**Supplementary Information for the Paper**

# Triflyl-Assisted Reductive Pd-Catalyzed Tsuji–Trost Type Reaction

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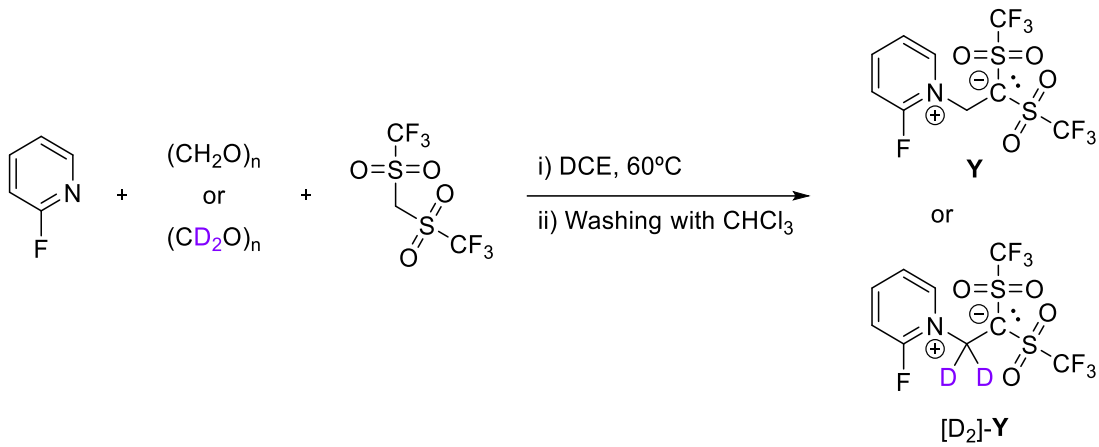
**General Methods:** $^{1}H$ NMR, $^{13}C$ NMR, and $^{19}F$ NMR spectra were recorded on a Bruker Avance AMX-700, Bruker AMX-500, or Bruker Avance-DPX 300. NMR spectra were recorded in $CDCl_3$, $C_6D_6$, or $CD_3CN$ solutions, except otherwise stated. Chemical shifts are given in ppm relative to TMS ($^{1}H$, 0.0 ppm), or $CDCl_3$ ($^{1}H$, 7.27 ppm; $^{13}C$, 76.9 ppm), or $C_6D_6$ ($^{1}H$, 7.16 ppm; $^{13}C$, 128.0 ppm), or $CD_3CN$ ($^{1}H$, 1.94 ppm; $^{13}C$, 118.2 ppm). Chemical shifts in $^{19}F$ are given in ppm relative to (trifluoromethyl)benzene ($C_6H_5CF_3$) in $CDCl_3$ ($^{19}F$, –63.7 ppm). Low and high resolution mass spectra were taken on an AGILENT 6520 Accurate-Mass QTOF LC/MS spectrometer using the electronic impact (EI) or electrospray modes (ES) unless otherwise stated. IR spectra were recorded on a Bruker Tensor 27 spectrometer. All commercially available compounds were used without further purification.

Azolium salt **Y** was synthesized according to a literature procedure: H. Yanai, Y. Takahashi, H. Fukaya, Y. Dobashi, T. Matsumoto, *Chem. Commun.* **2013**, *49*, 10091. Deuterated azolium salt [$D_2$]-**Y** was prepared adapting the same procedure: B. Alcaide, P. Almendros, C. Lázaro-Milla, *Chem. Eur. J.* **2019**, *25*, 7547.

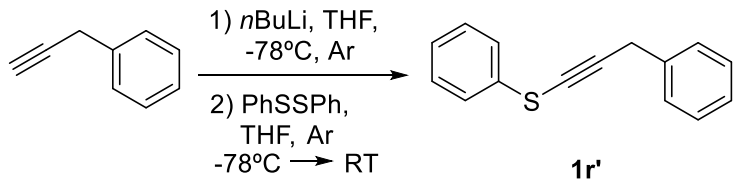



To a solution of $Tf_2CH_2$ (281 mg, 1.00 mmol) in 1,2-dichloroethane (6.0 mL), paraformaldehyde (90% purity, 73.0 mg, 2.19 mmol) or paraformaldehyde-$d_2$ (98% purity, 98 atom % D, 64 mg, 2.00 mmol) and 2-fluoropyridine (172 µL, 2.00 mmol) were added at room temperature. After being

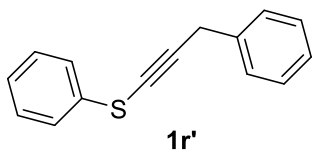
stirred for 8 h at 60 °C, the reaction mixture was concentrated under reduced pressure. The resulting residue was washed with $CHCl_3$ (1.0 mL x 3) to give zwitterion **Y** in 91% yield (356 mg, 0.915 mmol) or [$D_2$]-**Y** in 86% yield (336 mg, 0.858 mmol).

**Cyclobutenes 1a–o and 1q were readily obtained as described in the literature: 1a–i and 1q** (B. Alcaide, P. Almendros, C. Lázaro-Milla, *Adv. Synth. Catal.* **2017**, *359*, 2630); **1j–l** (B. Alcaide, P. Almendros, C. Lázaro-Milla, *Chem. Eur. J.* **2016**, *22*, 8998); **1m–o** (*Chem. Commun.* **2015**, *51*, 3395).

**Novel alkyne 1r' was prepared adapting a literature procedure (**X. Ye, J. Wang, S. Ding, S. Hosseyni, L. Wojtas, N. G. Akhmedov, X. Shi, *Chem. Eur. J.* **2017**, *23*, 10506**) as follow:**

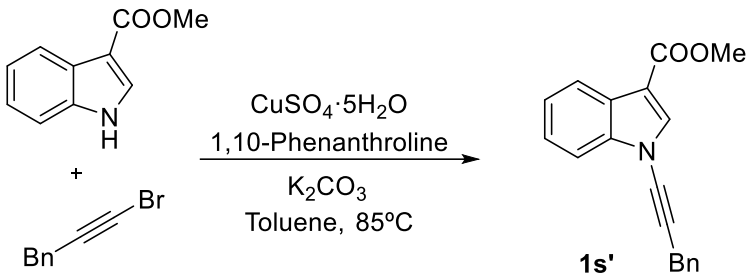



*n*BuLi (2.5 M in hexane, 2.4 mmol) was added dropwise to a THF solution (5 mL) of prop-2-yn-1-ylbenzene (2.2 mmol) cooled at –78ºC. The reaction mixture was allowed to react at –78ºC for an additional hour, and then a solution of diphenylsulfide (2.0 mmol) in THF (1 mL) was added at –78ºC. The reaction mixture was allowed to warm to RT and stirred overnight. The reaction was quenched using $K_2CO_3$ (aq. sat.), and was extracted with DCM (3 x 35 mL). The combined organic extract was dried over $MgSO_4$, and the desiccant was removed by filtration. After removal of the solvents in vacuum the residue was purified by column chromatography on silica gel to yield alkynylsulfide **1r'**.

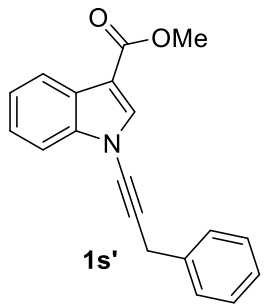


**Alkyne 1r'.** From 150 mg (1.29 mmol) of prop-2-yn-1-ylbenzene, and after flash chromatography of the residue using hexanes as eluent gave compound **1r'** (147 mg, 51%) as a colorless oil; $^{1}$H NMR (300 MHz, $C_6D_6$, 25 ºC): δ = 7.38 (m, 2H, $2CH^{Ar}$), 6.99 (m, 8H, $8CH^{Ar}$), 3.45 (s, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $C_6D_6$, 25 ºC): δ = 136.5 ($C^{Ar\text{-}q}$), 133.8 ($C^{Ar\text{-}q}$), 129.4 ($2CH^{Ar}$), 128.8 ($2CH^{Ar}$), 128.1 ($2CH^{Ar}$), 126.9 ($CH^{Ar}$), 126.4 ($CH^{Ar}$), 126.3 ($2CH^{Ar}$), 97.6 (*C*≡C), 68.1 (C≡*C*), 26.5 ($CH_2$); IR ($CH_2Cl_2$): ν = 2245 (C≡C) $cm^{-1}$. Alkyne **1r'** is not very stable at room temperature and should be used for next step inmediately after the purification.

**Novel alkyne 1s' was prepared adapting a literature procedure (**Y. Zhang, R. P. Hsung, M. R. Tracey, K. C. M. Kurtz, E. L. Vera, *Org. Lett*. **2004**, *6*, 1151**) as follow:**



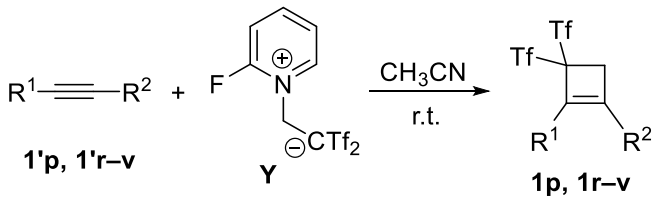

To a solution of (3-bromoprop-2-yn-1-yl)benzene (2.20 mmol) in 2 mL of freshly anhydrous toluene in a reaction vial were added methyl 1*H*-indole-3-carboxylate (2.00 mmol), $K_2CO_3$ (4.00 mmol), $CuSO_4 \cdot 5H_2O$ (0.20 mmol), and 1,10-phenanthroline (0.40 mmol). The reaction mixture was capped under a blanket of nitrogen and heated to 85 °C for 24 h. The progress of the reaction was monitored using TLC analysis. Upon completion, the reaction mixture was cooled to room temperature and diluted with 12 mL of AcOEt. The resulting mixture was filtered through a Celite pad and the filtrate was concentrated in vacuo. The crude residue was purified using silica gel column flash chromatography to yield alkyne **1s'**.




**1s'**

**Alkyne 1s'.** From 175 mg (1.0 mmol) of methyl 1*H*-indole-3-carboxylate, and after flash chromatography of the residue using hexanes/dichloromethane (6:4) as eluent gave compound **1s'** (130 mg, 45%) as a pale yellow oil; $^{1}$H NMR (300 MHz, $C_6D_6$, 25 ºC): δ = 8.52 (d, 1H, *J* = 7.3 Hz, $CH^{Ar}$), 7.59 (s, 1H, $CH^{Ar}$), 7.49 (d, 1H, *J* = 8.1 Hz, $CH^{Ar}$), 7.21 (m, 4H, $4CH^{Ar}$), 7.09 (m, 3H, $3CH^{Ar}$), 3.85 (s, 3H, $OCH_3$), 3.54 (s, 3H, $OCH_3$), 3.45 (s, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $C_6D_6$, 25 ºC): δ = 163.9 (C=O), 138.9 ($C^{Ar\text{-}q}$), 136.5 ($C^{Ar\text{-}q}$), 135.0 ($CH^{Ar}$), 128.9 ($2CH^{Ar}$), 128.1 ($2CH^{Ar}$), 127.1 ($CH^{Ar}$), 126.0 ($C^{Ar\text{-}q}$), 124.7 ($CH^{Ar}$), 123.8 ($CH^{Ar}$), 122.5 ($CH^{Ar}$), 111.5 ($CH^{Ar}$), 111.0 ($C^{Ar\text{-}q}$), 72.9 (*C*≡C), 69.6 (C≡*C*), 50.8 ($OCH_3$), 24.6 ($CH_2$); IR ($CH_2Cl_2$): ν = 2257 (C≡C), 1712 (C=O) $cm^{-1}$; HRMS (ES): calcd for $C_{19}H_{16}NO_2$ $[M + H]^+$: 290.11756; found: 290.11694.

**Novel cyclobutenes 1p and 1r–v were prepared as follow:**

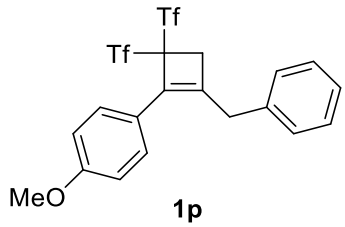



**1'p, 1'r–v** **Y** **1p, 1r–v**

**General procedure for the reaction of alkynes 1' and Yanais'reagent Y**.

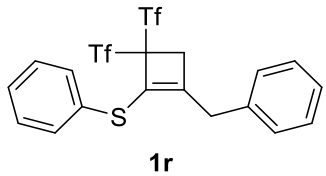
2-(2-Fluoropyridin-1-ium-1-yl)-1,1-bis[(trifluoromethyl)sulfonyl]ethan-1-ide **Y** (0.2 mmol) was added at room temperature to a solution of the appropriate alkyne **1'p and 1'r–v** (0.2 mmol) in acetonitrile (4 mL). The reaction was stirred at room temperature until disappearance of the starting material (TLC), and then the mixture was concentrated under reduced pressure. Chromatography of

the residue eluting with hexanes/diethyl ether mixtures gave analytically pure compounds. Spectroscopic and analytical data for bis(triflyl)cyclobutenes **1p** and **1r–v** follow.




**1p**

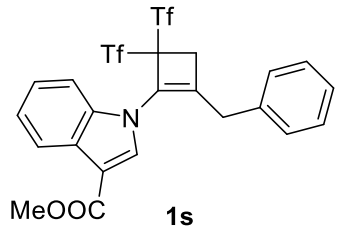
**1-(2-Benzyl-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 1p.** From 50 mg (0.22 mmol) of alkyne **1p'**, and after flash chromatography of the residue using hexanes/diethyl ether (95:5) as eluent gave compound **1p** (102 mg, 88%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.62 (m, 2H, $2CH^{Ar}$), 7.37 (m, 3H, $3CH^{Ar}$), 7.26 (m, 2H, $2CH^{Ar}$), 6.97 (m, 2H, $2CH^{Ar}$), 3.92 (s, 2H, $CH_2$), 3.86 (s, 3H, $OCH_3$), 3.24 (s, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.5 ($C^{Ar\text{-}q}$-OMe), 151.8 (*C*=C), 134.3 ($C^{Ar\text{-}q}$), 132.9 (C=*C*), 129.4 ($2CH^{Ar}$), 129.1 ($2CH^{Ar}$), 128.7 ($2CH^{Ar}$), 127.4 ($CH^{Ar}$), 122.0 ($C^{Ar\text{-}q}$), 119.7 (q, $J_{CF}$ = 331.3 Hz, $2CF_3$), 114.2 ($2CH^{Ar}$), 86.4 ($CTf_2$), 55.3 ($OCH_3$), 35.9 ($2CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –70.4 (s, 6F, $2CF_3$); IR ($CHCl_3$): ν = 1381, 1103 (O=S=O), 1204 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{20}H_{20}F_6NO_5S_2$ $[M + NH_4]^+$: 532.06816; found: 532.06649.




**1r**

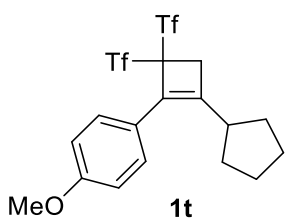
**(2-Benzyl-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)(phenyl)sulfane 1r.** From 20 mg (0.08 mmol) of alkyne **1r'**, and after flash chromatography of the residue using hexanes/diethyl ether (95:5) as eluent gave compound **1r** (38 mg, 87%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.63 (m, 2H, $2CH^{Ar}$), 7.38 (m, 3H, $3CH^{Ar}$), 7.29 (m, 3H, $3CH^{Ar}$), 7.02 (m, 2H, $2CH^{Ar}$), 3.29 (s, 2H, $CH_2$), 3.16 (s, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 161.5 (*C*=C), 134.3 ($C^{Ar\text{-}q}$),

133.8 (C=*C*), 132.8 (2$CH^{Ar}$), 129.9 ($C^{Ar\text{-}q}$), 129.6 (2$CH^{Ar}$), 129.1 ($CH^{Ar}$), 129.0 (2$CH^{Ar}$), 127.3 ($CH^{Ar}$), 126.2 ($C^{Ar\text{-}q}$), 119.6 (q, $J_{CF}$ = 330.8 Hz, $2CF_3$), 87.7 ($CTf_2$), 36.5 ($CH_2$), 35.6 ($CH_2$); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –70.0 (s, 6F, $2CF_3$); IR ($CHCl_3$): ν = 1380, 1104 (O=S=O), 1205 (C–F). 2257 (C≡C) $cm^{-1}$; HRMS (ES): calcd for $C_{19}H_{18}F_6NO_4S_3$ $[M + NH_4]^+$: 534.02967; found: 534.02798.



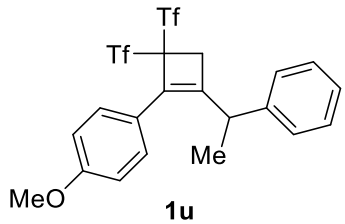

**1s**

**Methyl 1-(2-benzyl-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-1*H*-indole-3-carboxylate 1s.** From 43 mg (0.15 mmol) of alkyne **1s'**, and after flash chromatography of the residue using hexanes/diethyl ether (9:1) as eluent gave compound **1s** (58 mg, 67%) as a colorless oil; $^1H$ NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.20 (m, 1H, $CH^{Ar}$), 7.93 (s, 1H, $CH^{Ar}$), 7.47 (m, 1H, $CH^{Ar}$), 7.31 (m, 5H, 5$CH^{Ar}$), 7.12 (m, 2H, 2$CH^{Ar}$), 3.94 (s, 3H, $OCH_3$), 3.68 (s, 2H, $CH_2$), 3.26 (s, 2H, $CH_2$); $^{13}C$ NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 164.5 (C=O), 158.1 (*C*=C), 137.2 ($C^{Ar\text{-}q}$), 132.6 (C=*C*), 132.1 ($CH^{Ar}$), 129.2 (2$CH^{Ar}$), 128.6 (2$CH^{Ar}$), 127.7 ($CH^{Ar}$), 125.8 ($C^{Ar\text{-}q}$), 124.6 ($CH^{Ar}$), 124.0 ($C^{Ar\text{-}q}$), 123.4 ($CH^{Ar}$), 122.0 ($CH^{Ar}$), 119.5 (q, $J_{CF}$ = 330.8 Hz, $2CF_3$), 111.6 ($C^{Ar\text{-}q}$), 110.8 (2$CH^{Ar}$), 88.9 ($CTf_2$), 51.4 ($OCH_3$), 35.5 ($CH_2$), 32.8 ($CH_2$); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –70.0 (s, 6F, $2CF_3$); IR ($CHCl_3$): ν = 1709 (C=O), 1382, 1104 (O=S=O), 1205 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{23}H_{18}F_6NO_6S_2$ $[M + H]^+$: 582.04742; found: 582.04890.




**1t**

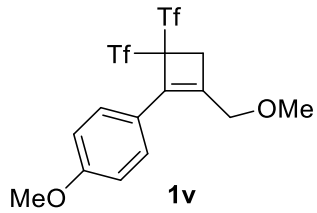
**1-(2-Cyclopentyl-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 1t.** From 30 mg (0.38 mmol) of alkyne **1t'**, and after flash chromatography of the residue using hexanes/diethyl ether (98:2) as eluent gave compound **1t** (70 mg, 95%) as a colorless solid; mp 63–65 ºC; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.52 (m, 2H, $2CH^{Ar}$), 6.93 (m, 2H, $2CH^{Ar}$), 3.83 (s, 3H, $OCH_3$), 3.33 (s, 2H, $CH_2$), 3.17 (p, 1H, *J* = 8.2 Hz, CH), 1.95 (m, 2H, $CH_2$), 1.71 (m, 4H, $2CH_2$), 1.56 (m, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.2 ($C^{Ar\text{-}q}$-OMe), 158.2 (*C*=C), 130.2 (C=*C*), 129.5 ($2CH^{Ar}$), 122.4 ($C^{Ar\text{-}q}$), 119.8 (q, $J_{CF}$ = 331.3 Hz, $2CF_3$), 114.0 ($2CH^{Ar}$), 86.2 ($CTf_2$), 55.2 ($OCH_3$), 39.2 (CH), 34.2 ($CH_2$), 30.6 ($CH_2$), 25.7 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –70.5 (s, 6F, $2CF_3$); IR ($CHCl_3$): ν = 1382, 1102 (O=S=O), 1207 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{18}H_{22}F_6NO_5S_2$ $[M + NH_4]^+$: 510.08381; found: 510.08535.




**1u**

**1-Methoxy-4-(2-(1-phenylethyl)-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 1u.** From 30 mg (0.12 mmol) of alkyne **1u'**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **1u** (55 mg, 88%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.53 (m, 2H, $2CH^{Ar}$), 7.39 (m, 2H, $2CH^{Ar}$), 7.30 (m, 3H, $3CH^{Ar}$), 6.95 (m, 2H, $2CH^{Ar}$), 4.22 (q, 1H, *J* = 7.1 Hz, CH), 3.85 (s, 3H, $OCH_3$), 3.34 (d, 1H, *J* = 15.5 Hz, C*H*H), 3.17 (dd, 1H, *J* = 15.5 Hz, CH*H*), 1.54 (d, 3H, *J* = 7.2 Hz, $CH_3$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.4 ($C^{Ar\text{-}q}$-OMe), 157.1 (*C*=C), 140.0 ($C^{Ar\text{-}q}$), 131.5 (C=*C*), 129.8 ($2CH^{Ar}$), 129.0 ($2CH^{Ar}$), 127.4 ($CH^{Ar}$), 127.1 ($2CH^{Ar}$), 122.1 ($C^{Ar\text{-}q}$), 119.8 (q, $J_{CF}$ = 331.4 Hz, $CF_3$), 119.7 (q, $J_{CF}$ = 331.1 Hz, $CF_3$), 114.1 ($2CH^{Ar}$), 86.4 ($CTf_2$), 55.3 ($OCH_3$), 39.4 (CH), 34.3 ($CH_2$), 17.9 ($CH_3$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –70.2 (s, 3F, $CF_3$), –70.5 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = –1383, 1103

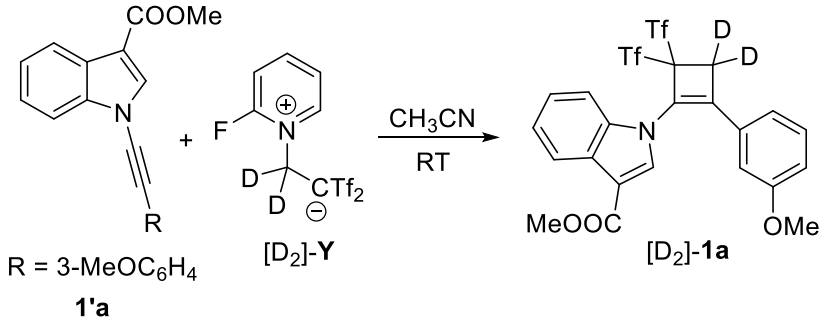
(O=S=O), 1205 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{21}H_{22}F_6NO_5S_2$ $[M + NH_4]^+$: 546.08381; found: 546.08515.




