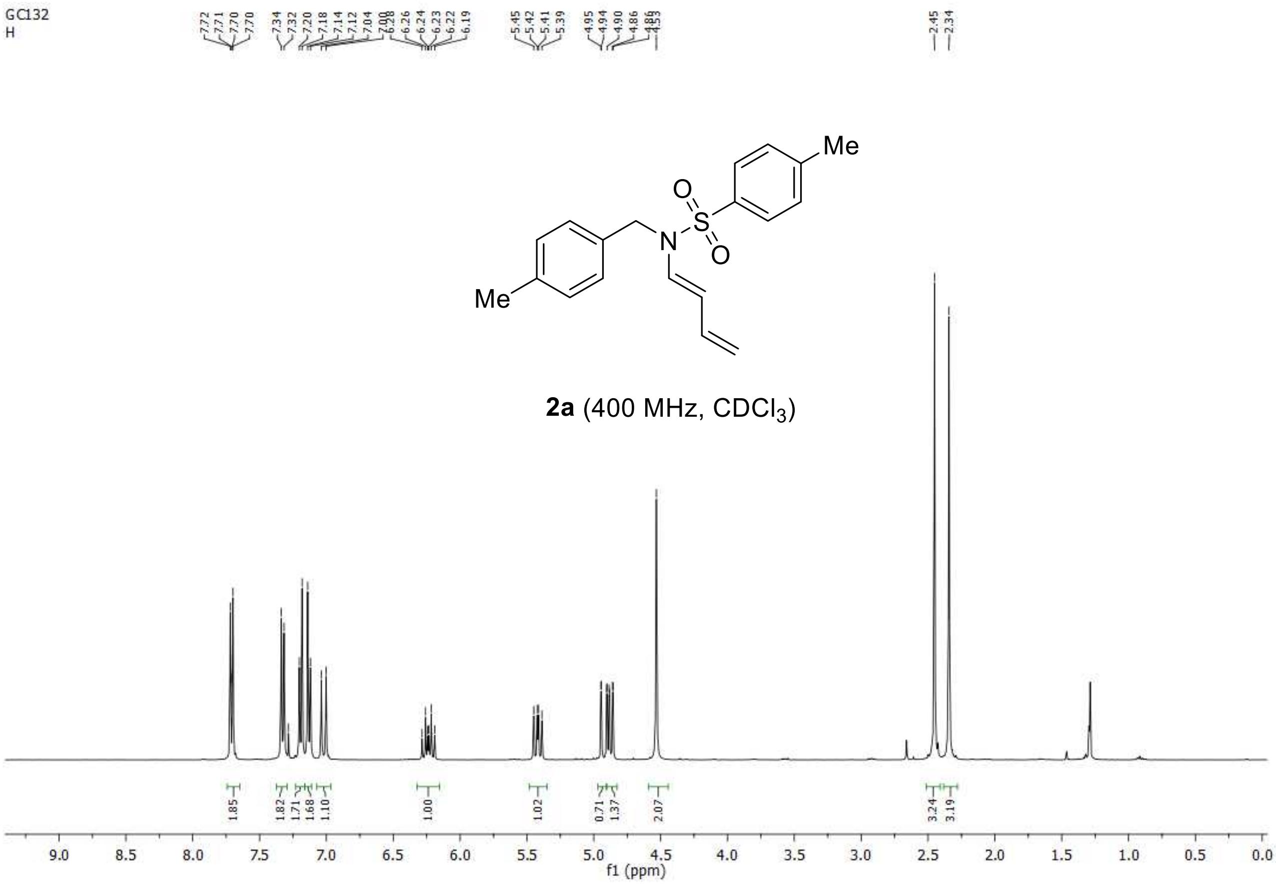

GC181
C
143.60
135.08
131.53
129.62
128.90
128.74
128.45
128.16
122.21
86.07
81.50
77.40
77.08
76.77
50.19
36.54
21.47
Me
O
S
O
N
1u (101 MHz, CDCl3)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


MS12
H
7.69 7.67 7.50 7.48 7.36 7.35 7.33 7.28 7.27 7.26 7.25
4.80
2.43
1.61 1.58
Me
O
S
O
N
Me
Me
Me
1v (300 MHz, CDCl3)
1.94 2.01 2.01 5.29
2.00
3.04
2.77 7.11
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
f1 (ppm)

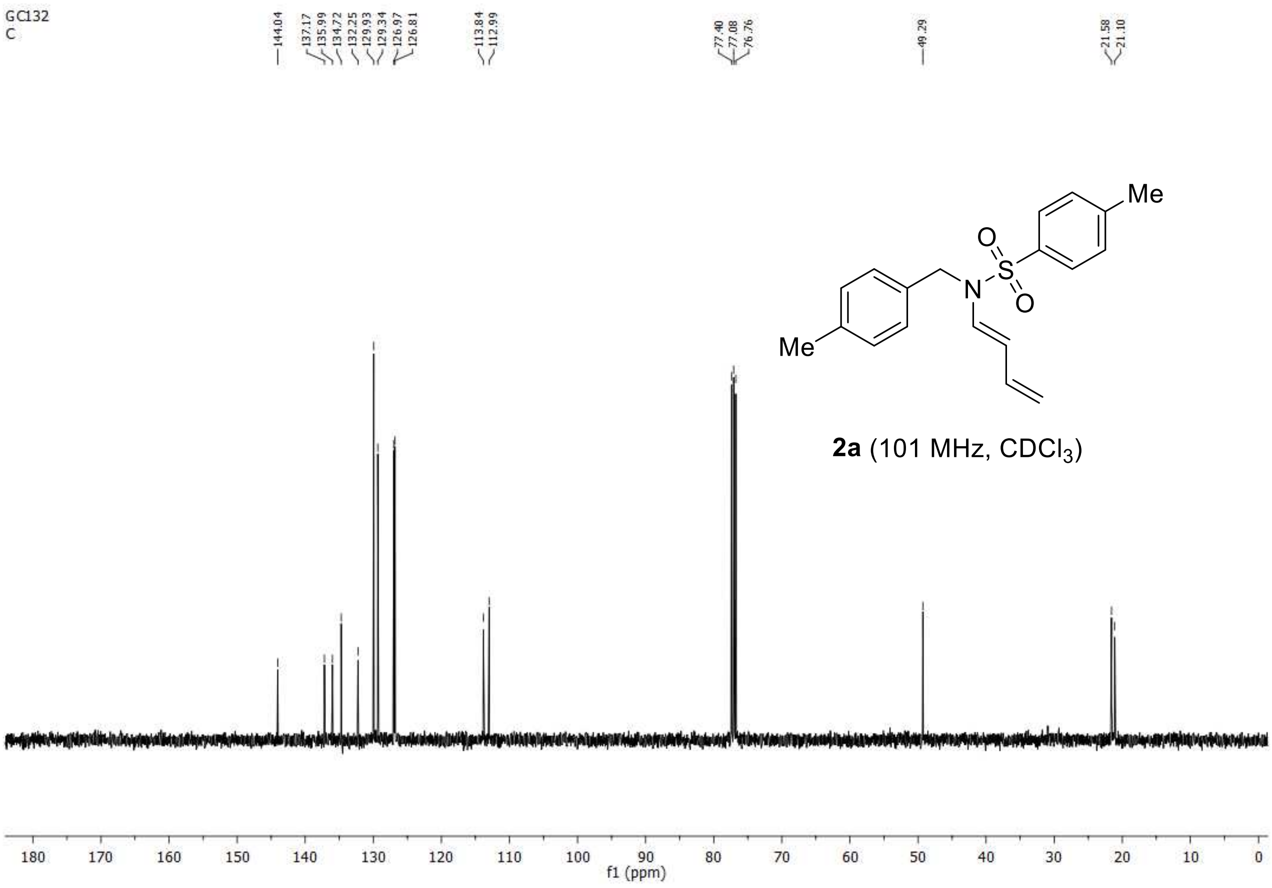

MS12A
C
142.75 139.89 139.45
129.16 128.22 127.51 126.89
81.73 79.97 77.38 77.06 76.75
57.37
52.01
31.25
21.47
3.39
Me
O
S
O
N
Me
Me
Me
1v (75 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MS13A
H
7.78 7.76 7.48 7.46 7.35 7.35 7.33 7.33 7.33 7.32 7.31 7.30 7.28 7.27
4.95 4.94 4.94 4.93 4.93 4.92 4.66 4.62
4.23 4.19
2.45 2.02 2.01 2.00 2.00 1.98 1.98 1.96 1.96
1.14 1.12 0.96 0.94 0.92
Me
O
S
O
N
Me
Me
1w (400 MHz, CDCl3)
1.98 2.02 5.15 1.00 1.02 1.02 3.09 2.02 3.10 3.06
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
f1 (ppm)

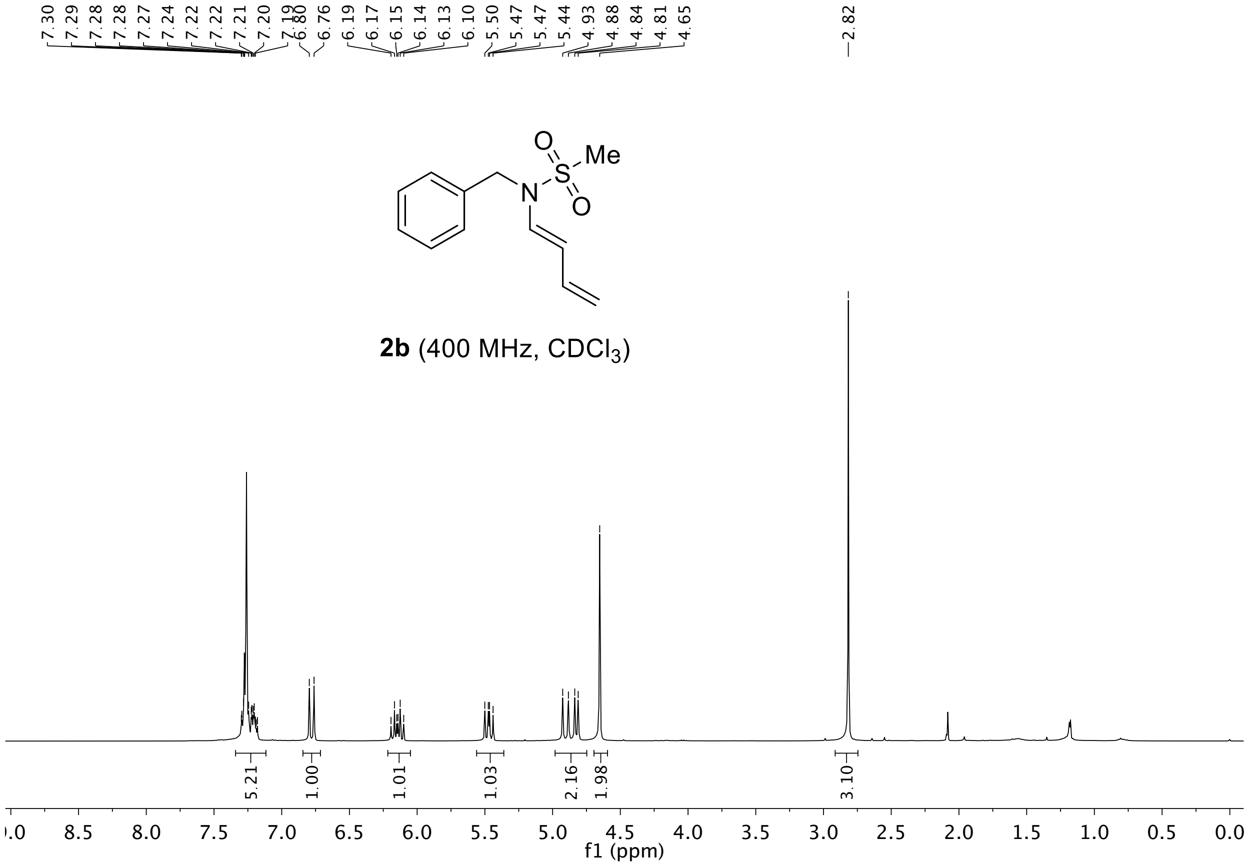

MS13A
C
143.21 138.72 136.41
129.36 128.31 127.90 127.74 127.25
87.46
77.39 77.08 76.76 76.56
48.30 47.18
23.31 21.50
13.62 12.12
Me
O
S
O
N
Me
Me
1w (101 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

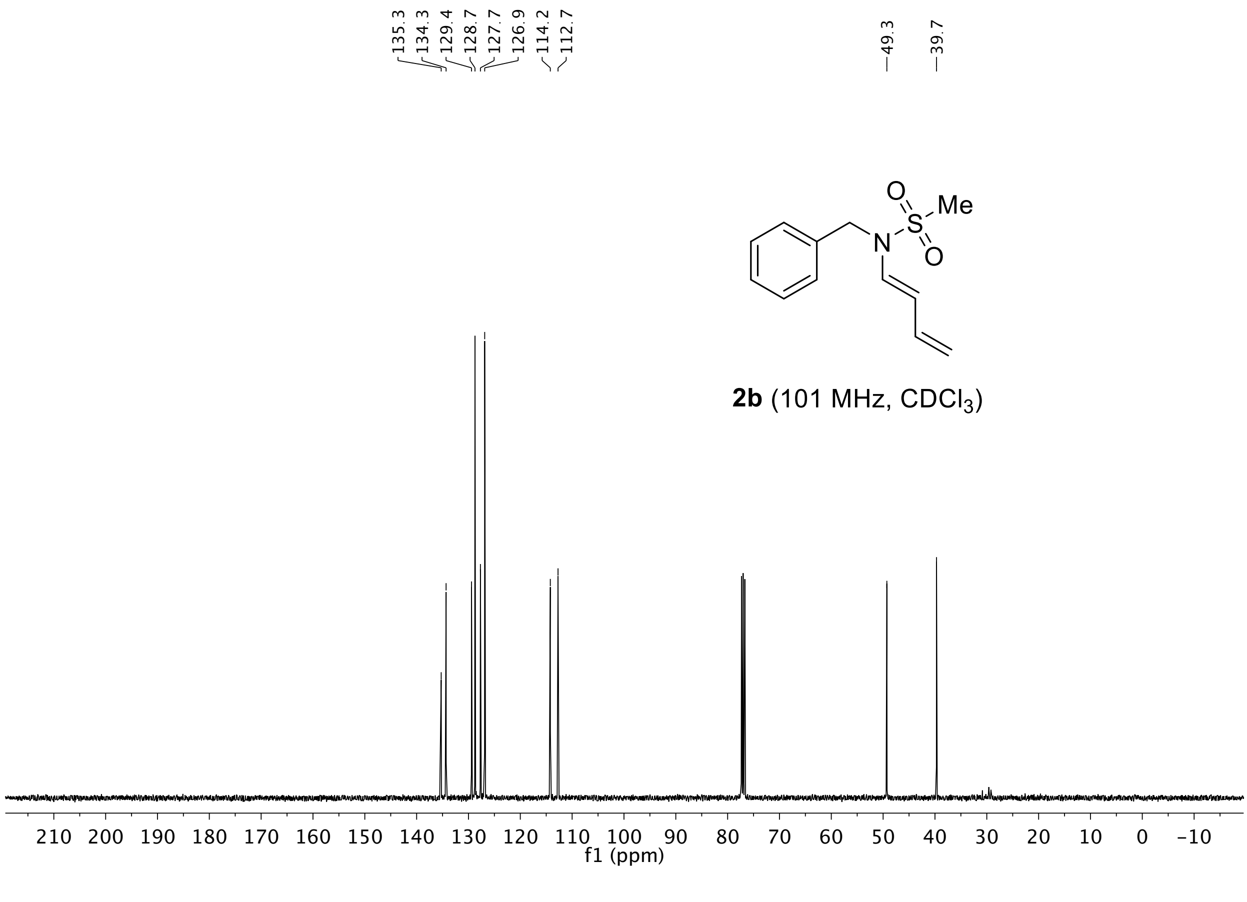


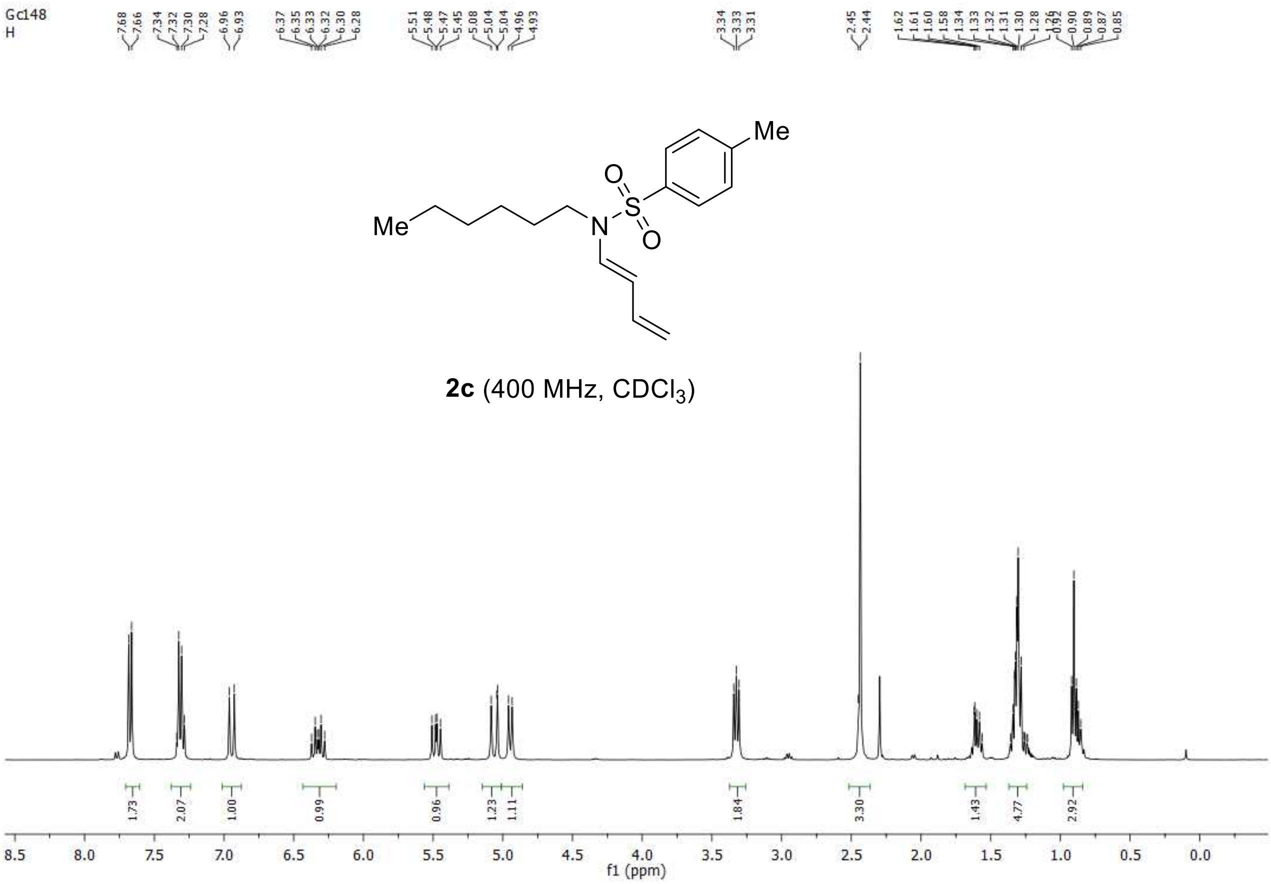
2a (400 MHz, $CDCl_3$)



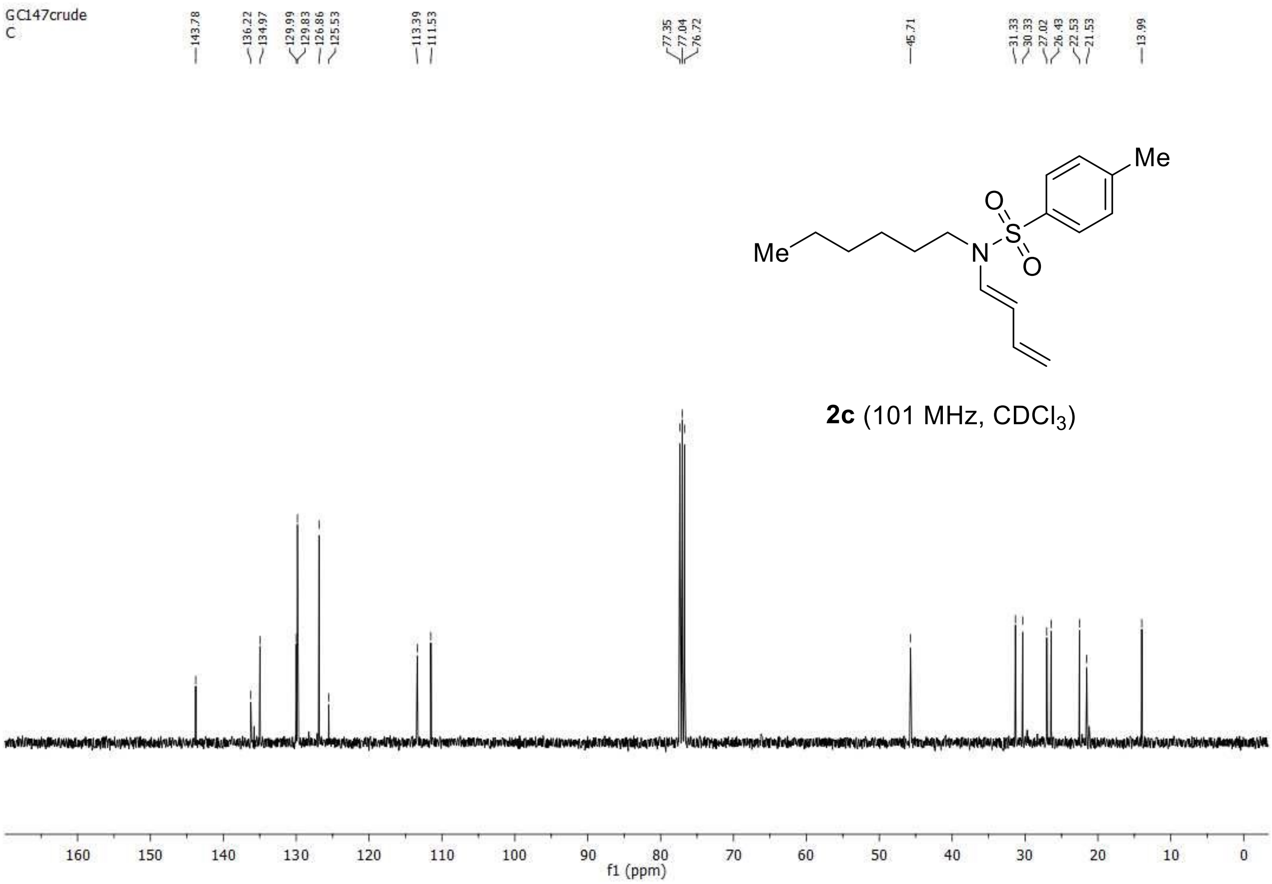
2a (101 MHz, $CDCl_3$)


7.30 7.29 7.28 7.28 7.27 7.24 7.22 7.22 7.21 7.20 7.19 6.80 6.76 6.19 6.17 6.15 6.14 6.13 6.10 5.50 5.47 5.47 5.44 4.93 4.88 4.84 4.81 4.65
2.82
O
S
Me
N
O
2b (400 MHz, CDCl3)
5.21 1.00 1.01 1.03 2.16 1.98 3.10
f1 (ppm)

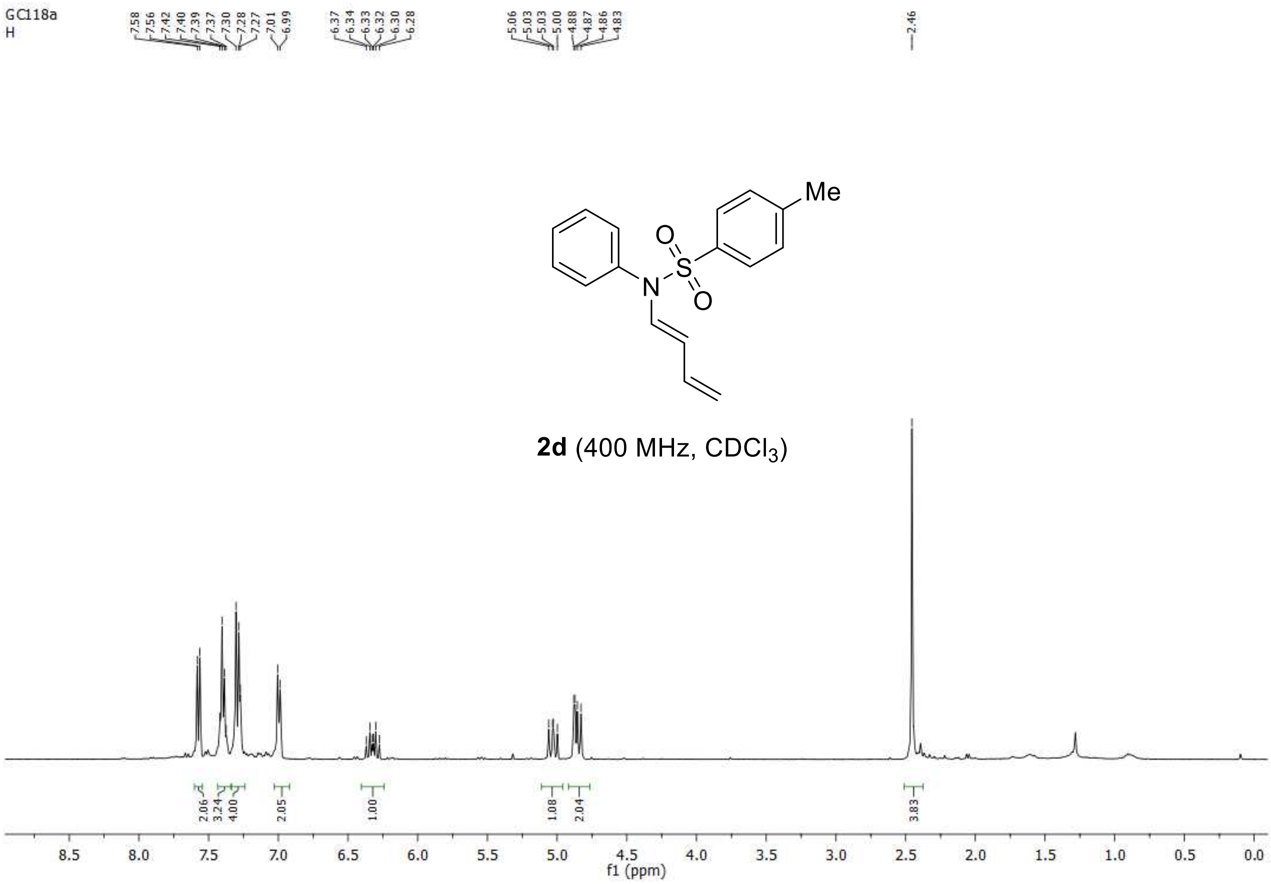

135.3 134.3 129.4 128.7 127.7 126.9 114.2 112.7
49.3
39.7
O
S
Me
N
O
2b (101 MHz, CDCl3)
f1 (ppm)



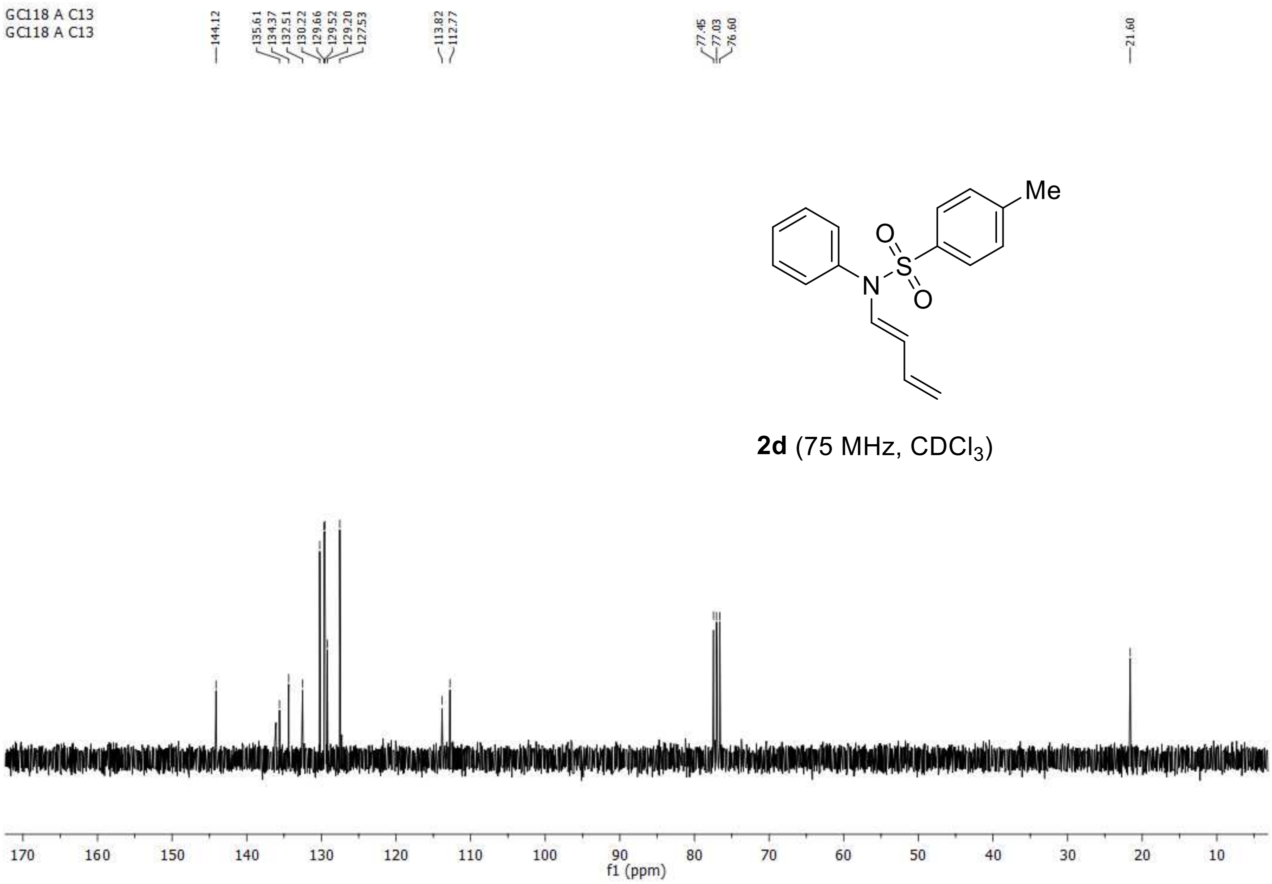
2c (400 MHz, $CDCl_3$)