**1v**

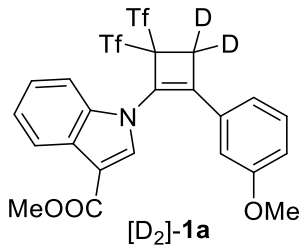
**1-Methoxy-4-(2-(methoxymethyl)-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 1v.** From 26 mg (0.15 mmol) of alkyne **1v'**, and after flash chromatography of the residue using hexanes/diethyl ether (85:15) as eluent gave compound **1v** (64 mg, 96%) as a pale yellow oil; $^1$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.48 (m, 2H, $2CH^{Ar}$), 6.94 (m, 2H, $2CH^{Ar}$), 4.37 (s, 2H, $CH_2$), 3.86 (s, 3H, $OCH_3$), 3.46 (s, 2H, $CH_2$), 3.41 (s, 3H, $OCH_3$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.6 ($C^{Ar\text{-}q}$-OMe), 149.3 (*C*=C), 133.0 (C=*C*), 129.6 ($2CH^{Ar}$), 121.7 ($C^{Ar\text{-}q}$), 119.8 (q, $J_{CF}$ = 331.3 Hz, $2CF_3$), 114.2 ($2CH^{Ar}$), 86.0 ($CTf_2$), 67.6 ($CH_2$), 59.0 ($OCH_3$), 55.3 ($OCH_3$), 35.6 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –70.3 (s, 6F, $2CF_3$); IR ($CHCl_3$): ν = 1382, 1109 (O=S=O), 1209 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{15}H_{18}F_6NO_6S_2$ $[M + NH_4]^+$: 486.04742; found: 486.04881.

**Novel cyclobutene [D2]-1a was prepared as follow:**




**General procedure for the reaction of alkynes 1' and deuterated Yanais'reagent [D2]-Y**.

2-(2-Fluoropyridin-1-ium-1-yl)-1,1-bis[(trifluoromethyl)sulfonyl]ethan-1-ide-2,2-*d*2 [D2]-**Y** (0.2 mmol) was added at room temperature to a solution of the appropriate alkyne **1'** (0.2 mmol) in acetonitrile (4 mL). The reaction was stirred at room temperature until disappearance of the starting material (TLC), and then the mixture was concentrated under reduced pressure. Chromatography of the residue eluting with hexanes/ethyl acetate mixtures gave analytically pure [D2]-**1**.

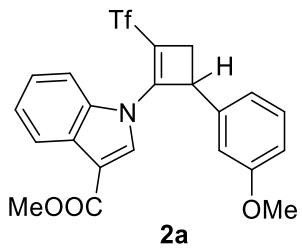



**Methyl 1-(2-(3-methoxyphenyl)-4,4-bis((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl-3,3-*d*2)-1*H*-indole-3-carboxylate [D2]-1a.** From 80 mg (0.26 mmol) of alkyne **1'a**, and after flash chromatography of the residue using hexanes/ethyl acetate (9:2) as eluent gave compound [D2]-**1a** (144 mg, 92%) as a colorless oil; $^{1}$H NMR (700 MHz, $CDCl_3$, 25 °C): δ = 8.26 (d, 1H, *J* = 8.0 Hz, $CH^{Ar}$), 8.03 (s, 1H, $CH^{Ar}$), 7.34 (m, 1H, $1CH^{Ar}$), 7.31 (m, 1H, $1CH^{Ar}$), 7.27 (m, 1H, $1CH^{Ar}$), 7.23 (m, 1H, $1CH^{Ar}$), 6.97 (m, 1H, $CH^{Ar}$), 6.71 (m, 1H, $CH^{Ar}$), 6.35 (m, 1H, $CH^{Ar}$), 3.94 (s, 3H, $OCH_3$), 3.33 (s, 3H, $OCH_3$); $^{13}$C NMR (175 MHz, $CDCl_3$, 25 °C): δ = 164.5 (C=O), 159.7 ($C^{Ar\text{-}q}$-$OCH_3$), 152.4

(C=*C*), 135.8 (*C*=C), 131.9 ($CH^{Ar}$), 130.1 ($CH^{Ar}$), 129.0 ($C^{Ar\text{-}q}$), 126.0 ($C^{Ar\text{-}q}$), 124.6 ($CH^{Ar}$), 123.5 ($CH^{Ar}$), 122.1 ($CH^{Ar}$), 120.6 ($CH^{Ar}$), 119.6 ($CH^{Ar}$), 119.5 (q, $J_{CF}$ = 330.6 Hz, $2CF_3$), 118.5 ($C^{Ar\text{-}q}$), 112.3 ($CH^{Ar}$), 112.0 ($CH^{Ar}$), 111.7 ($C^{Ar\text{-}q}$), 89.2 ($CTf_2$), 54.8 ($OCH_3$), 51.4 ($OCH_3$), 30.8 (m, $CD_2$-*low intensity*); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 °C): δ = –69.8 (s, 6F, $2CF_3$); D($^2H$) NMR (107 MHz, $CDCl_3$, 25 °C): δ = 3.72 (s, 2D, $CD_2$); IR ($CHCl_3$): ν = 1713 (C=O), 1381, 1105 (O=S=O), 1203 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{23}H_{16}D_2F_6NO_7S_2$ [*M* + H]$^+$: 600.05489; found: 600.05510.

**General procedure for the palladium-catalyzed allylic substitution reaction of bis(triflyl)cyclobutenes 1 using water as hydrogen donor. Synthesis of (triflyl)cyclobutenes 2, 4, and 5.**

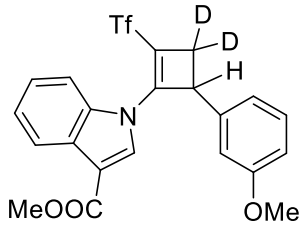
A solution of the appropriate bis(triflyl)cyclobutene **1** (1.0 mmol), $Pd(PPh_3)_4$ (0.05 mmol, 5.0 mol %), and $K_2CO_3$ (3.0 mmol) in a mixture of 1,4-dioxane/water (14 mL, 2:1) was heated in a sealed tube at 60 °C until disappearance of the starting material (TLC). The reaction mixture was allowed to cool to room temperature and was extracted with ethyl acetate (3 x 15 mL). The combined organic extract was dried over $MgSO_4$, and the desiccant was removed by filtration. After removal of the solvents in vacuum, the residue was purified by column chromatography on silica gel to give analytically pure compounds. Spectroscopic and analytical data for (triflyl)cyclobutenes **2**, **4**, and **5** follow.




**2a**

**Methyl 1-(4-(3-methoxyphenyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-1*H*-indole-3-carboxylate 2a.** From 55 mg (0.1 mmol) of bis(triflyl)cyclobutene **1a**, and after flash

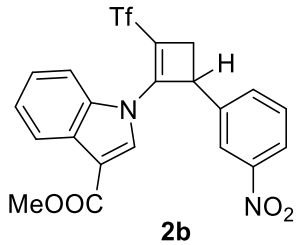
chromatography of the residue using dichloromethane as eluent gave compound **2a** (40 mg, 93%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.25 (d, 1H, *J* = 7.4 Hz, $CH^{Ar}$), 8.00 (s, 1H, $CH^{Ar}$), 7.29 (m, 4H, $4CH^{Ar}$), 6.92 (dd, 1H, *J* = 8.3, 2.1 Hz, $CH^{Ar}$), 6.77 (d, 1H, *J* = 7.6 Hz, $CH^{Ar}$), 6.58 (m, 1H, $CH^{Ar}$), 5.10 (dd, 1H, *J* = 4.4, 1.5 Hz, CH), 3.95 (s, 3H, $OCH_3$), 3.51 (s, 3H, $OCH_3$), 3.37 (dd, 1H, *J* = 13.4, 1.1 Hz, C*H*H), 3.25 (dd, 1H, *J* = 13.4, 4.6 Hz, CH*H*); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 164.7 (C=O), 159.6 ($C^{Ar\text{-}q}$-OMe), 143.7 (=C), 135.5 ($C^{Ar\text{-}q}$), 132.0 ($CH^{Ar}$), 130.9 ($C^{Ar\text{-}q}$), 129.9 ($CH^{Ar}$), 126.2 ($C^{Ar\text{-}q}$), 124.1 ($CH^{Ar}$), 123.2 ($CH^{Ar}$), 122.1 ($CH^{Ar}$), 119.9 ($CH^{Ar}$), 119.5 (=C-Tf), 119.5 (q, $J_{CF}$ = 328.3 Hz, $CF_3$), 117.2 ($CH^{Ar}$), 112.2 ($CH^{Ar}$), 111.9 ($CH^{Ar}$), 111.1 ($C^{Ar\text{-}q}$), 58.7 (CH), 55.0 ($OCH_3$), 51.3 ($OCH_3$), 26.5 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –77.2 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1710 (C=O), 1388, 1108 (O=S=O), 1210 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{22}H_{19}F_3NO_5S$ $[M + H]^+$: 466.09305; found: 466.09343.



[$D_2$]-**2a**

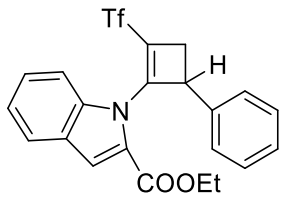
**Methyl 1-(4-(3-methoxyphenyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl-3,3-*d*$_2$)-1*H*-indole-3-carboxylate [D$_2$]-2a.** From 50 mg (0.08 mmol) of bis(triflyl)cyclobutene [$D_2$]-**1a**, and after flash chromatography of the residue using dichloromethane as eluent gave compound [$D_2$]-**2a** (34 mg, 89%) as a colorless oil; $^{1}$H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 8.25 (d, 1H, *J* = 7.9 Hz, $CH^{Ar}$), 7.98 (s, 1H, $CH^{Ar}$), 7.35 (t, 1H, *J* = 7.5 Hz, $CH^{Ar}$), 7.28 (m, 1H, $CH^{Ar}$), 7.23 (m, 2H, $2CH^{Ar}$), 6.92 (dd, 1H, *J* = 8.2, 2.4 Hz, $CH^{Ar}$), 6.77 (d, 1H, *J* = 7.7 Hz, $CH^{Ar}$), 6.58 (m, 1H, $CH^{Ar}$), 5.08 (s, 1H, CH), 3.95 (s, 3H, $OCH_3$), 3.51 (s, 3H, $OCH_3$); $^{13}$C NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 164.8 (C=O), 159.6 ($C^{Ar\text{-}q}$-OMe), 143.5 (=C), 135.5 ($C^{Ar\text{-}q}$), 132.0 ($CH^{Ar}$), 130.9 ($C^{Ar\text{-}q}$), 129.9 ($CH^{Ar}$), 126.3 ($C^{Ar\text{-}q}$), 124.1 ($CH^{Ar}$), 123.2 ($CH^{Ar}$), 122.1 ($CH^{Ar}$), 119.9 ($CH^{Ar}$), 119.6 (=C-Tf), 119.5 (q, $J_{CF}$ = 328.4

Hz, $CF_3$), 117.2 ($CH^{Ar}$), 112.2 ($CH^{Ar}$), 111.9 ($CH^{Ar}$), 111.1 ($C^{Ar\text{-}q}$), 58.5 (CH), 55.0 ($OCH_3$), 51.3 ($OCH_3$), 26.0 ($CD_2$-*low intensity*); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –76.9 (s, 3F, $CF_3$); D($^2H$) NMR (107 MHz, $CDCl_3$, 25 ºC): δ = 3.30 (m, 2D, $CD_2$); IR ($CHCl_3$): ν = 1710 (C=O), 1390, 1108 (O=S=O), 1211 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{22}H_{17}D_2F_3NO_5S$ [*M* + H]$^+$: 468.10561; found: 468.10478.



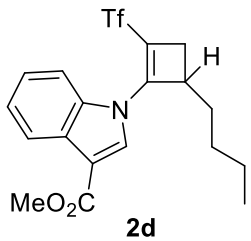

**2b**

**Methyl 1-(4-(3-nitrophenyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-1*H*-indole-3-carboxylate 2b.** From 52 mg (0.08 mmol) of bis(triflyl)cyclobutene **1b**, and after flash chromatography of the residue using hexanes/ethyl acetate (9:1 → 8:2) as eluent gave compound **2b** (24 mg, 61%) as a yellow oil; $^1H$ NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 8.28 (d, 1H, *J* = 8.0 Hz, $CH^{Ar}$), 8.24 (m, 1H, $CH^{Ar}$), 8.09 (t, 1H, *J* = 1.8 Hz, 1H, $CH^{Ar}$), 7.99 (s, 1H, $CH^{Ar}$), 7.47 (t, 1H, *J* = 8.0 Hz, $CH^{Ar}$), 7.38 (m, 1H, $CH^{Ar}$), 8.34 (d, 1H, *J* = 7.9 Hz, $CH^{Ar}$), 7.27 (m, 1H, $CH^{Ar}$), 7.10 (d, 1H, *J* = 8.2 Hz, $CH^{Ar}$), 5.15 (m, 1H, CH), 3.96 (s, 3H, $OCH_3$), 3.46 (d, 1H, *J* = 13.3 Hz, C*H*H), 3.35 (dd, 1H, *J* = 13.3, 4.6 Hz, CH*H*); $^{13}C$ NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 164.5 (C=O), 148.4 (=C), 139.6 ($C^{Ar\text{-}q}$), 135.1 ($C^{Ar\text{-}q}$), 133.1 ($CH^{Ar}$), 131.5 ($CH^{Ar}$), 131.4 ($C^{Ar\text{-}q}$), 130.1 ($CH^{Ar}$), 126.4 ($C^{Ar\text{-}q}$), 124.9 ($CH^{Ar}$), 124.5 ($CH^{Ar}$), 123.6 ($CH^{Ar}$), 122.6 (=C-Tf), 122.5 ($CH^{Ar}$), 122.0 ($CH^{Ar}$), 119.4 (q, $J_{CF}$ = 328.1 Hz, $CF_3$), 112.0 ($C^{Ar\text{-}q}$), 111.5 ($CH^{Ar}$), 58.6 (CH), 51.5 ($OCH_3$), 26.8 ($CH_2$); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –76.6 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1713 (C=O), 1539 (O=N=O), 1384, 1106 (O=S=O), 1204 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{21}H_{19}F_3N_3O_6S$ [*M* + $NH_4$]$^+$: 498.09412; found: 498.09552.




**2c**

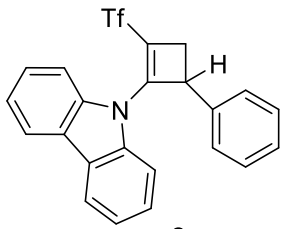
**Ethyl 1-(4-phenyl-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-1*H*-indole-2-carboxylate 2c.** From 35 mg (0.06 mmol) of bis(triflyl)cyclobutene **1c**, and after flash chromatography of the residue using hexanes/diethyl ether (95:5 → 9:1) as eluent gave compound **2c** (15 mg, 54%) as a colorless oil; $^{1}$H NMR (500 MHz, $CDCl_3$, 25 ºC): δ = 7.73 (d, 1H, *J* = 8.0 Hz, $CH^{Ar}$), 7.49 (s, 1H, $CH^{Ar}$), 7.33 (m, 3H, $3CH^{Ar}$), 7.24 (m, 3H, $3CH^{Ar}$), 7.04 (d, 2H, *J* = 7.4 Hz, $2CH^{Ar}$), 5.44 (d, 1H, *J* = 3.3 Hz, CH), 4.38 (s, 2H, $OCH_2$), 3.37 (dd, 1H, *J* = 13.1, 3.4 Hz, C*H*H), 3.28 (dd, 1H, *J* = 13.1, 4.7 Hz, CH*H*), 1.42 (t, 3H, *J* = 7.1 Hz, $CH_3$); $^{13}$C NMR (125 MHz, $CDCl_3$, 25 ºC): δ = 161.4 (C=O), 144.0 (=C), 137.7 ($C^{Ar\text{-}q}$), 130.1 ($C^{Ar\text{-}q}$), 130.1 ($CH^{Ar}$), 128.7 ($2CH^{Ar}$), 127.3 ($C^{Ar\text{-}q}$), 127.2 ($2CH^{Ar}$), 126.6 ($CH^{Ar}$), 126.6 ($C^{Ar\text{-}q}$), 127.7 ($CH^{Ar}$), 122.3 ($CH^{Ar}$), 121.2 (=C-Tf), 119.5 (q, $J_{CF}$ = 328.1 Hz, $CF_3$), 113.4 ($CH^{Ar}$), 112.8 ($CH^{Ar}$), 61.1 ($OCH_2$), 59.8 (CH), 25.6 ($CH_2$), 14.3 ($CH_3$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –77.9 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1705 (C=O), 1389, 1101 (O=S=O), 1209 (C–F) cm$^{-1}$; HRMS (ES): calcd for $C_{22}H_{19}F_3NO_4S$ [*M* + H]$^+$: 450.09814; found: 450.09925.




**2d**

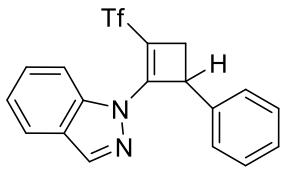
**Methyl 1-(4-butyl-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-1*H*-indole-3-carboxylate 2d.** From 35 mg (0.06 mmol) of bis(triflyl)cyclobutene **1d**, and after flash chromatography of the residue using hexanes/diethyl ether (9:1 → 8:2) as eluent gave compound **2d** (12 mg, 47%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.21 (m, 1H, $1CH^{Ar}$), 7.84 (s, 1H, $CH^{Ar}$), 7.34

(m, 3H, 3$CH^{Ar}$), 4.96 (d, 1H, $J$ = 1.6 Hz, CH), 3.94 (s, 3H, $OCH_3$), 2.92 (m, 2H, $CH_2$), 2.34 (m, 2H, $CH_2$), 1.45 (m, 4H, 2$CH_2$), 0.88 (t, 3H, $J$ = 7.2 Hz, $CH_3$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 164.9 (C=O), 149.9 (=C), 136.4 ($C^{Ar\text{-}q}$), 132.5 ($CH^{Ar}$), 126.1 ($C^{Ar\text{-}q}$), 124.0 ($CH^{Ar}$), 123.0 ($CH^{Ar}$), 122.4 ($C^{Ar\text{-}q}$), 122.0 ($CH^{Ar}$), 119.4 (q, $J_{CF}$ = 328.1 Hz, $CF_3$), 110.6 ($CH^{Ar}$), 110.4 (=C-Tf), 58.6 (CH), 51.3 ($OCH_3$), 28.2 ($CH_2$), 38.1 ($CH_2$), 22.4 ($CH_2$), 13.6 ($CH_3$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 °C): δ = –77.1 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1708 (C=O), 1382, 1109 (O=S=O), 1211 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{19}H_{24}F_3N_2O_4S$ [$M$ + $NH_4$]$^+$: 433.14034; found: 433.14139.



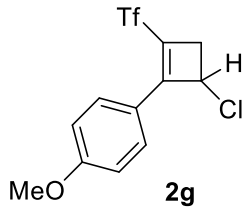

**2e**

**9-(4-Phenyl-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-9*H*-carbazole 2e.** From 34 mg (0.06 mmol) of bis(triflyl)cyclobutene **1e**, and after flash chromatography of the residue using hexanes/toluene (1:1) as eluent gave compound **2e** (11 mg, 42%) as a colorless oil; $^1$H NMR (500 MHz, $CDCl_3$, 25 °C): δ = 8.13 (d, 2H, $J$ = 7.7 Hz, 2$CH^{Ar}$), 7.36 (m, 9H, 9$CH^{Ar}$), 7.20 (m, 2H, 2$CH^{Ar}$), 5.31 (d, 1H, $J$ = 3.2 Hz, CH), 3.47 (d, 1H, $J$ = 13.3 Hz, C*H*H), 3.35 (dd, 1H, $J$ = 13.4, 4.7 Hz, CH*H*); $^{13}$C NMR (125 MHz, $CDCl_3$, 25 °C): δ = 145.0 (=C), 138.8 (2$C^{Ar\text{-}q}$), 130.5 ($C^{Ar\text{-}q}$), 130.3 (2$CH^{Ar}$), 128.7 (3$CH^{Ar}$), 127.6 (2$CH^{Ar}$), 126.4 (2$CH^{Ar}$), 124.1 (2$C^{Ar\text{-}q}$), 121.2 (2$CH^{Ar}$), 120.6 (2$CH^{Ar}$), 120.0 (=C-Tf), 119.4 (q, $J_{CF}$ = 328.4 Hz, $CF_3$), 58.1 (CH), 26.2 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 °C): δ = –77.4 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1390, 1100 (O=S=O), 1210 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{23}H_{20}F_3N_2O_2S$ [$M$ + $NH_4$]$^+$: 445.11921; found: 445.12097.




**2f**

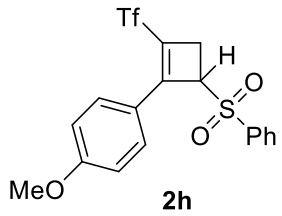
**1-(4-Phenyl-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-1*H*-indazole 2f.** From 40 mg (0.08 mmol) of bis(triflyl)cyclobutene **1f**, and after flash chromatography of the residue using hexanes/diethyl ether (95:5 → 9:1) as eluent gave compound **2f** (10 mg, 32%) as a colorless oil; $^{1}$H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 8.27 (s, 1H, $CH^{Ar}$), 7.82 (d, 1H, *J* = 8.0 Hz, $CH^{Ar}$), 7.39 (m, 2H, $2CH^{Ar}$), 7.33 (m, 2H, $2CH^{Ar}$), 7.29 (m, 1H, $CH^{Ar}$), 7.21 (m, 2H, $2CH^{Ar}$), 7.18 (d, 1H, *J* = 8.2 Hz, $CH^{Ar}$), 5.28 (d, 1H, *J* = 3.2 Hz, CH), 3.43 (d, 1H, *J* = 13.1 Hz, C*H*H), 3.24 (dd, 1H, *J* = 13.1, 4.7 Hz, CH*H*); $^{13}$C NMR (175 MHz, $CDCl_3$, 25 ºC): δ = 138.8 (=C), 138.2 ($C^{Ar\text{-}q}$), 137.5 ($2CH^{Ar}$), 130.5 ($C^{Ar\text{-}q}$), 130.2 ($CH^{Ar}$), 128.7 ($2CH^{Ar}$), 127.8 ($2CH^{Ar}$), 124.4 ($C^{Ar\text{-}q}$), 122.4 ($CH^{Ar}$), 121.4 ($CH^{Ar}$), 121.1 (=C-Tf), 119.5 (q, $J_{CF}$ = 328.2 Hz, $CF_3$), 111.5 ($2CH^{Ar}$), 58.0 (CH), 26.3 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –77.1 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1359, 1100 (O=S=O), 1211 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{18}H_{14}F_3N_2O_2S$ $[M + H]^+$: 379.07226; found: 379.07043.




**2g**

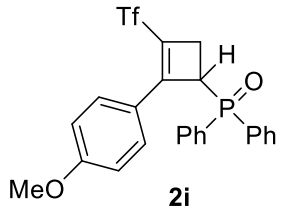
**1-(4-Chloro-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 2g.** From 30 mg (0.06 mmol) of bis(triflyl)cyclobutene **1g**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **2g** (12 mg, 55%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.70 (m, 2H, $2CH^{Ar}$), 6.94 (m, 2H, $2CH^{Ar}$), 4.83 (m, 1H, CH), 3.84 (s, 3H, $OCH_3$), 3.20 (m, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.5 ($C^{Ar\text{-}q}$-OMe), 132.9 (=C), 128.5 ($2CH^{Ar}$), 124.6 (=C-Tf), 122.4 ($C^{Ar\text{-}q}$), 119.8 (q, $J_{CF}$ = 329.1 Hz, $CF_3$), 114.1 ($2CH^{Ar}$),

56.0 (CH), 55.3 ($OCH_3$), 36.1 ($CH_2$); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.9 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1380, 1110 (O=S=O), 1210 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{12}H_{14}ClF_3NO_3S$ [*M* + $NH_4$]$^+$: 344.03295; found: 344.03207.




**2h**

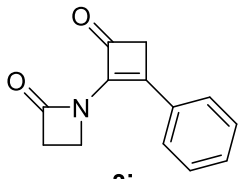
**1-Methoxy-4-(4-(phenylsulfonyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 2h.** From 30 mg (0.05 mmol) of bis(triflyl)cyclobutene **1h**, and after flash chromatography of the residue using hexanes/ethyl acetate (9:1 → 8:2) as eluent gave compound **2h** (15 mg, 67%) as a colorless oil; $^1H$ NMR (500 MHz, $CDCl_3$, 25 ºC): δ = 7.93 (m, 2H, $2CH^{Ar}$), 7.69 (m, 3H, $3CH^{Ar}$), 7.52 (m, 2H, $2CH^{Ar}$), 6.97 (m, 2H, $2CH^{Ar}$), 4.84 (d, 1H, *J* = 3.7 Hz, CH), 3.91 (s, 3H, $OCH_3$), 3.21 (dd, 1H, *J* = 14.0, 4.9 Hz, C*H*H), 2.93 (dd, 1H, *J* = 14.0, 1.6 Hz, CH*H*); $^{13}C$ NMR (125 MHz, $CDCl_3$, 25 ºC): δ = 163.7 ($C^{Ar\text{-}q}$-OMe), 159.2 (=C), 135.1 ($C^{Ar\text{-}q}$), 134.7 ($CH^{Ar}$), 132.9 ($2CH^{Ar}$), 129.2 ($2CH^{Ar}$), 129.1 ($2CH^{Ar}$), 121.3 (=C-Tf), 121.0 ($C^{Ar\text{-}q}$), 119.8 (q, $J_{CF}$ = 326.9 Hz, $CF_3$), 114.4 ($2CH^{Ar}$), 60.6 (CH), 55.6 ($OCH_3$), 31.5 ($CH_2$); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –78.2 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1387, 1107 (O=S=O), 1209 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{18}H_{19}F_3NO_5S_2$ [*M* + $NH_4$]$^+$: 450.06513; found: 450.06531.




**2i**

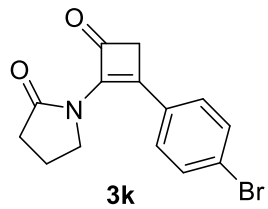
**(2-(4-Methoxyphenyl)-3-((trifluoromethyl)sulfonyl)cyclobut-2-en-1-yl)diphenylphosphine oxide 2i.** From 35 mg (0.06 mmol) of bis(triflyl)cyclobutene **1i**, and after flash chromatography of

the residue using hexanes/ethyl acetate (1:1) as eluent gave compound **2i** (19 mg, 63%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.87 (m, 4H, 4$CH^{Ar}$), 7.70 (m, 2H, 2$CH^{Ar}$), 7.54 (m, 6H, 6$CH^{Ar}$), 6.84 (m, 2H, 2$CH^{Ar}$), 5.00 (s, 1H, CH), 3.80 (s, 3H, $OCH_3$), 2.87 (d, 1H, *J* = 14.0 Hz, C*H*H), 2.79 (dd, 1H, *J* = 14.1, 4.2 Hz, CH*H*); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 161.7 ($C^{Ar\text{-}q}$-OMe), 150.3 (d, $J_{CP}$ = 2.3 Hz, =C), 133.7 (d, $J_{CP}$ = 90.2 Hz, $C^{Ar\text{-}q}$), 132.7 (d, $J_{CP}$ = 2.6 Hz, $CH^{Ar}$), 132.4 (d, $J_{CP}$ = 2.6 Hz, $CH^{Ar}$), 131.8 ($C^{Ar\text{-}q}$), 131.5 (d, $J_{CP}$ = 8.1 Hz, 2$CH^{Ar}$), 131.4 (d, $J_{CP}$ = 7.5 Hz, 2$CH^{Ar}$), 130.8 (2$CH^{Ar}$), 130.1 (d, $J_{CP}$ = 38.0 Hz, $C^{Ar\text{-}q}$), 129.1 (d, $J_{CP}$ = 12.6 Hz, 2$CH^{Ar}$), 128.9 (d, $J_{CP}$ = 12.3 Hz, 2$CH^{Ar}$), 123.2 (=C-Tf), 119.8 (q, $J_{CF}$ = 329.5 Hz, $CF_3$), 113.9 (2$CH^{Ar}$), 57.8 (d, $J_{CP}$ = 26.4 Hz, CH), 55.4 ($OCH_3$), 31.5 (d, $J_{CP}$ = 7.6 Hz, $CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –75.7 (s, 3F, $CF_3$); $^{31}$P NMR (121 MHz, $CDCl_3$, 25 ºC): δ = 18.2 (s, P, P(=O)$Ph_2$); IR ($CHCl_3$): ν = 1389, 1109 (O=S=O), 1210 (C–F) cm$^{-1}$; HRMS (ES): calcd for $C_{24}H_{21}F_3O_4PS$ [*M* + H]$^+$: 493.08448; found: 493.08588.



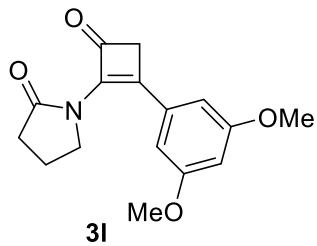

**3j**

**1-(4-Oxo-2-phenylcyclobut-1-en-1-yl)azetidin-2-one 3j.** From 30 mg (0.06 mmol) of bis(triflyl)cyclobutene **1j**, and after flash chromatography of the residue using hexanes/ethyl acetate (9:1 → 8:2) as eluent gave compound **3j** (9 mg, 73%) as a colorless solid; mp 122–124 ºC; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.74 (m, 2H, 2$CH^{Ar}$), 7.50 (m, 3H, 3$CH^{Ar}$), 3.86 (t, 2H, *J* = 4.8 Hz, $CH_2$), 3.41 (s, 2H, $CH_2$), 3.19 (t, 2H, *J* = 4.8 Hz, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 184.0 (C=O), 164.3 (NC=O), 149.9 (C=*C*), 131.1 ($CH^{Ar}$), 131.0 ($C^{Ar\text{-}q}$), 130.5 (2$CH^{Ar}$), 128.7 (2$CH^{Ar}$), 128.3 (*C*=C), 46.1 ($CH_2$), 39.8 ($CH_2$), 38.2 ($CH_2$); IR ($CHCl_3$): ν = 1772 (NC=O), 1745 (C=O), 1602 (C=C) cm$^{-1}$; HRMS (ES): calcd for $C_{13}H_{11}NNaO_2$ [*M* + Na]$^+$: 236.06820; found: 236.06793.




**3k**

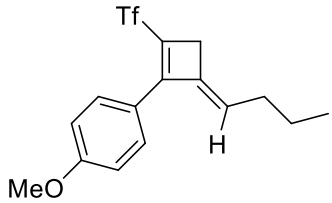
**1-(2-(4-Bromophenyl)-4-oxocyclobut-1-en-1-yl)pyrrolidin-2-one 3k.** From 40 mg (0.07 mmol) of bis(triflyl)cyclobutene **1k**, and after flash chromatography of the residue using hexanes/ethyl acetate (9:1 → 8:2) as eluent gave compound **3k** (12 mg, 55%) as a colorless oil; $^{1}$H NMR (500 MHz, $CDCl_3$, 25 °C): δ = 7.61 (m, 2H, $2CH^{Ar}$), 7.33 (m, 2H, $2CH^{Ar}$), 3.98 (t, 2H, *J* = 7.1 Hz, $CH_2$), 3.43 (s, 2H, $CH_2$), 2.53 (t, 2H, *J* = 8.1 Hz, $CH_2$), 2.22 (m, 2H, $CH_2$); $^{13}$C NMR (125 MHz, $CDCl_3$, 25 °C): δ = 185.3 (C=O), 173.7 (NC=O), 153.2 (C=*C*), 132.3 ($2CH^{Ar}$), 131.7 ($2CH^{Ar}$), 130.5 (*C*=C), 130.4 ($C^{Ar\text{-}q}$), 126.0 ($C^{Ar\text{-}q}$), 47.0 ($CH_2$), 46.2 ($CH_2$), 30.6 ($CH_2$), 19.1 ($CH_2$); IR ($CHCl_3$): ν = 1739 (C=O), 1726 (NC=O) $cm^{-1}$; HRMS (ES): calcd for $C_{14}H_{13}BrNO_2$ [*M* + H]$^+$: 306.01242; found: 306.01294.




**3l**

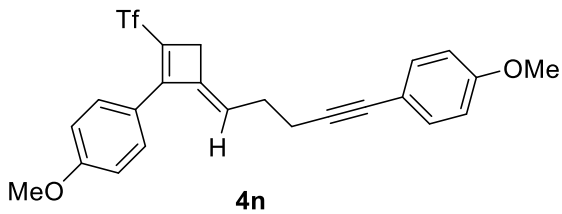
**1-(2-(3,5-Dimethoxyphenyl)-4-oxocyclobut-1-en-1-yl)pyrrolidin-2-one 3l.** From 38 mg (0.07 mmol) of bis(triflyl)cyclobutene **1l**, and after flash chromatography of the residue using hexanes/ethyl acetate (8:2 → 7:3) as eluent gave compound **3l** (14 mg, 69%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 6.67 (d, 2H, *J* = 2.2 Hz, $2CH^{Ar}$), 7.33 (t, 1H, *J* = 2.2 Hz, $CH^{Ar}$), 3.94 (t, 2H, *J* = 7.1 Hz, $CH_2$), 3.83 (s, 6H, $2OCH_3$), 3.40 (s, 2H, $CH_2$), 2.52 (t, 2H, *J* = 8.1 Hz, $CH_2$), 2.21 (m, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 185.9 (C=O), 173.6 (NC=O), 160.5 ($2C^{Ar\text{-}q}$-OMe), 156.0 (*C*=C), 132.9 ($C^{Ar\text{-}q}$), 130.7 (C=*C*), 108.9 ($2CH^{Ar}$), 103.5 ($CH^{Ar}$), 55.5 ($2OCH_3$), 47.1

($CH_2$), 46.2 ($CH_2$), 30.6 ($CH_2$), 19.1 ($CH_2$); IR ($CHCl_3$): ν = 1771 (NC=O), 1743 (C=O) $cm^{-1}$; HRMS (ES): calcd for $C_{16}H_{18}NO_4$ [*M* + H]$^+$: 288.12303; found: 288.12264.




**4m**

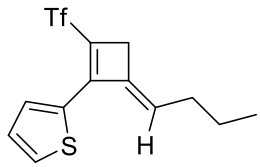
**(*E*)-1-(4-Butylidene-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 4m.** From 30 mg (0.06 mmol) of bis(triflyl)cyclobutene **1m**, and after flash chromatography of the residue using hexanes/dichloromethane (9:1 → 85:15) as eluent gave compound **4m** (15 mg, 71%) as a pale yellow oil; $^1$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.78 (m, 2H, $2CH^{Ar}$), 6.97 (m, 2H, $2CH^{Ar}$), 6.17 (t, 1H, *J* = 7.7 Hz, =CH), 3.87 (s, 3H, $OCH_3$), 3.41 (s, 2H, $CH_2$), 2.19 (q, 2H, *J* = 7.4 Hz, $CH_2$), 1.53 (m, 2H, $CH_2$), 0.97 (t, 3H, *J* = 7.4 Hz, $CH_3$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 162.3 ($C^{Ar\text{-}q}$-OMe), 162.2 (=C), 134.1 ($C^{Ar\text{-}q}$), 131.7 ($2CH^{Ar}$), 128.9 (=CH), 121.7 (=C), 120.2 (q, $J_{CF}$ = 326.5 Hz, $CF_3$), 119.5 (=C-Tf), 114.2 ($2CH^{Ar}$), 55.4 ($OCH_3$), 35.9 ($CH_2$), 30.8 ($CH_2$), 22.4 ($CH_2$), 13.8 ($CH_3$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –78.3 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1381, 1109 (O=S=O), 1212 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{16}H_{18}F_3O_3S$ [*M* + H]$^+$: 347.09233; found: 347.09131.




**4n**

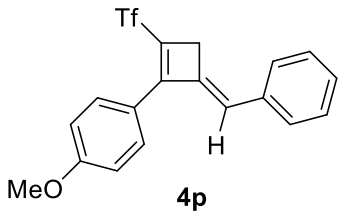
**(*E*)-1-Methoxy-4-(5-(2-(4-methoxyphenyl)-3-((trifluoromethyl)sulfonyl)cyclobut-2-en-1-ylidene)pent-1-yn-1-yl)benzene 4n.** From 36 mg (0.06 mmol) of bis(triflyl)cyclobutene **1n**, and after flash chromatography of the residue using hexanes/diethyl ether (9:1 → 8:2) as eluent gave compound **4n** (11 mg, 42%) as a pale yellow oil; $^1$H NMR (700 MHz, $CDCl_3$, 25 ºC): δ = 7.81 (m,

2H, 2CH$^{Ar}$), 7.31 (m, 2H, 2CH$^{Ar}$), 6.97 (m, 2H, 2CH$^{Ar}$), 6.83 (m, 2H, 2CH$^{Ar}$), 6.28 (t, 1H, $J$ = 7.6 Hz, =CH), 3.87 (s, 3H, $OCH_3$), 3.81 (s, 3H, $OCH_3$), 3.47 (s, 2H, $CH_2$), 2.61 (t, 2H, $J$ = 6.9 Hz, $CH_2$), 2.52 (m, 2H, $CH_2$); $^{13}$C NMR (175 MHz, $CDCl_3$, 25 °C): δ = 162.3 ($C^{Ar\text{-}q}$-OMe), 161.9 ($C^{Ar\text{-}q}$-OMe), 159.3 (=C), 135.1 ($C^{Ar\text{-}q}$), 132.8 (2CH$^{Ar}$), 131.7 (2CH$^{Ar}$), 126.7 (=CH), 121.6 (=C-Tf), 120.1 (=C), 120.2 (q, $J_{CF}$ = 326.8 Hz, $CF_3$), 115.5 ($C^{Ar\text{-}q}$), 114.2 (2CH$^{Ar}$), 113.9 (2CH$^{Ar}$), 86.7 ($C$≡C), 81.6 (C≡$C$), 55.4 ($OCH_3$), 55.3 ($OCH_3$), 35.9 ($CH_2$), 28.2 ($CH_2$), 19.5 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 °C): δ = –78.3 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1381, 1108 (O=S=O), 1208 (C–F) cm$^{-1}$; HRMS (ES): calcd for $C_{24}H_{22}F_3O_4S$ [$M$ + H]$^+$: 463.11854; found: 463.11844.



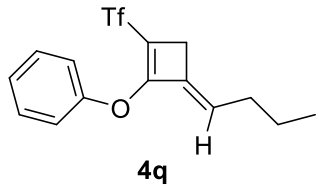

**4o**

**(*E*)-2-(4-Butylidene-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)thiophene 4o.** From 50 mg (0.11 mmol) of bis(triflyl)cyclobutene **1o**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **4o** (32 mg, 91%; containing *ca.* 5% of its *Z* isomer) as a pale yellow solid; mp 55–57 °C; $^1$H NMR (300 MHz, $CDCl_3$, 25 °C): δ = 8.01 (d, 1H, $J$ = 3.5 Hz, CH$^{Ar}$), 7.64 (dd, 1H, $J$ = 5.0, 0.8 Hz, CH$^{Ar}$), 7.18 (dd, 1H, $J$ = 5.0, 3.4 Hz, CH$^{Ar}$), 6.32 (t, 1H, $J$ = 7.7 Hz, =CH), 3.43 (s, 2H, $CH_2$), 2.20 (q, 2H, $J$ = 7.4 Hz, $CH_2$), 1.54 (m, 2H, $CH_2$), 0.98 (t, 3H, $J$ = 7.4 Hz, $CH_3$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 °C): δ = 153.7 (=C), 134.2 (CH$^{Ar}$), 132.8 ($C^{Ar\text{-}q}$), 132.3 (CH$^{Ar}$), 130.2 ($C^{Ar\text{-}q}$), 129.3 (CH$^{Ar}$), 128.4 (=CH), 120.3 (q, $J_{CF}$ = 326.5 Hz, $CF_3$), 117.3 (=C-Tf), 35.9 ($CH_2$), 30.8 ($CH_2$), 22.3 ($CH_2$), 13.8 ($CH_3$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 °C): δ = –78.6 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1382, 1111 (O=S=O), 1213 (C–F) cm$^{-1}$; HRMS (ES): calcd for $C_{13}H_{14}F_3O_2S_2$ [$M$ + H]$^+$: 323.03818; found: 323.03757.




**4p**

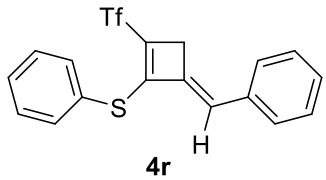
**(*E*)-1-(4-Benzylidene-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 4p.** From 45 mg (0.09 mmol) of bis(triflyl)cyclobutene **1p**, and after flash chromatography of the residue using hexanes/diethyl ether (95:5) as eluent gave compound **4p** (25 mg, 75%) as a pale orange solid; mp 135–137 ºC; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.81 (m, 2H, $2CH^{Ar}$), 7.42 (m, 5H, $5CH^{Ar}$), 7.02 (m, 2H, $2CH^{Ar}$), 6.93 (t, 1H, *J* = 7.7 Hz, =CH), 3.90 (s, 3H, $OCH_3$), 3.81 (s, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 163.8 (=C), 162.4 ($C^{Ar\text{-}q}$-OMe), 135.1 ($C^{Ar\text{-}q}$), 134.9 ($C^{Ar\text{-}q}$), 131.5 ($2CH^{Ar}$), 129.2 ($CH^{Ar}$), 129.0 ($2CH^{Ar}$), 128.6 ($2CH^{Ar}$), 126.4 (=CH), 121.5 (=C-Tf), 121.2 (=C), 120.2 (q, $J_{CF}$ = 326.5 Hz, $CF_3$), 114.3 ($2CH^{Ar}$), 55.4 ($OCH_3$), 38.3 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –78.2 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1379, 1110 (O=S=O), 1211 (C–F) cm$^{-1}$; HRMS (ES): calcd for $C_{19}H_{16}F_3O_3S$ [*M* + H]$^+$: 381.07668; found: 381.07648.