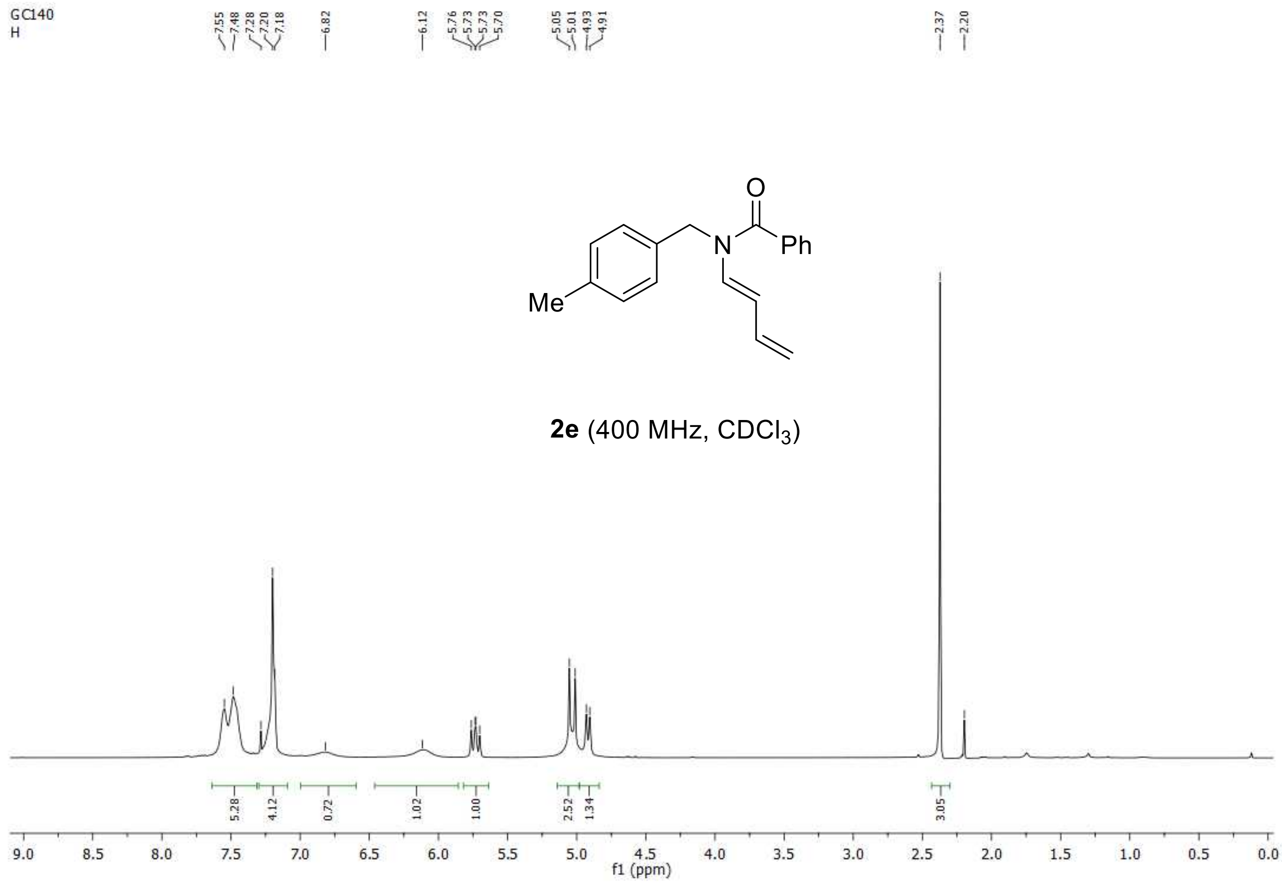
2c (101 MHz, $CDCl_3$)



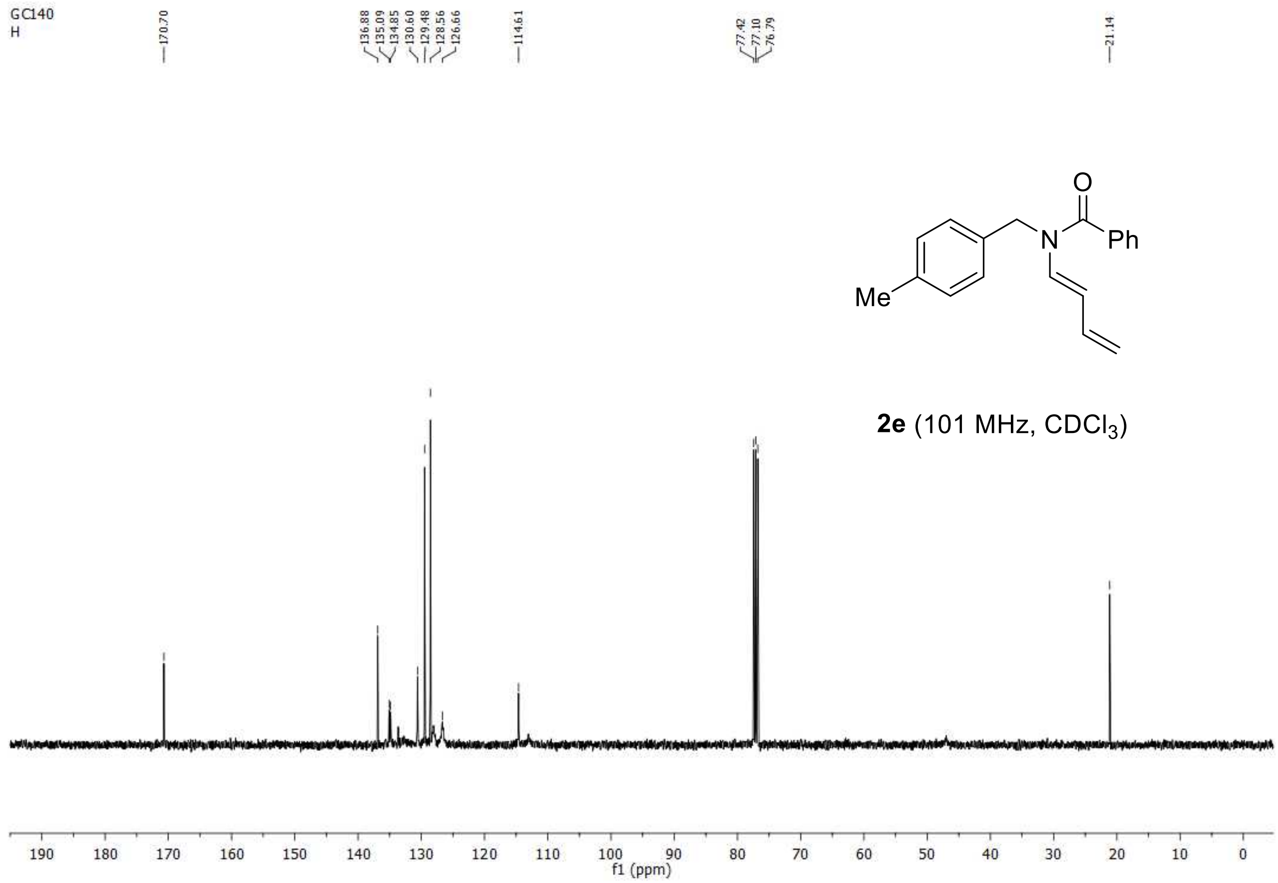
2d (400 MHz, $CDCl_3$)



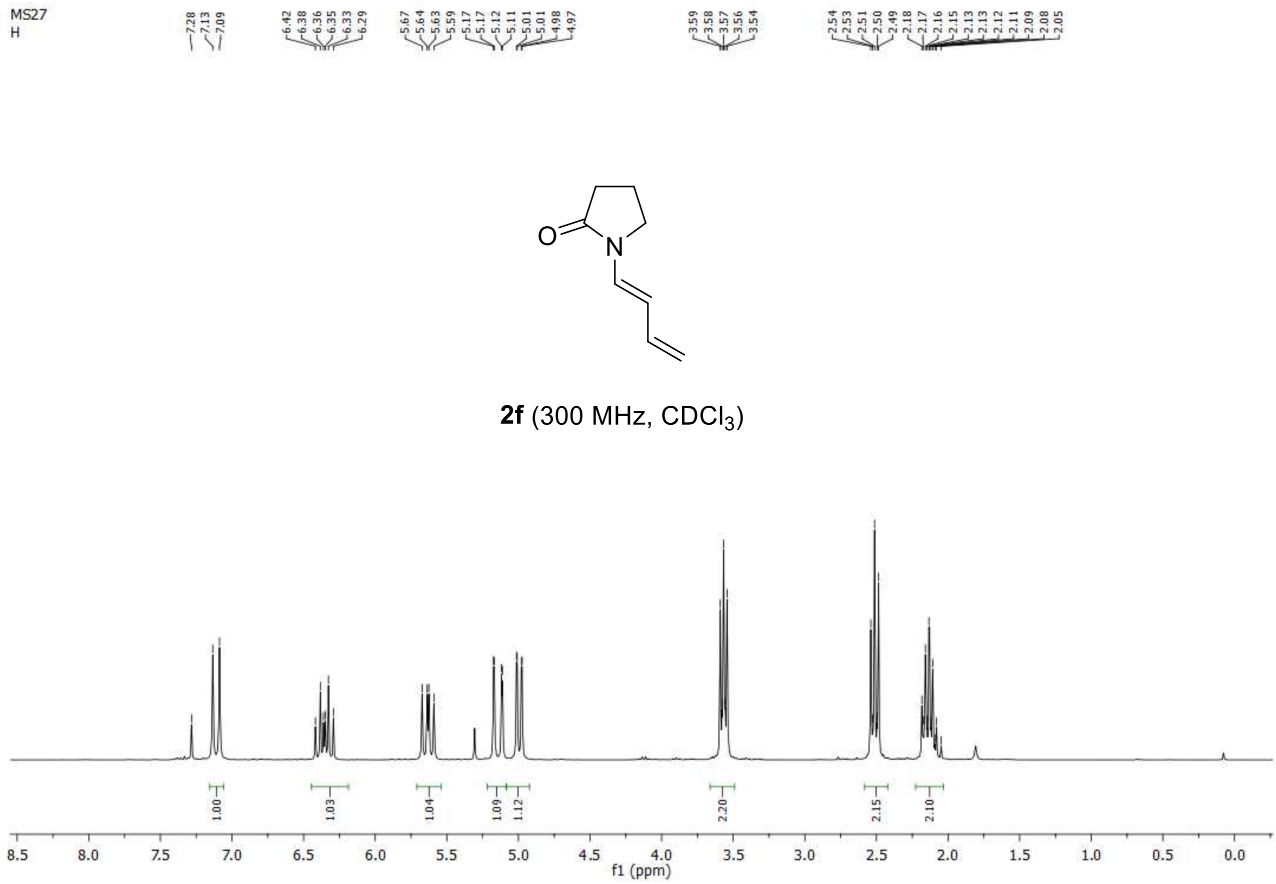
2d (75 MHz, $CDCl_3$)



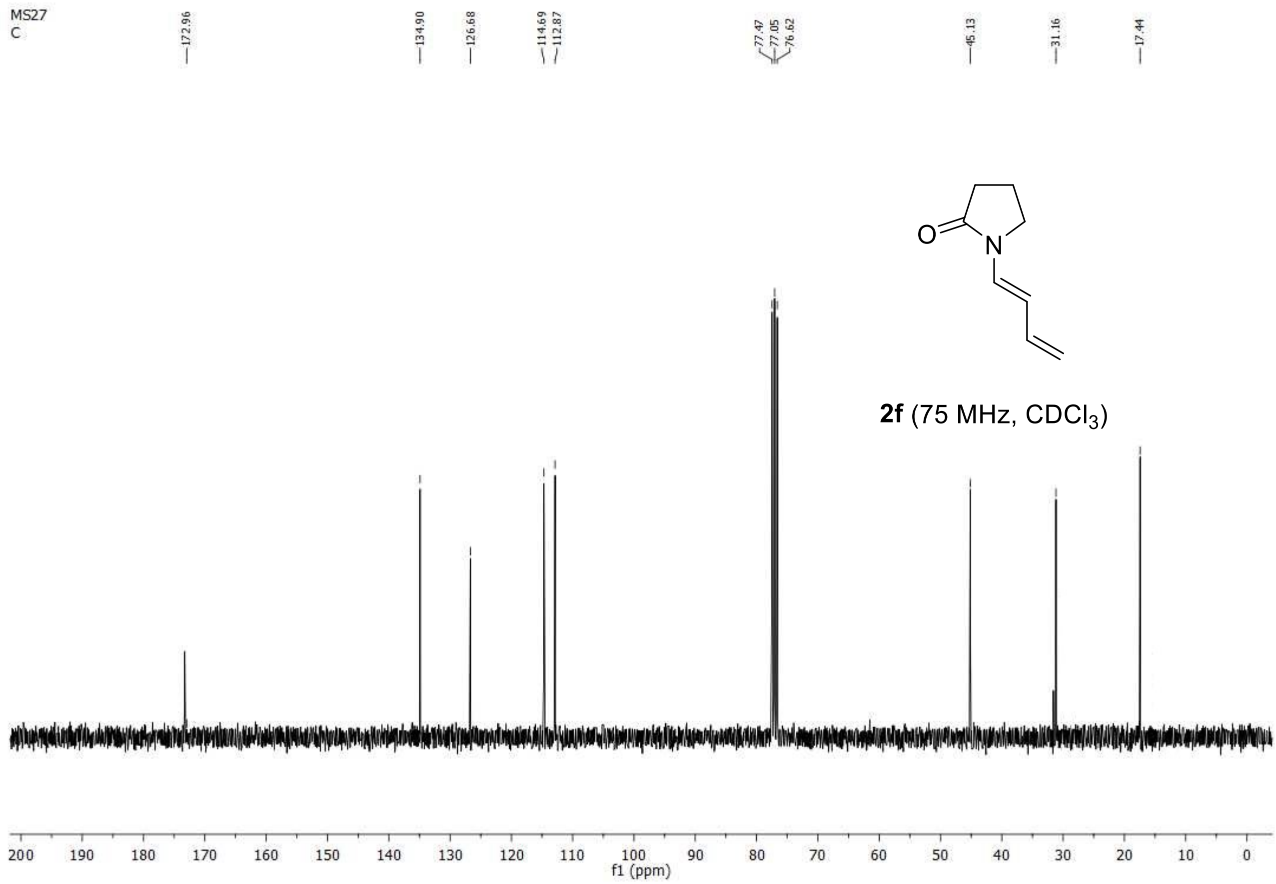
2e (400 MHz, $CDCl_3$)



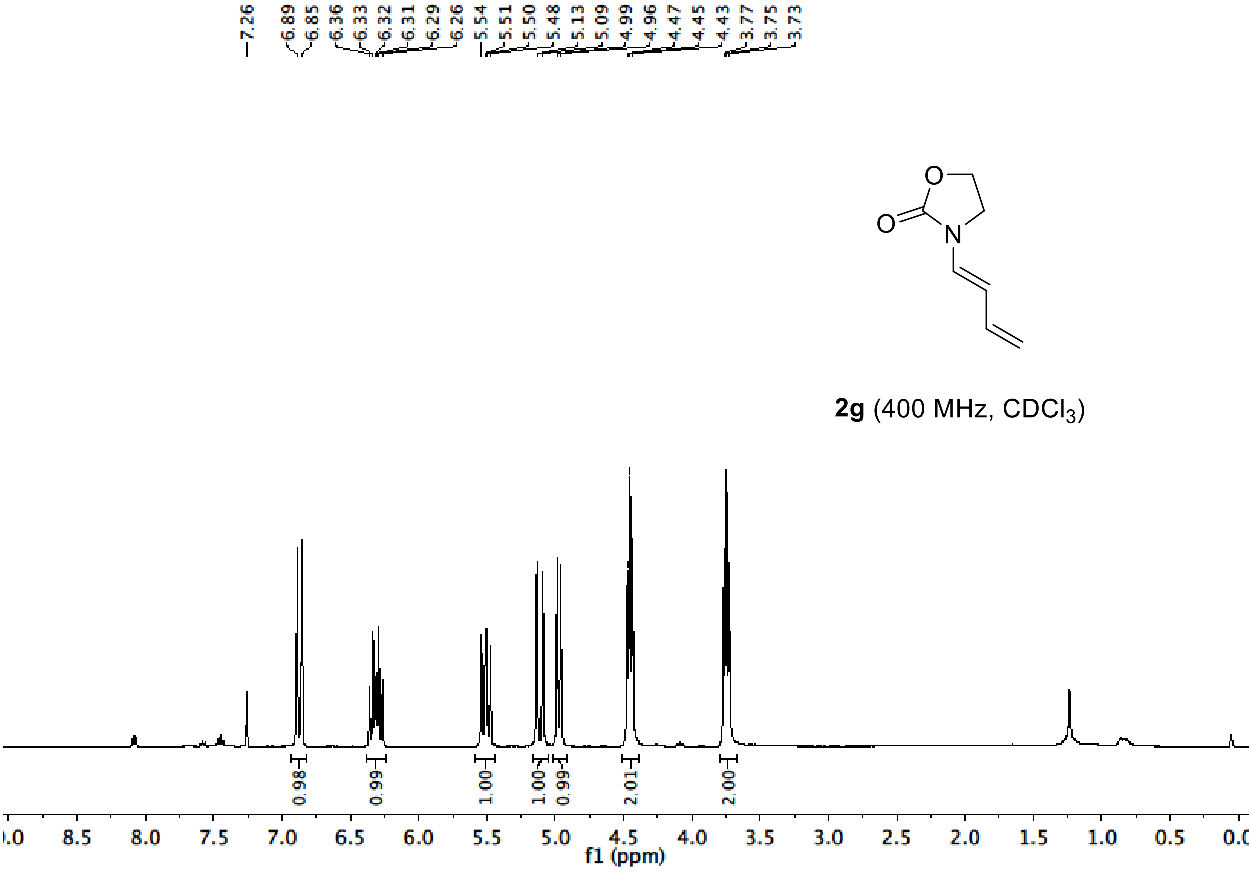
2e (101 MHz, $CDCl_3$)



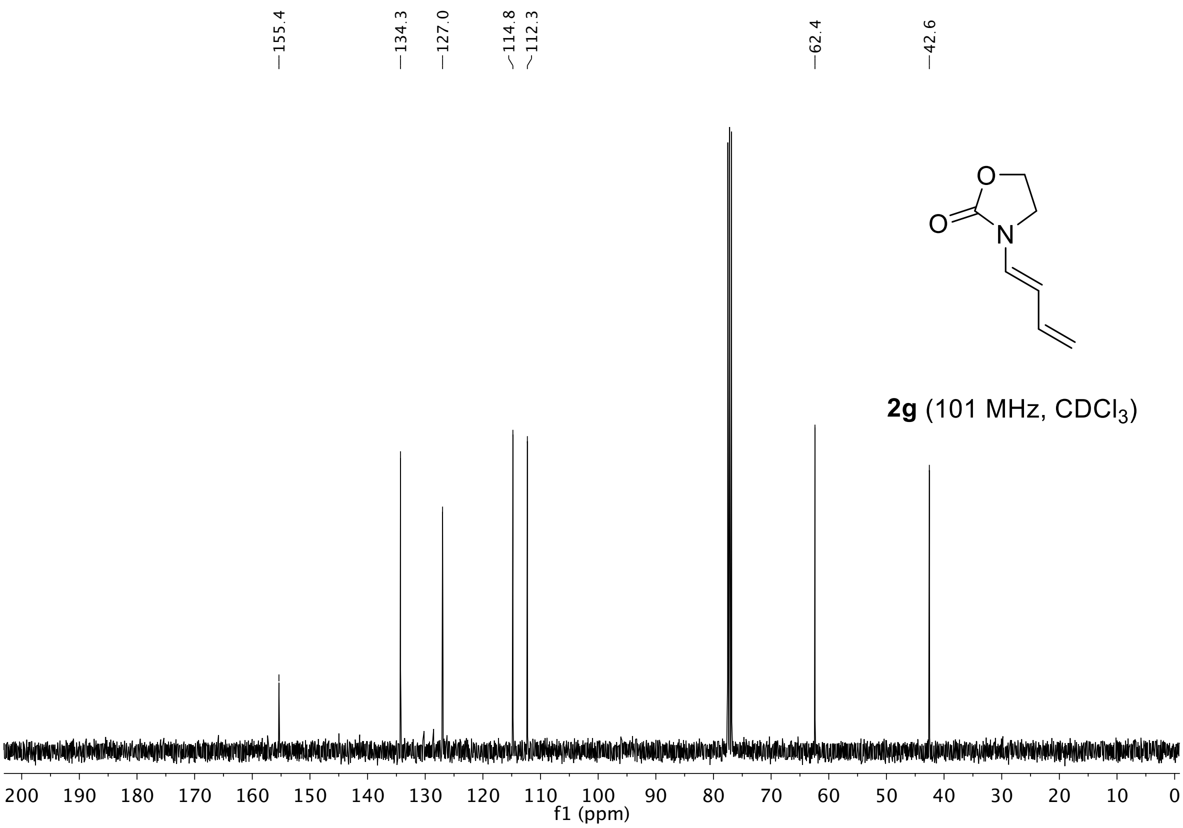
2f (300 MHz, $CDCl_3$)



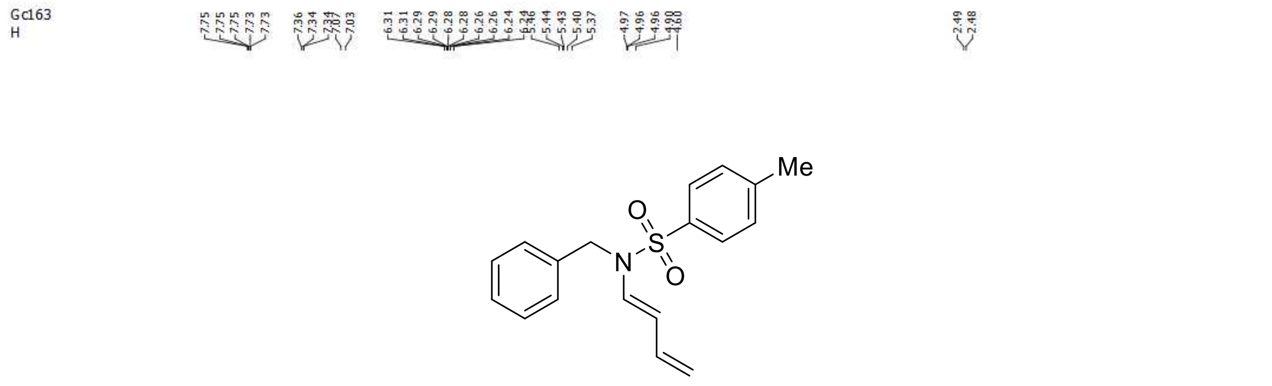
2f (75 MHz, $CDCl_3$)



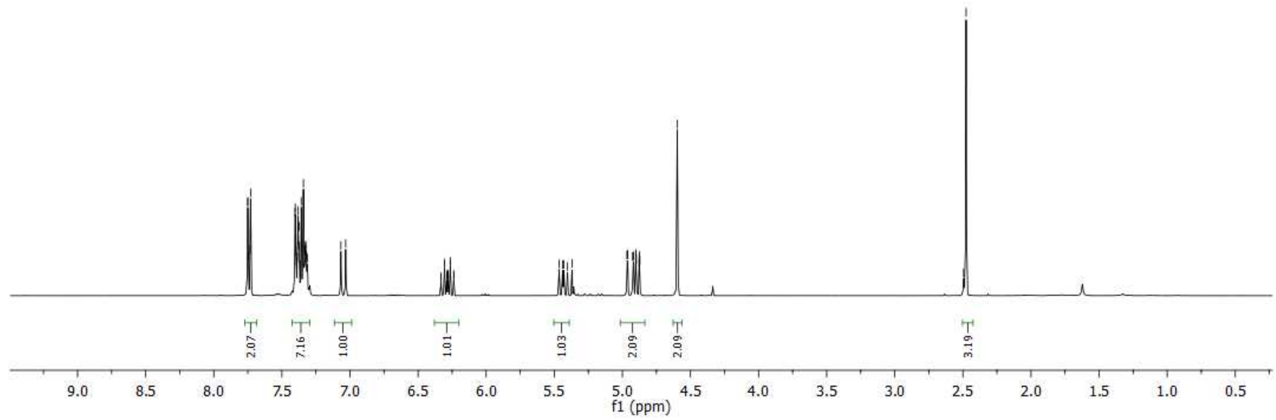
2g (400 MHz, $CDCl_3$)

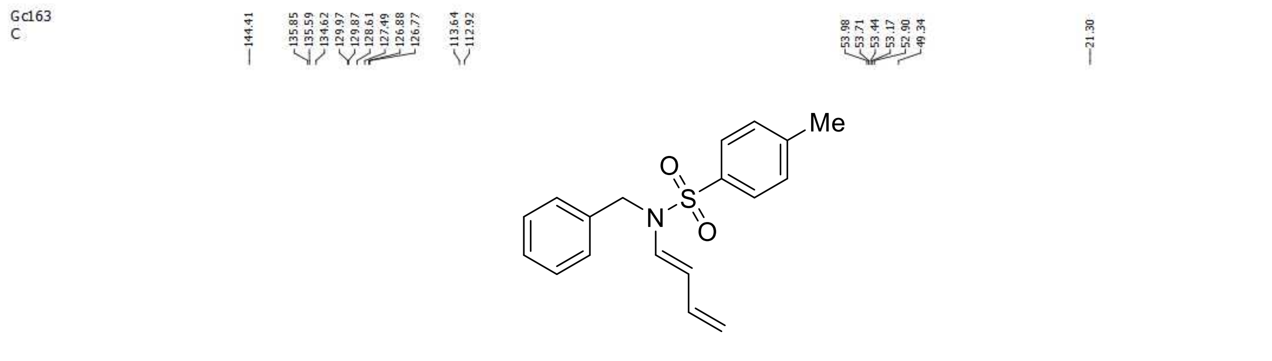


2g (101 MHz, $CDCl_3$)