**4q**

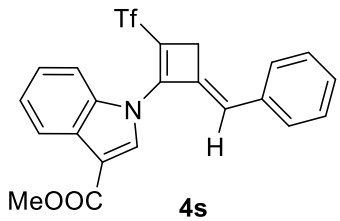
**(*E*)-((4-Butylidene-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)oxy)benzene 4q.** From 47 mg (0.10 mmol) of bis(triflyl)cyclobutene **1q**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **4q** (21 mg, 64%) as a colorless oil; $^{1}$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.42 (m, 2H, $2CH^{Ar}$), 7.32 (m, 1H, $CH^{Ar}$), 7.22 (m, 2H, $2CH^{Ar}$), 5.01 (t, 1H, *J* = 7.8 Hz, =CH), 3.07 (s, 2H, $CH_2$), 1.96 (q, 2H, *J* = 7.4 Hz, $CH_2$), 1.31 (m, 2H, $CH_2$), 0.82 (t, 3H, *J* = 7.4 Hz, $CH_3$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 160.3 (=C), 153.6 ($C^{Ar\text{-}q}$), 131.1 (=CH), 130.6 (=C), 129.9 ($2CH^{Ar}$), 126.9 ($CH^{Ar}$), 120.3 ($2CH^{Ar}$), 120.3 ($2CH^{Ar}$), 120.1 (q, $J_{CF}$ =

325.5 Hz, $CF_3$), 101.4 (=C-Tf), 30.9 ($CH_2$), 29.8 ($CH_2$), 21.9 ($CH_2$), 13.6 ($CH_3$); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –79.0 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1379, 1111 (O=S=O), 1207 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{15}H_{16}F_3O_3S$ $[M + H]^+$: 333.07668; found: 333.07818.



**4r**

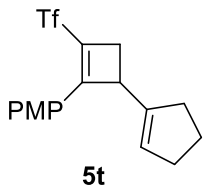
**(*E*)-(4-Benzylidene-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)(phenyl)sulfane 4r.** From 45 mg (0.09 mmol) of bis(triflyl)cyclobutene **1r**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **4r** (25 mg, 74%) as a colorless solid; mp 120–122 ºC; $^1H$ NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.66 (m, 2H, $2CH^{Ar}$), 7.50 (m, 1H, $CH^{Ar}$), 7.38 (m, 2H, $2CH^{Ar}$), 7.18 (m, 3H, $3CH^{Ar}$), 6.93 (m, 2H, $2CH^{Ar}$), 5.24 (t, 1H, =CH), 3.64 (s, 2H, $CH_2$); $^{13}C$ NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 163.3 (=C), 135.4 ($2CH^{Ar}$), 134.4 (=C), 134.1 ($C^{Ar\text{-}q}$), 130.7 ($CH^{Ar}$), 129.7 ($2CH^{Ar}$), 129.4 ($CH^{Ar}$), 128.9 ($2CH^{Ar}$), 128.5 ($2CH^{Ar}$), 127.5 (=CH), 126.8 ($C^{Ar\text{-}q}$), 121.2 (=C-Tf), 120.2 (q, $J_{CF}$ = 325.3 Hz, $CF_3$), 38.7 ($CH_2$); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –78.3 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1375, 1110 (O=S=O), 1211 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{18}H_{14}F_3O_2S_2$ $[M + H]^+$: 383.03818; found: 383.04009.



**4s**

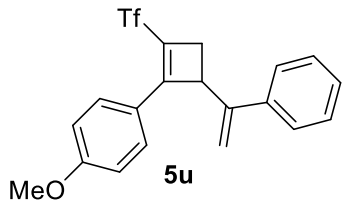
**Methyl (*E*)-1-(4-benzylidene-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-1*H*-indole-3-carboxylate 4s.** From 35 mg (0.06 mmol) of bis(triflyl)cyclobutene **1s**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **4s** (12 mg, 45%) as a pale yellow oil; $^1H$ NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 8.29 (m, 1H, $CH^{Ar}$), 8.20 (s,

1H, $CH^{Ar}$), 7.79 (m, 1H, $CH^{Ar}$), 7.40 (m, 7H, $7CH^{Ar}$), 7.01 (s, 1H, =CH), 3.96 (s, 3H, $OCH_3$), 3.83 (s, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 164.2 (C=O), 150.1 (=C), 135.7 ($C^{Ar\text{-}q}$), 134.0 ($C^{Ar\text{-}q}$), 133.8 ($CH^{Ar}$), 131.0 ($C^{Ar\text{-}q}$), 130.2 ($CH^{Ar}$), 129.4 (=CH), 129.3 ($2CH^{Ar}$), 128.9 ($2CH^{Ar}$), 127.4 (=C), 124.7 ($CH^{Ar}$), 124.4 ($CH^{Ar}$), 122.4 ($CH^{Ar}$), 119.9 (q, $J_{CF}$ = 326.0 Hz, $CF_3$), 114.2 (=C-Tf), 113.2 ($C^{Ar\text{-}q}$), 112.6 ($CH^{Ar}$), 51.6 ($OCH_3$), 35.5 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –78.0 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1711 (C=O), 1372, 1110 (O=S=O), 1213 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{22}H_{20}F_3N_2O_4S$ $[M + NH_4]^+$: 465.10904; found: 465.10894.

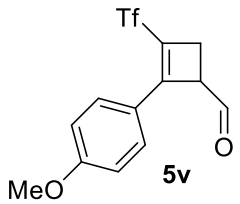



**5t**

**1-(4-(Cyclopent-1-en-1-yl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)-4-methoxybenzene 5t.** From 40 mg (0.08 mmol) of bis(triflyl)cyclobutene **1t**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3 → 95:5) as eluent gave compound **5t** (23 mg, 80%) as a colorless solid; mp 123–125 ºC; $^1$H NMR (300 MHz, $CDCl_3$, 25 ºC): δ = 7.41 (m, 2H, $2CH^{Ar}$), 6.89 (m, 2H, $2CH^{Ar}$), 6.05 (s, 1H, =CH), 4.84 (d, 1H, *J* = 2.9 Hz, CH), 3.83 (s, 3H, $OCH_3$), 3.04 (d, 1H, *J* = 13.6 Hz, C*H*H), 2.94 (dd, 1H, *J* = 13.7, 4.6 Hz, CH*H*), 2.62 (m, 1H, C*H*H), 2.39 (m, 3H, CH*H*, $CH_2$), 1.95 (m, 2H, $CH_2$); $^{13}$C NMR (75 MHz, $CDCl_3$, 25 ºC): δ = 159.7 ($C^{Ar\text{-}q}$-OMe), 140.1 (=C), 138.1 ($C^{Ar\text{-}q}$), 135.5 (=CH), 129.3 ($2CH^{Ar}$), 128.3 (=C), 125.3 (=C-Tf), 119.9 (q, $J_{CF}$ = 329.3 Hz, $CF_3$), 113.7 ($2CH^{Ar}$), 57.1 (CH), 55.2 ($OCH_3$), 33.3 ($CH_2$), 32.6 ($CH_2$), 29.2 ($CH_2$), 24.0 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –76.3 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1379, 1110 (O=S=O), 1211 (C–F) $cm^{-1}$.




**1-Methoxy-4-(4-(1-phenylvinyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl)benzene 5u.** From 45 mg (0.08 mmol) of bis(triflyl)cyclobutene **1u**, and after flash chromatography of the residue using hexanes/diethyl ether (97:3) as eluent gave compound **5u** (21 mg, 62%) as a pale yellow oil; $^{1}$H NMR (500 MHz, $CDCl_3$, 25 ºC): δ = 7.31 (m, 2H, 2CH$^{Ar}$), 7.25 (m, 3H, 3CH$^{Ar}$), 7.04 (m, 2H, 2CH$^{Ar}$), 6.62 (m, 2H, 2CH$^{Ar}$), 5.60 (s, 1H, =C*H*H), 5.50 (s, 1H, =CH*H*), 4.92 (d, 1H, *J* = 3.2 Hz, CH), 3.74 (s, 3H, $OCH_3$), 3.18 (d, 1H, *J* = 13.9 Hz, C*H*H), 3.08 (dd, 1H, *J* = 13.9, 4.6 Hz, CH*H*); $^{13}$C NMR (125 MHz, $CDCl_3$, 25 ºC): δ = 159.7 (*C*$^{Ar\text{-}q}$-OMe), 143.5 (=C), 141.3 (=C), 137.6 (*C*$^{Ar\text{-}q}$), 131.8 (*C*$^{Ar\text{-}q}$), 129.5 (2CH$^{Ar}$), 128.5 (2CH$^{Ar}$), 128.2 (CH$^{Ar}$), 127.5 (2CH$^{Ar}$), 124.1 (=C-Tf), 119.9 (q, $J_{CF}$ = 329.5 Hz, $CF_3$), 118.7 (=$CH_2$), 113.2 (2CH$^{Ar}$), 56.5 (CH), 55.2 ($OCH_3$), 30.5 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 ºC): δ = –76.0 (s, 3F, $CF_3$); IR ($CHCl_3$): ν = 1382, 1108 (O=S=O), 1210 (C–F) cm$^{-11}$; HRMS (ES): calcd for $C_{20}H_{18}F_3O_3S$ [*M* + H]$^+$: 395.09233; found: 395.09109.

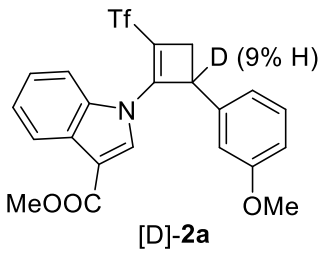



**2-(4-Methoxyphenyl)-3-((trifluoromethyl)sulfonyl)cyclobut-2-ene-1-carbaldehyde 5v.** From 40 mg (0.09 mmol) of bis(triflyl)cyclobutene **1v**, and after flash chromatography of the residue using hexanes/diethyl ether (95:5) as eluent gave compound **5v** (12 mg, 43%) as a pale yellow oil; $^{1}$H NMR (500 MHz, $C_6D_6$, 25 ºC): δ = 9.48 (s, 1H, CHO), 7.46 (m, 2H, 2CH$^{Ar}$), 6.56 (m, 2H, 2CH$^{Ar}$), 3.87 (dd, 1H, *J* = 4.7, 1.5 Hz, CH), 3.17 (s, 3H, $OCH_3$), 2.87 (d, 1H, *J* = 14.1 Hz, C*H*H), 2.32 (dd, 1H, *J* = 14.1, 4.8 Hz, CH*H*); $^{13}$C NMR (125 MHz, $C_6D_6$, 25 ºC): δ = 184.0 (HC=O), 162.7 (*C*$^{Ar\text{-}q}$-OMe),

146.0 (=C), 137.2 ($C^{Ar\text{-}q}$), 131.4 ($2CH^{Ar}$), 123.5 (=C-Tf), 120.3 (q, $J_{CF}$ = 329.3 Hz, $CF_3$), 114.5 ($2CH^{Ar}$), 56.4 (CH), 54.9 ($OCH_3$), 27.9 ($CH_2$); $^{19}F$ NMR (282 MHz, $C_6D_6$, 25 °C): δ = –76.2 (s, 3F, $CF_3$); IR ($CH_2Cl_2$): ν = 1731 (C=O), 1382, 1108 (O=S=O), 1210 (C–F) $cm^{-11}$; HRMS (ES): calcd for $C_{13}H_{12}F_3O_4S$ [*M* + H]$^+$: 321.04029; found: 321.04118.

**General procedure for the palladium-catalyzed allylic substitution reaction of bis(triflyl)cyclobutenes 1 using heavy water as deuterium donor. Synthesis of deuterated (triflyl)cyclobutenes [D]-2a and [D$_3$]-2a.**

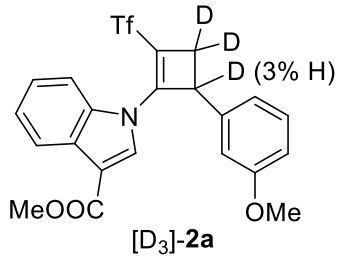
A solution of the appropriate bis(triflyl)cyclobutene **1** (1.0 mmol), $Pd(PPh_3)_4$ (0.05 mmol, 5.0 mol %), and $K_2CO_3$ (3.0 mmol) in a mixture of 1,4-dioxane/heavy water (14 mL, 2:1) was heated in a sealed tube at 60 °C until disappearance of the starting material (TLC). The reaction mixture was allowed to cool to room temperature and was extracted with ethyl acetate (3 x 15 mL). The combined organic extract was dried over $MgSO_4$, and the desiccant was removed by filtration. After removal of the solvents in vacuum, the residue was purified by column chromatography on silica gel to give analytically pure compounds. Spectroscopic and analytical data for deuterated (triflyl)cyclobutenes [D]-**2a** and [$D_3$]-**2a** follow.



[D]-**2a**

**Methyl 1-(4-(3-methoxyphenyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl-4-*d*)-1*H*-indole-3-carboxylate [D]-2a.** From 35 mg (0.06 mmol) of bis(triflyl)cyclobutene **1a**, and after flash chromatography of the residue using dichloromethane as eluent gave compound [D]-**2a** (20 mg, 74%; containing *ca.* 9% of **2a**) as a colorless oil; $^1H$ NMR (700 MHz, $CDCl_3$, 25 °C): δ = 8.25 (d, 1H, *J* =

8.0 Hz, $CH^{Ar}$), 7.98 (s, 1H, $CH^{Ar}$), 7.36 (t, 1H, *J* = 7.5 Hz, $CH^{Ar}$), 7.29 (m, 1H, $CH^{Ar}$), 7.23 (m, 2H, $2CH^{Ar}$), 6.92 (dd, 1H, *J* = 8.2, 2.3 Hz, $CH^{Ar}$), 6.78 (d, 1H, *J* = 7.7 Hz, $CH^{Ar}$), 6.58 (m, 1H, $CH^{Ar}$), 3.95 (s, 3H, $OCH_3$), 3.51 (s, 3H, $OCH_3$), 3.36 (d, 1H, *J* = 13.3 Hz, C*H*H), 3.25 (d, 1H, *J* = 13.3 Hz, CH*H*); $^{13}$C NMR (175 MHz, $CDCl_3$, 25 °C): δ = 164.7 (C=O), 159.6 ($C^{Ar\text{-}q}$-OMe), 143.8 (=C), 135.5 ($C^{Ar\text{-}q}$), 132.0 ($CH^{Ar}$), 130.9 ($C^{Ar\text{-}q}$), 129.9 ($CH^{Ar}$), 126.3 ($C^{Ar\text{-}q}$), 124.1 ($CH^{Ar}$), 123.2 ($CH^{Ar}$), 122.1 ($CH^{Ar}$), 119.9 ($CH^{Ar}$), 119.5 (q, $J_{CF}$ = 328.3 Hz, $CF_3$), 119.4 (=C-Tf), 117.2 ($CH^{Ar}$), 112.2 ($CH^{Ar}$), 111.9 ($CH^{Ar}$), 111.1 ($C^{Ar\text{-}q}$), 58.4 (t, $J_{CD}$ = 24.1 Hz, CD), 55.0 ($OCH_3$), 51.3 ($OCH_3$), 26.4 ($CH_2$); $^{19}$F NMR (282 MHz, $CDCl_3$, 25 °C): δ = –76.9 (s, 3F, $CF_3$); D($^2$H) NMR (107 MHz, $CDCl_3$, 25 °C): δ = 5.07 (s, 1D, CD); IR ($CHCl_3$): ν = 1711 (C=O), 1388, 1108 (O=S=O), 1210 (C–F) cm$^{-1}$; HRMS (ES): calcd for $C_{22}H_{18}DF_3NO_5S$ [*M* + H]$^+$: 467.09933; found: 467.09995.

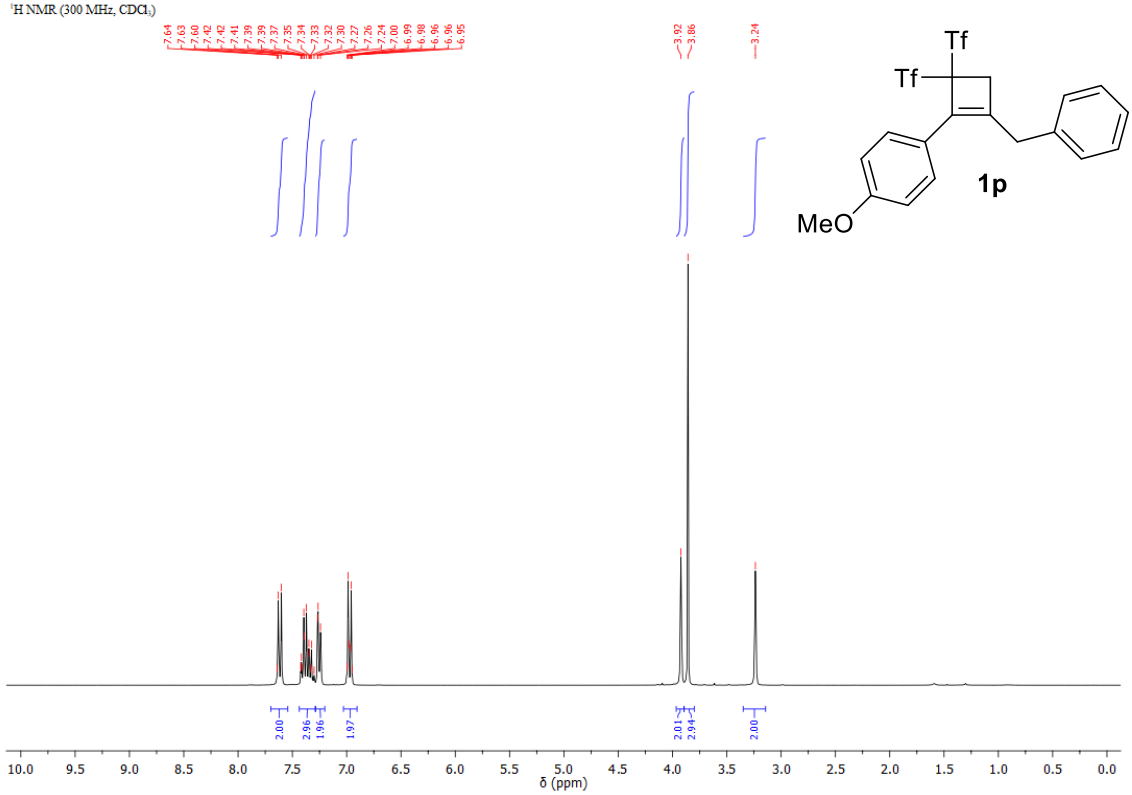


[$D_3$]-**2a**

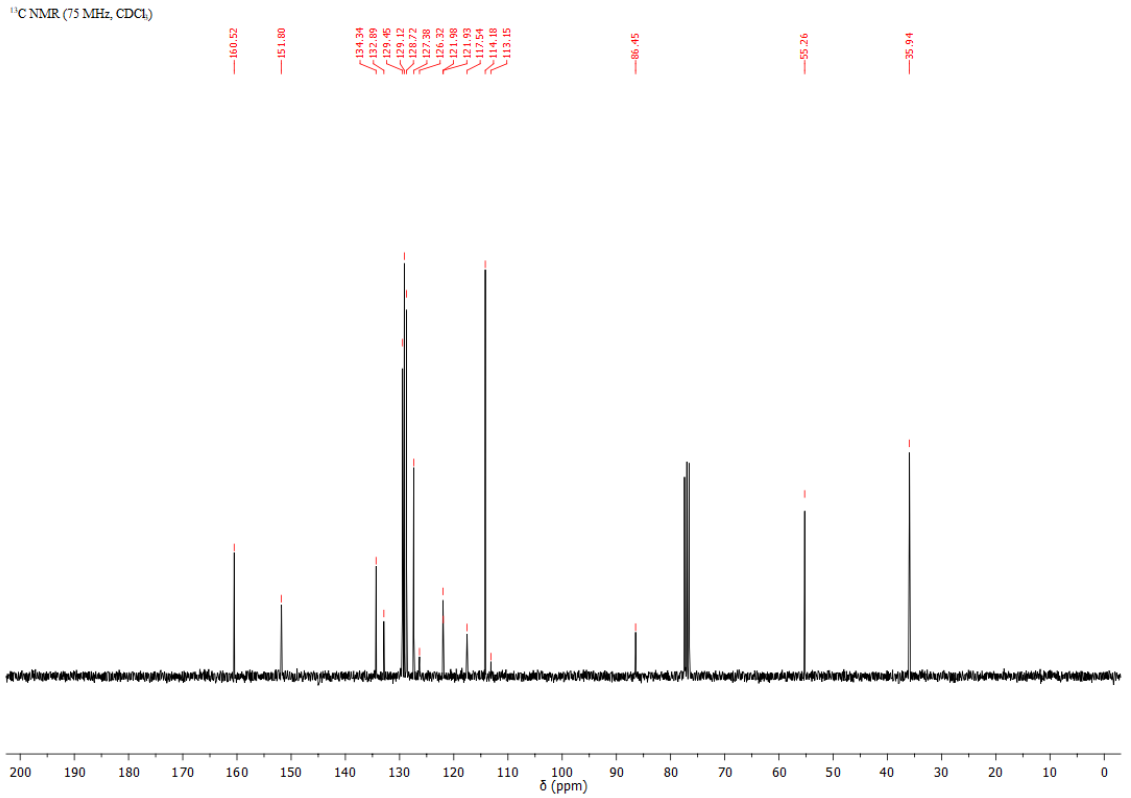
**Methyl 1-(4-(3-methoxyphenyl)-2-((trifluoromethyl)sulfonyl)cyclobut-1-en-1-yl-3,3,4-*d*$_3$)-1*H*-indole-3-carboxylate [D$_3$]-2a.** From 50 mg (0.08 mmol) of bis(triflyl)cyclobutene [$D_2$]-**1a**, and after flash chromatography of the residue using dichloromethane as eluent gave compound [$D_3$]-**2a** (32 mg, 82%; containing *ca.* 3% of [$D_2$]-**2a**) as a colorless oil; $^1$H NMR (700 MHz, $CDCl_3$, 25 °C): δ = 8.25 (d, 1H, *J* = 8.0 Hz, $CH^{Ar}$), 7.98 (s, 1H, $CH^{Ar}$), 7.35 (m, 1H, $CH^{Ar}$), 7.29 (m, 1H, $CH^{Ar}$), 7.23 (m, 2H, $2CH^{Ar}$), 6.92 (dd, 1H, *J* = 8.2, 2.4 Hz, $CH^{Ar}$), 6.77 (d, 1H, *J* = 7.7 Hz, $CH^{Ar}$), 6.58 (m, 1H, $CH^{Ar}$), 3.95 (s, 3H, $OCH_3$), 3.51 (s, 3H, $OCH_3$); $^{13}$C NMR (175 MHz, $CDCl_3$, 25 °C): δ = 164.8 (C=O), 159.6 ($C^{Ar\text{-}q}$-OMe), 143.5 (=C), 135.5 ($C^{Ar\text{-}q}$), 132.0 ($CH^{Ar}$), 130.9 ($C^{Ar\text{-}cq}$), 129.9 ($CH^{Ar}$), 126.3 ($C^{Ar\text{-}q}$), 124.1 ($CH^{Ar}$), 123.2 ($CH^{Ar}$), 122.1 ($CH^{Ar}$), 119.9 ($CH^{Ar}$), 119.5 (=C-Tf), 119.5 (q, $J_{CF}$ = 328.1 Hz, $CF_3$), 117.2 ($CH^{Ar}$), 112.2 ($CH^{Ar}$), 111.9 ($CH^{Ar}$), 111.1 ($C^{Ar\text{-}q}$), 58.5 (m, CD-*low intensity*), 55.0

($OCH_3$), 51.3 ($OCH_3$), 26.0 (m, $CD_2$-*low intensity*); $^{19}F$ NMR (282 MHz, $CDCl_3$, 25 °C): δ = –76.9 (s, 3F, $CF_3$); D($^2H$) NMR (107 MHz, $CDCl_3$, 25 °C): δ = 5.10 (s, 1D, CD), 3.30 (m, 2D, $CD_2$); IR ($CHCl_3$): ν = 1709 (C=O), 1393, 1108 (O=S=O), 1209 (C–F) $cm^{-1}$; HRMS (ES): calcd for $C_{22}H_{16}D_3F_3NO_5S$ $[M + H]^+$: 469.11188; found: 469.11099.

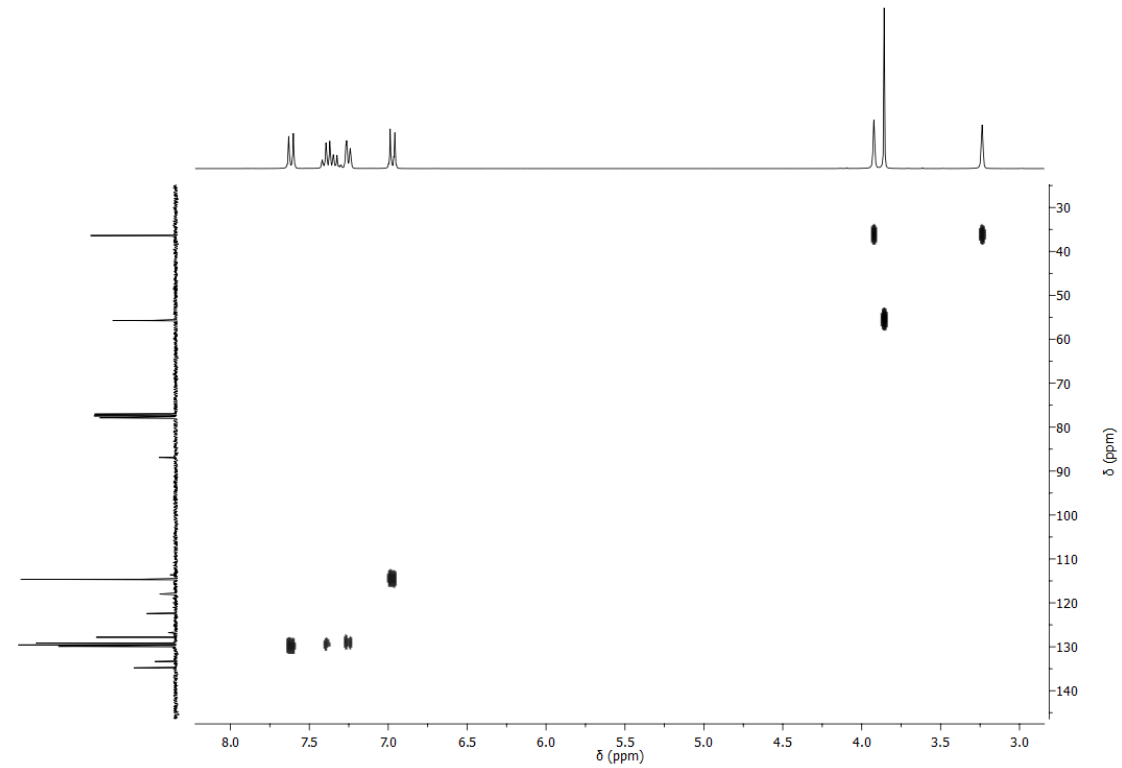
$^1$H NMR (300 MHz, $CDCl_3$)



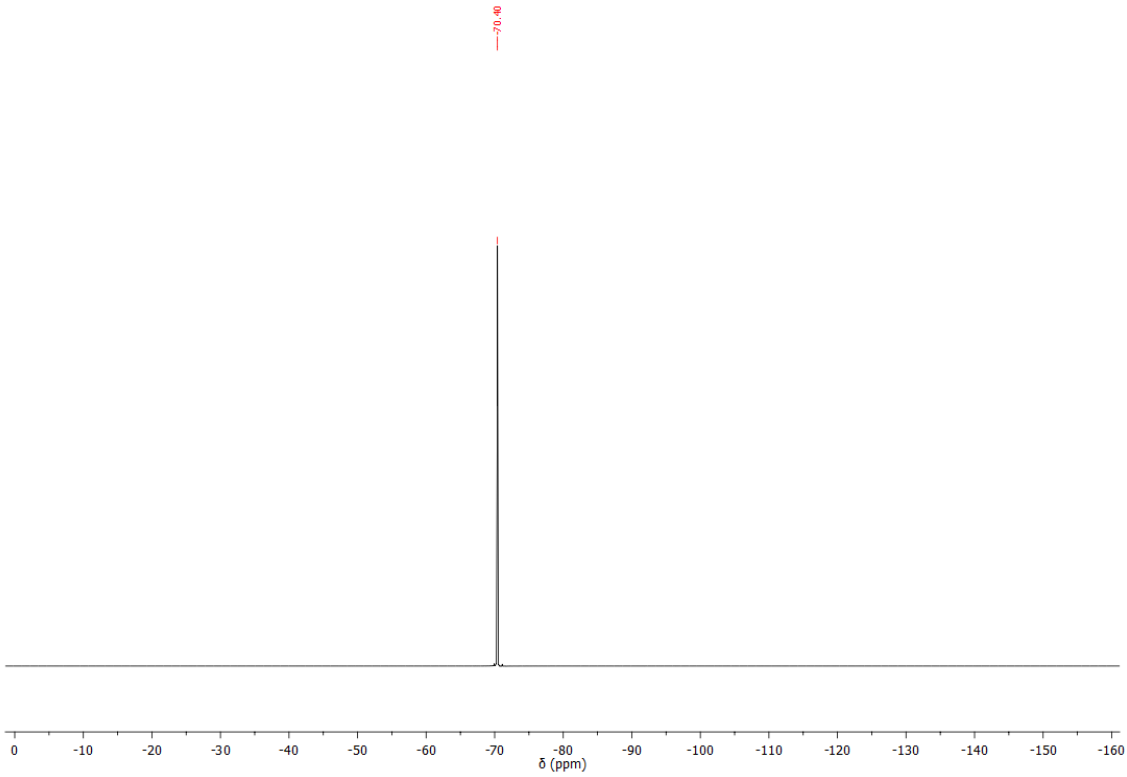

$^{13}$C NMR (75 MHz, $CDCl_3$)



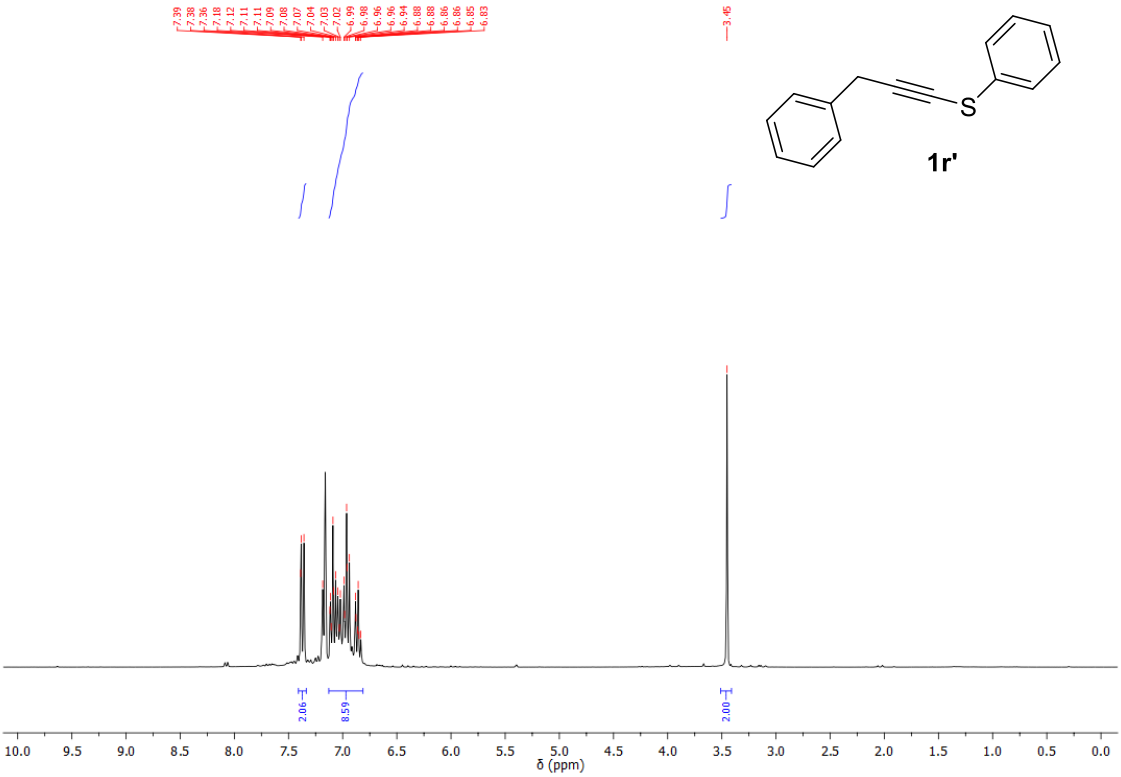
2D-HMQC NMR ($CDCl_3$)




$^{19}F$ NMR (282 MHz, $CDCl_3$)



$^1$H NMR (300 MHz, $C_6D_6$)

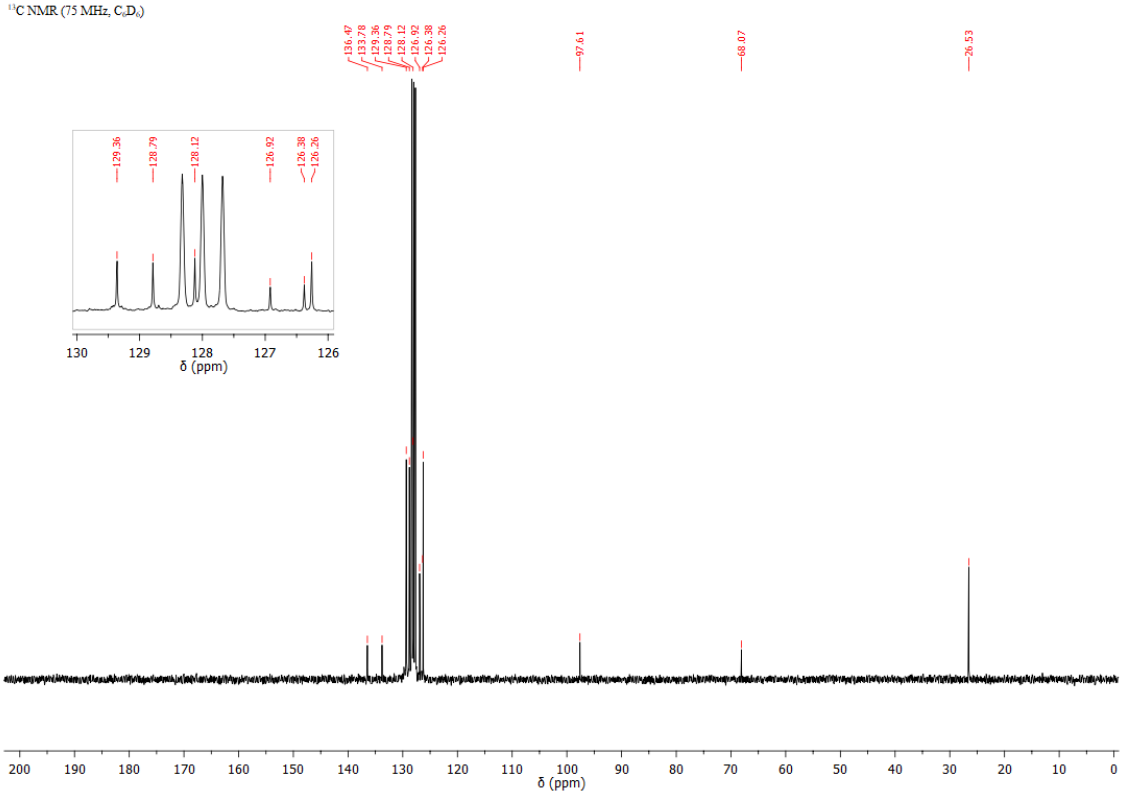




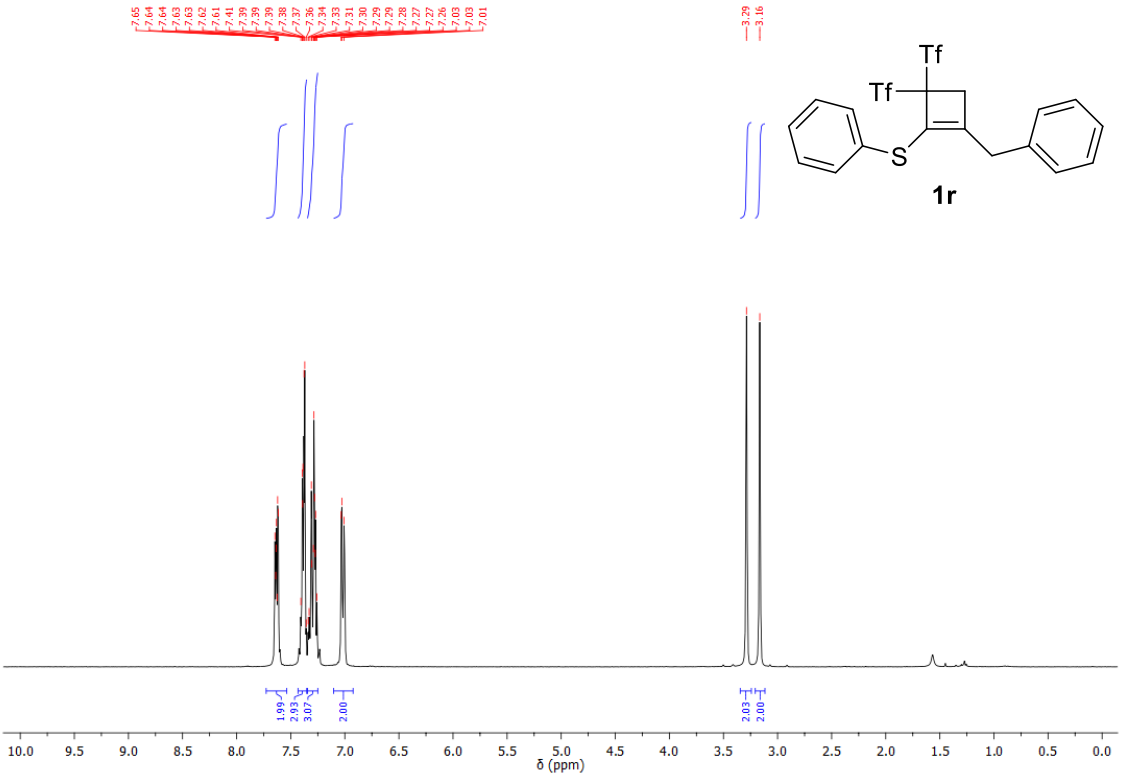


**1r'**

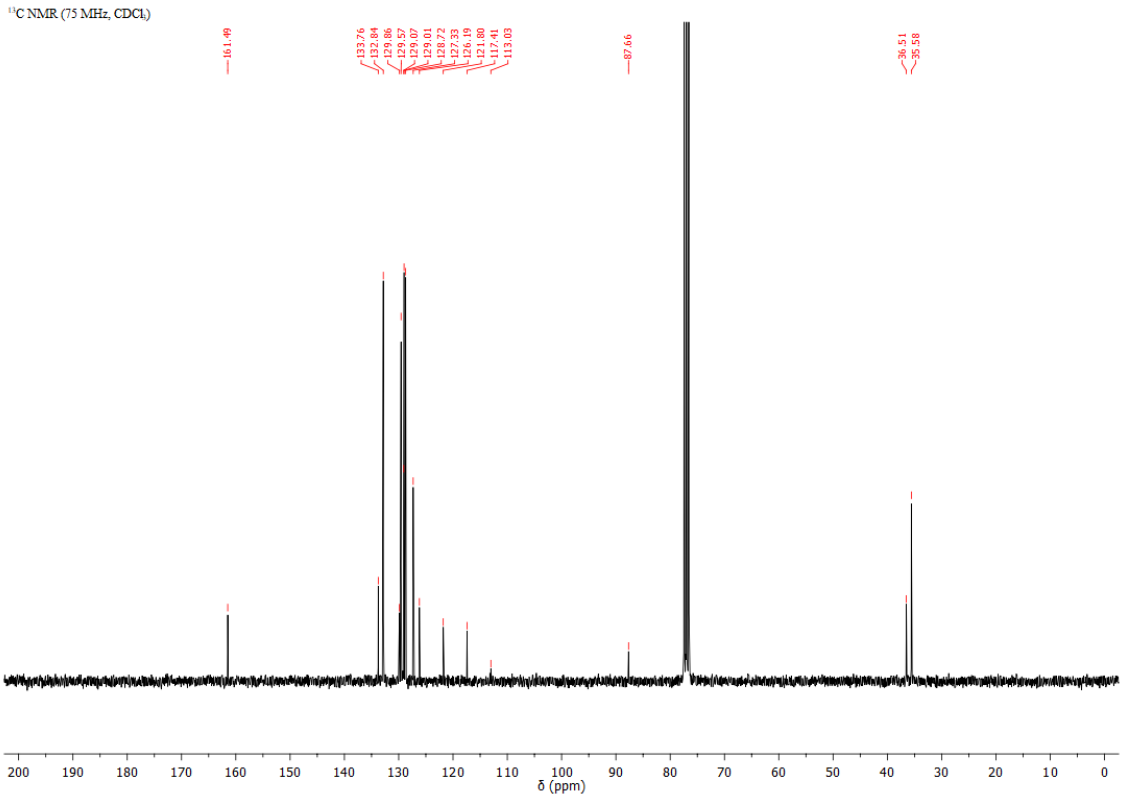
$^{13}$C NMR (75 MHz, $C_6D_6$)



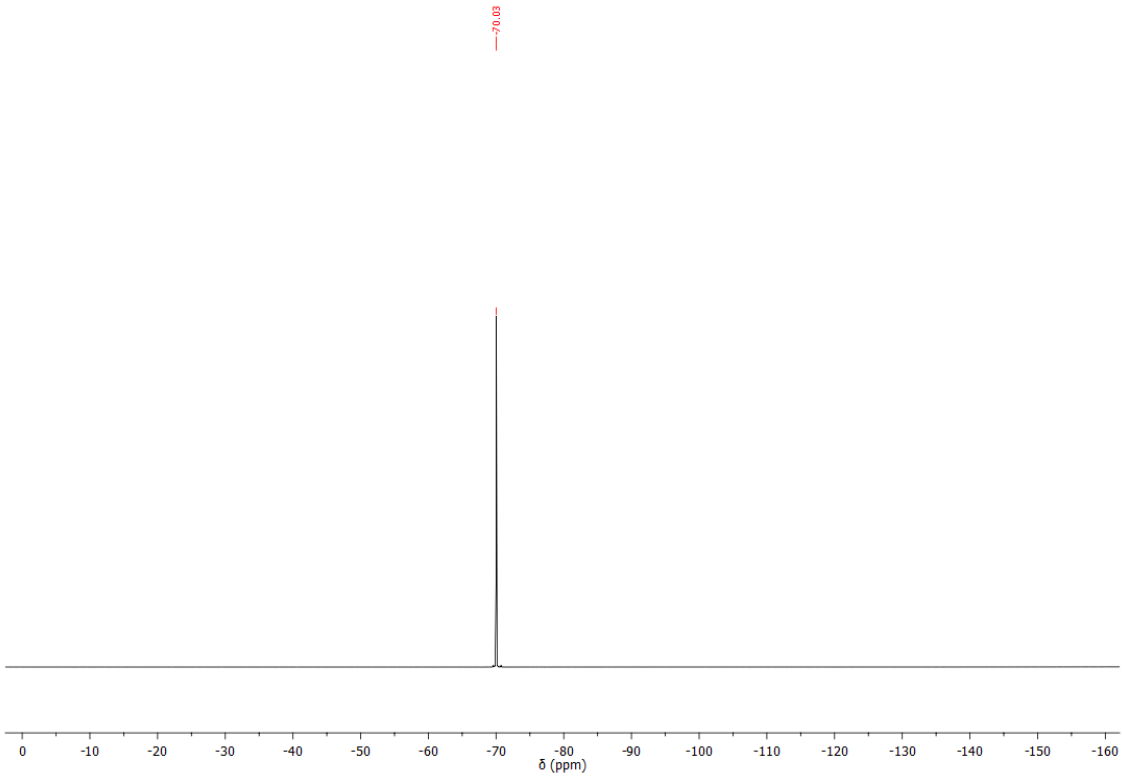
$^1$H NMR (300 MHz, $CDCl_3$)