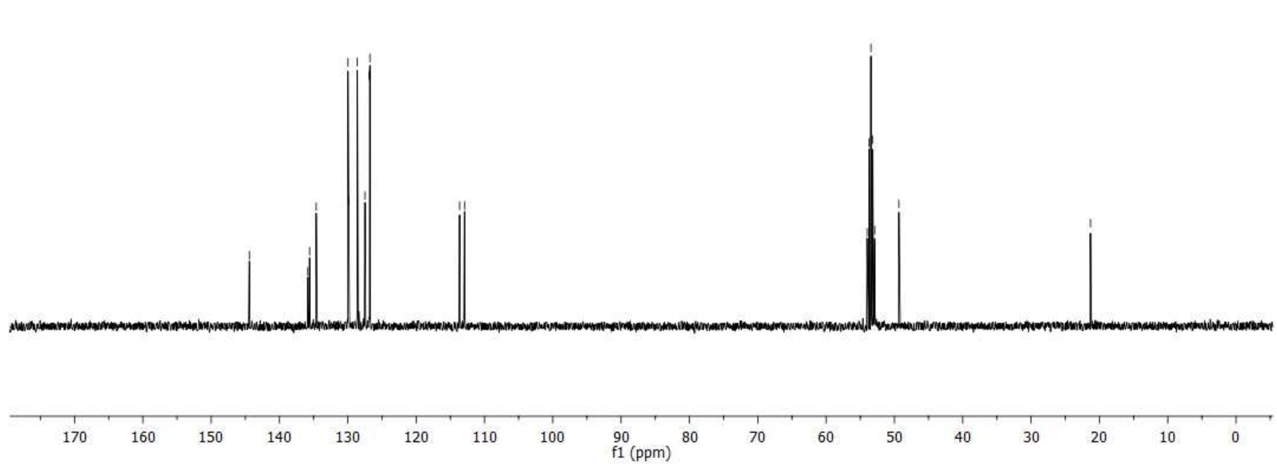


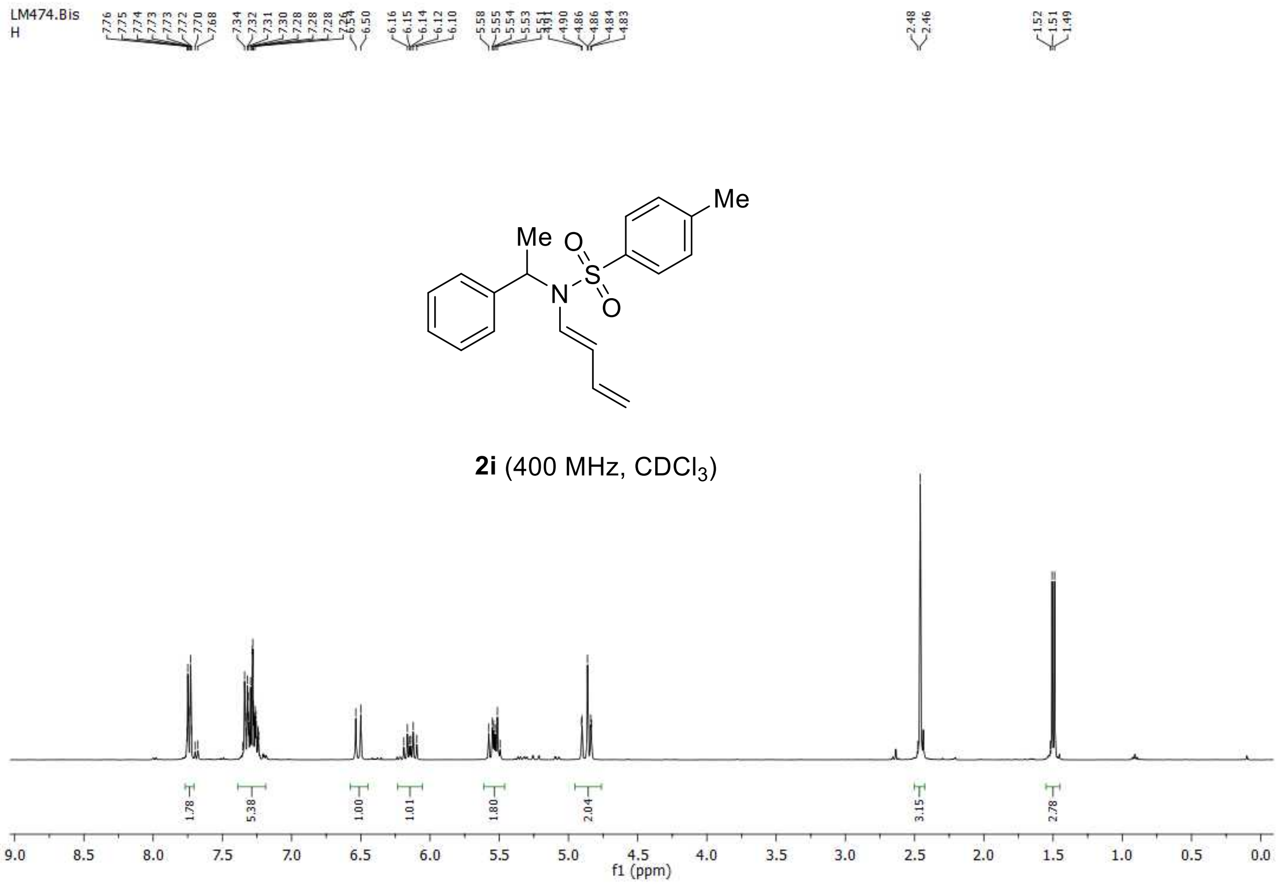
2h (400 MHz, CD_2Cl_2)



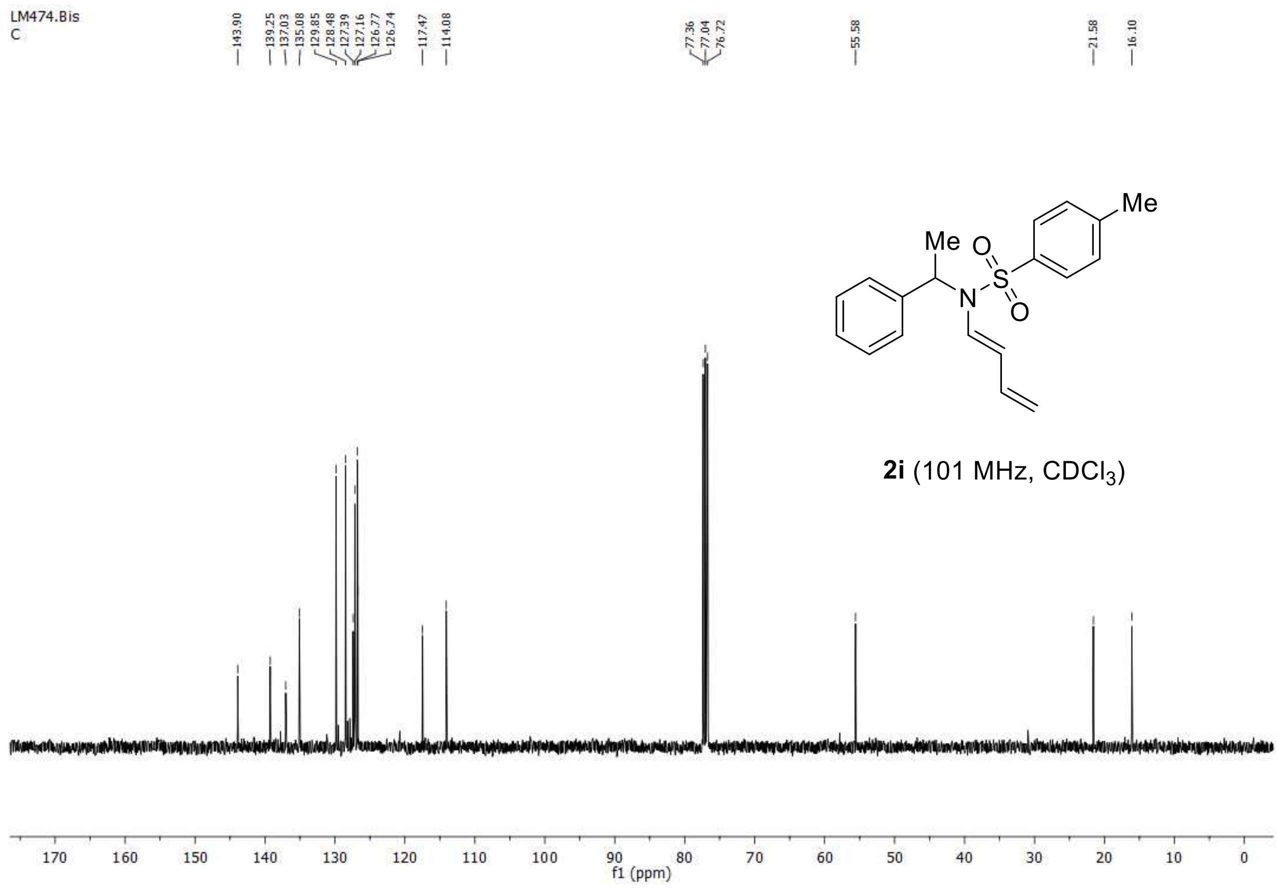


2h (101 MHz, CD_2Cl_2)

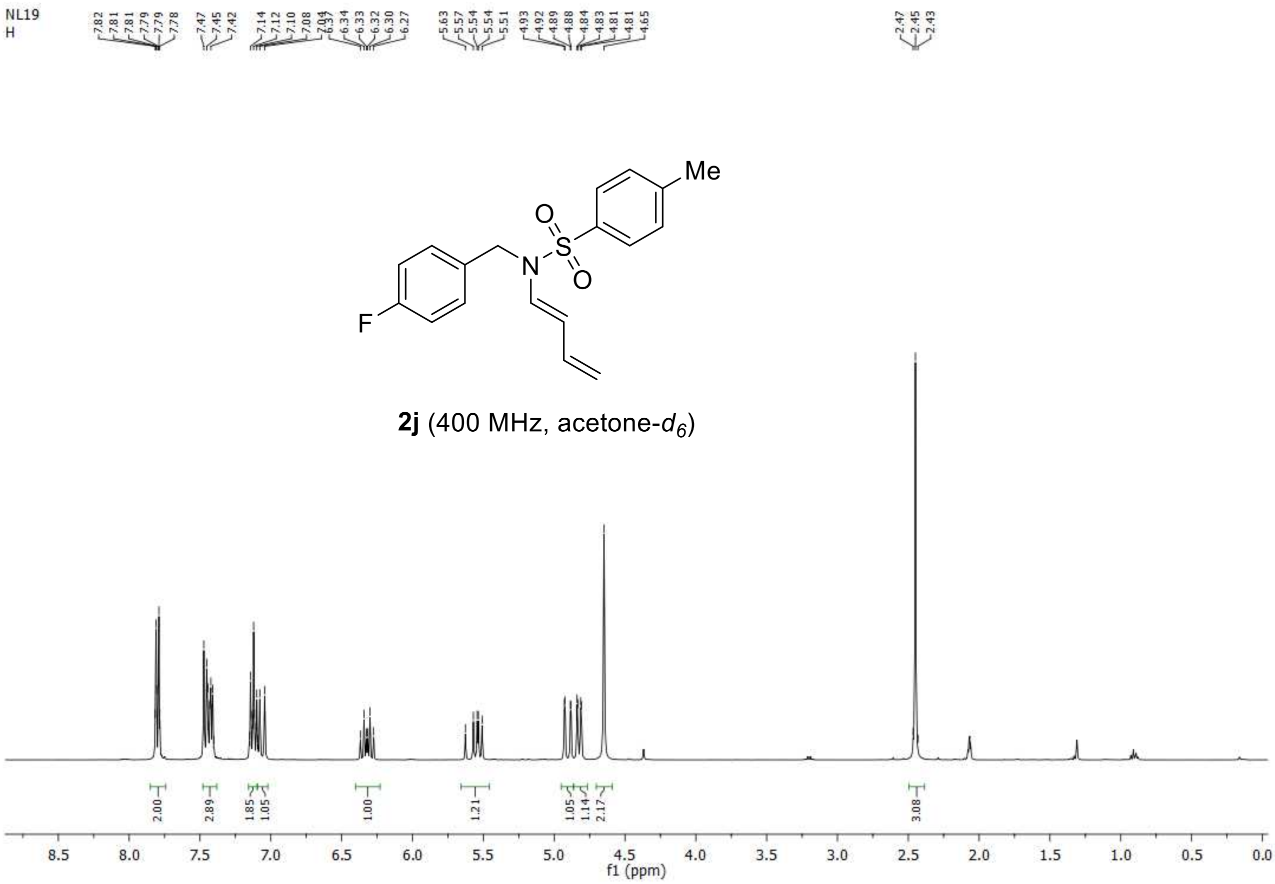




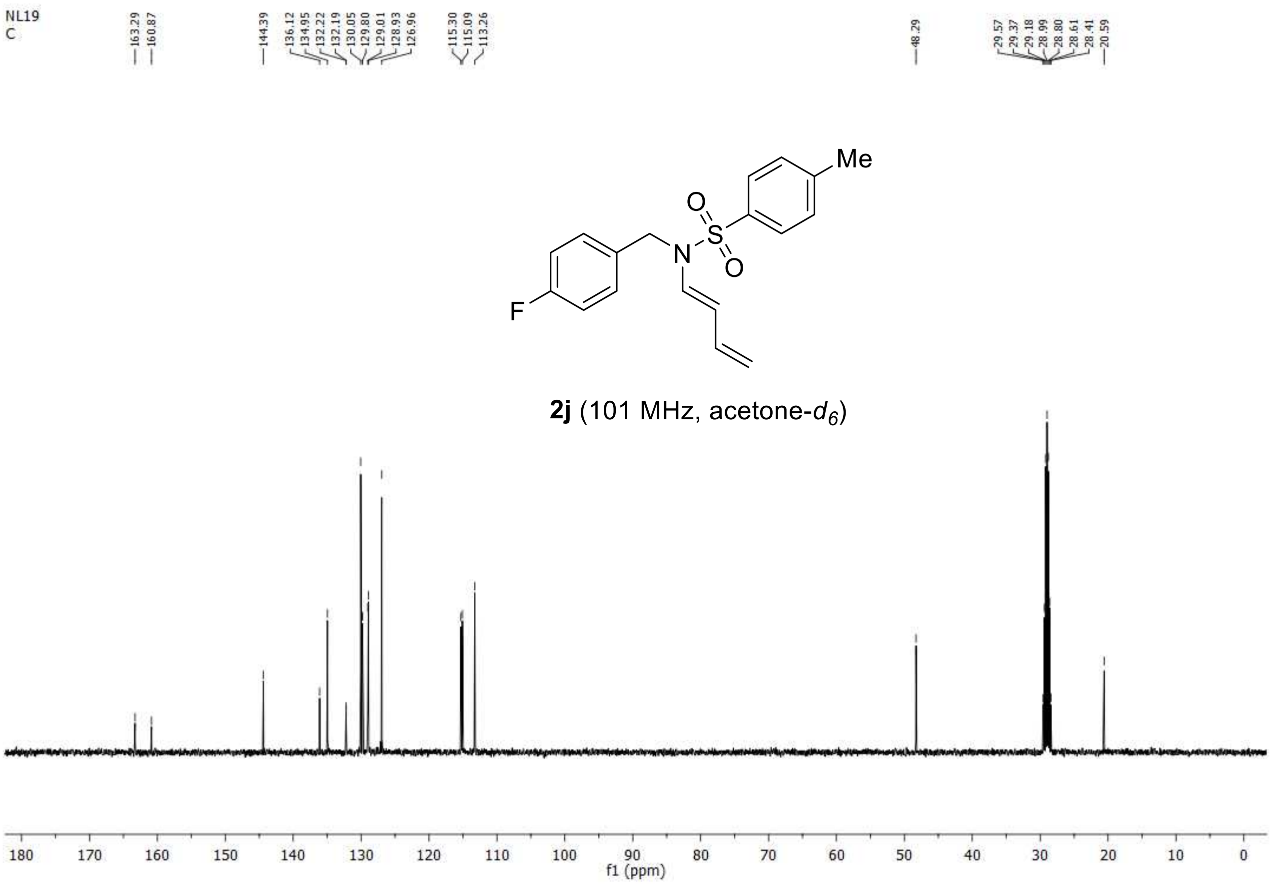
2i (400 MHz, $CDCl_3$)



2i (101 MHz, $CDCl_3$)

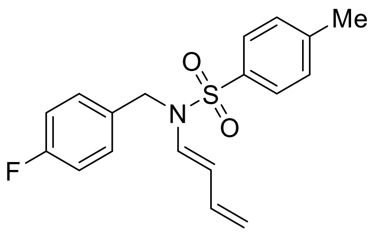


2j (400 MHz, acetone-d_6)

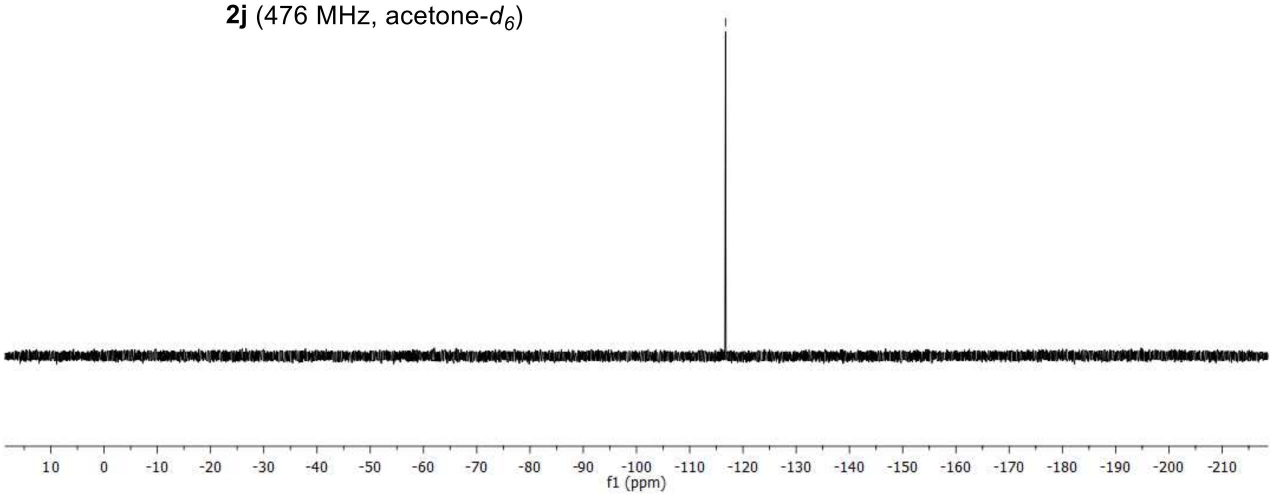


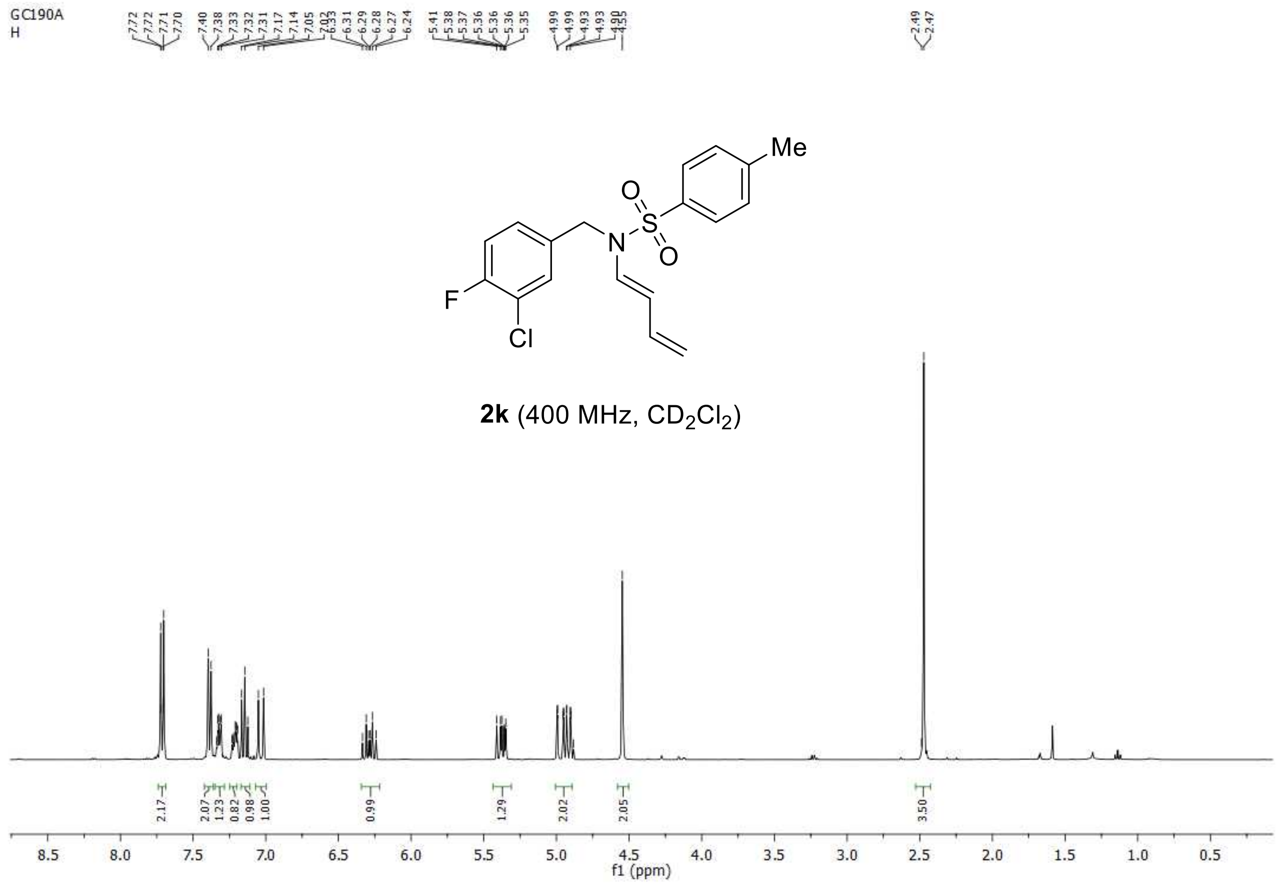
2j (101 MHz, acetone-d_6)

NL19
F

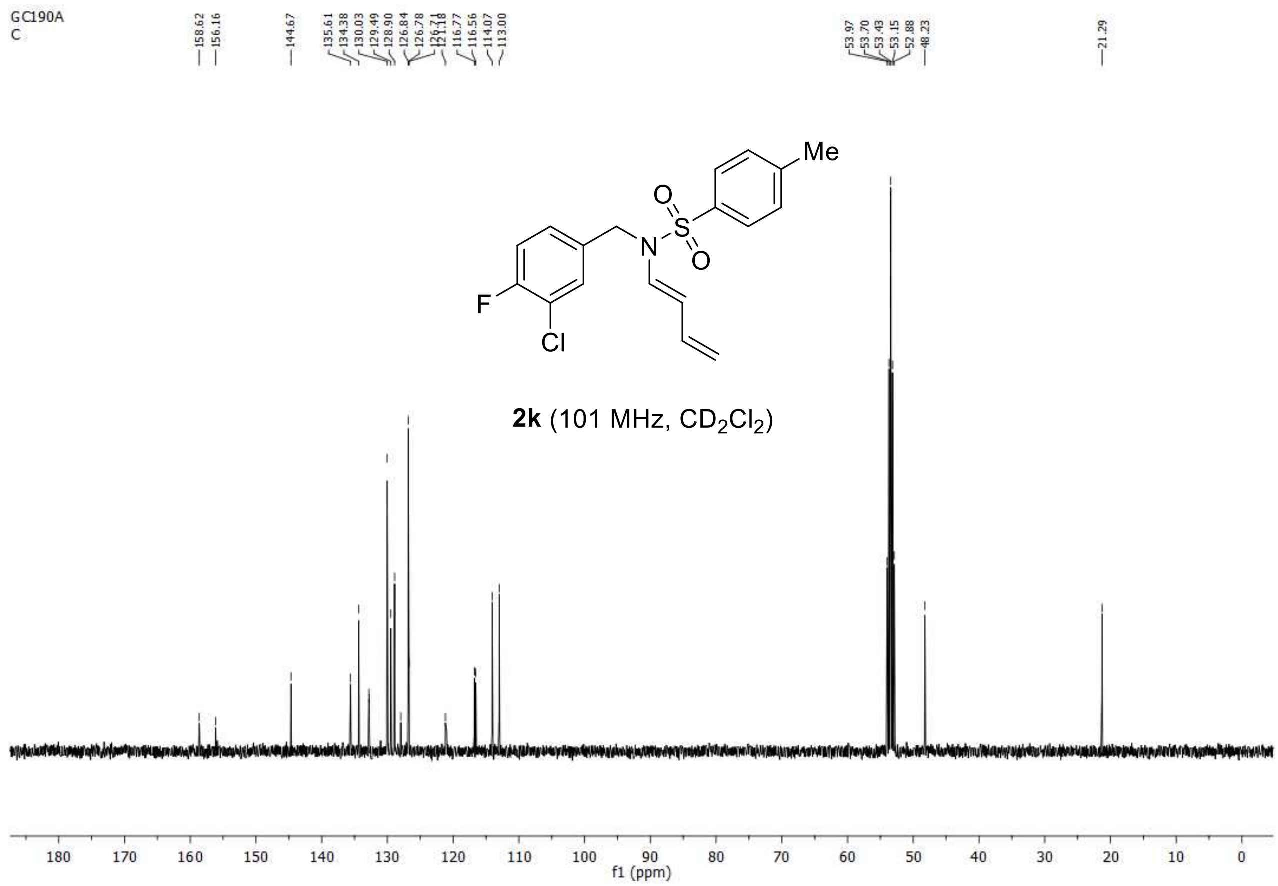


2j (476 MHz, acetone-d_6)