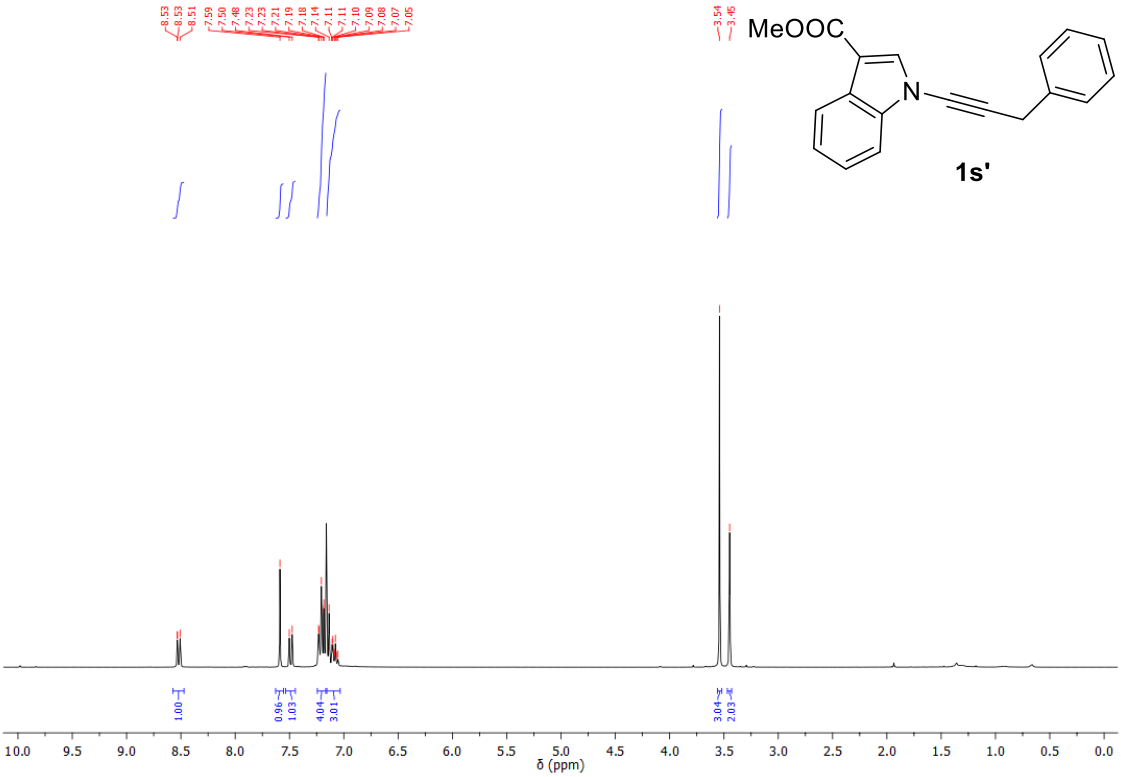

$^{13}$C NMR (75 MHz, $CDCl_3$)



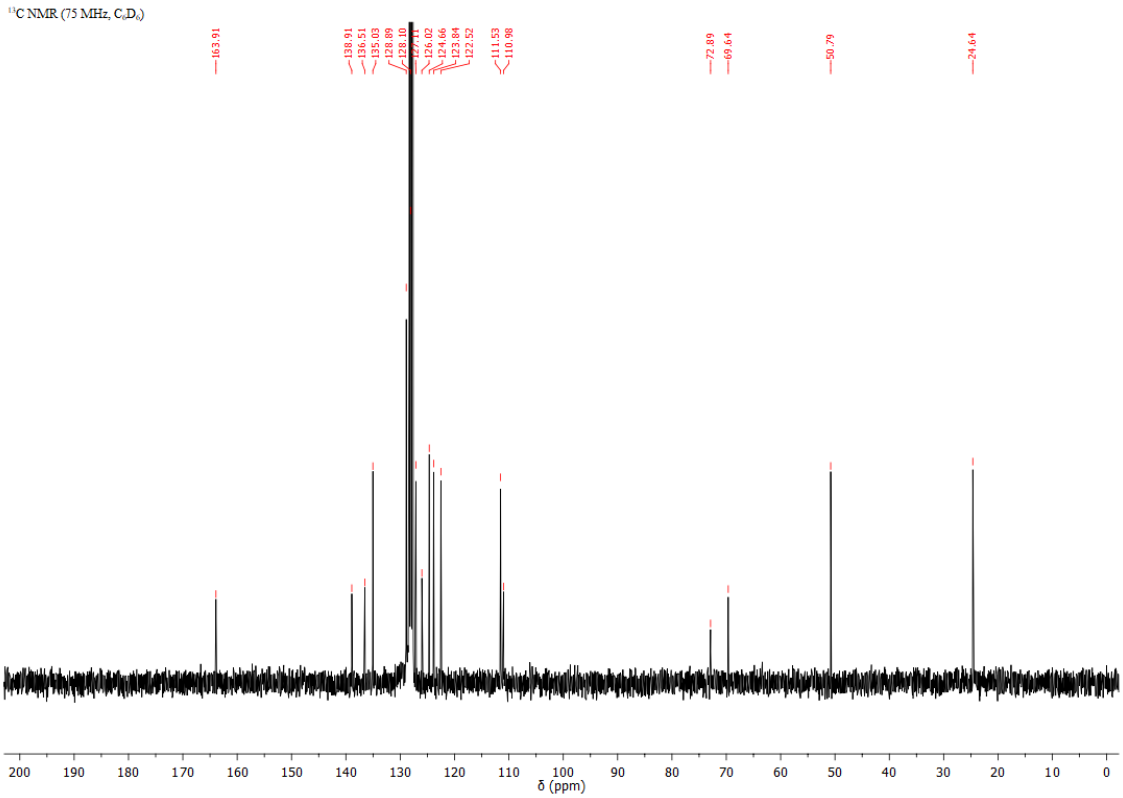
$^{19}$F NMR (282 MHz, $CDCl_3$)



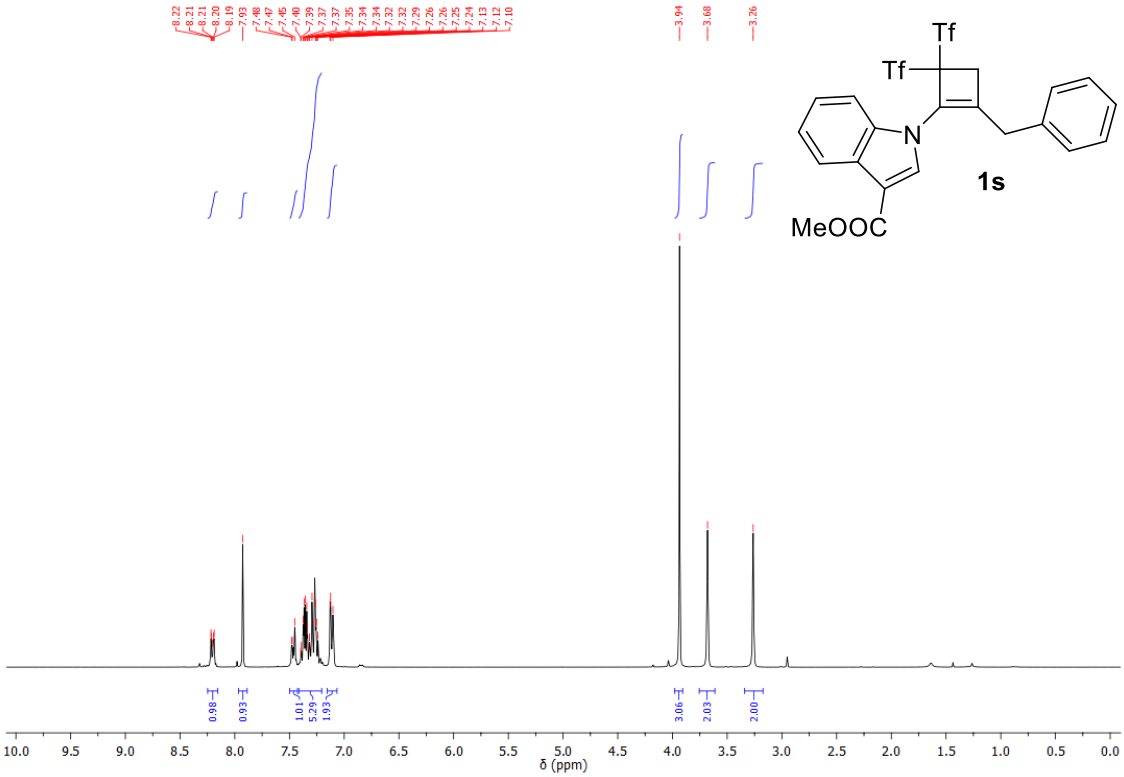
$^1$H NMR (300 MHz, $C_5D_5N$)



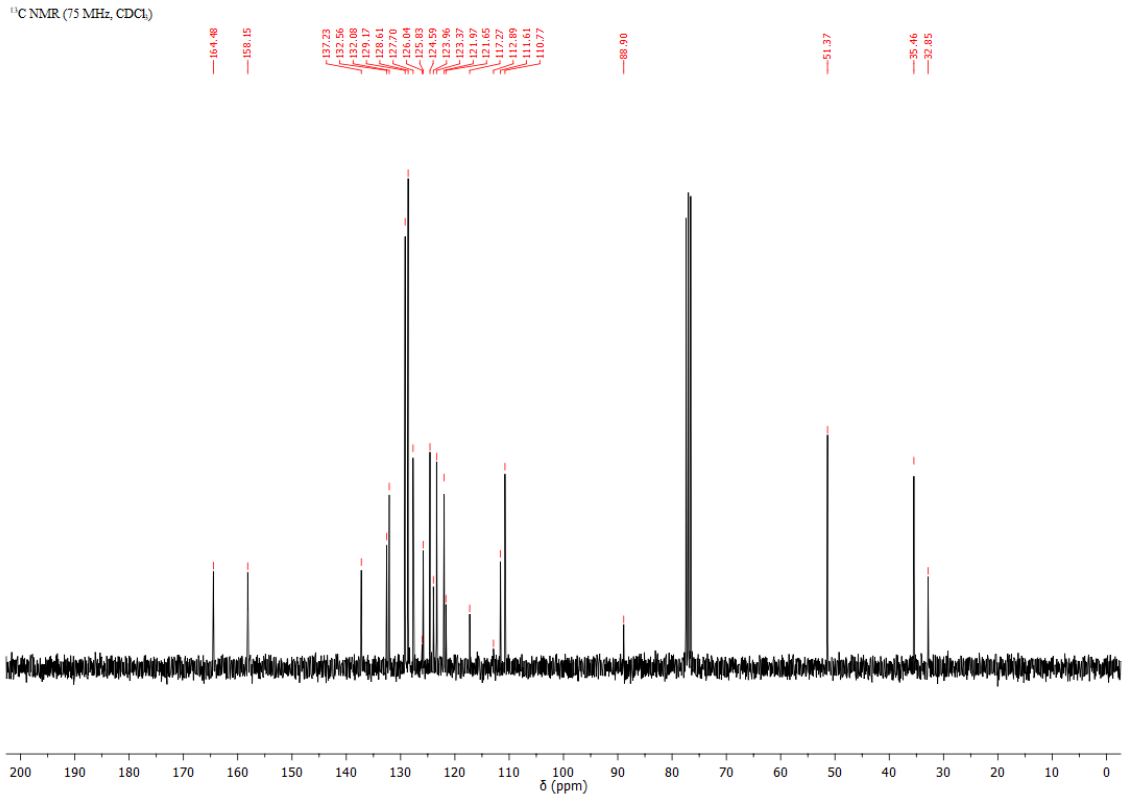

$^{13}$C NMR (75 MHz, $C_5D_5N$)



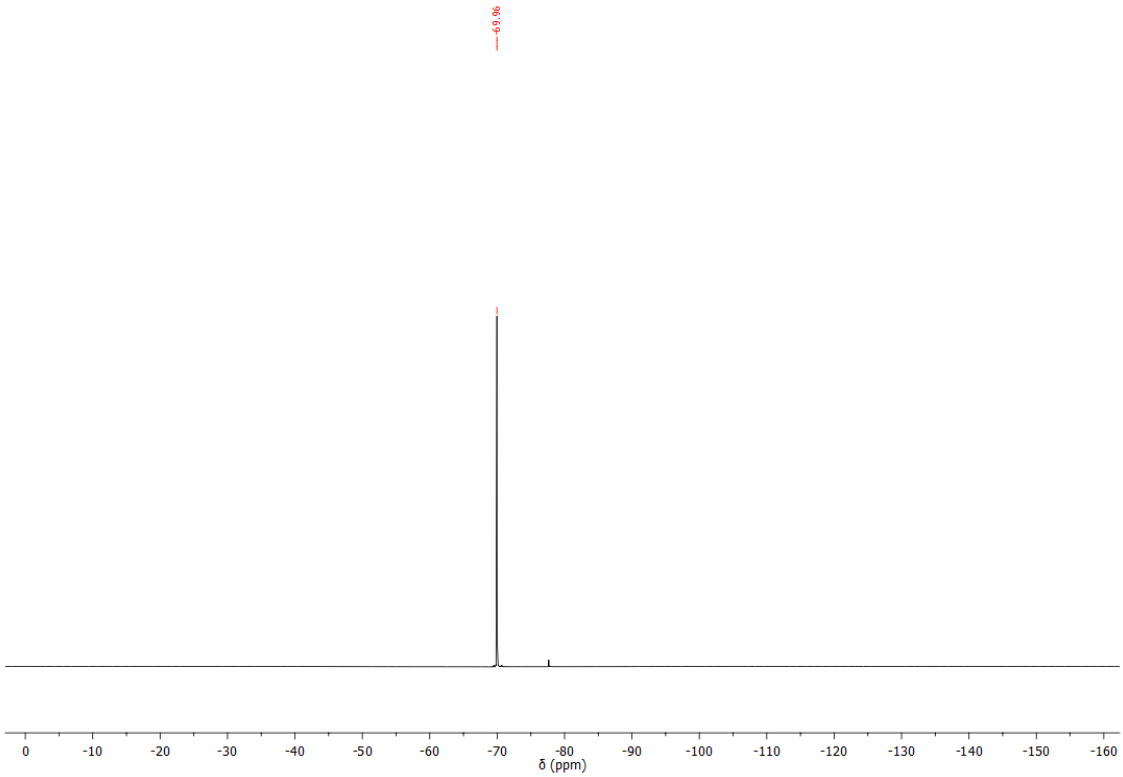
$^1$H NMR (300 MHz, $CDCl_3$)



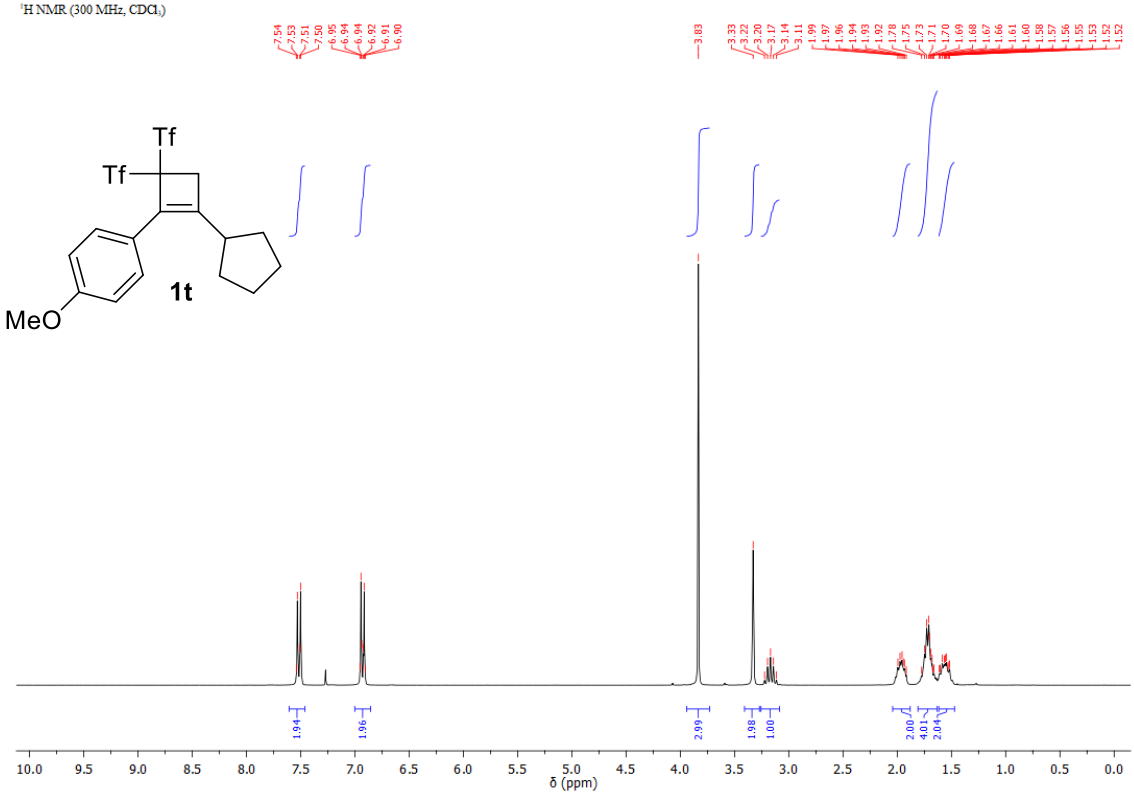

$^{13}$C NMR (75 MHz, $CDCl_3$)



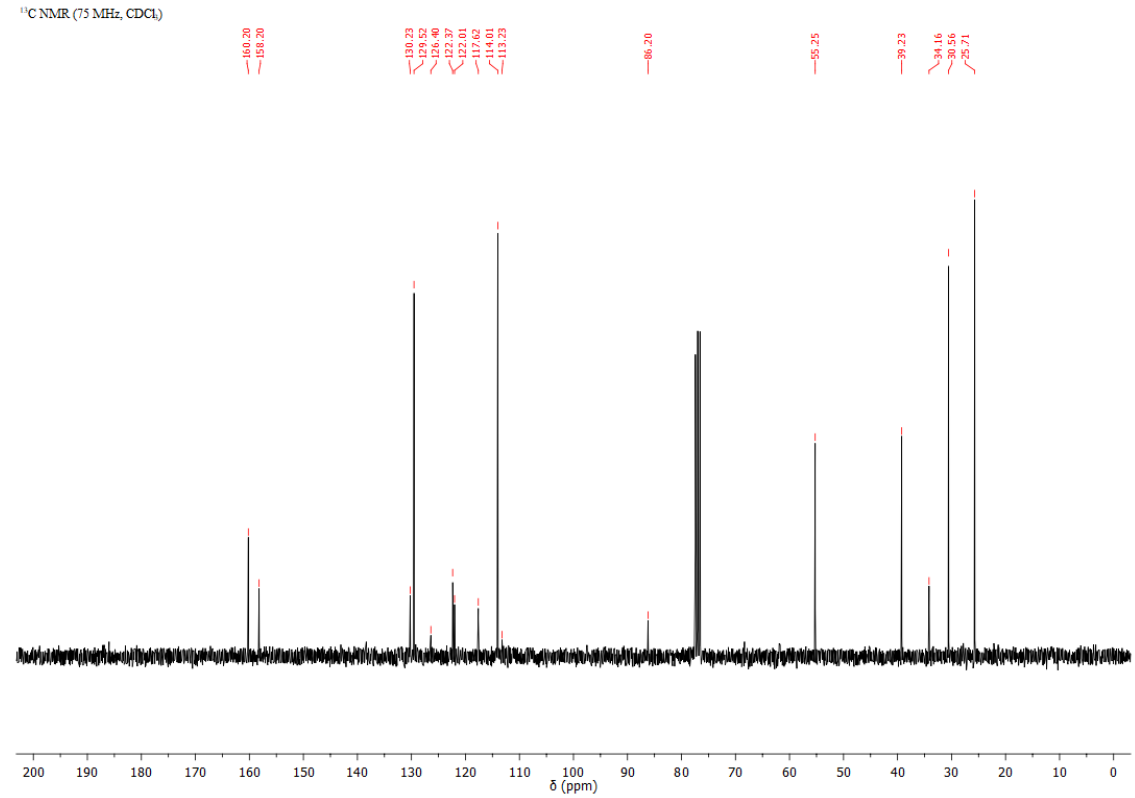
$^{19}$F NMR (282 MHz, $CDCl_3$)