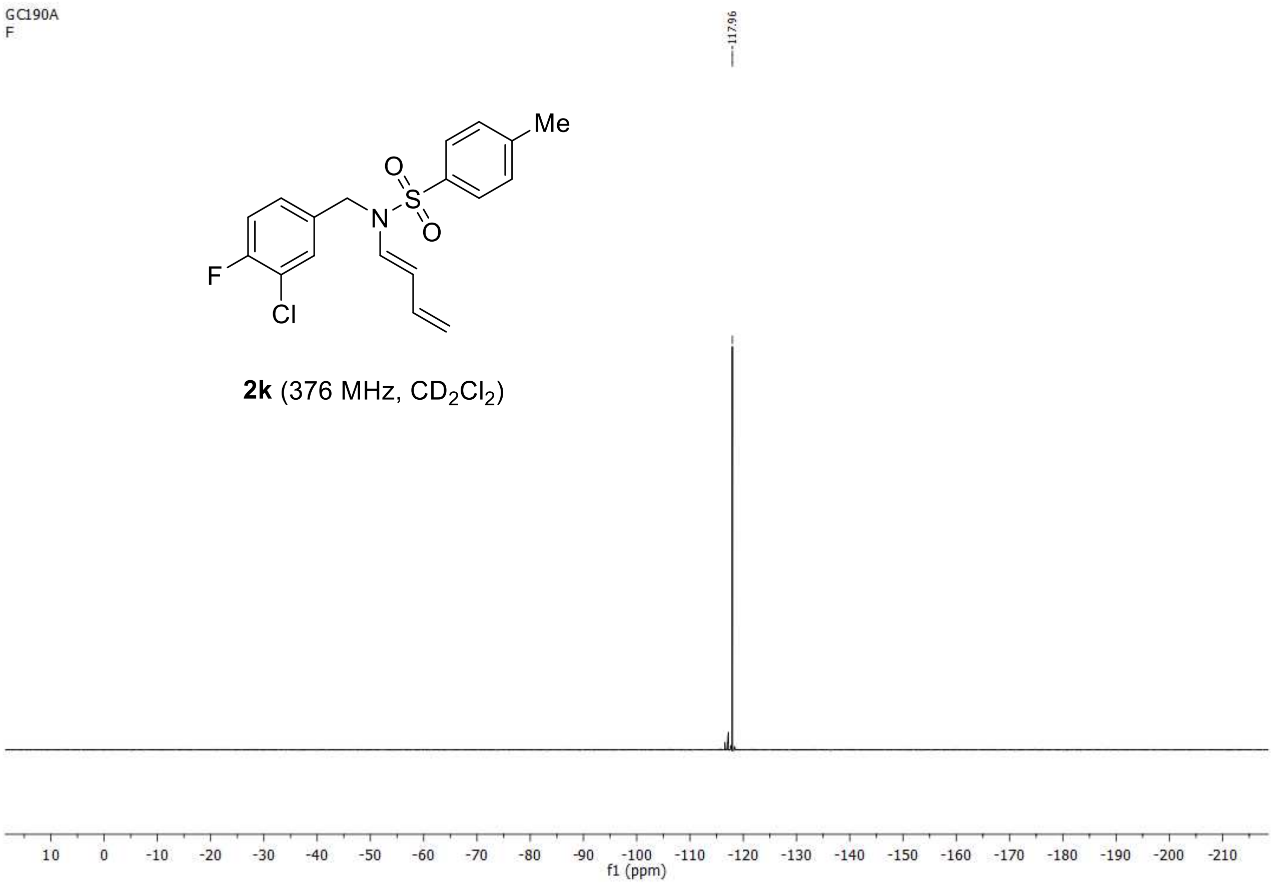


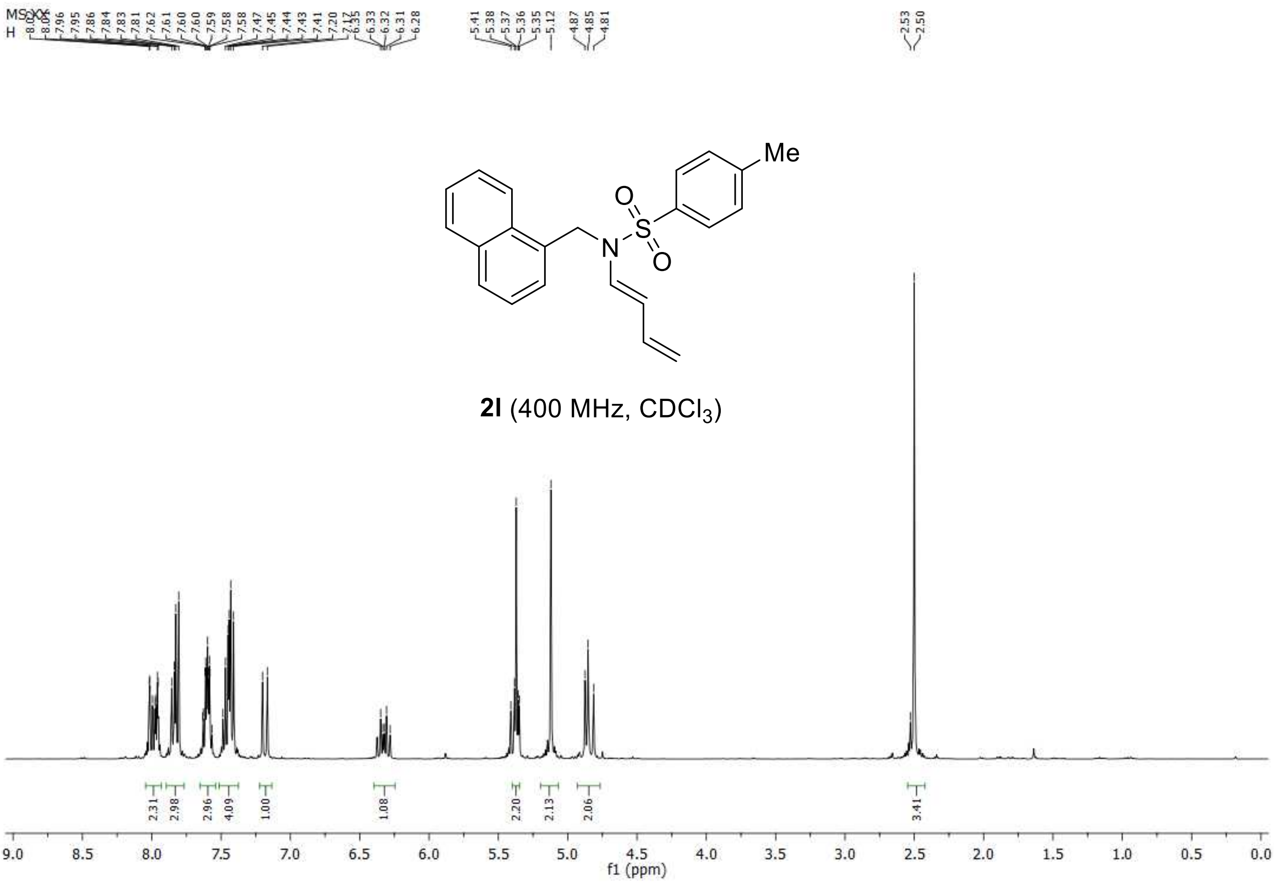


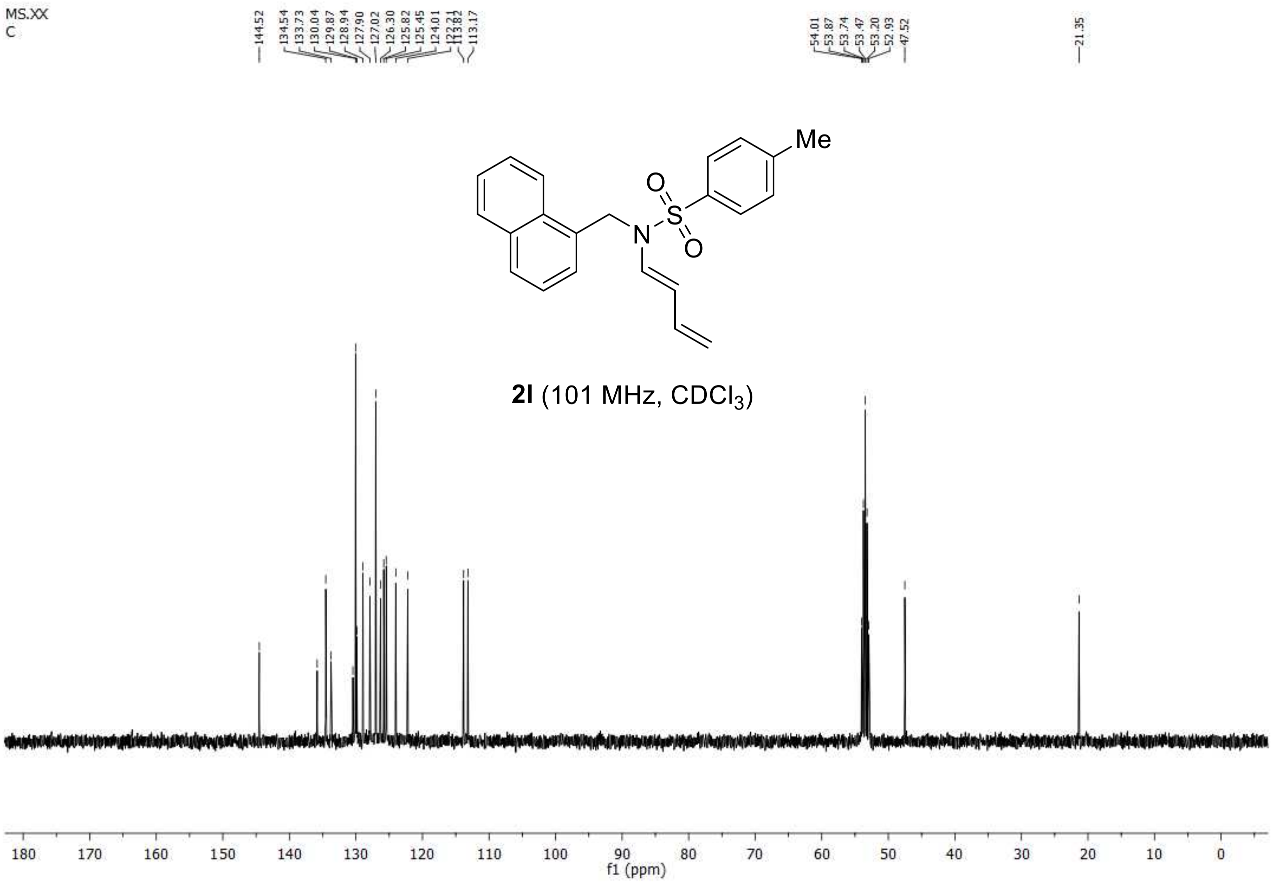
2k (400 MHz, CD_2Cl_2)

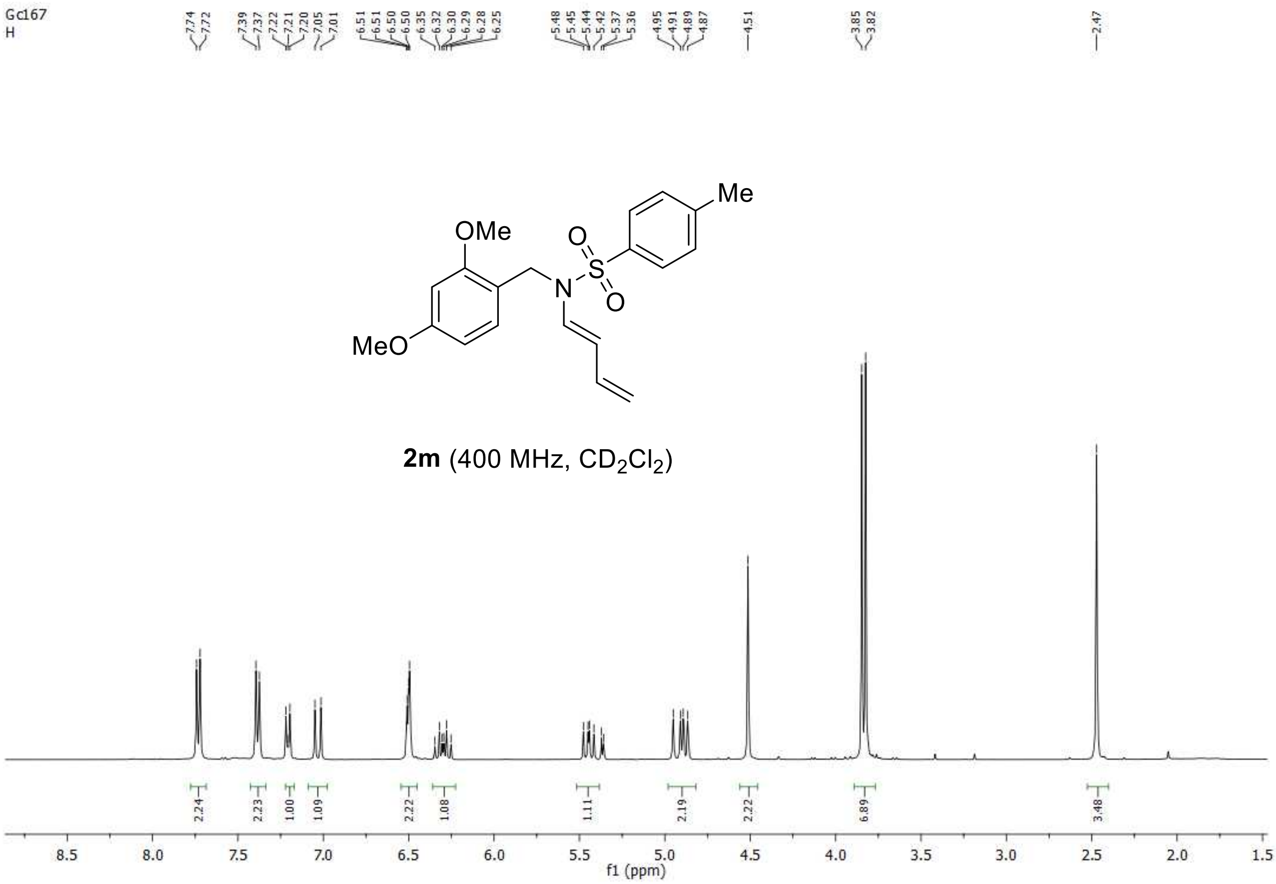


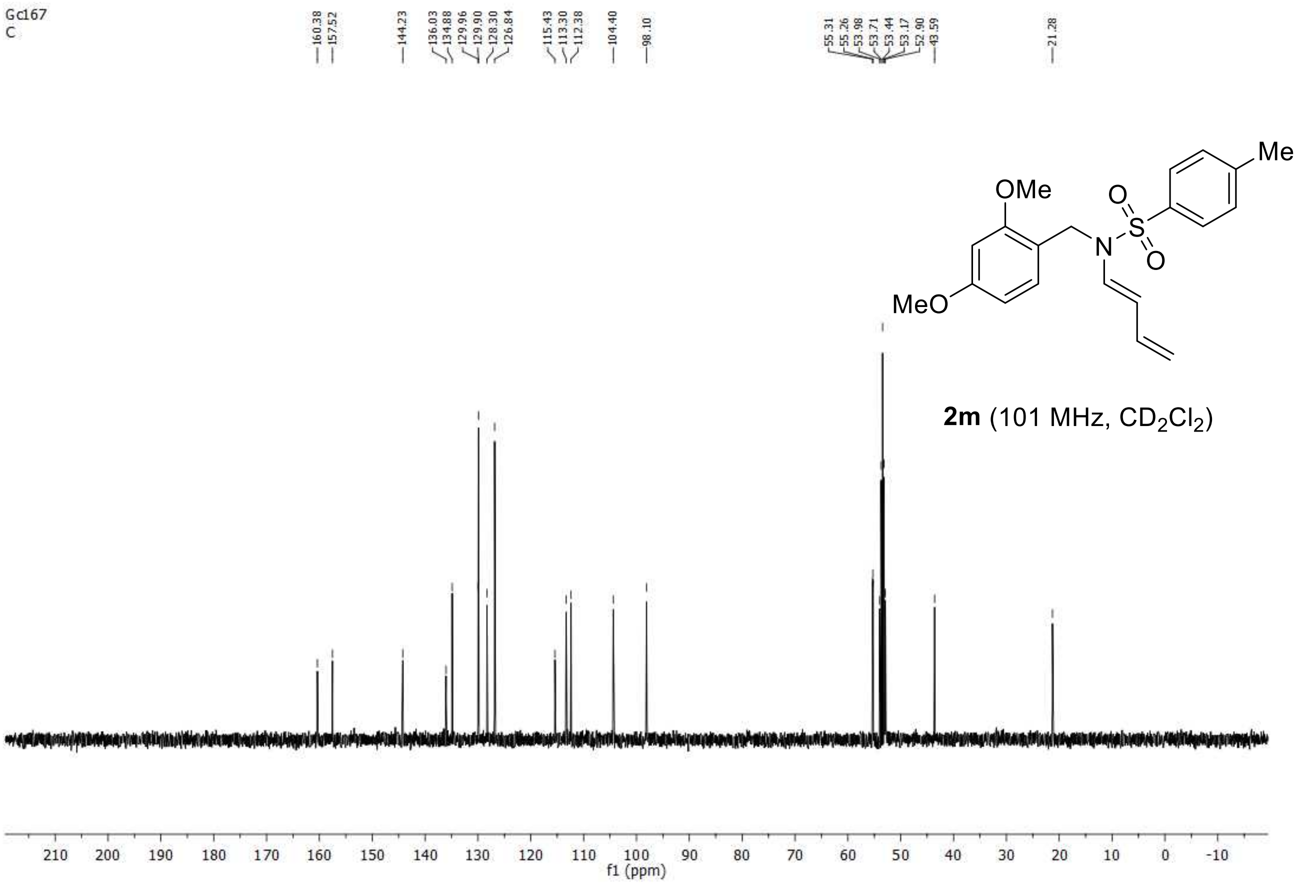
2k (101 MHz, CD_2Cl_2)


GC190A
F
-117.96
Me
O
S
O
N
F
Cl
2k (376 MHz, CD2Cl2)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


MS.XX
H
2I (400 MHz, CDCl3)
f1 (ppm)

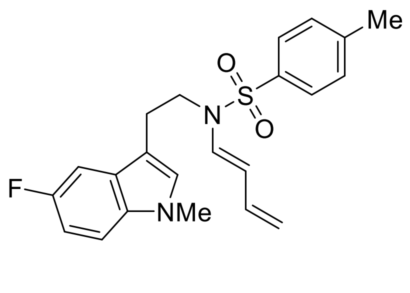

MS.XX
C
2I (101 MHz, CDCl3)
f1 (ppm)


Gc167
H
7.74
7.72
7.39
7.37
7.22
7.21
7.20
7.05
7.01
6.51
6.51
6.50
6.50
6.35
6.32
6.30
6.29
6.28
6.25
5.48
5.45
5.44
5.42
5.37
5.36
4.95
4.91
4.89
4.87
4.51
3.85
3.82
2.47
OMe
Me
MeO
N
S
O
O
2m (400 MHz, CD2Cl2)
2.24
2.23
1.00
1.09
2.22
1.08
1.11
2.19
2.22
6.89
3.48
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
f1 (ppm)

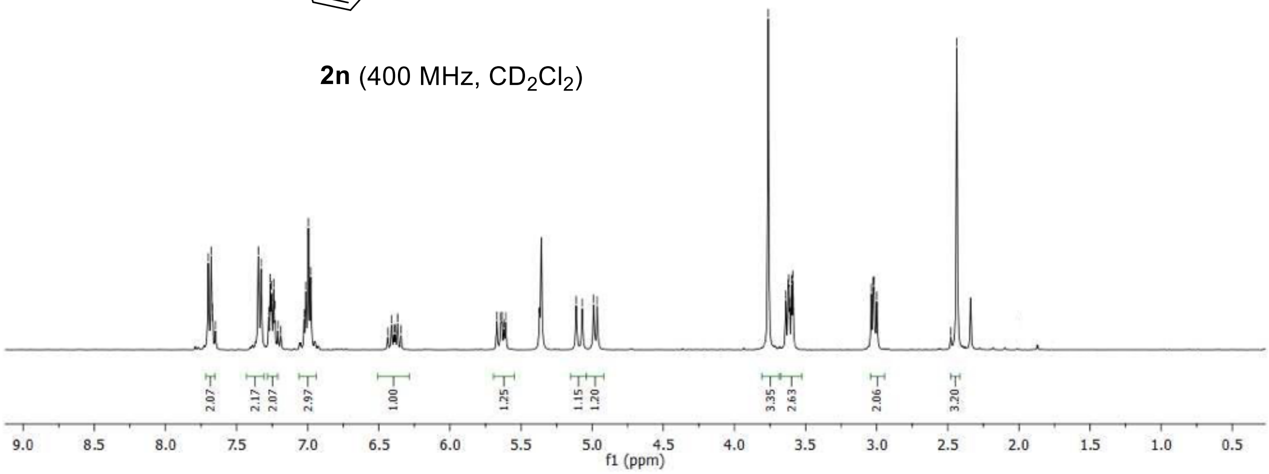

Gc167
C
160.38
157.52
144.23
136.03
134.88
129.96
129.90
128.30
126.84
115.43
113.30
112.38
104.40
98.10
55.31
55.26
53.98
53.71
53.44
53.17
52.90
43.59
21.28
OMe
Me
MeO
N
S
O
O
2m (101 MHz, CD2Cl2)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

GC161bis
H

7.70 7.68 7.67 7.65 7.35 7.33 7.26 7.26 7.24 6.99 6.98 6.98 6.41 6.40 6.39 6.37 6.34 5.67 5.64 5.63 5.62 5.61 5.11 5.07 4.99 4.96 3.76 3.64 3.62 3.62 3.61 3.60 3.59 3.04 3.02 3.02 3.00 2.48 2.44

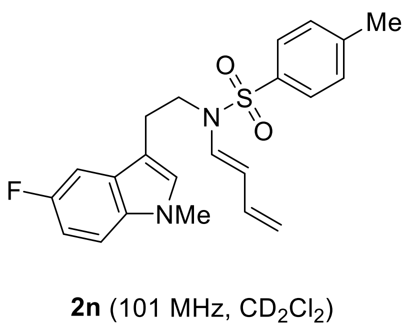


2n (400 MHz, CD_2Cl_2)

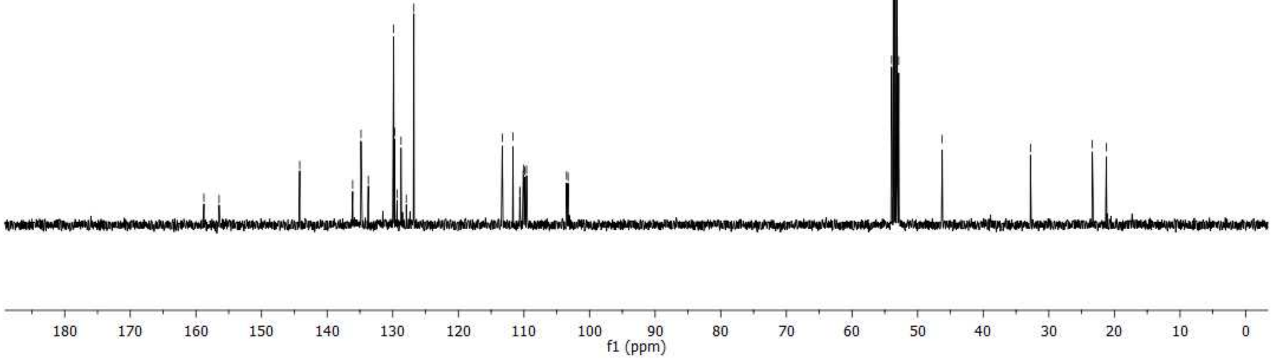


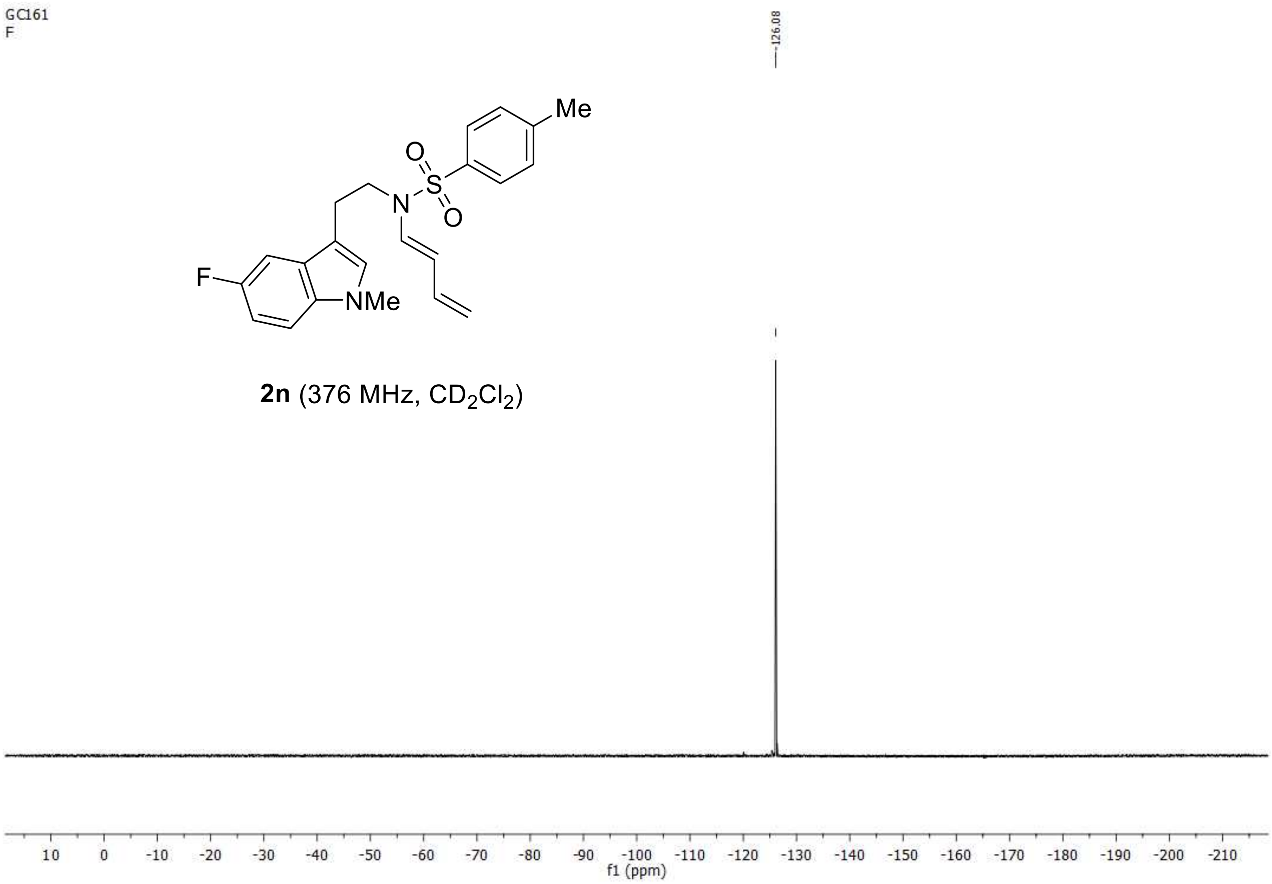
GC161
C

158.78 156.46 144.18 136.11 134.84 133.71 129.85 129.72 129.34 128.73 127.93 126.77 113.31 111.67 110.13 110.03 109.86 103.60 103.50 103.27 53.96 53.69 53.42 53.15 52.88 46.25 32.80 23.38 21.24

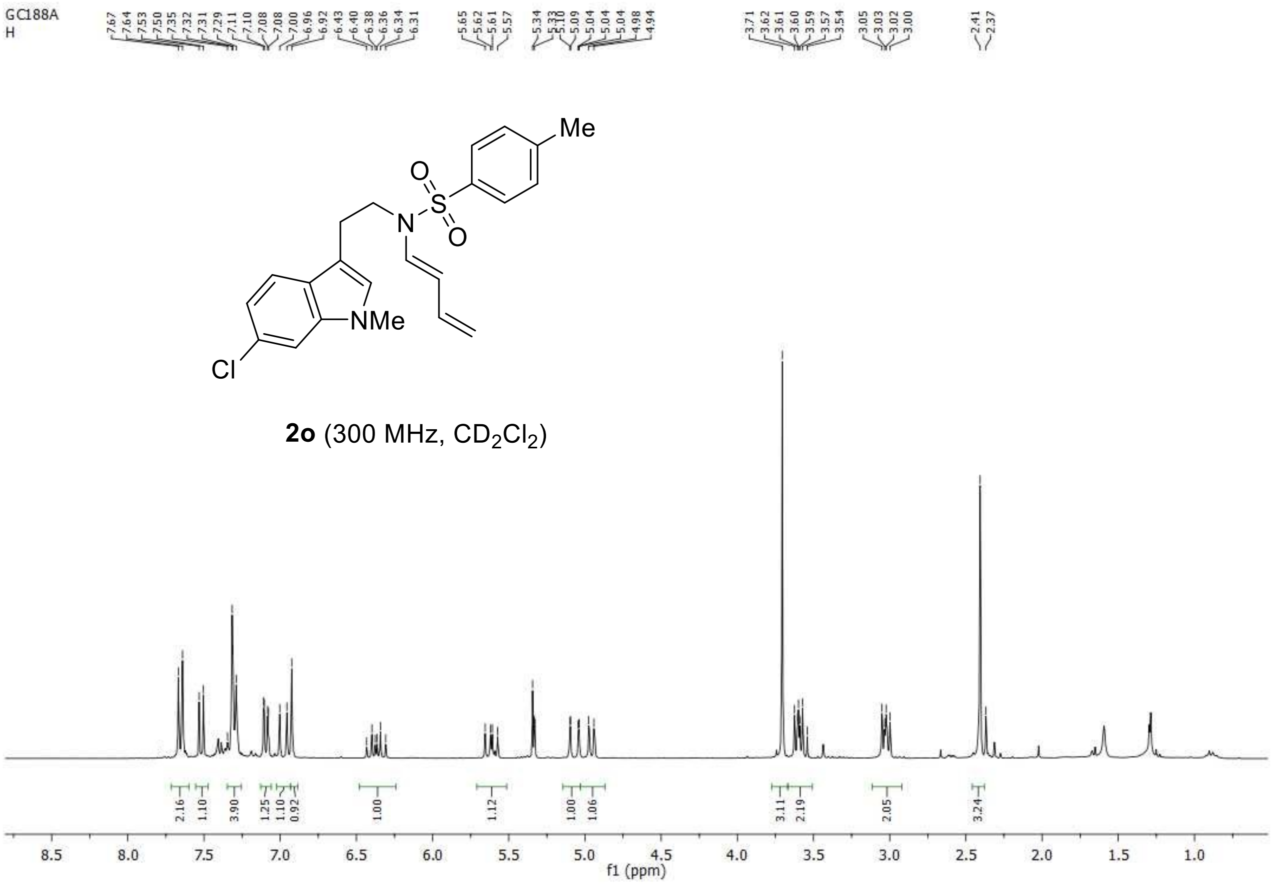


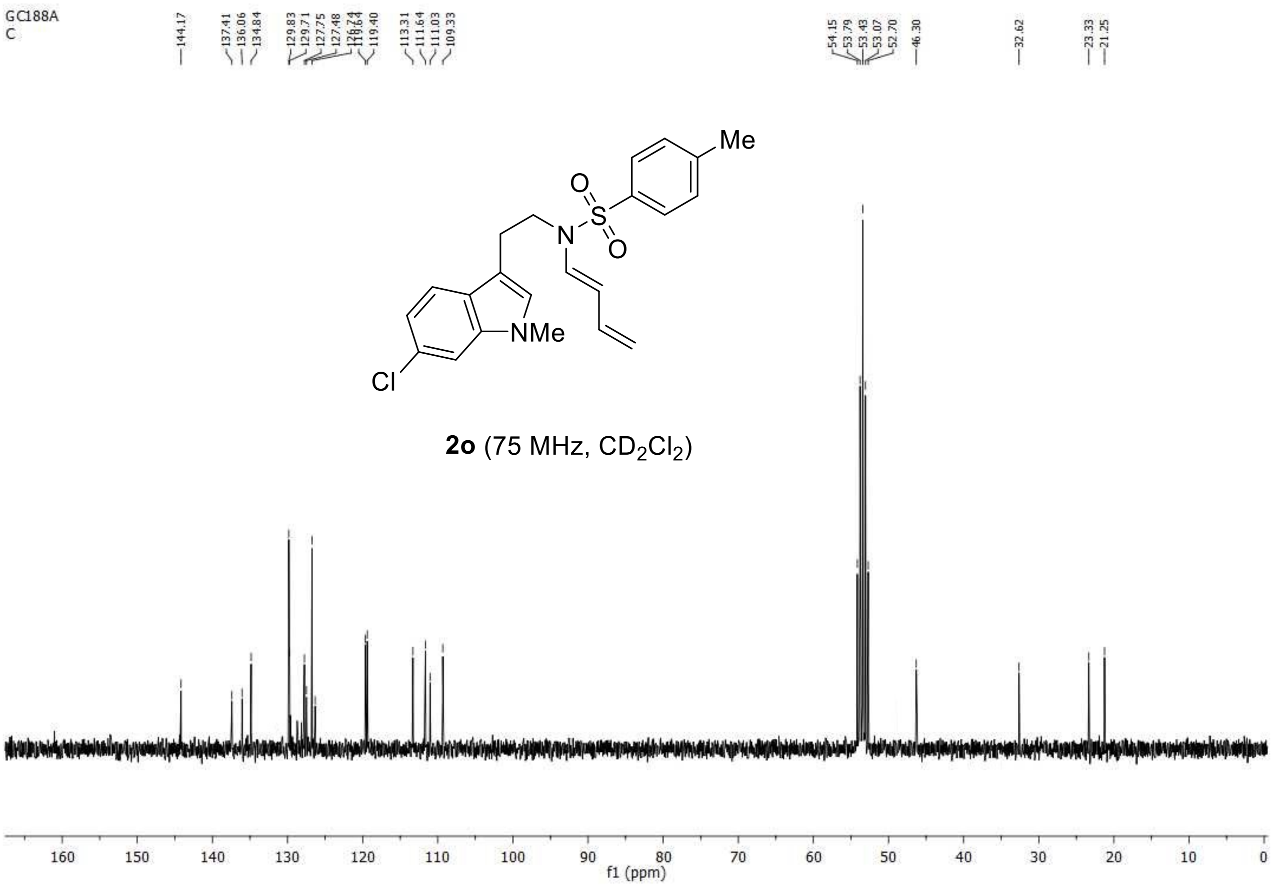
2n (101 MHz, CD_2Cl_2)