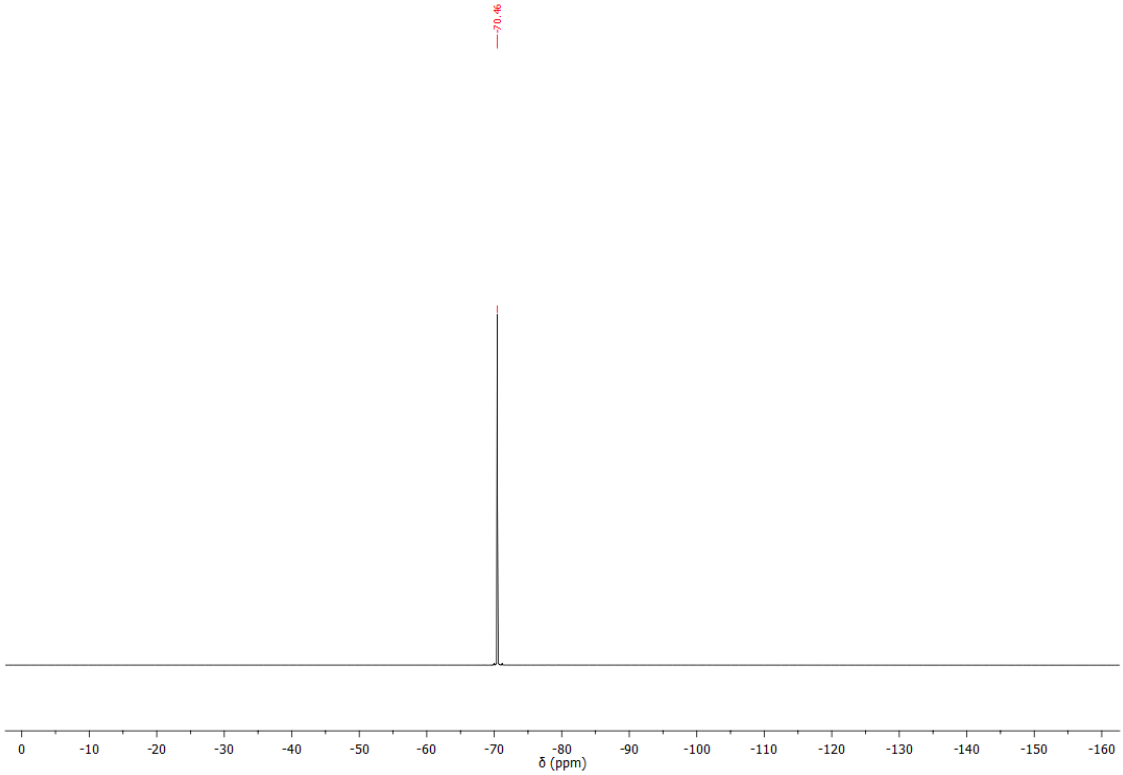
$^1$H NMR (300 MHz, $CDCl_3$)



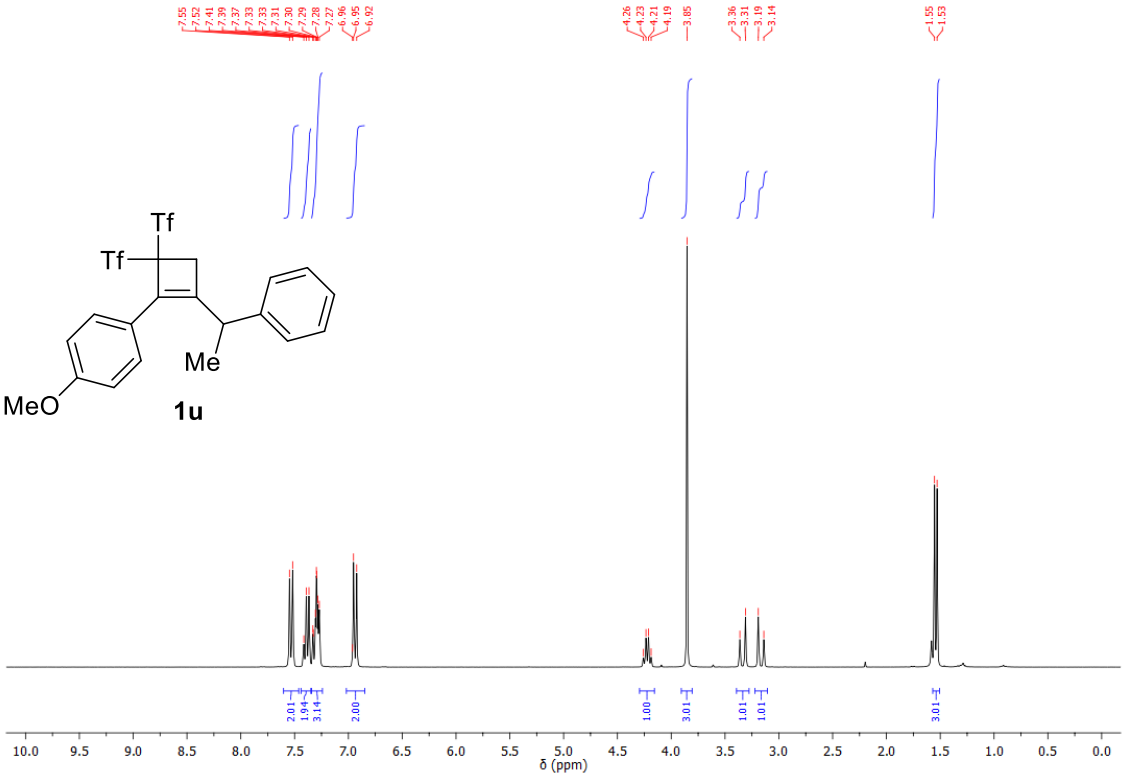

$^{13}$C NMR (75 MHz, $CDCl_3$)



$^{19}$F NMR (282 MHz, $CDCl_3$)



$^1$H NMR (300 MHz, $CDCl_3$)

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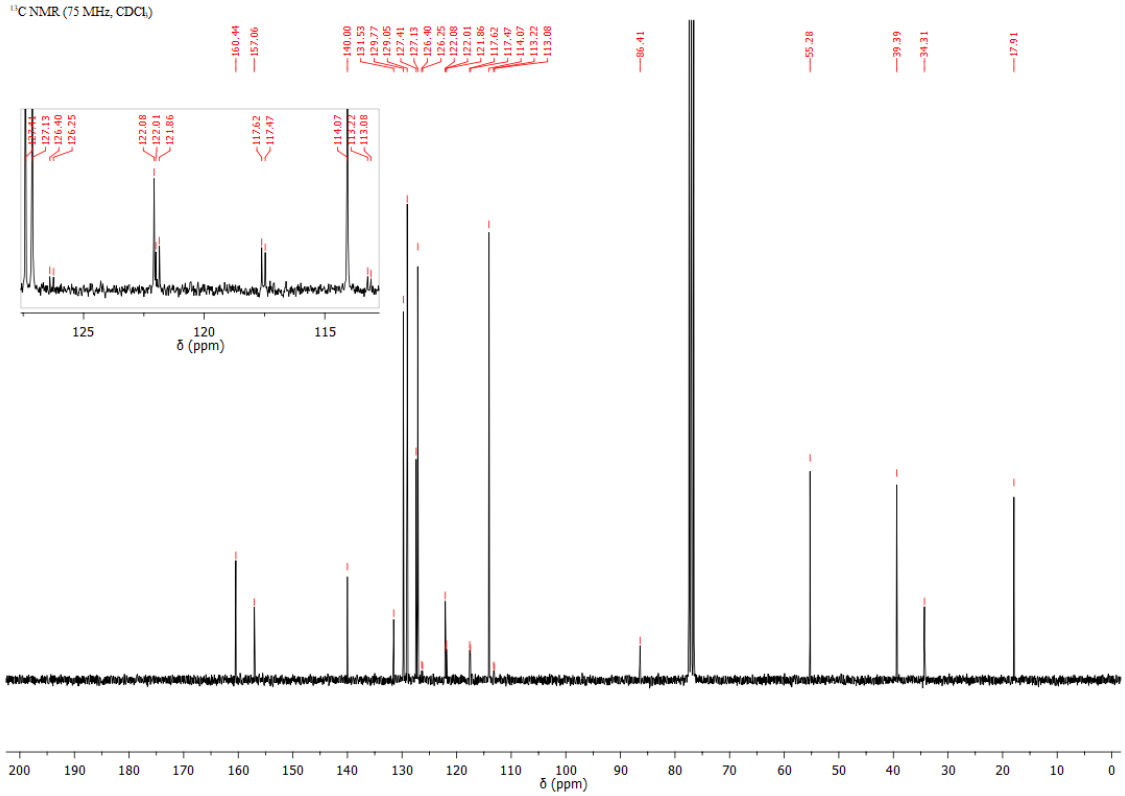

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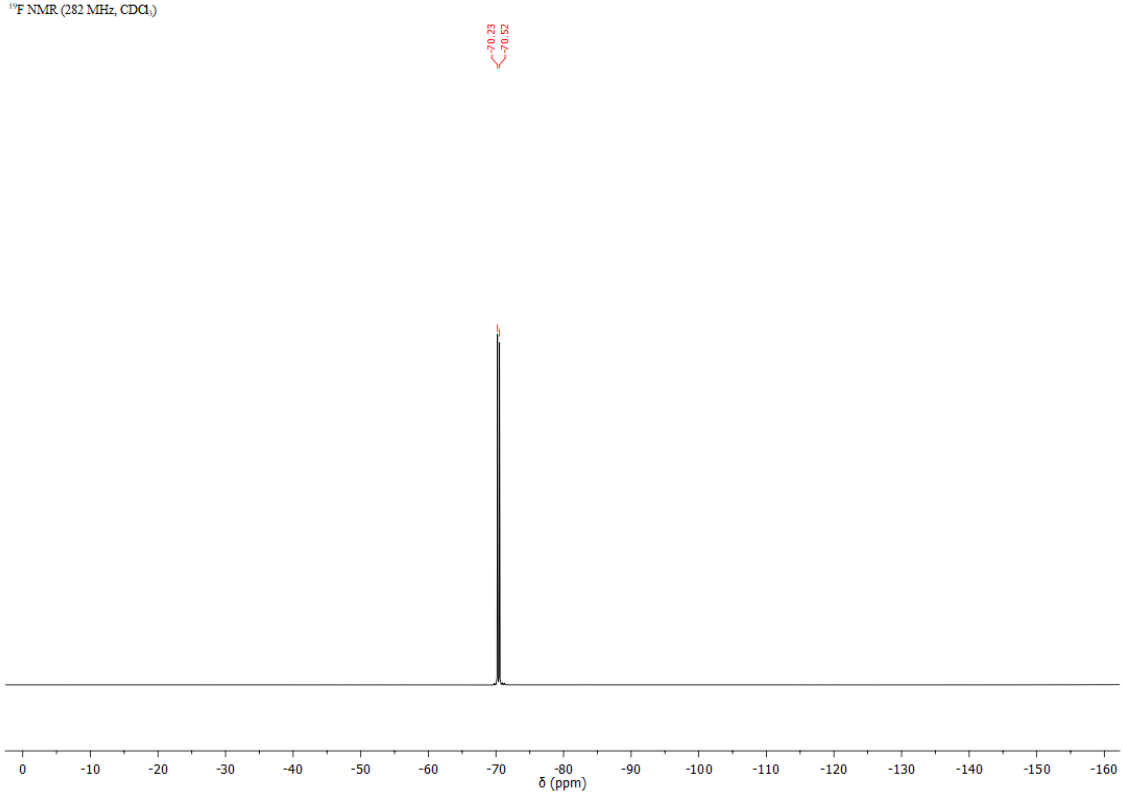
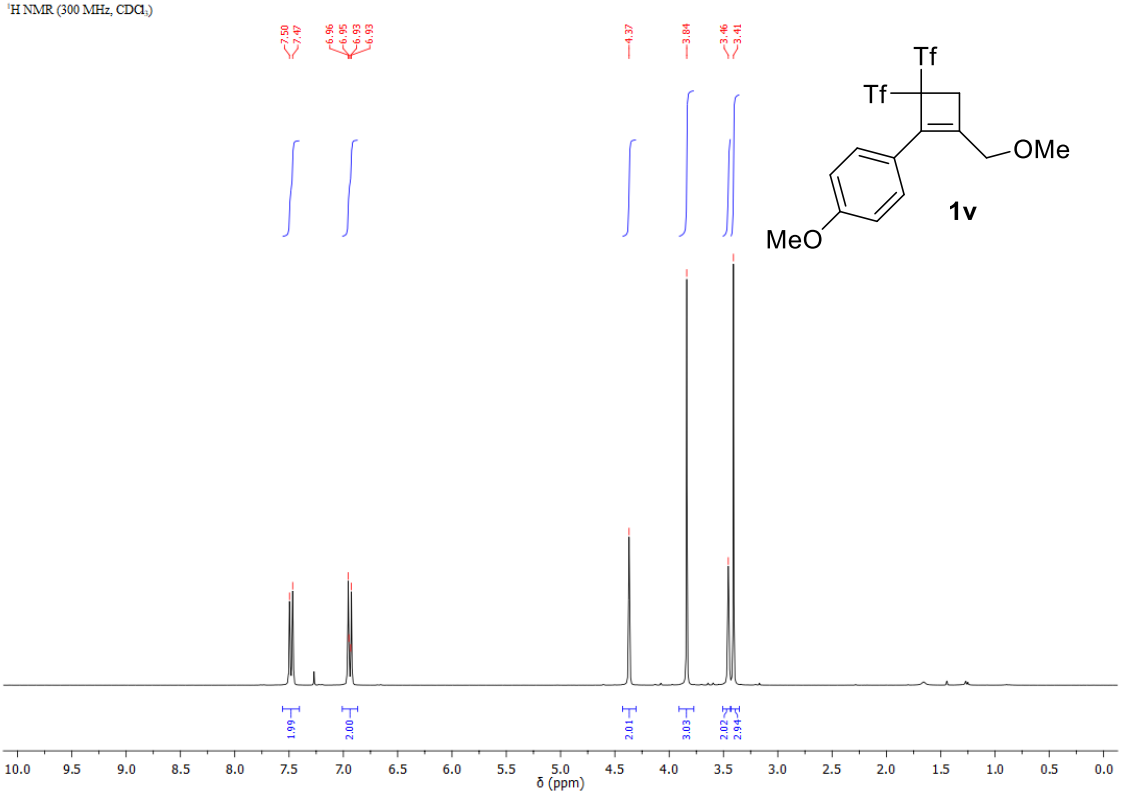
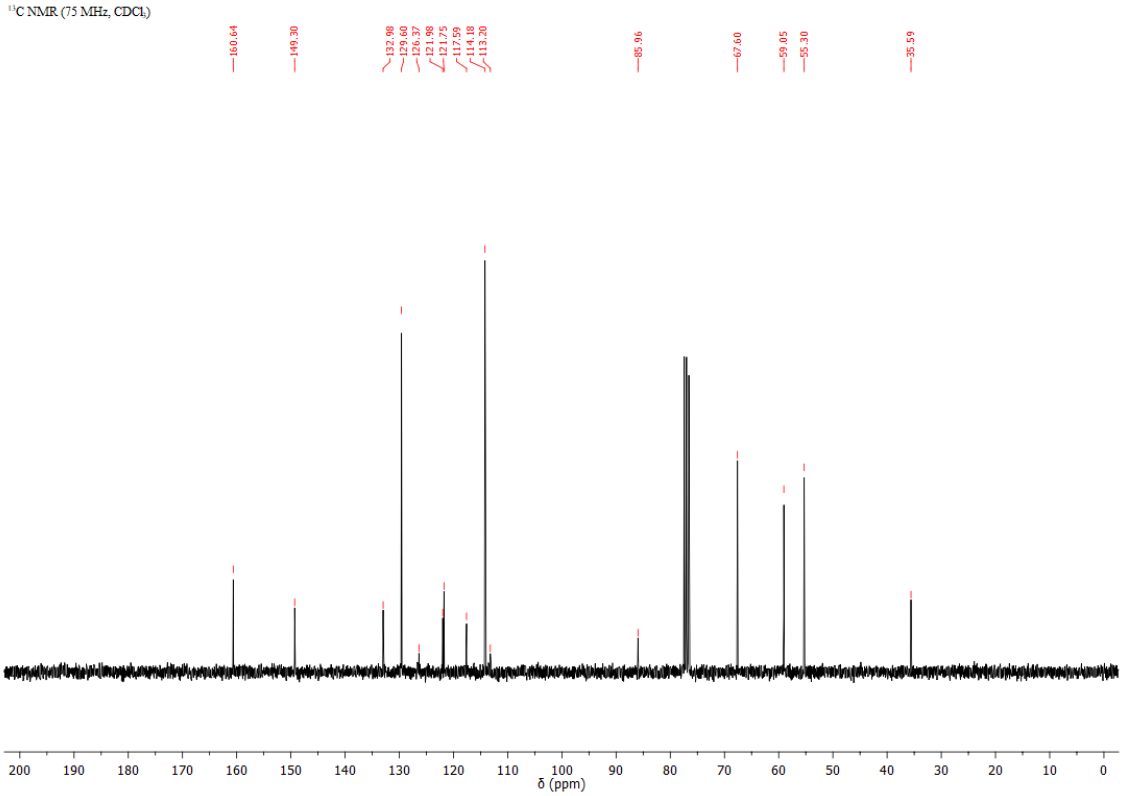


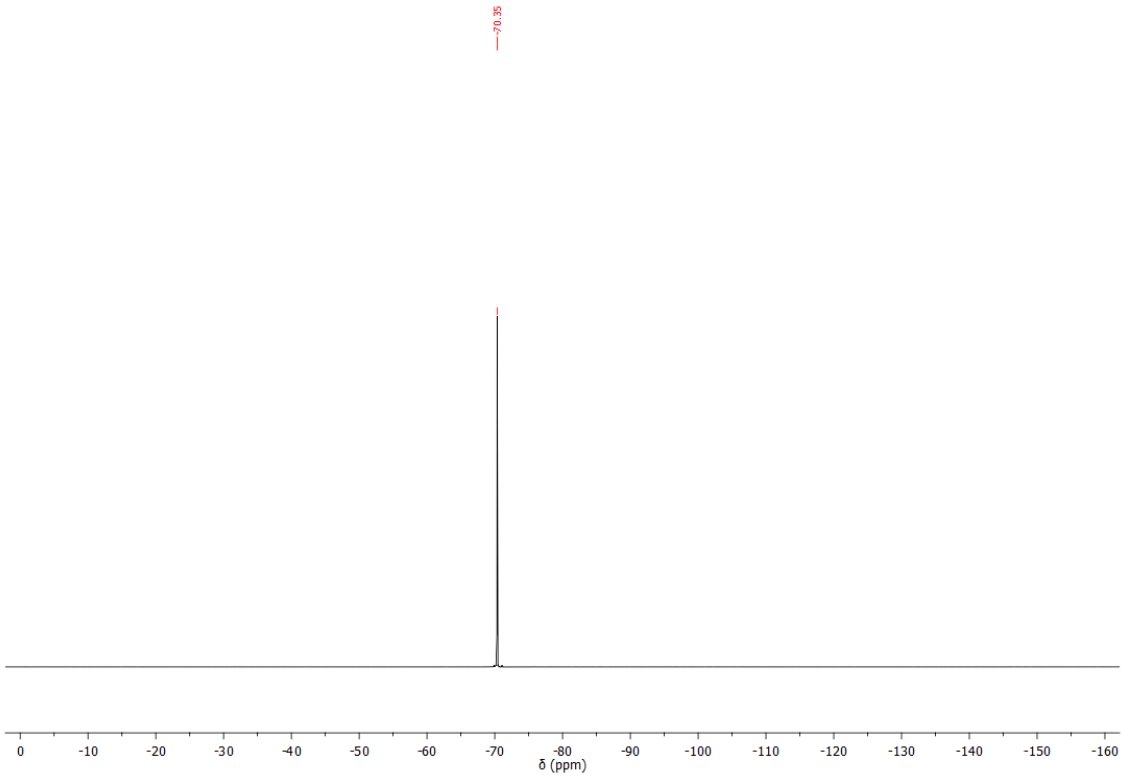
$^1$H NMR (300 MHz, $CDCl_3$)