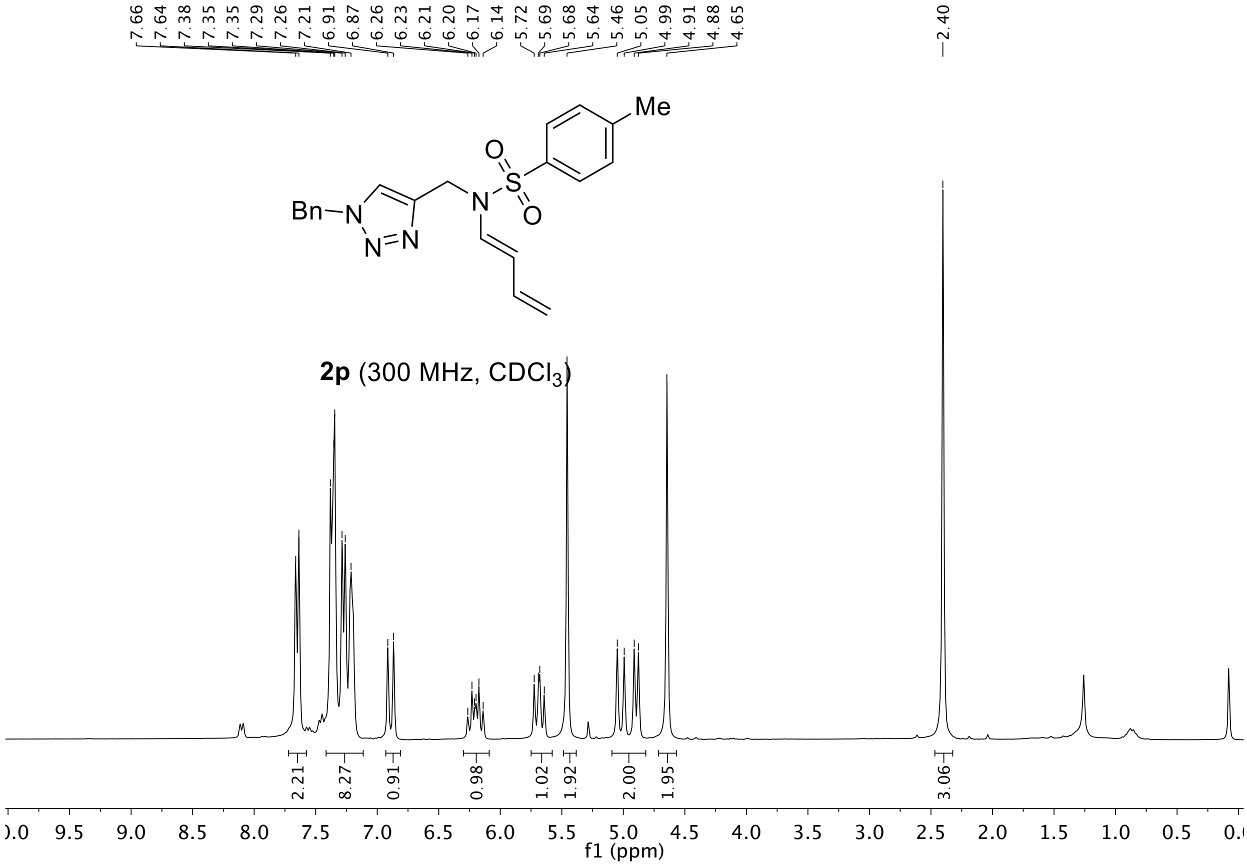




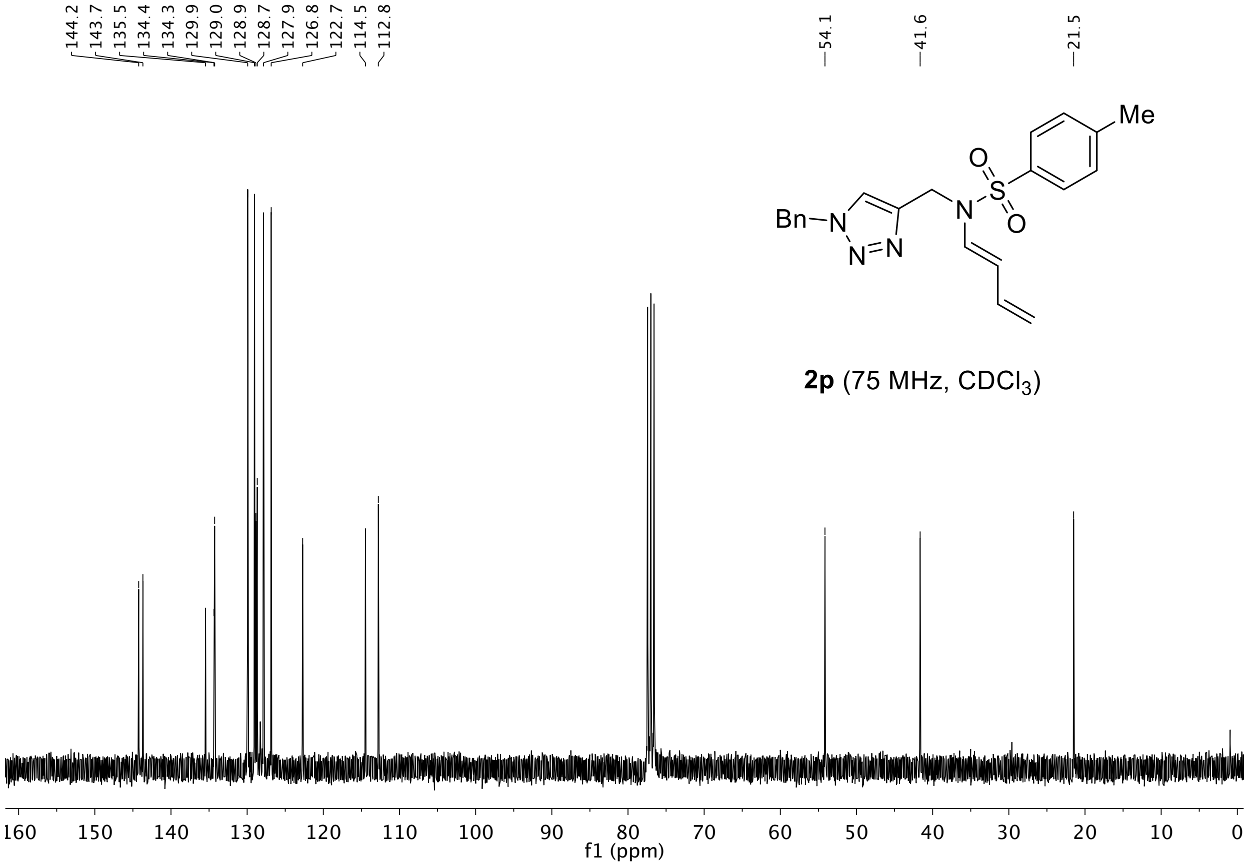
2n (376 MHz, CD_2Cl_2)


GC188A
H
NMe
Cl
Me
O
S
O
N
2o (300 MHz, CD$_2$Cl$_2$)
f1 (ppm)

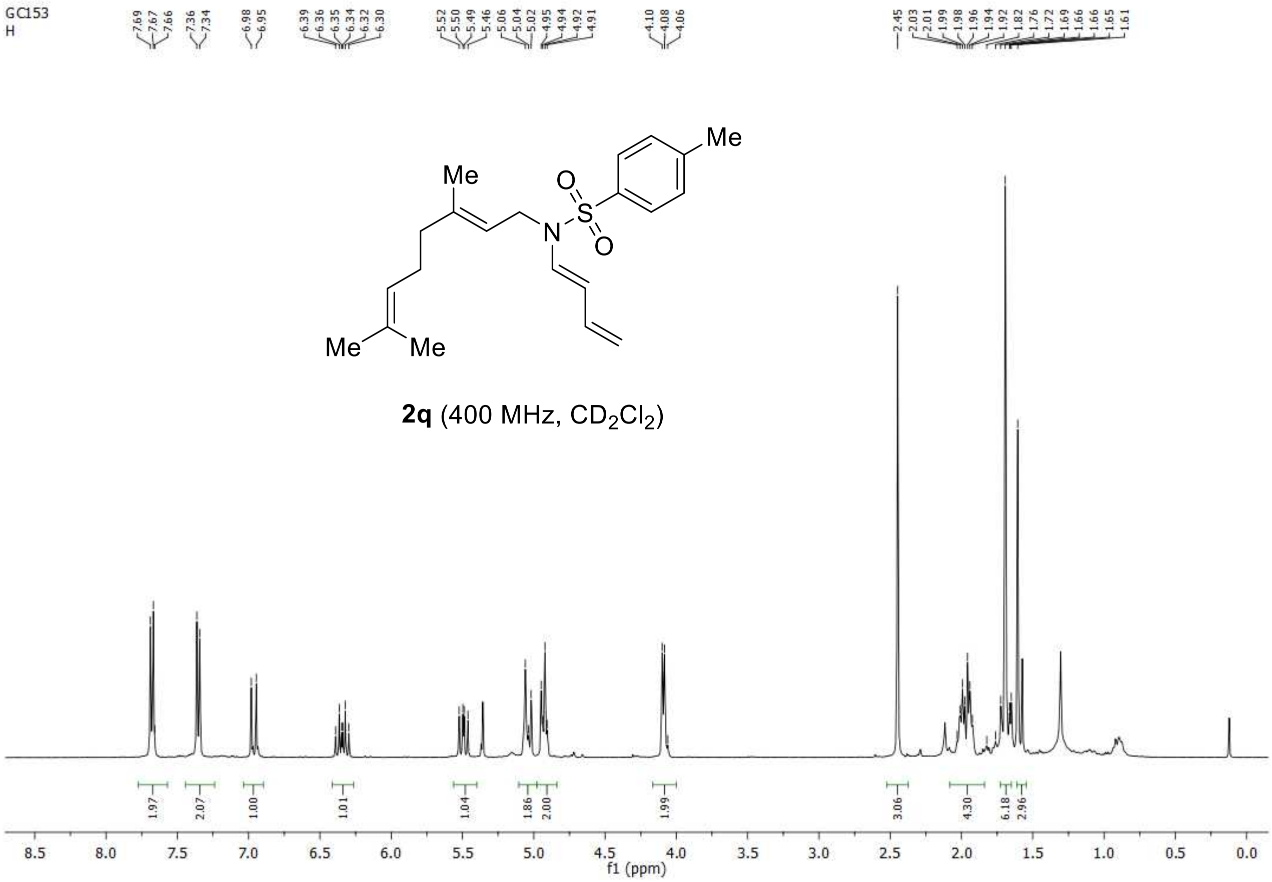

GC188A
C
NMe
Cl
Me
O
S
O
N
2o (75 MHz, CD$_2$Cl$_2$)
f1 (ppm)



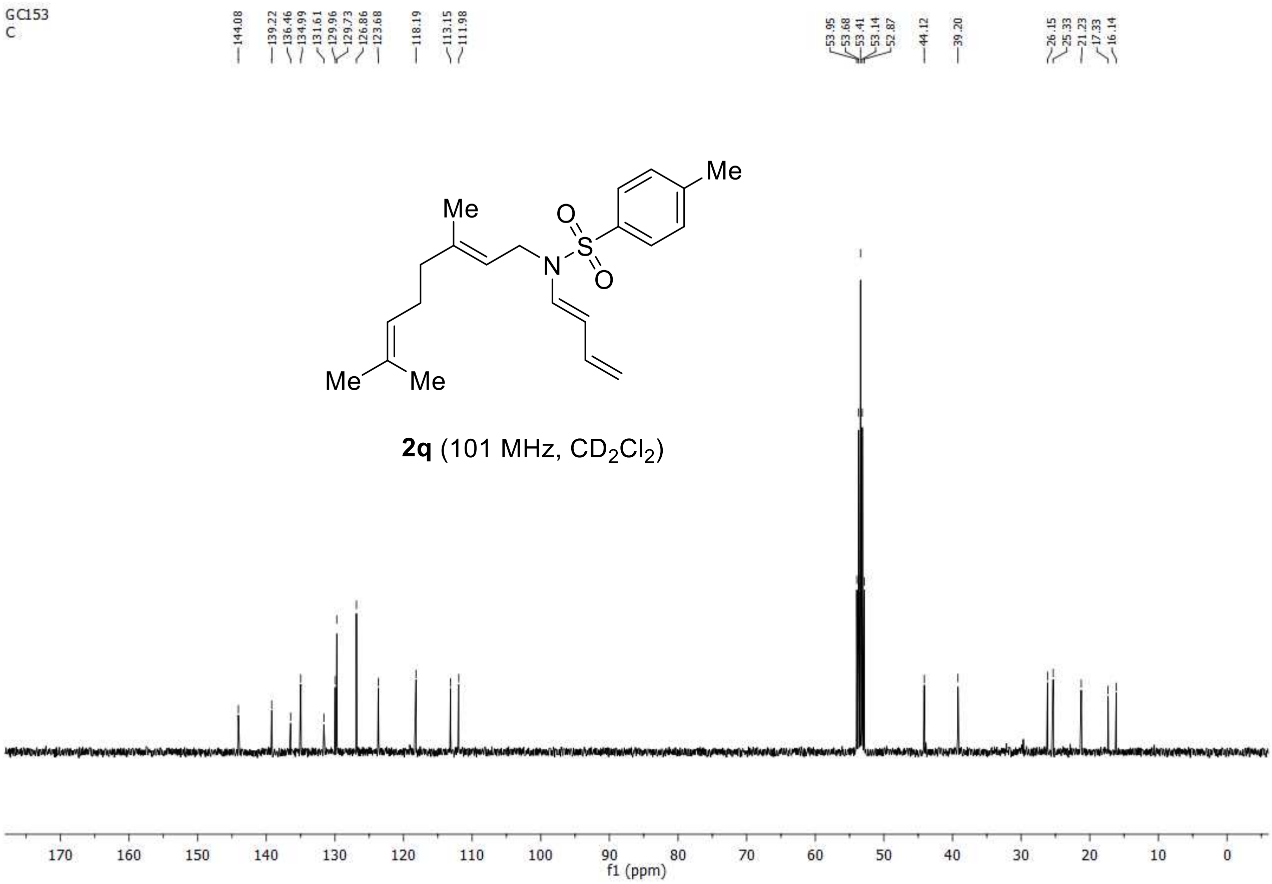
2p (300 MHz, $CDCl_3$)



2p (75 MHz, $CDCl_3$)

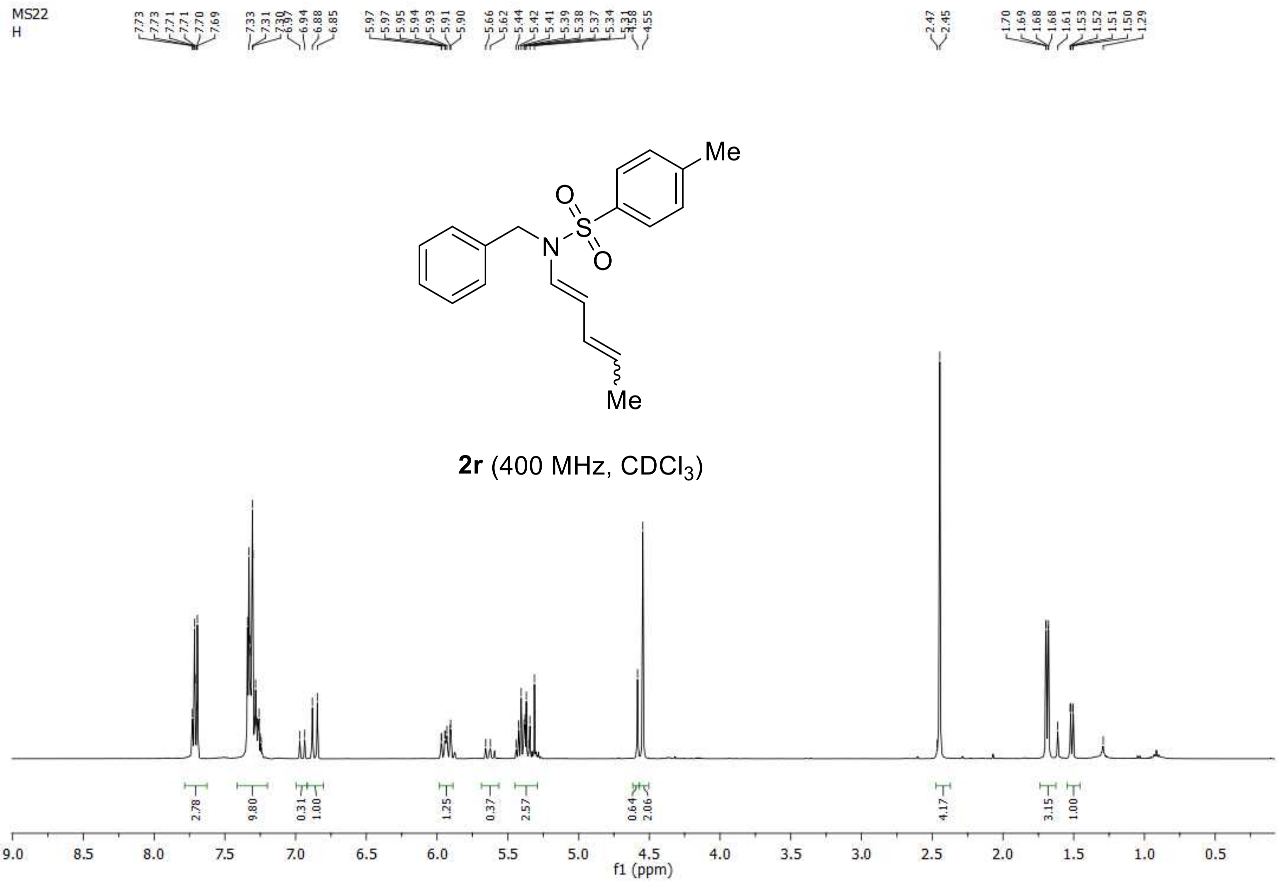


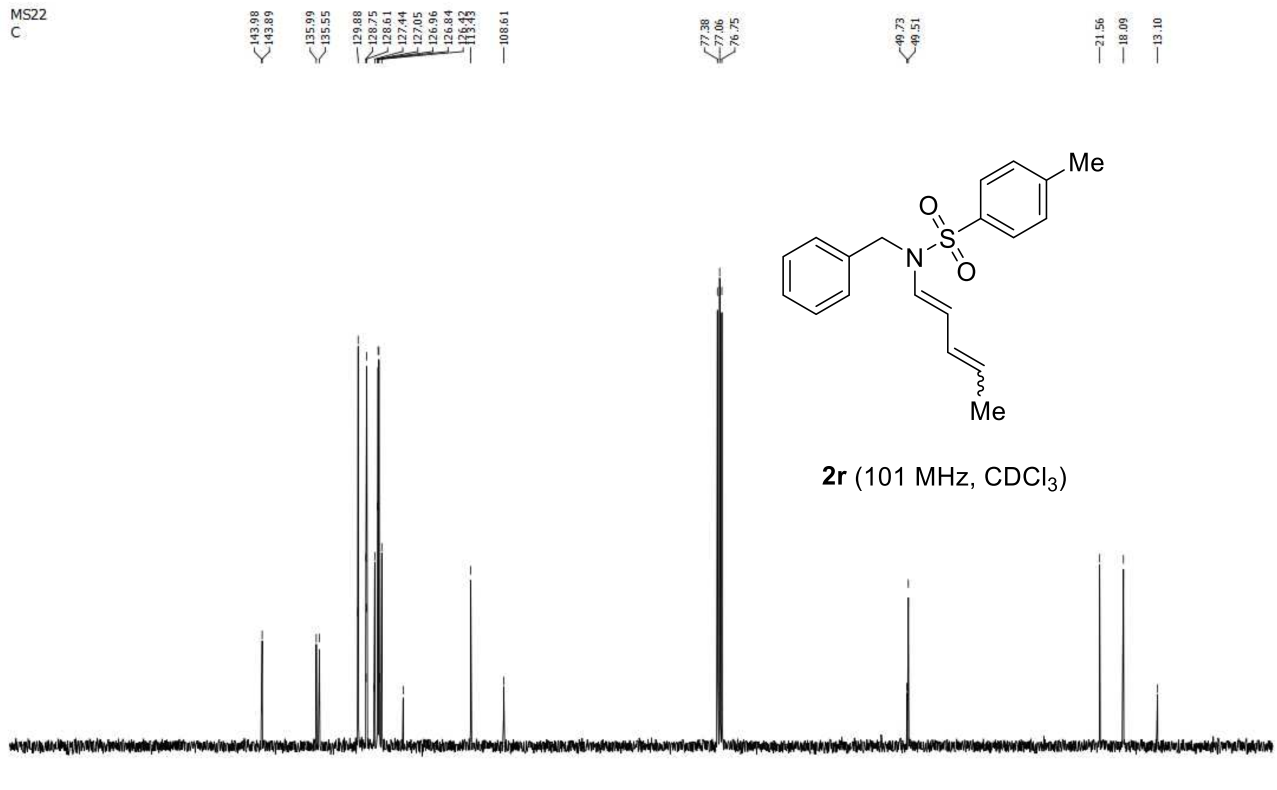
2q (400 MHz, CD_2Cl_2)

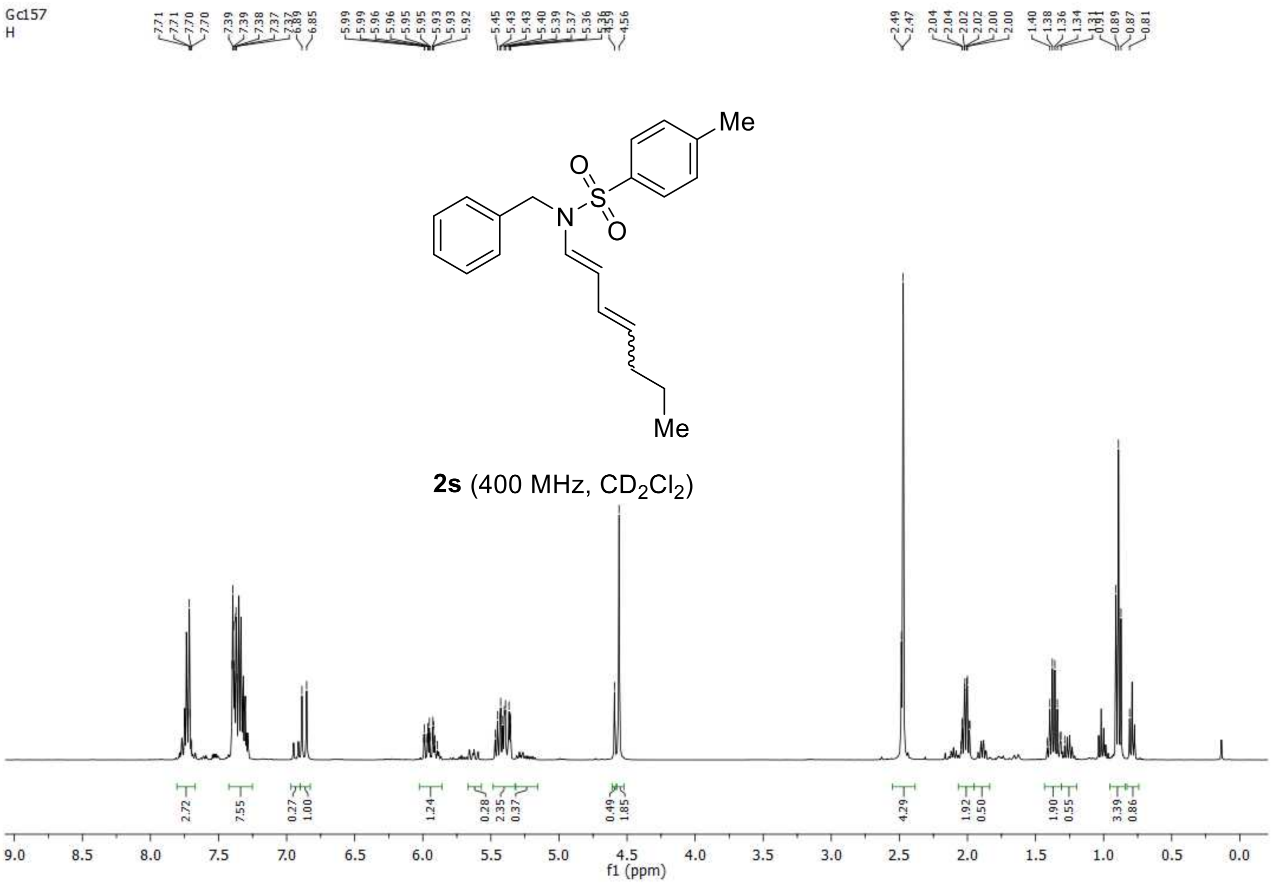


2q (101 MHz, CD_2Cl_2)

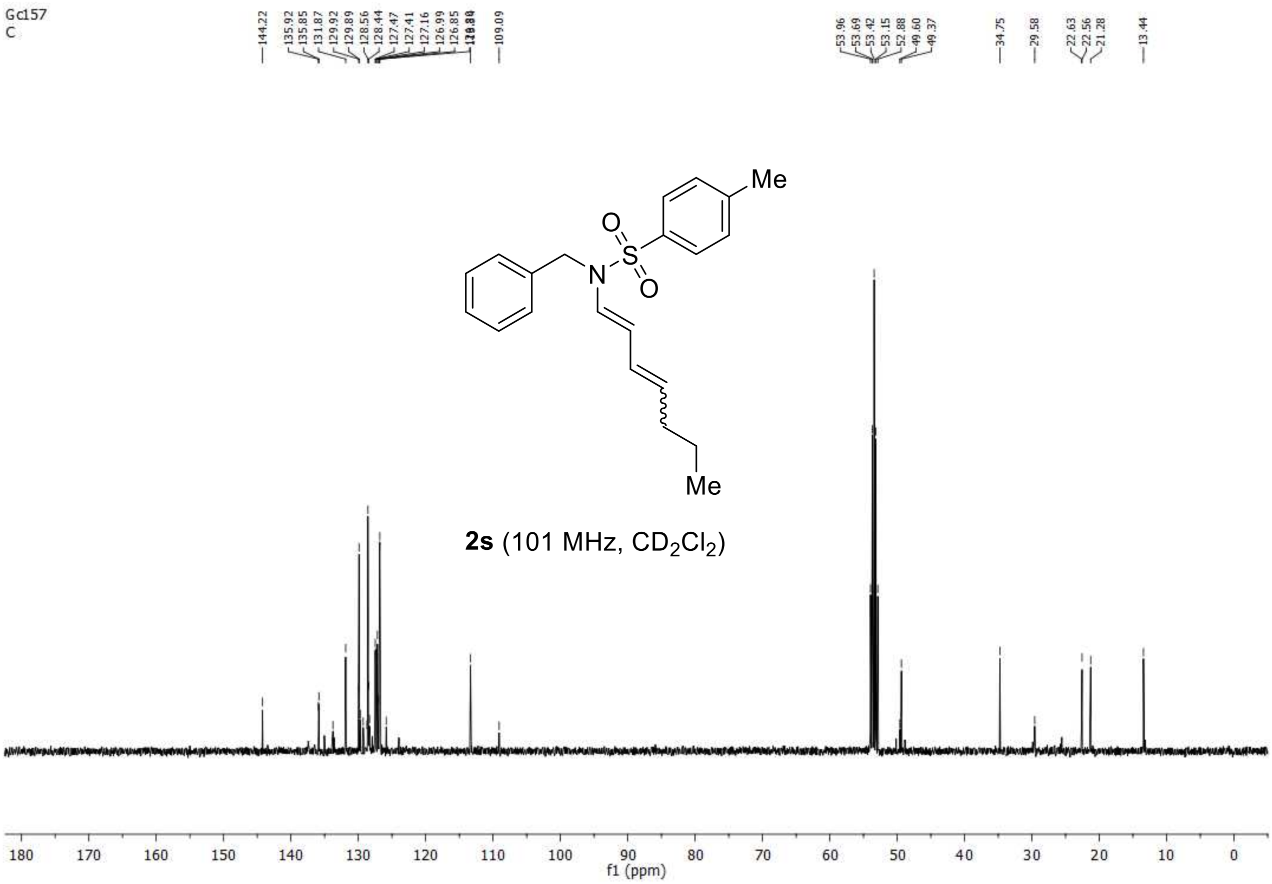
ù



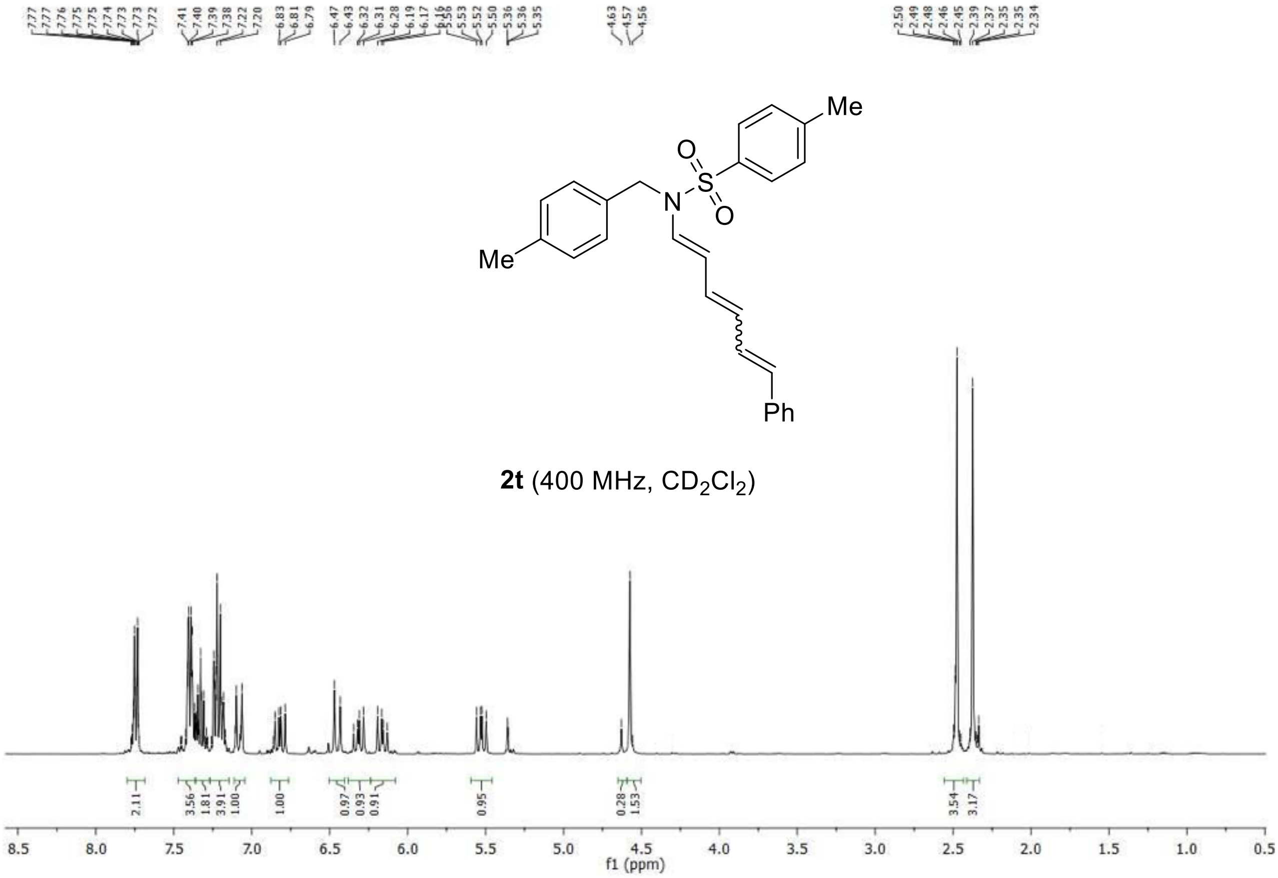




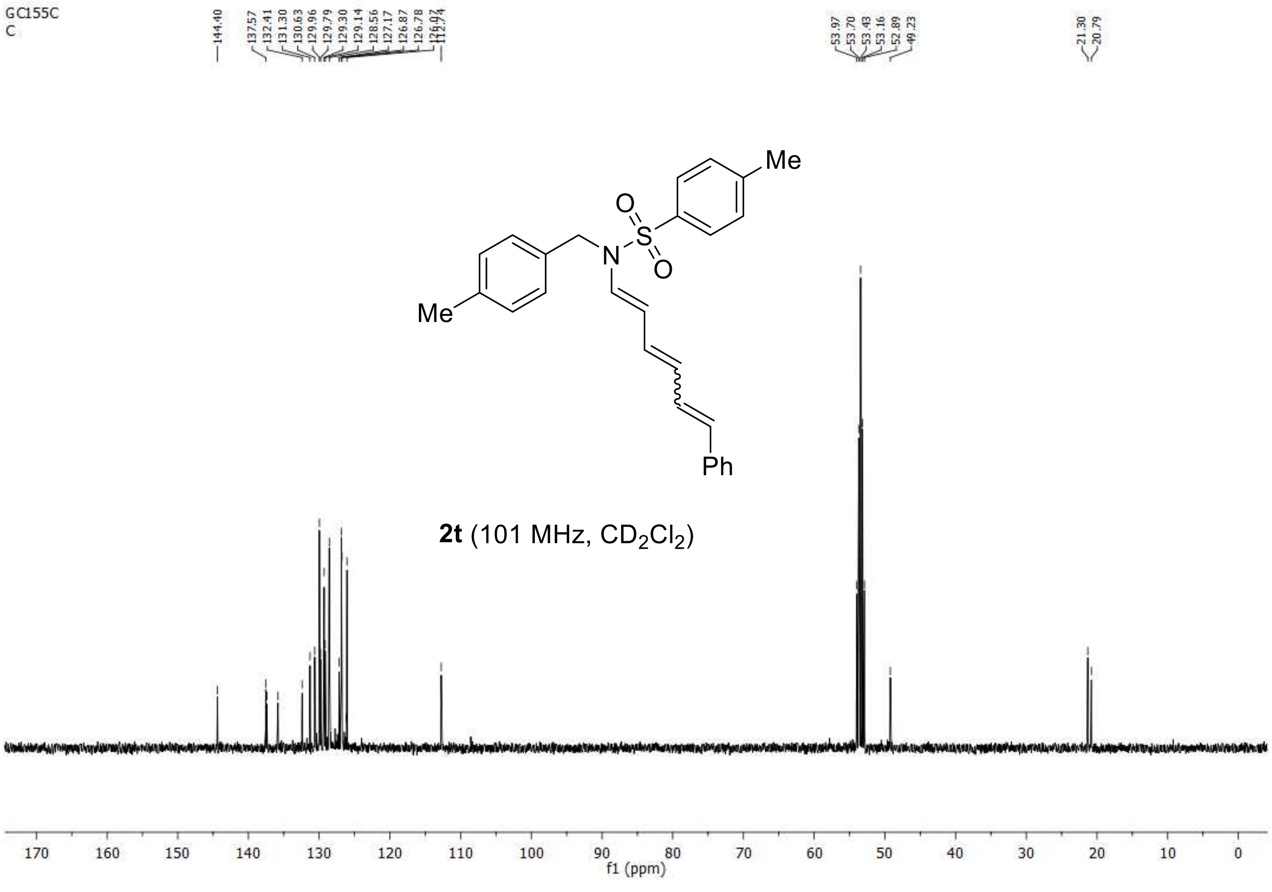
2s (400 MHz, CD_2Cl_2)



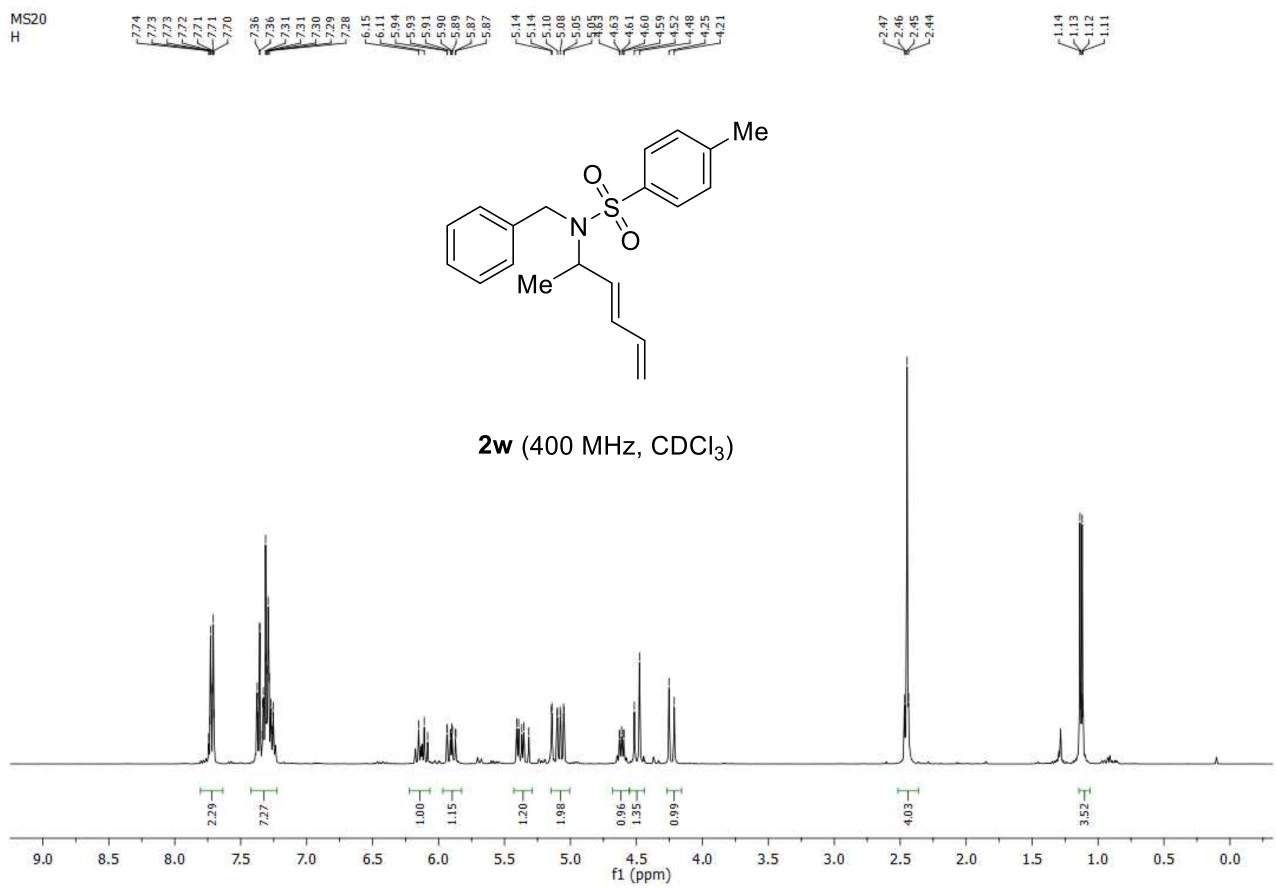
2s (101 MHz, CD_2Cl_2)



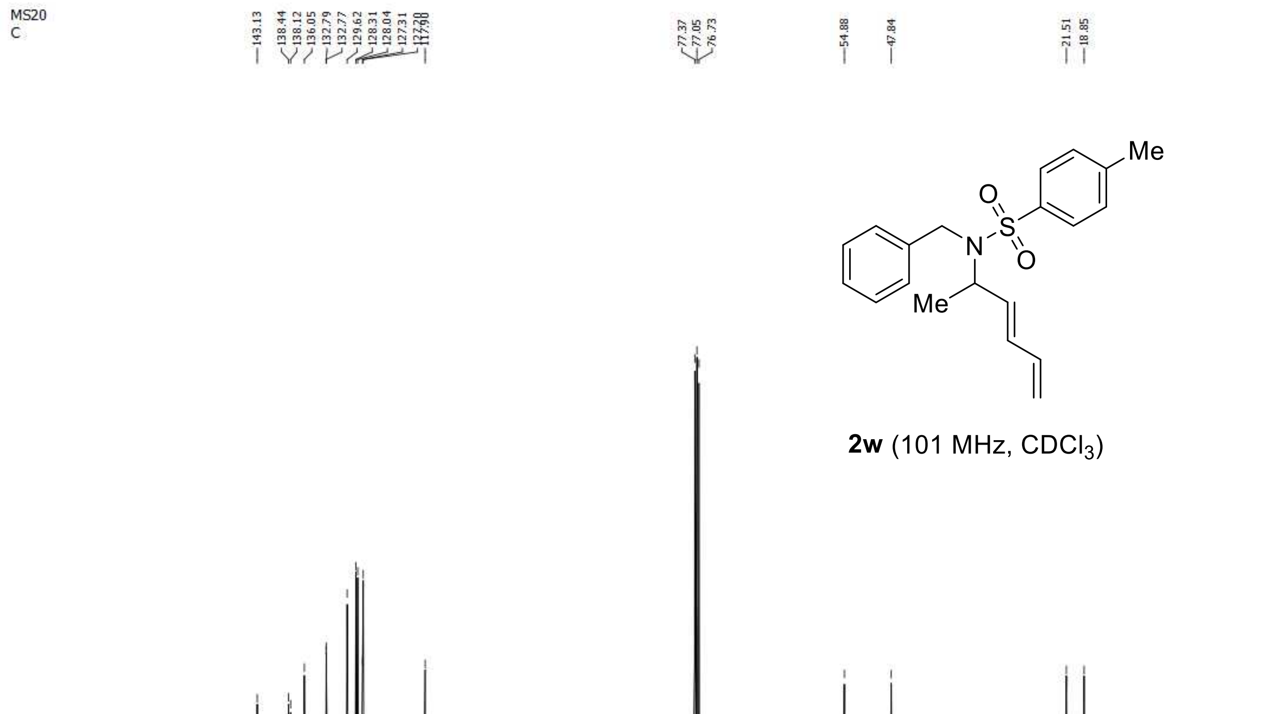
2t (400 MHz, CD_2Cl_2)



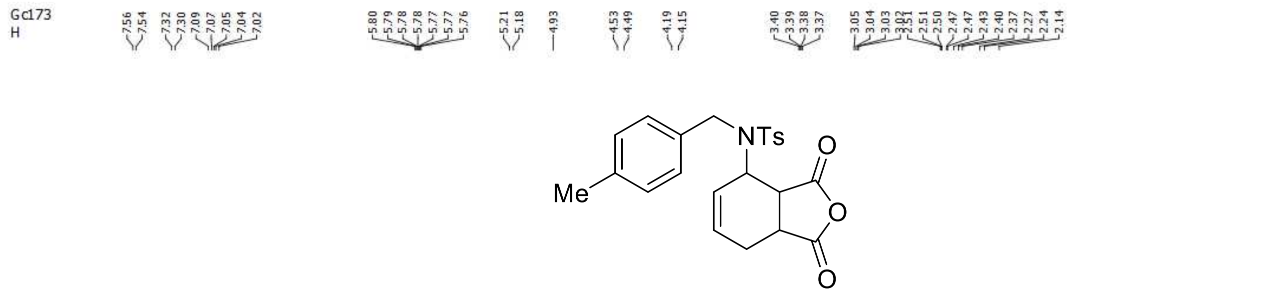
2t (101 MHz, CD_2Cl_2)



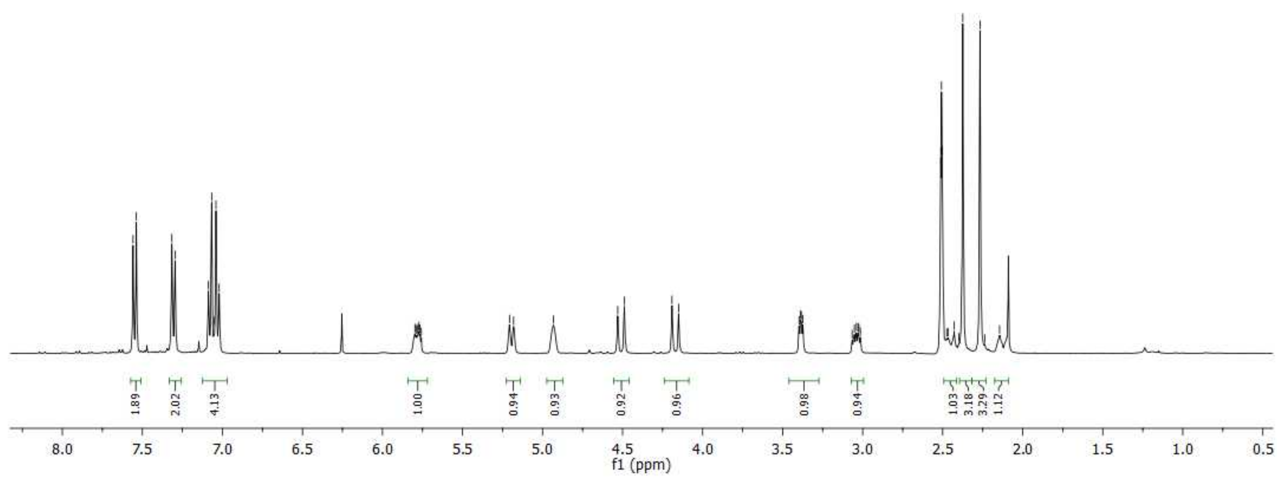
2w (400 MHz, $CDCl_3$)

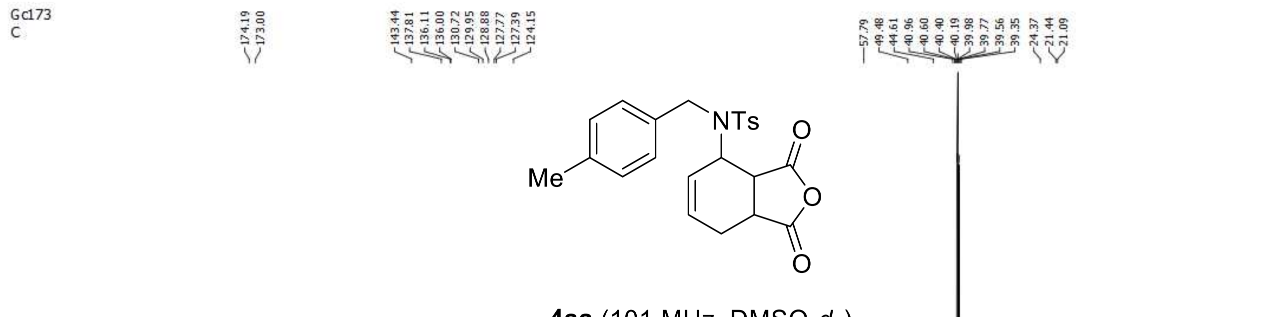


2w (101 MHz, $CDCl_3$)

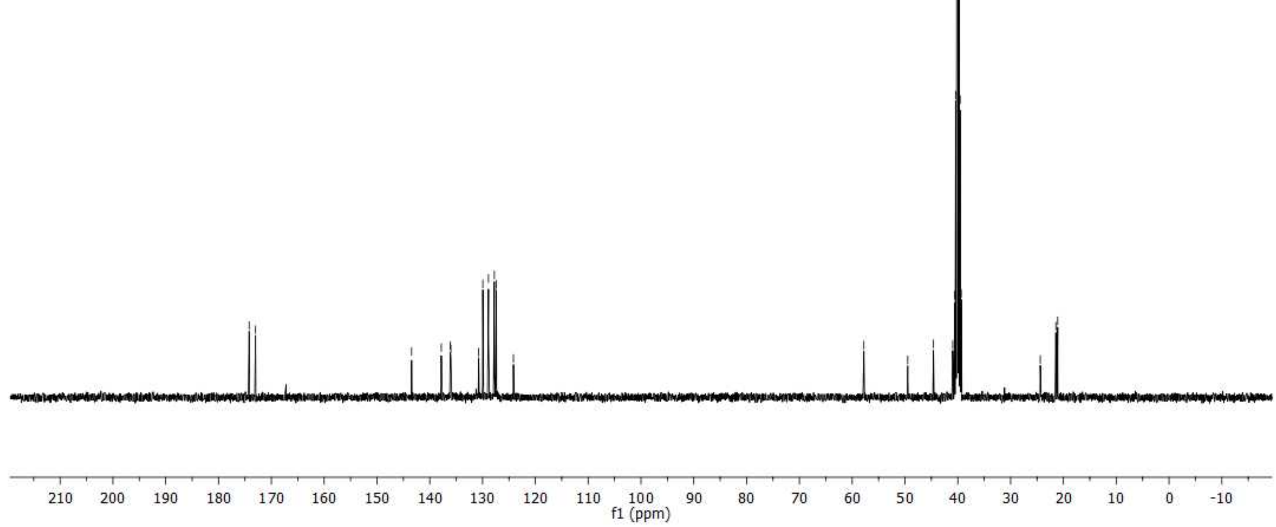


4aa (400 MHz, DMSO-d_6)





4aa (101 MHz, DMSO-d_6)



XYZ coordinates

M06-CPCM- Def2-svp

AcOH
8
scf done: -228.779032

C	15.723275	2.005402	3.611597
C	15.069115	3.152178	4.317813
O	14.417693	3.062860	5.326045
O	15.285141	4.322939	3.699826
H	14.827169	5.014118	4.219479
H	16.270476	2.323953	2.711248
H	16.414849	1.502257	4.309494
H	14.950948	1.266100	3.336851

PMe3
13
scf done: -460.757990

C	15.090836	6.627135	8.698990
P	15.521747	6.104720	6.972918
C	16.291922	7.687162	6.389501
C	17.075495	5.165385	7.350541
H	17.054234	8.067557	7.099010
H	16.771236	7.531691	5.404846
H	15.511219	8.460075	6.261587
H	17.771348	5.751036	7.984326
H	16.827770	4.223543	7.874743
H	17.592827	4.898448	6.410182
H	15.947584	7.102947	9.217498
H	14.248782	7.343684	8.676252
H	14.765909	5.748542	9.287050

Reag 1
31
scf done: -1068.442660

C	8.017025	10.549343	3.771146
C	8.213300	10.034302	2.372309
N	8.760431	8.681998	2.381119
C	10.121742	8.523198	2.878942
C	11.130610	9.241308	2.097090
C	11.956661	9.847404	1.447113
C	12.961785	10.564076	0.680470
S	8.190393	7.598015	1.244390
C	8.816056	8.170871	-0.321360
O	8.813496	6.313072	1.530351
O	6.740064	7.737035	1.216049
H	7.240159	9.993822	1.850341
H	8.876296	10.719223	1.799321
H	10.344119	7.442651	2.920694
H	12.498113	11.257719	-0.044831
H	13.608079	9.871540	0.110521
H	13.616214	11.164879	1.338541
H	10.130982	8.878658	3.929165
H	8.440697	7.477653	-1.092843
H	8.435672	9.190390	-0.503577
H	9.918311	8.158601	-0.282455
C	8.692729	11.681848	4.226169
C	8.497947	12.146793	5.528010
C	7.629965	11.473357	6.384088
C	6.958545	10.332529	5.937700
C	7.152682	9.872443	4.639155
H	9.382783	12.204794	3.550292
H	9.032930	13.038464	5.875073
H	7.476127	11.835869	7.407167
H	6.275852	9.799640	6.609737
H	6.633472	8.974612	4.277670

Diene 2
31
scf done: -1885.971803

C	1.238586	-0.454698	-0.736494
C	0.049437	-0.268817	-0.026650
C	0.071223	-0.010603	1.355128
C	1.312334	0.060744	2.006551
C	2.504591	-0.128597	1.298081
C	2.470755	-0.386643	-0.075310
C	-1.211704	0.206014	2.139437
N	-1.935062	1.443302	1.807296
C	-3.085354	1.484698	1.025153
C	-3.640956	0.474001	0.312546
C	-4.908414	0.653272	-0.381559
C	-5.522486	-0.345681	-1.186809
S	-1.365471	2.905322	2.490610
C	-0.238437	3.570539	1.253038
O	-0.576223	2.532399	3.663276
O	-2.496080	3.828119	2.580484
H	-0.990689	0.227515	3.215837
H	-1.921746	-0.618659	1.972874
H	-4.965229	-1.270282	-1.389415
H	-6.167817	-0.020168	-2.011245
H	-5.253589	1.686600	-0.508617
H	0.141920	4.517987	1.668461
H	0.580031	2.852833	1.093500
H	-0.802363	3.753912	0.325769
H	-3.191535	-0.524675	0.287738
H	-3.579546	2.459525	1.045575
H	1.343018	0.277373	3.078815
H	3.463258	-0.071980	1.823242
H	3.401943	-0.535189	-0.630963
H	1.203657	-0.657837	-1.811531
H	-0.907609	-0.320836	-0.554617

Allenamide 5
31
scf done: -1885.960942

C	8.430878	5.898020	8.641265
C	8.565302	4.733828	7.875376
C	7.436526	4.144483	7.293536
C	6.173325	4.719331	7.477586
C	6.038901	5.883523	8.243475
C	7.167677	6.472868	8.825314
C	9.873617	4.138450	7.684753
N	10.957038	4.868635	8.354528
S	11.380817	4.408745	9.957200
O	11.926496	5.589800	10.599342
C	11.837470	5.668540	7.678500
C	11.798721	5.916666	6.333704
C	11.327916	6.688543	5.370337
C	11.597263	6.540305	3.911409
O	10.197444	3.742892	10.481897
C	12.672145	3.212386	9.712773
H	9.871625	3.108551	8.066447
H	10.136499	4.106405	6.618222
H	12.643796	6.079221	8.295462
H	12.161658	5.622330	3.703586
H	12.175072	7.393080	3.528050
H	10.655122	6.512811	3.344412
H	10.688996	7.527234	5.670528
H	12.921719	2.816240	10.702562
H	12.278105	2.418705	9.067898
H	13.532883	3.727216	9.260022
H	7.541089	3.238908	6.697784
H	5.295299	4.260905	7.024998
H	5.056311	6.330673	8.386639
H	7.063114	7.378444	9.421066
H	9.308904	6.356446	9.093852

Allene 6
31
scf done: -1885.947899

C	17.297317	3.363506	8.125707
C	16.035070	3.249906	7.524867
C	15.918093	3.113757	6.124834
C	17.092699	3.099724	5.346237
C	18.358243	3.215840	5.945207
C	18.462009	3.346718	7.338562
C	14.554028	2.993954	5.456536
N	13.842665	1.699091	5.645615
C	14.589300	0.477851	5.316874
C	14.643663	0.135222	3.832010
C	14.381208	0.946915	2.763287
C	14.588215	1.842612	1.805835
S	12.874258	1.569886	7.074471
C	11.457894	0.631506	6.451562
O	13.537739	0.745740	8.121406
O	12.430343	2.952891	7.397817
H	13.867163	3.775648	5.820043
H	14.658535	3.124670	4.365437
H	14.147650	-0.380286	5.850912
H	13.825620	2.112014	1.070741
H	15.565382	2.338414	1.724050
H	10.807471	0.455309	7.323545
H	10.953267	1.250138	5.695431
H	11.799780	-0.327083	6.022718
H	17.012337	3.006070	4.255411
H	19.260709	3.203704	5.323271
H	19.446656	3.437414	7.811116
H	17.371701	3.469968	9.213801
H	15.131482	3.265246	8.144394
H	15.639735	0.554269	5.676601
H	15.151922	-0.819029	3.623148

Reag 1z
34
scf done: -1107.689791

C	-0.060595	-0.177597	0.081721
C	-0.022251	-0.009235	1.470379
C	1.212064	0.026038	2.120168
C	2.396727	-0.116971	1.396123
C	2.351249	-0.290959	0.015075
C	1.118694	-0.320035	-0.642362
C	-1.308188	0.157716	2.231230
N	-2.014229	1.361700	1.804409
S	-3.679862	1.291360	1.682665
O	-4.001133	0.037855	1.012275
C	-1.395254	2.640268	2.135410
C	-1.271792	2.877563	3.575043
C	-1.178692	3.038198	4.774373
C	-1.115120	3.226137	6.219263
C	-4.282909	1.178990	3.355110
O	-4.120750	2.567257	1.136001
H	-1.974220	-0.701816	2.035842
H	-1.107630	0.191322	3.324807
H	-1.979769	3.439148	1.646745
H	-0.237880	2.683426	6.623828
C	-2.385785	2.764593	6.926152
H	-0.927695	4.296025	6.437894
H	-0.395514	2.654753	1.656850
H	-5.381346	1.096020	3.297869
H	-3.854190	0.278983	3.828522
H	-3.983576	2.091541	3.898275
H	1.244385	0.170962	3.208469
H	3.361508	-0.087300	1.915774
H	3.280520	-0.401664	-0.555792
H	1.079533	-0.455957	-1.729375
H	-1.035629	-0.193039	-0.423988
H	-2.300858	2.903932	8.018394
H	-3.264681	3.336215	6.575809
H	-2.580544	1.693440	6.732624

Dienamide 2z

34

scf done: -1107.715803

C	-0.036899	0.010426	0.022964
C	-0.022251	0.030778	1.418479
C	1.189327	0.030407	2.105209
C	2.403547	0.011258	1.406277
C	2.377764	-0.011373	0.009283
C	1.165640	-0.012404	-0.680596
C	3.720343	0.079541	2.134886
N	3.917545	1.324878	2.877526
S	4.169508	2.741034	1.983811
O	4.888929	3.673290	2.839261
C	3.692235	1.447509	4.247045
C	3.240040	0.501147	5.095568
C	3.094766	0.749202	6.516288
C	2.659182	-0.153074	7.413004
C	2.541824	3.412936	1.728258
O	4.711582	2.321729	0.700631
H	4.553709	-0.029794	1.421093
H	3.825721	-0.737921	2.869666
H	2.396181	-1.160793	7.050555
C	2.502660	0.101099	8.871433
H	3.365422	1.759434	6.867887
H	2.684179	4.394399	1.244630
H	1.964019	2.734138	1.079557
H	2.059764	3.534999	2.713299
H	2.975086	-0.505813	4.740539
H	3.957881	2.439138	4.639069
H	3.324943	-0.007537	-0.544196
H	1.162307	-0.026299	-1.776453
H	-0.990644	0.011928	-0.517345
H	-0.964850	0.045429	1.977901
H	1.192891	0.057673	3.202358
H	3.132800	-0.580179	9.477381
H	2.780240	1.139179	9.131825
H	1.459692	-0.065760	9.207120

Diene 2’z

34

scf done: -1107.704910

C	-0.251220	0.076250	0.388101
C	-0.214761	-0.046497	1.776542
C	1.009811	-0.068214	2.443315
C	2.210981	0.040093	1.733166
C	2.162807	0.152021	0.338387
C	0.940384	0.169771	-0.331035
C	3.533242	0.084458	2.451490
N	3.901018	1.408718	2.958470
S	4.512134	2.546129	1.902559
O	5.292154	3.497231	2.684309
C	3.269770	1.889944	4.183310
C	3.646305	1.049587	5.356992
C	2.770252	0.483428	6.202384
C	3.150944	-0.312684	7.356645
C	3.111449	3.444984	1.262205
O	5.121119	1.811613	0.799669
H	4.345307	-0.263388	1.792915
H	3.519081	-0.584734	3.332691
H	4.231800	-0.444707	7.520521
C	2.277109	-0.877444	8.201322
H	1.688874	0.626816	6.034580
H	3.519188	4.215529	0.585933
H	2.450826	2.753241	0.712863
H	2.580848	3.924529	2.102175
H	4.727769	0.908415	5.512932
H	3.625759	2.925488	4.345540
H	3.103566	0.234539	-0.221590
H	0.917172	0.252491	-1.423836
H	-1.213123	0.088971	-0.137435
H	-1.148128	-0.134813	2.344695
H	1.037767	-0.189887	3.534953

H	2.606816	-1.474469	9.060305
H	1.192936	-0.759932	8.059725
H	2.162291	1.934877	4.076328

Int I
27
scf done: -1049.506231

C	3.823590	-1.252823	-0.636798
P	2.096617	-0.613399	-0.615968
C	2.149507	0.552413	-2.041079
Pd	1.268462	0.195468	1.390664
P	0.394532	0.994191	3.381847
C	-0.660571	2.501041	3.289460
C	1.202370	-2.034223	-1.373758
C	-0.714165	-0.133557	4.326291
C	1.575328	1.491613	4.704888
H	2.549827	0.062092	-2.950882
H	1.131484	0.929116	-2.248589
H	2.785186	1.419858	-1.786293
H	4.109724	-1.612635	-1.645251
H	4.518775	-0.451986	-0.326043
H	3.919513	-2.082957	0.086322
H	1.670855	-2.344375	-2.329203
H	1.205430	-2.888865	-0.673213
H	0.149735	-1.753285	-1.559390
H	-1.083622	0.347001	5.254232
H	-1.576414	-0.417515	3.695989
H	-0.167099	-1.057396	4.588141
H	-1.028665	2.799127	4.291594
H	-0.080451	3.334002	2.852507
H	-1.523979	2.306852	2.627564
H	1.042425	1.864638	5.602225
H	2.201378	0.625966	4.988057
H	2.245880	2.283587	4.324998

Int II
35
scf done: -1278.301881

C	15.946335	6.970252	5.542910
P	15.467870	5.654463	6.715438
C	15.189146	6.582427	8.273145
C	17.043116	4.787858	7.056466
Pd	13.666912	4.343774	6.012978
O	14.802552	2.675508	5.278409
C	15.751701	2.939538	4.463588
C	16.501820	1.718181	3.960764
P	11.669897	3.325026	5.394666
C	10.660178	2.690636	6.784057
C	10.480701	4.377175	4.484238
C	11.847484	1.866191	4.307041
O	16.103419	4.067642	4.107345
H	16.781065	7.573227	5.949703
H	16.248122	6.484673	4.599342
H	15.079060	7.626529	5.348731
H	17.790655	5.492673	7.469191
H	16.874150	3.969415	7.779321
H	17.413339	4.361805	6.108226
H	16.082400	7.174053	8.552991
H	14.326318	7.261278	8.148073
H	14.952180	5.877104	9.090272
H	12.772301	5.516517	6.593457
H	10.857672	1.453906	4.031522
H	12.396016	2.156998	3.393367
H	12.444385	1.093902	4.822601
H	9.735408	2.204888	6.417014
H	11.249836	1.959215	7.365208
H	10.392953	3.526782	7.455038
H	9.569766	3.807797	4.216579
H	10.202792	5.243220	5.111503
H	10.954028	4.760267	3.562359
H	17.130965	1.973013	3.091847
H	17.155160	1.336964	4.768441

H 15.803275 0.903461 3.700487

Int III
53
scf done: -1885.963261

C	16.009184	3.482477	4.377793
P	15.120850	2.986084	5.891213
C	15.007956	1.168931	5.775617
Pd	13.237772	4.228586	6.147419
O	14.596767	5.921016	6.173208
C	14.696500	6.458452	7.335505
C	15.680445	7.601883	7.440006
C	11.534243	5.715358	6.167109
C	11.042288	4.720497	6.707789
C	10.213379	3.719489	7.371480
C	11.741702	7.054481	5.589915
N	10.965941	8.079867	6.265256
S	11.736409	9.240392	7.188911
O	13.053885	9.446016	6.597332
C	9.536365	7.870873	6.433947
C	8.827143	7.825069	5.107532
O	10.803453	10.355661	7.312437
C	11.948103	8.518061	8.795126
O	14.028062	6.126587	8.320252
C	16.332083	3.271203	7.225830
H	17.254682	2.689015	7.038717
H	16.574728	4.347758	7.260839
H	15.901014	2.976673	8.199052
H	16.985378	2.965204	4.309520
H	15.400709	3.238366	3.488868
H	16.163297	4.575362	4.410855
H	16.010136	0.721469	5.633086
H	14.556480	0.766141	6.699845
H	14.358293	0.893082	4.926016
H	12.496293	2.842591	6.021274
H	16.092699	7.663270	8.461810
H	16.492438	7.514277	6.698273
H	15.128861	8.539065	7.233719
H	9.149754	8.713909	7.034315
H	9.341881	6.939032	7.008318
H	12.810478	7.332087	5.608077
H	9.263260	4.181277	7.702377
H	10.715872	3.297460	8.259614
H	9.972362	2.882964	6.690938
H	11.449366	7.027436	4.519326
H	12.366826	9.304376	9.446516
H	10.954758	8.209142	9.164201
H	12.644663	7.658780	8.714914
C	8.086934	6.709596	4.715420
C	7.434085	6.691562	3.481517
C	7.526497	7.789903	2.630074
C	8.274076	8.906270	3.013011
C	8.921425	8.922588	4.244181
H	8.024575	5.841999	5.386536
H	6.853143	5.810893	3.183324
H	7.015945	7.777468	1.660004
H	8.348570	9.771634	2.344144
H	9.515475	9.791637	4.557612

Int III*
53
scf done: -1885.967409

C	8.906169	9.520862	5.573554
C	8.664505	8.144328	5.647856
C	7.572886	7.603123	4.968248
C	6.722361	8.426629	4.228656
C	6.965218	9.796501	4.162447
C	8.060325	10.343221	4.836385
C	9.603061	7.274638	6.437755
N	10.961053	7.342364	5.909029
S	12.221492	7.481935	6.996760
C	12.180176	6.016642	8.005004

C	11.187539	6.872153	4.554974
C	11.021697	5.418131	4.384004
C	10.664244	4.255961	4.193442
C	10.086012	2.943334	3.944756
Pd	12.859390	4.165251	4.977043
O	11.902713	3.006613	6.537109
C	12.330933	1.804712	6.661396
O	13.292935	1.325935	6.055691
P	15.042929	3.861018	5.551537
C	15.912487	2.563251	4.615482
C	15.311840	3.419527	7.302383
C	16.076755	5.351315	5.335649
C	11.551423	0.963205	7.654166
O	13.455619	7.479622	6.215909
O	11.907841	8.603262	7.875052
H	16.967263	2.493030	4.943633
H	15.390018	1.608453	4.796418
H	15.877647	2.797999	3.536821
H	16.394954	3.427158	7.530880
H	14.796258	4.144855	7.956925
H	14.896860	2.412502	7.475275
H	17.094485	5.191274	5.740586
H	16.140787	5.597474	4.260467
H	15.594395	6.203141	5.849131
H	13.577262	5.014577	3.862954
H	11.943853	-0.065789	7.697429
H	11.606334	1.420476	8.659157
H	10.481731	0.940259	7.375418
H	9.636684	7.628800	7.484383
H	9.242793	6.222736	6.452558
H	12.192782	7.190554	4.235457
H	9.109976	3.035276	3.433268
H	9.935786	2.411208	4.901301
H	10.750710	2.322702	3.316575
H	10.463193	7.397296	3.899626
H	13.045751	6.094001	8.685957
H	11.247748	6.022573	8.593691
H	12.242123	5.106286	7.377712
H	7.389474	6.521189	5.017083
H	5.867535	7.992251	3.697332
H	6.300714	10.444444	3.579073
H	8.252677	11.421206	4.785826
H	9.775811	9.933806	6.102608

TS (III-IV)
53
scf done: -1885.955630

Pd	-0.110441	0.001198	0.267177
C	-0.012498	0.485384	2.439866
C	1.129551	0.369873	1.903882
C	2.605786	0.392639	1.939086
N	3.181733	-0.934525	1.848751
O	1.544771	-0.332644	-1.017177
P	-1.725590	-0.235765	-1.425707
H	-1.238874	0.249336	1.395884
C	2.756963	-1.949040	2.800855
C	2.952885	-1.531355	4.235744
C	4.216643	-1.126726	4.681235
C	4.406137	-0.746298	6.006604
C	3.335374	-0.765128	6.903078
C	2.074360	-1.164279	6.466253
C	1.885775	-1.541396	5.135725
S	4.498573	-1.231744	0.865058
O	4.874940	0.042308	0.260040
C	-0.869568	0.754553	3.610903
C	1.676853	0.491013	-1.999052
O	0.850610	1.339241	-2.328051
C	-3.252036	-1.138655	-0.953464
C	-1.196001	-1.119791	-2.935089
C	-2.376051	1.344844	-2.069076
O	5.480748	-1.990077	1.638806
C	3.882588	-2.308749	-0.399944

C	2.968439	0.313368	-2.771654
H	-3.959939	-1.199760	-1.802647
H	-2.997152	-2.162248	-0.623567
H	-3.744084	-0.619305	-0.110861
H	-2.048095	-1.245265	-3.630217
H	-0.406139	-0.523223	-3.421922
H	-0.787184	-2.111644	-2.671465
H	-3.140207	1.167654	-2.850130
H	-2.824686	1.928036	-1.244747
H	-1.526960	1.912387	-2.487007
H	3.826264	0.299823	-2.074118
H	2.955859	-0.659896	-3.298622
H	3.094494	1.118275	-3.513908
H	3.340679	-2.865960	2.598081
H	1.691021	-2.197711	2.618373
H	2.998906	0.997315	1.104365
H	-0.232648	1.006251	4.478138
H	-1.484108	-0.126265	3.873351
H	-1.559058	1.598095	3.427426
H	2.926145	0.885166	2.883138
H	4.725316	-2.506151	-1.084569
H	3.549487	-3.247942	0.072713
H	3.048963	-1.779002	-0.897275
H	0.890670	-1.849086	4.785164
H	1.229052	-1.179830	7.164354
H	3.486782	-0.466261	7.946897
H	5.400474	-0.433904	6.346651
H	5.052816	-1.119194	3.969624

TS (III-IV)*
53
scf done: -1885.954579

C	-0.015064	0.038822	0.010315
C	0.002518	0.038307	1.407222
C	1.214930	0.024245	2.089259
C	2.421945	0.006279	1.381436
C	2.398612	0.014266	-0.013247
C	1.182992	0.027976	-0.699689
C	3.719711	-0.011636	2.140845
N	3.826341	1.129588	3.042225
S	4.417652	0.851073	4.582147
O	4.500012	2.156302	5.234358
C	3.942813	2.450937	2.444214
C	5.308656	2.735144	1.916767
C	6.191758	2.564018	1.023931
C	6.753363	2.176816	-0.269690
Pd	7.301259	3.297471	2.660256
O	9.162838	3.140567	1.657987
C	9.915006	2.217718	2.131831
O	9.650739	1.508024	3.106564
P	8.211294	3.994603	4.703292
C	8.134485	2.713297	6.002554
C	7.378472	5.422080	5.492257
C	9.973259	4.475395	4.682169
O	3.614628	-0.219052	5.160304
C	6.065361	0.204941	4.380146
C	11.227030	2.013337	1.398017
H	10.288388	4.857484	5.671992
H	10.570200	3.583147	4.422946
H	10.144307	5.250603	3.914353
H	8.558787	3.086526	6.954502
H	7.079198	2.422469	6.161042
H	8.707414	1.834934	5.654984
H	7.857732	5.685075	6.454864
H	7.410258	6.297889	4.819435
H	6.318524	5.163128	5.672361
H	5.833419	3.427576	3.295399
H	11.443146	2.828211	0.687990
H	12.050646	1.916698	2.127473
H	11.182703	1.059449	0.840125
H	3.768463	-0.928381	2.757758
H	4.582967	-0.039267	1.438660

H	3.615151	3.204915	3.175783
H	5.985096	1.746685	-0.940620
H	7.563558	1.438732	-0.127424
H	7.213089	3.047881	-0.770967
H	3.223590	2.481317	1.603126
H	6.419280	-0.059768	5.391532
H	6.018039	-0.702895	3.756169
H	6.720727	0.968795	3.920025
H	3.345986	0.009752	-0.569842
H	1.173877	0.034236	-1.795597
H	-0.970850	0.051036	-0.526307
H	-0.939426	0.047612	1.967896
H	1.247707	0.029965	3.186859

Int IV
53
scf done: -1886.008332

C	-1.033678	2.954042	1.102650
P	0.290153	1.716404	1.331604
C	1.387521	1.979714	-0.107073
Pd	0.029657	-0.496046	1.652669
O	0.413130	-2.640654	1.959279
C	1.611925	-2.393943	2.294160
C	2.528987	-3.536346	2.611942
O	2.042665	-1.208353	2.316794
C	-1.872987	-0.483071	1.046573
C	-2.920688	-0.010145	1.733064
C	-2.907010	0.728792	3.028817
C	1.252184	2.382976	2.734021
C	-2.030706	-1.375985	-0.152184
N	-1.302631	-0.896217	-1.323226
S	-0.478895	-2.015895	-2.253347
O	-0.146844	-1.356572	-3.514562
C	-1.764237	0.343018	-1.925849
C	-3.201593	0.312476	-2.382352
C	1.031835	-2.289227	-1.360174
O	-1.209198	-3.280548	-2.268919
H	-1.661662	-2.390222	0.094922
H	-0.577081	3.950895	0.952506
H	-1.659635	2.706842	0.227306
H	-1.683918	2.985909	1.993453
H	1.700272	3.039428	-0.174975
H	2.282650	1.340839	0.006191
H	0.871006	1.692481	-1.041345
H	1.589221	3.417273	2.528992
H	0.629110	2.374239	3.646849
H	2.127992	1.732208	2.908849
H	1.981217	-4.347794	3.119338
H	2.927694	-3.946937	1.665032
H	3.379613	-3.200402	3.226834
H	-1.093580	0.573291	-2.772693
H	-1.635201	1.149756	-1.177593
H	-3.110115	-1.498442	-0.398989
H	-1.875075	0.930300	3.375292
H	-3.402489	0.135066	3.822331
H	-3.464783	1.685250	2.970391
H	-3.924859	-0.239409	1.328572
H	1.599915	-3.034504	-1.942555
H	1.579507	-1.333922	-1.301817
H	0.800782	-2.676197	-0.351046
C	-4.102086	1.289864	-1.953516
C	-5.429204	1.276383	-2.383280
C	-5.870353	0.273400	-3.243495
C	-4.979921	-0.713744	-3.669256
C	-3.655121	-0.695080	-3.241593
H	-3.756871	2.073808	-1.264639
H	-6.124277	2.050042	-2.036389
H	-6.913606	0.255781	-3.579735
H	-5.322062	-1.508708	-4.341992
H	-2.962911	-1.479748	-3.573163

Int IV*
53
scf done: -1886.001645

C	-1.567179	2.181612	-0.027605
P	-0.101802	1.503424	0.819715
C	0.090998	2.583652	2.280354
C	1.300975	1.973315	-0.252945
Pd	0.068428	-0.666476	1.383726
C	-1.905952	-0.858964	1.151468
C	-2.478593	-1.220791	-0.004696
C	-1.785691	-1.352147	-1.324288
N	-2.182527	-0.345740	-2.331794
S	-3.776927	-0.380230	-2.861383
O	0.682604	-2.657149	2.047501
C	1.886777	-2.276771	2.135729
O	2.210538	-1.088836	1.857223
C	2.930294	-3.266972	2.561773
C	-2.638058	-0.771193	2.450038
H	-1.401765	3.246899	-0.278594
H	-1.777116	1.597045	-0.944131
H	-2.447534	2.094700	0.635568
H	1.326161	3.067571	-0.417928
H	2.242925	1.647894	0.224692
H	1.216408	1.458512	-1.227721
H	0.129338	3.648105	1.978877
H	-0.756693	2.431421	2.972629
H	1.022772	2.317323	2.810950
H	2.603659	-3.789454	3.477728
H	3.046301	-4.036100	1.776767
H	3.901015	-2.774373	2.731996
C	-1.147109	0.034743	-3.292752
H	-3.543736	-1.515658	0.017049
H	-3.705194	-1.053929	2.336887
H	-2.187166	-1.440449	3.209412
H	-2.597578	0.254072	2.872302
H	-0.696726	-1.209868	-1.180371
H	-1.920873	-2.372452	-1.739134
C	-4.598348	0.817970	-1.839488
O	-3.811030	0.138652	-4.227815
O	-4.348517	-1.689401	-2.562218
H	-5.661773	0.799141	-2.133001
H	-4.480200	0.535632	-0.780622
H	-4.157471	1.807448	-2.040937
H	-1.598993	0.737267	-4.013886
H	-0.370341	0.597545	-2.734932
C	-0.506602	-1.125297	-4.013253
C	-1.270697	-1.963426	-4.834881
C	-0.677504	-3.040179	-5.488257
C	0.686504	-3.293190	-5.332514
C	1.453242	-2.467082	-4.514496
C	0.855318	-1.391885	-3.856229
H	-2.342633	-1.765343	-4.963978
H	-1.286856	-3.688722	-6.128448
H	1.151708	-4.141366	-5.848306
H	2.523467	-2.662557	-4.380265
H	1.459136	-0.748117	-3.200639

TS (IV-V)*
53
scf done: -1885.953752

C	0.023729	0.030435	-0.037842
C	0.008989	-0.040876	1.356807
C	1.203223	-0.066551	2.070944
C	2.430587	-0.021241	1.398336
C	2.436575	0.054103	0.004155
C	1.240163	0.076230	-0.714405
C	3.723968	-0.036979	2.172470
N	3.830284	1.053281	3.139680
S	3.751378	0.680325	4.775369
O	2.971124	-0.549228	4.917383
C	3.631016	2.418098	2.698635
C	4.772656	3.052861	1.944042

C	5.741863	2.420876	1.173139
C	6.073524	1.912140	-0.006343
Pd	6.592872	3.079181	3.068992
O	5.598326	4.327604	4.458781
C	5.694066	4.009169	5.695938
O	6.424015	3.118452	6.145629
P	8.702664	3.057743	4.144256
C	9.099147	1.647385	5.235918
C	9.093950	4.519720	5.168459
C	10.106334	3.036389	2.960553
C	5.422381	0.293611	5.221267
O	3.347371	1.886282	5.489018
C	4.859865	4.839389	6.645343
H	7.193053	2.144650	1.920397
H	3.812425	-0.986933	2.729563
H	4.581058	0.004468	1.473017
H	3.410628	3.040178	3.583018
H	7.075370	1.535769	-0.244449
H	5.310798	1.858019	-0.797122
H	5.384719	-0.122144	6.242820
H	5.807656	-0.458558	4.511407
H	6.003659	1.235642	5.214301
H	11.077687	3.075117	3.490556
H	10.064908	2.116260	2.349450
H	10.033573	3.903365	2.278950
H	10.155333	4.493948	5.481919
H	8.905022	5.443544	4.592640
H	8.442699	4.510581	6.057638
H	10.141120	1.728487	5.600856
H	8.401000	1.662376	6.088836
H	8.981802	0.696085	4.685219
H	4.069836	5.399099	6.118912
H	4.411573	4.181951	7.409050
H	5.515464	5.559828	7.169916
H	3.396183	0.092226	-0.529556
H	1.260653	0.134409	-1.808895
H	-0.918423	0.051486	-0.597999
H	-0.946343	-0.079063	1.893326
H	1.197970	-0.125399	3.166997
H	2.722263	2.463071	2.056168
H	4.593590	4.119146	1.719270

TS (IV-V)**
53
scf done: -1885.956325

C	-2.621751	2.656996	-1.142653
P	-0.929000	1.986770	-1.302714
C	-0.858033	1.410667	-3.038319
Pd	-0.379769	0.420990	0.412283
C	-0.050196	-0.629537	2.163782
C	-0.247904	-1.859786	2.625454
C	-0.733643	-3.040139	1.860073
C	0.400991	0.632509	2.601769
N	1.774020	0.868666	2.768989
S	2.303343	2.446549	3.069066
O	1.143520	3.180776	3.552051
O	-0.661512	-1.263695	-0.844156
C	-1.827011	-1.359774	-1.372057
O	-2.723092	-0.519694	-1.277179
C	0.075551	3.524540	-1.374468
C	2.757140	-0.120147	2.334064
C	2.896090	-1.278185	3.287248
O	3.523423	2.346015	3.853643
C	2.733748	3.070068	1.461056
C	-2.042216	-2.638021	-2.157708
H	-0.072000	1.660083	1.416579
H	3.730012	0.397575	2.238197
H	2.475274	-0.479877	1.322376
H	-0.232072	1.242685	3.262231
H	-0.862449	-2.793990	0.793021
H	-1.693380	-3.409258	2.271765
H	-0.013076	-3.876885	1.952477

H	-0.007378	-2.033414	3.691295
H	3.023550	4.125353	1.599849
H	3.582448	2.490483	1.063404
H	1.851439	2.991686	0.804088
H	-0.284775	4.195323	-2.178460
H	0.001686	4.060474	-0.409843
H	1.137672	3.284275	-1.566027
H	-1.038158	2.253566	-3.732792
H	0.130259	0.964914	-3.251072
H	-1.635523	0.641525	-3.182635
H	-2.827601	3.396111	-1.940718
H	-3.327888	1.812606	-1.209923
H	-2.737745	3.142730	-0.156665
H	-1.213762	-2.799349	-2.870255
H	-2.041746	-3.500680	-1.465350
H	-3.003482	-2.611485	-2.696165
C	3.008885	-2.581469	2.798960
C	3.134652	-3.656996	3.676338
C	3.144485	-3.435319	5.053080
C	3.041027	-2.134311	5.545748
C	2.922380	-1.059675	4.666887
H	2.970724	-2.756519	1.715256
H	3.214137	-4.676725	3.281592
H	3.233030	-4.279995	5.746070
H	3.053832	-1.954301	6.626968
H	2.841064	-0.035199	5.050885

Int V

53

scf done: -1885.961828

Pd	12.438121	8.275870	5.743077
O	14.123268	7.036639	6.268910
C	14.611200	7.265309	7.428776
O	14.208448	8.127806	8.216138
H	11.317309	9.319086	5.372815
P	13.562997	10.274536	6.011319
C	15.384457	10.149594	6.035564
C	13.251337	11.519066	4.707232
C	13.152576	11.145274	7.558388
C	10.808106	7.041478	4.915147
C	11.438043	6.243896	5.811978
C	10.988025	6.002733	7.220221
C	9.982725	7.371389	3.931638
N	9.034072	6.485706	3.390993
C	8.830374	5.170253	3.972184
C	9.975500	4.214641	3.745046
C	10.781097	4.301523	2.608437
C	11.837725	3.411609	2.425294
C	12.093229	2.418322	3.370271
C	11.281977	2.316086	4.499717
C	10.231287	3.212212	4.684801
C	15.823068	6.425711	7.783451
S	8.080778	6.988221	2.098099
O	8.785102	8.078863	1.441281
O	7.689899	5.792626	1.366740
C	6.629098	7.660900	2.870466
H	7.901524	4.752335	3.541020
H	8.653272	5.291399	5.061400
H	10.002999	8.356187	3.452600
H	10.197801	6.712466	7.523164
H	11.830882	6.085617	7.931244
H	10.588498	4.970829	7.303874
H	12.256687	5.598885	5.447462
H	5.965613	8.010891	2.061818
H	6.135341	6.867200	3.455399
H	6.933465	8.502600	3.514232
H	9.599670	3.138550	5.581053
H	11.473074	1.537548	5.247474
H	12.926927	1.721583	3.226290
H	12.469937	3.495852	1.533882
H	10.586287	5.083382	1.864396
H	13.843916	12.436204	4.888450

H	13.521867	11.101876	3.720590
H	12.176737	11.774083	4.688951
H	13.722181	12.091103	7.636442
H	12.069928	11.361936	7.588652
H	13.410040	10.472350	8.394151
H	15.834373	11.160351	6.008936
H	15.681039	9.631478	6.963268
H	15.735945	9.564884	5.167005
H	16.715566	6.880084	7.311012
H	15.982314	6.408115	8.874230
H	15.732940	5.399160	7.389174

Int V*
53
scf done: -1885.959501

C	16.064297	2.745995	7.516353
C	15.841394	3.034631	6.164096
C	16.922843	3.421810	5.369889
C	18.204072	3.532019	5.911207
C	18.415399	3.246687	7.258063
C	17.341871	2.851718	8.058874
C	14.463018	2.911898	5.567918
N	13.885269	1.570280	5.672412
S	12.866618	1.244262	6.980046
O	13.479385	0.238877	7.845526
C	14.678018	0.450937	5.201396
C	14.794631	0.324468	3.705860
C	14.444900	1.222563	2.759142
C	14.533157	2.218560	1.901884
Pd	12.779340	-0.277420	2.851370
O	13.568371	-2.240558	3.289142
C	12.925139	-2.848068	4.210872
O	11.945140	-2.387585	4.812137
P	10.707779	-1.060733	2.211388
C	10.032786	-0.299287	0.692958
C	9.383668	-0.834743	3.442235
C	10.669897	-2.847970	1.842163
C	13.398632	-4.255745	4.503195
O	12.481755	2.534924	7.545107
C	11.447965	0.513081	6.214690
H	12.052900	1.076942	2.498937
H	13.760708	3.602111	6.065333
H	14.485549	3.196411	4.500114
H	14.262221	-0.488880	5.608859
H	13.736424	2.473079	1.193649
H	15.446915	2.833186	1.878681
H	10.756631	0.263294	7.038120
H	11.005115	1.265821	5.542061
H	11.739193	-0.406929	5.667061
H	9.068142	-0.765460	0.415588
H	9.884932	0.782832	0.857805
H	10.750134	-0.426577	-0.137491
H	9.706192	-3.117234	1.369462
H	11.502236	-3.114742	1.167560
H	10.784081	-3.401315	2.789688
H	8.441587	-1.290630	3.082188
H	9.705915	-1.321200	4.380023
H	9.218903	0.242539	3.622987
H	12.998487	-4.932791	3.723815
H	14.498850	-4.324429	4.458468
H	13.031873	-4.599675	5.484065
H	16.756567	3.643858	4.306623
H	19.042628	3.837741	5.274556
H	19.420603	3.329353	7.687771
H	17.502334	2.624921	9.119315
H	15.225039	2.428531	8.148892
H	15.711735	0.503425	5.614615
H	15.401970	-0.538075	3.386467

Int V**
53
scf done: -1885.970005

C	16.181345	2.633755	6.517806
P	14.787504	2.898500	5.367035
C	15.578042	3.645874	3.901271
Pd	13.191794	4.323549	6.217717
O	14.799083	5.742900	6.500176
C	15.262327	5.850913	7.686627
C	16.449260	6.783512	7.826955
C	11.784282	5.395455	7.915646
C	11.542372	5.695636	6.604742
C	10.846611	6.356243	5.693122
C	10.935842	6.192085	4.214746
N	11.052591	4.480353	8.630353
S	11.596988	4.055220	10.203690
O	10.520545	3.261464	10.778258
C	9.900473	3.818450	8.038258
C	8.731245	4.748566	7.845755
C	13.007402	3.036829	9.884685
O	12.032215	5.287852	10.837973
C	14.328981	1.215733	4.825647
O	14.846430	5.237710	8.676164
H	12.101982	3.236913	5.863213
H	9.625926	2.982504	8.705712
H	10.213944	3.386362	7.064698
H	12.599168	5.877721	8.481106
H	11.691596	5.435075	3.937676
H	11.198481	7.145571	3.717628
H	9.954867	5.881004	3.802423
H	10.111561	7.093181	6.063996
H	13.374885	2.702129	10.870265
H	12.678969	2.177493	9.275769
H	13.760694	3.666335	9.366600
H	15.203808	0.675099	4.416832
H	13.916939	0.649972	5.680487
H	13.544879	1.283301	4.050375
H	16.431636	3.034781	3.550445
H	14.838058	3.745207	3.087126
H	15.926927	4.656222	4.180845
H	16.948394	1.979794	6.060357
H	16.629367	3.613232	6.762771
H	15.818743	2.176617	7.455699
H	16.372090	7.641491	7.137976
H	16.548991	7.132252	8.867983
H	17.370642	6.228932	7.562631
C	7.950869	4.662491	6.690537
C	6.870804	5.521595	6.498842
C	6.565346	6.483008	7.462075
C	7.339432	6.572292	8.619058
C	8.414567	5.706985	8.811920
H	8.209169	3.923138	5.920092
H	6.269661	5.448621	5.584894
H	5.723298	7.167951	7.309434
H	7.106010	7.325441	9.380519
H	9.029540	5.784252	9.718431

TS (V-VI)
53
scf done: -1885.955473

C	-0.398197	0.376860	0.485190
C	-0.217471	0.418843	1.865483
C	0.981634	-0.012988	2.440233
C	2.005593	-0.472837	1.610928
C	1.824132	-0.521872	0.229652
C	0.621878	-0.101410	-0.337046
C	1.138973	0.035255	3.939724
N	2.149110	-0.869064	4.460544
C	1.936519	-2.251193	4.506579
C	0.833621	-2.854278	4.057439
Pd	0.115127	-4.840891	3.642840
O	-1.399029	-5.304654	2.218867

C	-2.313341	-6.098822	2.632733
O	-2.318926	-6.677791	3.722648
S	3.635217	-0.250225	4.972948
O	3.837468	1.003078	4.264076
C	3.365599	0.117624	6.689044
O	4.604055	-1.332527	4.888376
C	-0.357787	-2.763632	3.345703
C	-1.694339	-2.452157	3.951369
P	0.697885	-7.074296	4.136609
C	2.495636	-7.342268	4.391148
C	-0.028754	-7.765659	5.662677
C	0.294310	-8.322585	2.863635
C	-3.473059	-6.302536	1.676109
H	1.199375	-4.364182	4.692243
H	1.407003	1.060620	4.256142
H	0.175110	-0.207371	4.431689
H	2.769898	-2.811652	4.945132
H	-1.707212	-2.651722	5.038206
H	-2.490253	-3.050549	3.470384
H	-1.947604	-1.382407	3.791536
H	-0.283607	-2.633235	2.251127
H	4.310913	0.527743	7.082990
H	2.559334	0.865198	6.768999
H	3.100244	-0.815914	7.212075
H	-1.027488	0.784152	2.512076
H	-1.345964	0.712768	0.048530
H	0.479227	-0.145849	-1.422756
H	2.631948	-0.894907	-0.410359
H	2.950834	-0.811252	2.053807
H	2.716265	-8.406605	4.602628
H	3.053473	-7.030713	3.489317
H	2.844468	-6.724683	5.238896
H	0.319331	-8.804075	5.824409
H	0.260111	-7.144885	6.529914
H	-1.125922	-7.742196	5.553232
H	0.748361	-9.298278	3.123240
H	-0.802713	-8.423708	2.812077
H	0.671380	-7.993161	1.878855
H	-3.744519	-7.372085	1.635676
H	-4.355836	-5.762925	2.067224
H	-3.252054	-5.927270	0.663449

TS (V-VI)*
53
scf done: -1885.954142

C	-0.051766	-0.034663	0.007034
C	-0.029105	-0.020830	1.402388
C	1.182864	-0.029582	2.095767
C	2.380260	-0.062315	1.370859
C	2.359913	-0.078970	-0.020517
C	1.143574	-0.064132	-0.706940
C	1.203746	-0.009067	3.603003
N	1.918520	-1.140256	4.189612
C	1.537277	-2.490189	3.827925
C	0.255356	-3.009985	4.429568
Pd	0.290170	-2.976860	6.570968
O	1.915303	-4.331348	6.469435
C	2.941280	-4.078326	7.195414
C	4.153239	-4.930297	6.897168
S	3.399223	-0.849465	4.923446
O	4.135398	-2.107880	4.956973
O	3.993741	0.326826	4.289019
C	2.986066	-0.388907	6.584563
C	-0.853125	-2.284702	4.849516
C	-2.000671	-1.707644	4.517869
P	0.140355	-2.856782	8.930474
C	0.681743	-4.338845	9.852421
C	-1.587323	-2.651650	9.518921
C	0.997682	-1.477443	9.767207
O	2.996999	-3.199033	8.062191
H	-0.919674	-1.938531	6.477663
H	1.696757	0.915204	3.954418

H	0.168782	0.011995	3.994200
H	2.351103	-3.174730	4.121439
H	-2.691308	-1.266063	5.245853
H	-2.285426	-1.662831	3.455982
H	3.925444	-0.060971	7.062022
H	2.263592	0.444401	6.544143
H	2.584600	-1.279389	7.103587
H	-1.635667	-2.645441	10.624885
H	-2.000347	-1.701406	9.133521
H	-2.213993	-3.477820	9.136316
H	0.408374	-4.245676	10.921098
H	0.200772	-5.239659	9.430351
H	1.775469	-4.435057	9.752929
H	0.784131	-1.495451	10.853267
H	2.081174	-1.587297	9.594561
H	0.655343	-0.513370	9.347837
H	4.822618	-4.976830	7.772236
H	3.869660	-5.944921	6.570093
H	4.703470	-4.444336	6.069535
H	-0.971401	0.003040	1.967058
H	-1.010610	-0.025678	-0.524549
H	1.129933	-0.077182	-1.802886
H	3.303366	-0.100155	-0.578559
H	3.332972	-0.068683	1.916165
H	1.456861	-2.562921	2.719376
H	0.073899	-4.072350	4.188524

TS (V-VI)**
53
scf done: -1885.963065

Pd	0.256491	0.108630	-0.187356
C	0.293376	-0.256648	1.962139
C	1.571153	0.106427	1.532133
C	2.825073	0.238060	1.958417
N	-0.515780	0.590920	2.732173
C	-0.096310	1.947348	3.058786
O	-1.806406	-0.460677	-0.129556
C	-2.071728	-1.620327	-0.619310
O	-1.306647	-2.286266	-1.314732
P	0.309577	0.353704	-2.542491
H	1.773808	0.583721	-0.029583
C	4.016000	0.706359	1.204469
S	-2.024973	0.044619	3.284368
O	-2.052718	-1.394328	3.062575
C	1.041564	2.016989	4.047199
C	1.063357	1.186563	5.170993
C	2.123498	1.252974	6.073044
C	3.167432	2.155192	5.866794
C	3.143746	2.996504	4.755032
C	2.085775	2.923607	3.850154
C	1.220042	-1.007414	-3.355069
C	1.098905	1.855641	-3.238773
C	-1.312977	0.310261	-3.382676
C	-3.451188	-2.129878	-0.252391
O	-2.187228	0.592030	4.627288
C	-3.224876	0.814813	2.233920
H	-0.975263	2.477810	3.469918
H	0.180946	2.469477	2.119946
H	-0.006686	-1.313868	2.005281
H	3.778366	0.937817	0.149576
H	4.819545	-0.054167	1.220924
H	4.436464	1.616915	1.675223
H	2.993553	-0.020815	3.017466
H	-4.207592	0.482154	2.611536
H	-3.134221	1.909493	2.328211
H	-3.025109	0.456561	1.206552
H	1.198745	-0.899579	-4.456788
H	2.268975	-1.019547	-3.008056
H	0.740172	-1.957955	-3.062045
H	-1.192873	0.458445	-4.472990
H	-1.765192	-0.678184	-3.186378
H	-1.978014	1.091507	-2.973749

H	1.091053	1.835625	-4.345628
H	0.560533	2.756192	-2.891762
H	2.143684	1.923333	-2.884275
H	-3.505415	-2.245368	0.846970
H	-4.223903	-1.394101	-0.542353
H	-3.659689	-3.098009	-0.736110
H	2.078139	3.569782	2.961459
H	3.958836	3.710314	4.586809
H	4.001081	2.204445	6.576917
H	2.132415	0.594437	6.949450
H	0.238054	0.483152	5.335040

VI

53

scf done: -1886.020477

C	0.931245	-1.907061	0.954046
C	0.633541	-1.322245	2.188497
C	1.659160	-1.174731	3.130519
C	2.951408	-1.609825	2.844603
C	3.235899	-2.202536	1.612765
C	2.223343	-2.349642	0.667667
C	-0.764598	-0.860932	2.520641
N	-1.485042	-1.747870	3.443820
S	-1.714115	-1.212582	5.025778
C	-3.215631	-0.262271	4.957370
C	-2.178126	-2.931420	3.057758
C	-3.049558	-3.138184	1.924080
C	-2.746218	-2.856789	0.590292
C	-3.519843	-3.437886	-0.545635
Pd	-1.169708	-4.139687	1.636438
P	0.233365	-5.236616	3.157214
C	-0.509794	-6.753526	3.851868
O	-0.343185	-4.938578	-0.158295
C	-0.201429	-6.210240	-0.224651
C	0.428699	-6.698605	-1.516187
O	-0.491063	-7.011943	0.665492
C	1.855290	-5.778641	2.514894
C	0.697376	-4.292108	4.654938
O	-1.971915	-2.379205	5.862088
O	-0.623436	-0.299803	5.341902
H	-3.836746	-3.891866	2.091042
H	-0.714592	0.134480	2.993933
H	-1.367236	-0.732939	1.604966
H	-2.495164	-3.478808	3.955873
H	-4.142599	-4.289504	-0.216459
H	-2.832941	-3.803900	-1.330883
H	-4.181912	-2.684407	-1.016962
H	-2.098736	-2.008847	0.331797
H	-3.414093	0.105975	5.977952
H	-3.067943	0.582261	4.263935
H	-4.031862	-0.920869	4.616495
H	0.152115	-2.021313	0.190050
H	2.429266	-2.818291	-0.301587
H	4.252999	-2.545770	1.389076
H	3.745113	-1.483148	3.590330
H	1.429531	-0.718545	4.102338
H	1.321305	-4.915396	5.324660
H	1.269106	-3.392302	4.360754
H	-0.203361	-3.958898	5.203210
H	0.185145	-7.239733	4.563605
H	-1.446178	-6.494221	4.379597
H	-0.739923	-7.430615	3.012026
H	2.467313	-6.216187	3.327082
H	1.686659	-6.533209	1.728075
H	2.384136	-4.908369	2.083104
H	1.509393	-6.460426	-1.500659
H	0.310803	-7.789345	-1.624372
H	-0.003493	-6.180323	-2.389822

VI*
53
scf done: -1886.005439

C	-0.944636	2.918875	1.066965
C	-0.047882	1.861426	1.258967
C	0.920140	1.612185	0.284053
C	0.987991	2.390747	-0.871460
C	0.087123	3.436597	-1.057424
C	-0.877920	3.699825	-0.083542
C	-0.133605	0.996996	2.491724
N	-0.176567	1.736692	3.741558
S	-1.655529	2.014431	4.477386
O	-1.849178	3.451254	4.653839
C	0.904946	2.673269	4.025530
C	2.264771	2.011251	4.125086
C	3.336459	2.930574	4.545601
C	4.570289	2.970856	4.017708
Pd	2.167892	0.799482	5.789909
O	1.910528	0.109998	7.910422
C	1.594821	1.282906	8.246766
C	1.324022	1.605353	9.686775
P	2.687406	-1.069074	4.646352
C	3.817904	-2.070424	5.674287
C	3.487074	-1.077779	3.002432
C	1.235041	-2.160694	4.435463
O	1.525569	2.210229	7.383628
O	-2.650687	1.235594	3.744192
C	-1.467572	1.298520	6.090070
H	0.681410	3.205469	4.969478
H	3.767884	-2.111937	2.726888
H	2.802967	-0.680610	2.230589
H	4.396093	-0.449694	3.020743
H	1.531336	-3.144156	4.021931
H	0.759189	-2.308305	5.422236
H	0.495305	-1.688980	3.763108
H	3.982067	-3.069327	5.226259
H	4.786162	-1.549090	5.779204
H	3.377731	-2.182342	6.681769
H	2.239599	2.034008	10.134915
H	0.529235	2.365051	9.774054
H	1.055821	0.698180	10.252371
H	-1.038939	0.364961	2.454792
H	0.730191	0.302290	2.516236
H	0.935837	3.461448	3.236042
H	4.854769	2.316448	3.179662
H	5.336334	3.659274	4.396252
H	3.085876	3.620805	5.368612
H	-2.419071	1.474415	6.620278
H	-1.276493	0.219076	5.970984
H	-0.630250	1.794065	6.612976
H	1.635645	0.790907	0.431227
H	1.754309	2.183031	-1.627384
H	0.137849	4.054122	-1.961723
H	-1.587831	4.523465	-0.221707
H	-1.699419	3.135558	1.834300
H	2.540897	1.490685	3.189753

VI**
53
scf done: -1886.017558

C	0.250335	1.078167	3.877933
P	-0.119453	-0.418385	2.894151
C	-1.721885	-0.996590	3.549783
C	1.071065	-1.655569	3.521517
Pd	0.217932	-0.053041	0.687542
C	-1.612482	-0.836698	0.181490
N	-1.318295	-1.841161	-0.809605
C	-1.395585	-1.573585	-2.244723
C	-2.815246	-1.404888	-2.723981
O	1.065860	0.334932	-1.338652
C	2.153454	0.747047	-0.835235
O	2.337654	0.758906	0.409045

C	3.224185	1.259647	-1.757836
C	-2.313235	0.355276	-0.326603
C	-3.449317	0.836476	0.205367
C	-4.160610	2.049016	-0.280819
S	-0.649101	-3.289289	-0.301849
O	-0.929249	-3.413670	1.126895
O	-1.087747	-4.326273	-1.229127
C	1.110912	-3.117093	-0.511809
H	-1.856108	0.889807	-1.175039
H	0.254054	0.856000	4.962459
H	1.240039	1.469116	3.578584
H	-0.503455	1.857821	3.666529
H	1.011471	-1.751115	4.622922
H	0.846708	-2.630661	3.051978
H	2.093981	-1.350498	3.232771
H	-1.687691	-1.050707	4.654314
H	-2.529097	-0.304164	3.246950
H	-1.940569	-2.001152	3.142854
H	3.277644	0.642034	-2.670522
H	2.965292	2.287722	-2.072179
H	4.203902	1.286947	-1.253931
H	-0.931680	-2.432830	-2.763852
H	-0.777620	-0.689178	-2.491826
H	-2.145399	-1.298556	1.026602
H	-3.615461	2.529296	-1.113996
H	-4.292464	2.801906	0.521378
H	-5.177537	1.794397	-0.640012
H	-3.913820	0.282237	1.038569
H	1.549412	-4.101322	-0.274091
H	1.317207	-2.843151	-1.560100
H	1.480875	-2.334398	0.174284
C	-3.158703	-0.344543	-3.564639
C	-4.475989	-0.171217	-3.987848
C	-5.464346	-1.060118	-3.569193
C	-5.125601	-2.128871	-2.737297
C	-3.809141	-2.300813	-2.319185
H	-2.382365	0.367172	-3.877235
H	-4.733549	0.671024	-4.640895
H	-6.502651	-0.922191	-3.893144
H	-5.897383	-2.835474	-2.409741
H	-3.538827	-3.134837	-1.659776

TS (VI-VII)
53
scf done: -1885.976484

C	-0.082613	-0.061588	0.149956
C	-0.079770	0.097246	1.541936
C	1.144707	0.144127	2.213484
C	2.345099	0.034579	1.511953
C	2.332639	-0.118720	0.127029
C	1.114563	-0.166932	-0.553242
C	-1.364627	0.289726	2.303969
N	-2.102725	1.491601	1.911847
S	-1.432658	2.990571	2.342297
O	-0.594356	2.739907	3.503911
C	-3.193083	1.476025	1.052340
C	-3.694503	0.409888	0.388833
C	-4.904758	0.529289	-0.402206
C	-5.445706	-0.525666	-1.171035
Pd	-6.571937	-0.279007	0.766464
O	-6.250783	1.008111	2.450626
C	-6.223907	2.268852	2.198634
O	-6.459087	2.786420	1.106203
P	-8.364033	-1.086766	2.028038
C	-9.556308	0.254709	2.378210
C	-7.846718	-1.616713	3.700186
C	-9.429530	-2.464112	1.459973
C	-5.799072	3.136352	3.366047
O	-2.518256	3.959420	2.386328
C	-0.392385	3.431762	0.969173
H	-1.158314	0.352745	3.385230
H	-6.712247	-1.281664	-0.483471

H	-8.722874	-1.851968	4.335011
H	-7.197328	-2.507771	3.629981
H	-7.263883	-0.794907	4.152719
H	-10.228359	-2.679230	2.195702
H	-9.891954	-2.203566	0.490856
H	-8.817155	-3.372415	1.315246
H	-10.365015	-0.091058	3.050693
H	-9.006453	1.086825	2.853376
H	-9.995780	0.625591	1.434945
H	-6.271003	4.131261	3.298356
H	-6.025170	2.665437	4.337712
H	-4.703259	3.287349	3.302401
H	-2.058697	-0.557499	2.166380
H	-4.866915	-1.458202	-1.263827
H	-6.044331	-0.272630	-2.057134
H	-5.271227	1.550130	-0.579737
H	-0.019559	4.448841	1.178990
H	0.440335	2.712271	0.899348
H	-1.006833	3.428620	0.052803
H	-3.237894	-0.588361	0.466505
H	-3.705915	2.446143	0.965616
H	1.152670	0.292831	3.300346
H	3.297730	0.077417	2.052449
H	3.275368	-0.199340	-0.426404
H	1.098071	-0.287702	-1.642528
H	-1.036021	-0.084993	-0.393765

TS (VI-VII)*
53
scf done: -1885.971670

C	-2.404774	-0.701377	0.643025
C	-1.415860	-0.502863	1.609379
C	-0.222561	0.126909	1.245693
C	-0.020496	0.543975	-0.067654
C	-1.011036	0.340305	-1.030072
C	-2.206380	-0.280904	-0.671614
C	-1.652395	-0.942832	3.027296
N	-0.508768	-1.635784	3.624349
S	0.006721	-1.068061	5.145197
O	0.018648	0.383189	5.048173
C	-0.265209	-2.984730	3.340231
C	-0.523795	-3.563139	2.047027
C	0.243176	-4.745185	1.642866
C	0.493407	-5.096640	0.373235
Pd	-2.220577	-4.217714	3.113802
O	-3.819990	-4.783089	4.408619
C	-4.338036	-3.758604	4.980525
C	-5.468447	-4.064097	5.943204
P	-3.618347	-4.894910	1.341862
C	-5.329636	-4.272861	1.507266
C	-3.820733	-6.710896	1.380762
C	-3.182026	-4.550718	-0.399799
O	-3.975479	-2.589816	4.816860
C	-1.278736	-1.563534	6.266918
O	1.217272	-1.807305	5.472702
H	-1.259792	-3.793734	4.320920
H	-3.929276	-4.982999	-1.092386
H	-3.119274	-3.459669	-0.567647
H	-2.191320	-4.990651	-0.617591
H	-5.972333	-4.633241	0.681628
H	-5.732682	-4.627691	2.472667
H	-5.331662	-3.167798	1.523283
H	-4.562794	-7.059980	0.637266
H	-2.845088	-7.190856	1.178629
H	-4.145779	-7.000401	2.396915
H	-5.918453	-5.053152	5.754799
H	-5.070544	-4.060214	6.975322
H	-6.238349	-3.275510	5.887866
H	-1.852393	-0.051012	3.649077
H	-2.548264	-1.595180	3.112882
H	0.593521	-3.380539	3.903124
H	0.148658	-4.476938	-0.467975

H	1.071616	-5.996485	0.130693
H	0.629438	-5.373831	2.462278
H	-1.051963	-1.072475	7.228561
H	-2.266644	-1.262074	5.877898
H	-1.242603	-2.660292	6.373016
H	-3.339843	-1.202431	0.930816
H	-2.989265	-0.442201	-1.422489
H	-0.849679	0.668494	-2.063423
H	0.919028	1.036682	-0.343929
H	0.549182	0.284479	2.010282
H	-0.820799	-2.882647	1.234785

VII
53
scf done: -1885.983127

C	-8.618089	-0.724966	-1.654278
P	-7.468737	-2.126194	-1.439600
C	-8.396435	-3.290739	-0.381070
Pd	-5.353178	-1.473391	-0.868913
O	-5.644229	0.192295	-2.211889
C	-5.253918	0.023775	-3.424191
C	-5.490897	1.226646	-4.317119
C	-3.217967	-0.540480	-0.721513
C	-3.290147	-1.667652	0.068851
C	-3.346920	0.815936	-0.234825
C	-3.271723	1.858939	-1.090589
N	-3.450379	3.200616	-0.802466
S	-2.994032	4.348388	-1.970689
O	-3.152100	3.726035	-3.277104
C	-3.860502	3.701010	0.510894
H	-4.631921	4.473989	0.358020
C	-1.252101	4.586834	-1.708418
O	-3.690930	5.577024	-1.626557
O	-4.723359	-0.997065	-3.865353
C	-7.434683	-2.944305	-3.070137
H	-5.428848	-2.697827	0.125270
H	-9.588448	-1.075781	-2.055078
H	-8.779545	-0.224827	-0.682485
H	-8.156957	0.004542	-2.342611
H	-9.391275	-3.507995	-0.814957
H	-7.826567	-4.231773	-0.281611
H	-8.525907	-2.857527	0.626919
H	-8.460184	-3.102468	-3.455582
H	-6.844905	-2.327035	-3.772086
H	-6.923954	-3.919206	-2.972057
H	-5.222118	0.998896	-5.361850
H	-6.550205	1.539640	-4.264040
H	-4.886947	2.084382	-3.963587
C	-2.718473	4.255756	1.319992
H	-4.358374	2.858981	1.022381
H	-3.399536	-1.577770	1.158870
H	-2.944678	-2.636977	-0.310068
H	-2.930249	-0.658646	-1.777870
H	-0.909187	5.257172	-2.514937
H	-1.095996	5.047580	-0.718920
H	-0.751207	3.606554	-1.782118
H	-3.556592	0.950640	0.836330
H	-3.072635	1.663554	-2.153802
C	-2.679957	5.615681	1.638522
C	-1.593408	6.153406	2.328498
C	-0.530429	5.333762	2.702681
C	-0.560726	3.973369	2.390386
C	-1.648125	3.438001	1.705320
H	-3.506338	6.263528	1.320538
H	-1.575182	7.222721	2.568391
H	0.326716	5.755690	3.240022
H	0.272232	3.324129	2.684001
H	-1.659868	2.370035	1.450271

VII*
53
scf done: -1885.989536

C	-4.661241	1.661506	2.101496
C	-4.293184	2.388679	0.968103
C	-5.290322	2.913900	0.140084
C	-6.633947	2.709661	0.440168
C	-6.995494	1.980416	1.574477
C	-6.007332	1.459193	2.406749
C	-2.842071	2.626843	0.647570
N	-2.535479	2.327807	-0.754906
S	-1.900988	3.562804	-1.728823
O	-2.579110	4.792090	-1.346334
C	-2.529696	1.034516	-1.251605
C	-2.678859	-0.107217	-0.492878
C	-2.991524	-1.399597	-1.091583
C	-3.291397	-2.496069	-0.381092
Pd	-0.395543	0.045632	-0.824959
O	-0.309069	0.873859	1.164005
C	0.318084	0.185785	2.046504
C	0.212106	0.738088	3.455411
P	1.844549	-0.287009	-1.154319
C	2.372866	-2.005379	-0.862347
C	2.948704	0.716333	-0.102932
C	2.440587	0.079573	-2.844950
O	0.983191	-0.826415	1.819360
C	-0.204910	3.666961	-1.209203
O	-1.937500	3.082109	-3.101963
H	-0.426707	-0.508763	-2.302121
H	3.537347	-0.052025	-2.915304
H	1.942150	-0.592819	-3.565639
H	2.182383	1.119744	-3.116312
H	3.458415	-2.114960	-1.048595
H	2.137770	-2.251652	0.187171
H	1.812337	-2.684544	-1.528892
H	4.005066	0.527658	-0.375066
H	2.726452	1.791108	-0.232337
H	2.772742	0.431745	0.948391
H	0.633949	0.033019	4.190100
H	0.762389	1.695323	3.519723
H	-0.841796	0.957391	3.707101
H	-2.599402	3.693105	0.807826
H	-2.165529	2.039778	1.297922
H	-3.306629	-2.474795	0.717711
H	-3.527781	-3.448501	-0.870143
H	-2.979951	-1.443806	-2.191574
H	0.258082	4.484912	-1.786925
H	-0.176528	3.881702	-0.127956
H	0.273371	2.694355	-1.425257
H	-3.879469	1.244608	2.751439
H	-6.284333	0.882699	3.297105
H	-8.054021	1.817237	1.808265
H	-7.407976	3.124963	-0.215688
H	-4.996518	3.492664	-0.745458
H	-2.776899	-0.033245	0.598419
H	-2.574558	0.975990	-2.346569

Comprehensive table in atomic units

M06/def2-svp CPCM tol				
	H (Hartrees)	ZPC (Hartees)	S (cal/K*mol)	Imaginary freq (cm^{-1})
AcOH	-228,717717	0,061315	64,545	
Reagent **1**	-1068,193810	0,24885	131,114	
PMe_3	-460,646928	0,111062	77,183	
Diene **2**	-1068,213513	0,249439	125,342	
Allene **6**	-1068,189087	0,24817	129,39	
Allenamide **5**	-1068,193733	0,247646	131,262	
Diene ***1r***	-1107,412585	0,277206	139,477	
Dienamide ***2r***	-1107,438857	0,276946	134,44	
Diene ***2'r***	-1107,427450	0,27746	134,3	
I	-1049,281323	0,224908	132,72	
II *trans*	-1278,017140	0,284741	159,146	
III *trans*	-1885,540871	0,42239	205,161	
TS (III-IV)	-1885,533412	0,422218	195,902	-542,314
IV	-1885,580609	0,427723	195,322	
TS (IV-V)**	-1885,534678	0,421647	193,17	-540,2303
V**	-1885,548965	0,421041	204,396	
TS (V-VI)**	-1885,542184	0,420881	195,005	-480,1693
VI**	-1885,590315	0,427243	200,913	
I	-1049,281323	0,224908	132,72	
II *trans*	-1278,017140	0,284741	159,146	
III *trans*	-1885,540871	0,42239	205,161	
TS (III-IV)	-1885,533412	0,422218	195,902	-542,314
IV	-1885,580609	0,427723	195,322	
TS (IV-V)**	-1885,534678	0,421647	193,17	-540,2303
V**	-1885,548965	0,421041	204,396	
V	-1885,540186	0,421642	205,246	
TS (V-VI)	-1885,535999	0,419474	196,626	-570,0259
VI	-1885,59334	0,427138	195,442	
TS (VI-VII)	-1885,554125	0,422359	197,875	-506,6901
VII	-1885,559134	0,423993	197,32	
I	-1049,281323	0,224908	132,72	
II *trans*	-1278,017140	0,284741	159,146	
III *trans*	-1885,540871	0,42239	205,161	
TS (III-IV)*	-1885,53281	0,421769	194,105	-482,1328
IV*	-1885,574068	0,427577	196,228	
TS (IV-V)*	-1885,532765	0,420986	192,819	-534,2421

V*	-1885,536303	0,423198	197,162	
TS (V-VI)*	-1885,533635	0,420508	191,25	-542,4177
VI*	-1885,577133	0,428306	193,221	
TS (VI-VII)*	-1885,549724	0,421947	191,19	-519,1945
VII*	-1885,566843	0,422692	201,91	

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