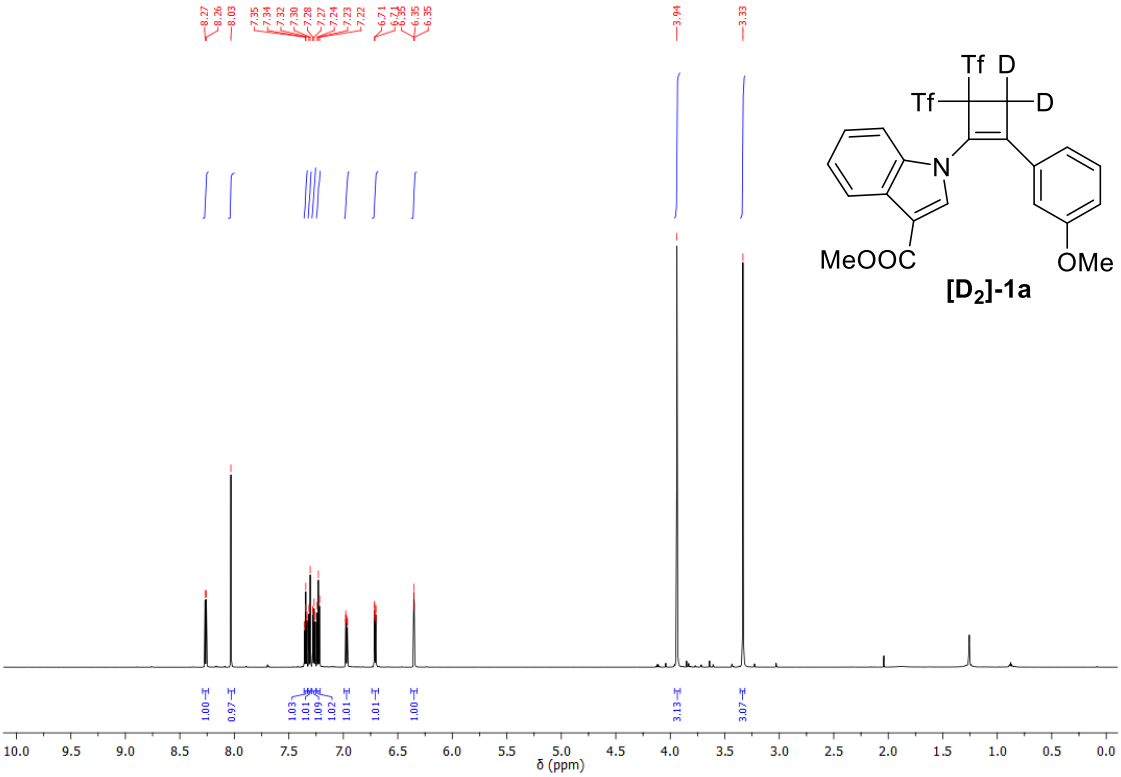

$^{13}$C NMR (75 MHz, $CDCl_3$)



$^{19}$F NMR (282 MHz, $CDCl_3$)



$^1$H NMR (700 MHz, $CDCl_3$)

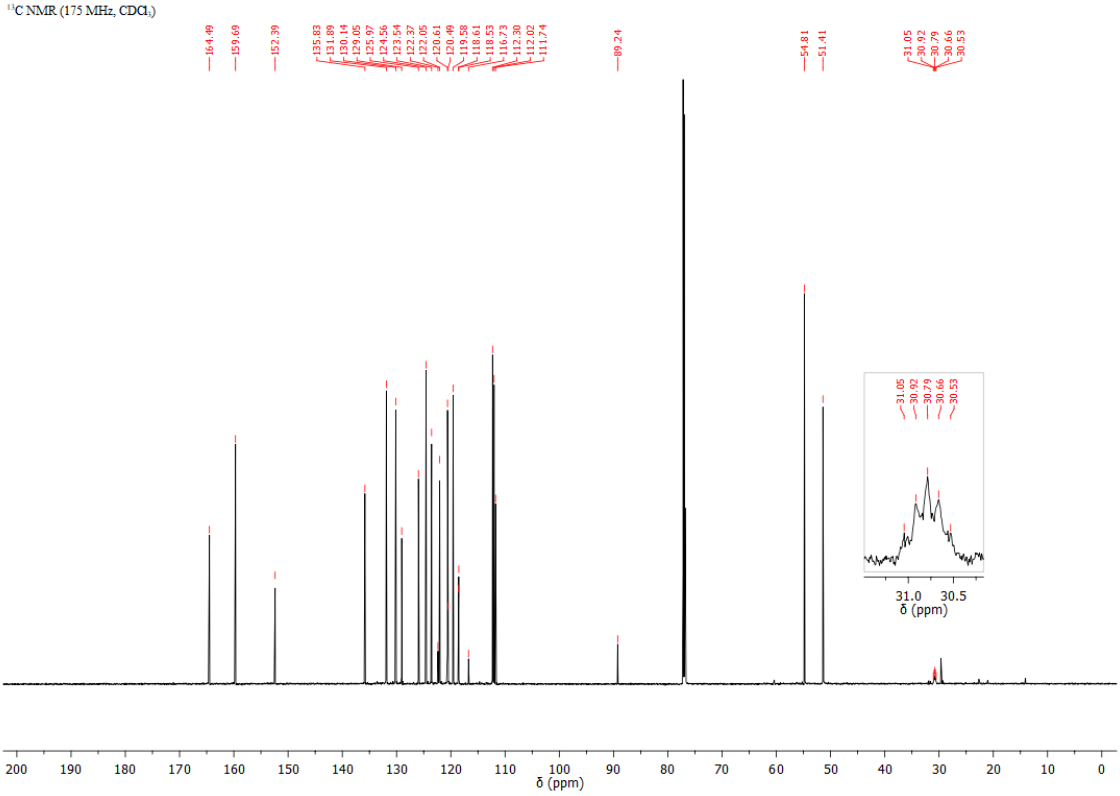




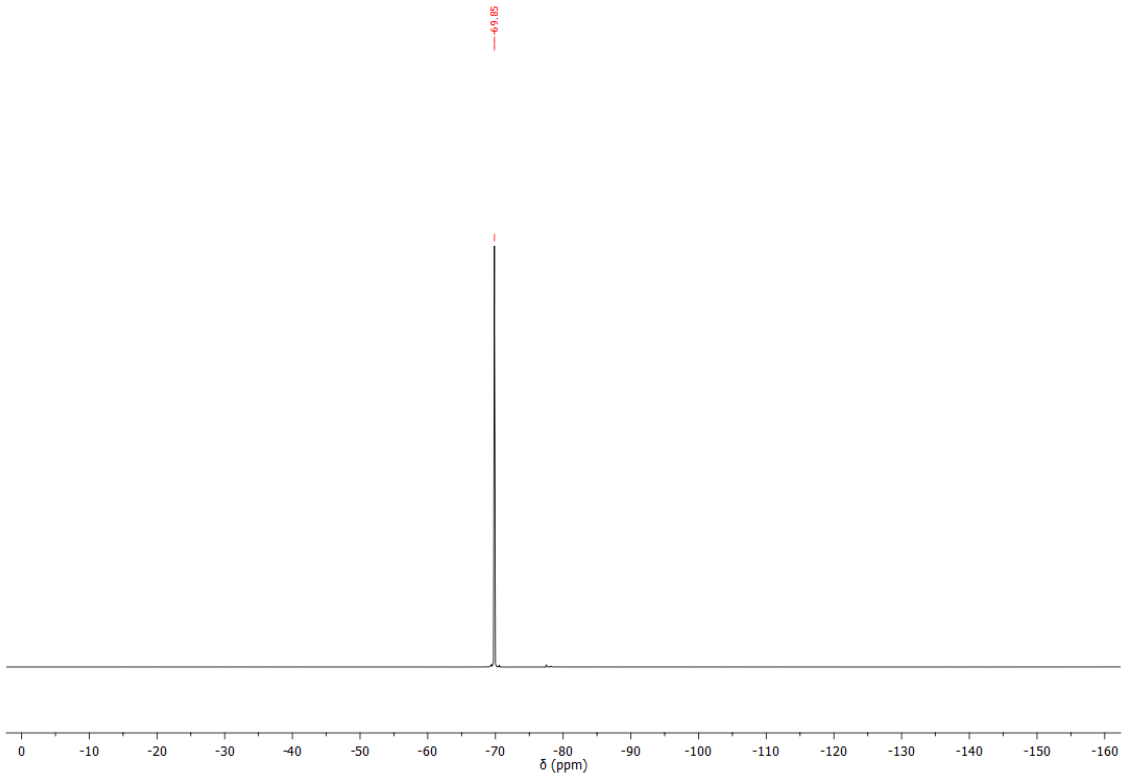


**[$D_2$]-1a**

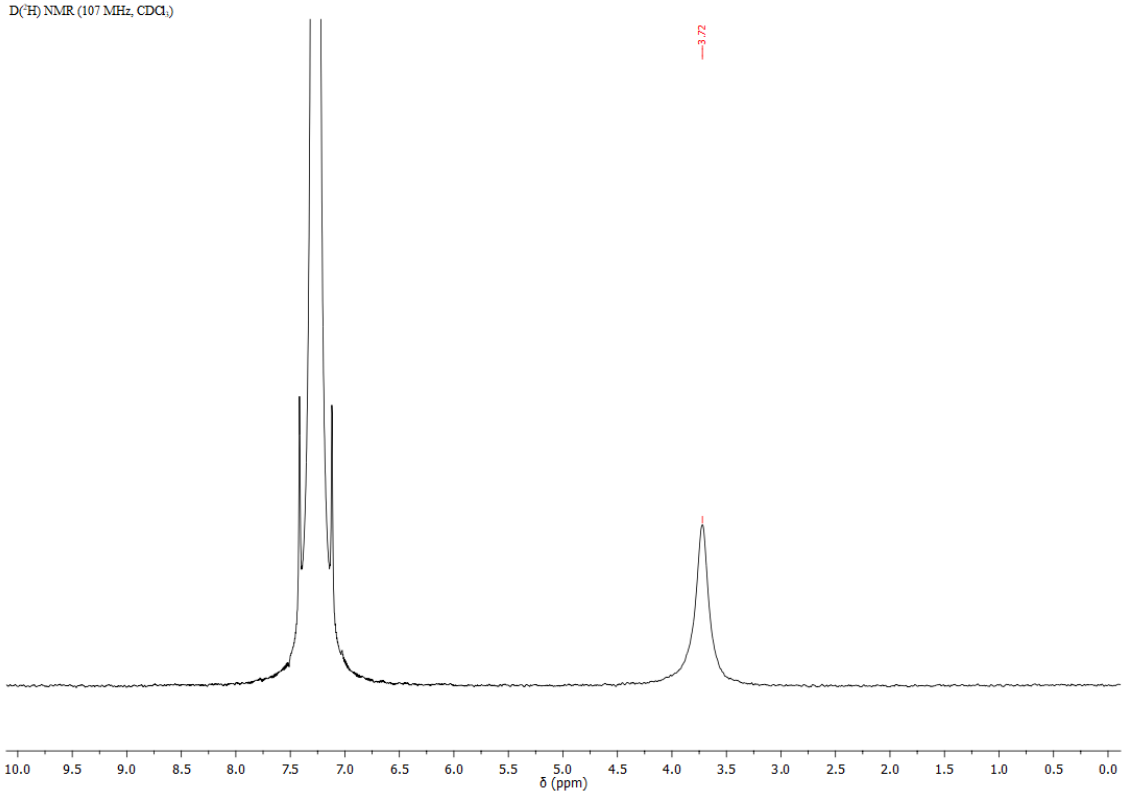
$^{13}$C NMR (175 MHz, $CDCl_3$)



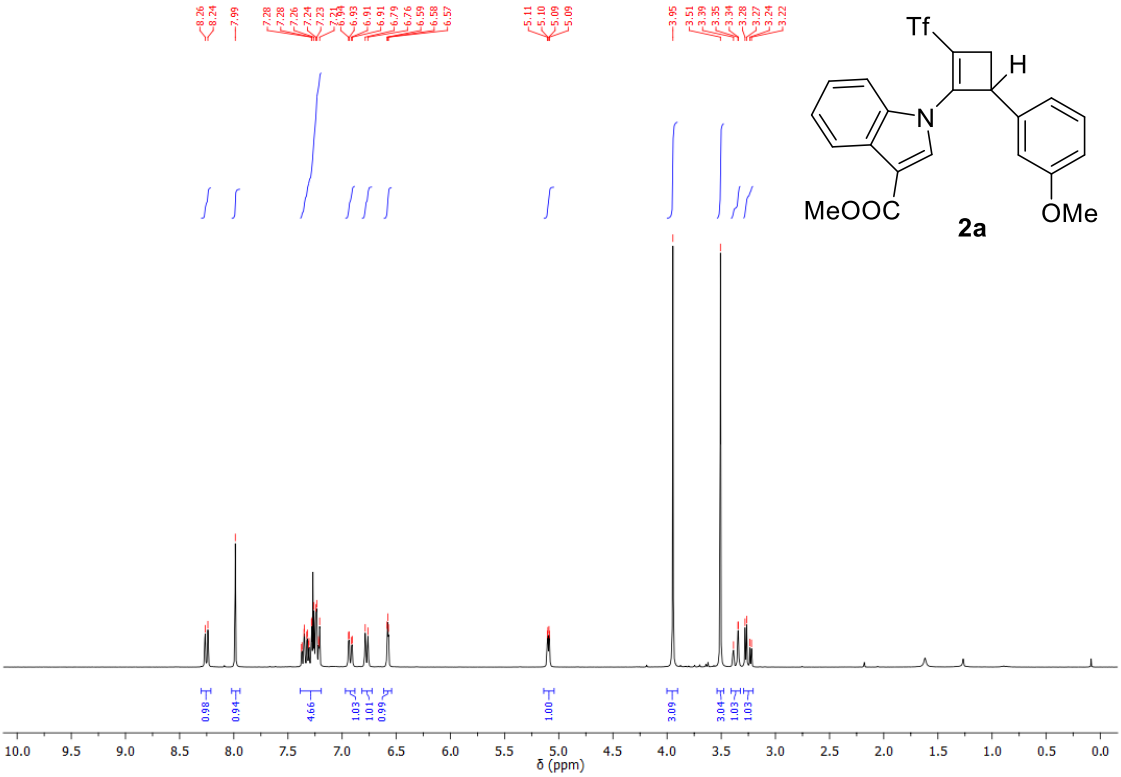
$^{19}$F NMR (282 MHz, $CDCl_3$)



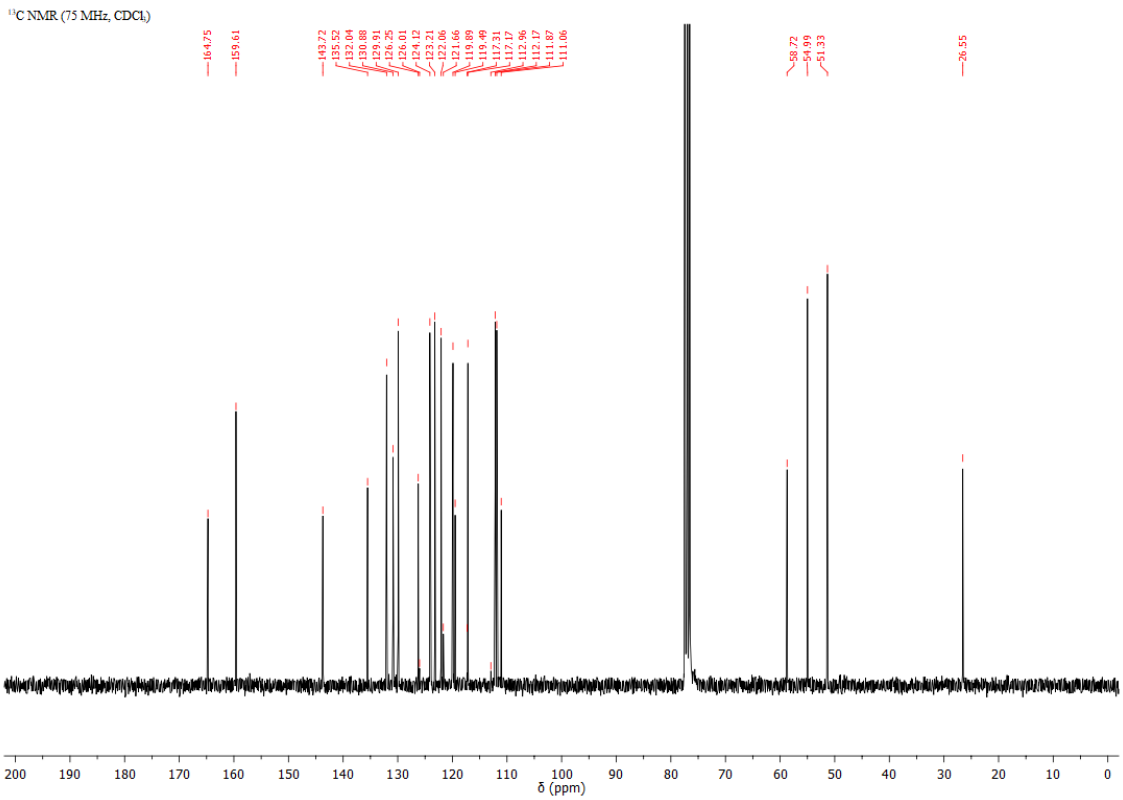

D($^2$H) NMR (107 MHz, $CDCl_3$)



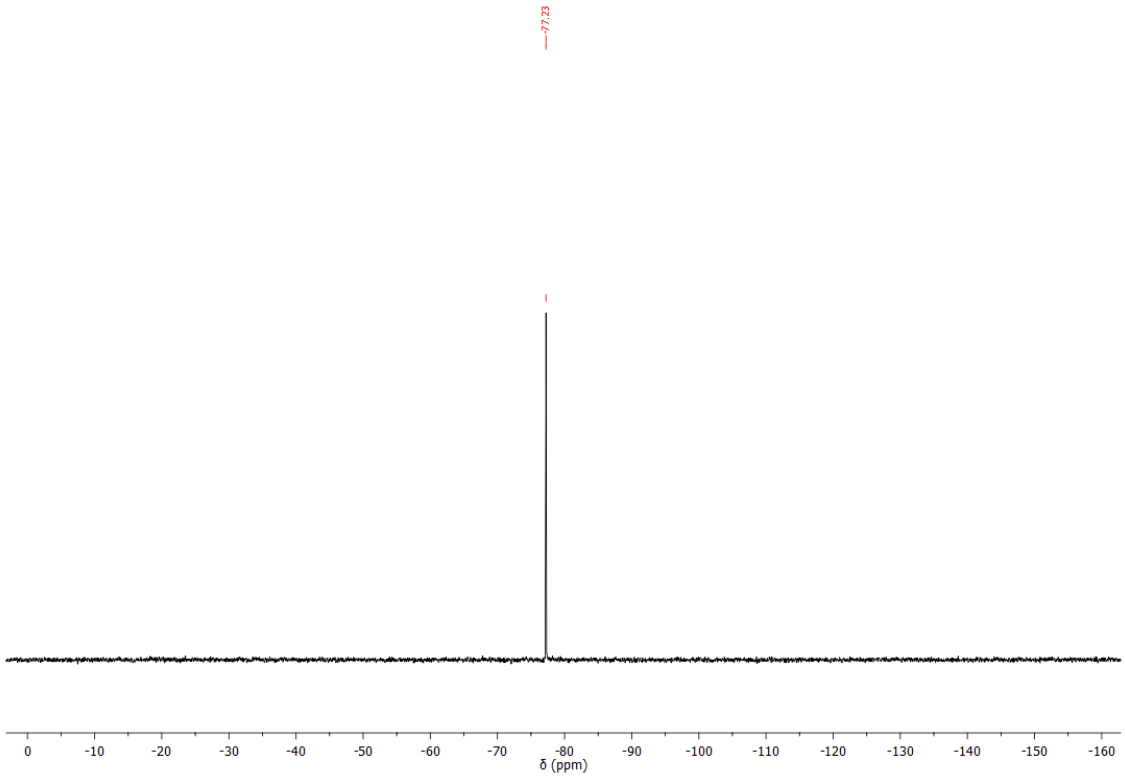
$^1$H NMR (300 MHz, CDCl$_3$)



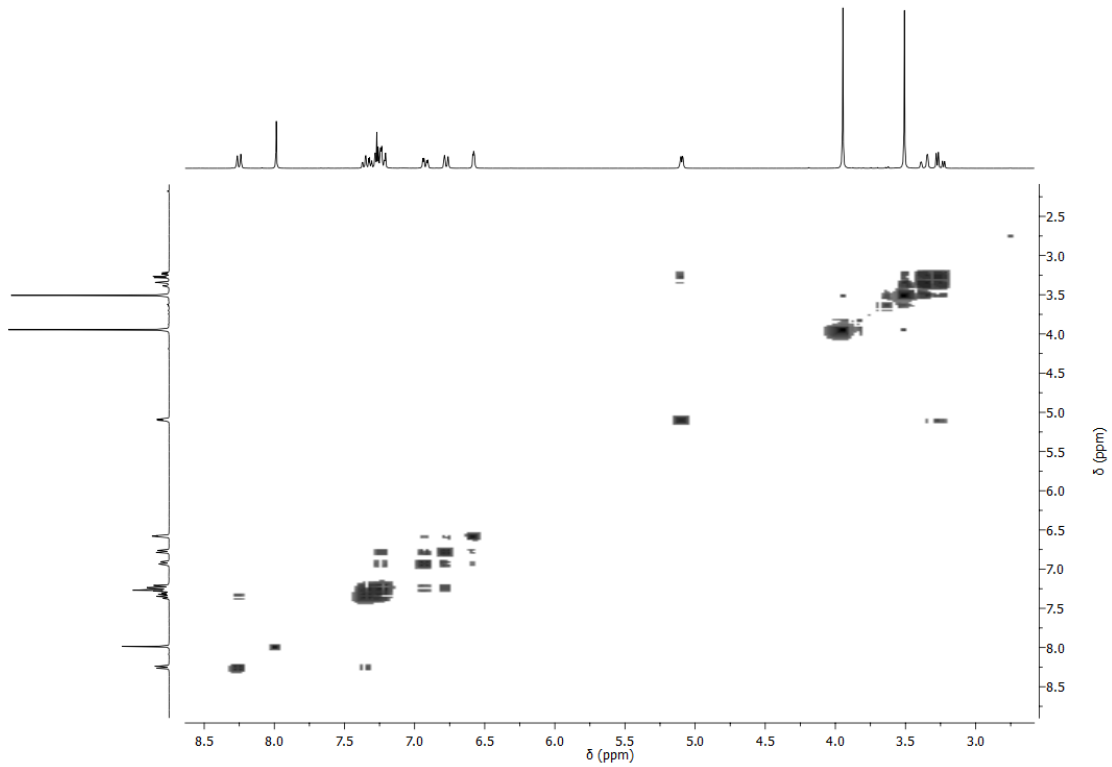

$^{13}$C NMR (75 MHz, CDCl$_3$)



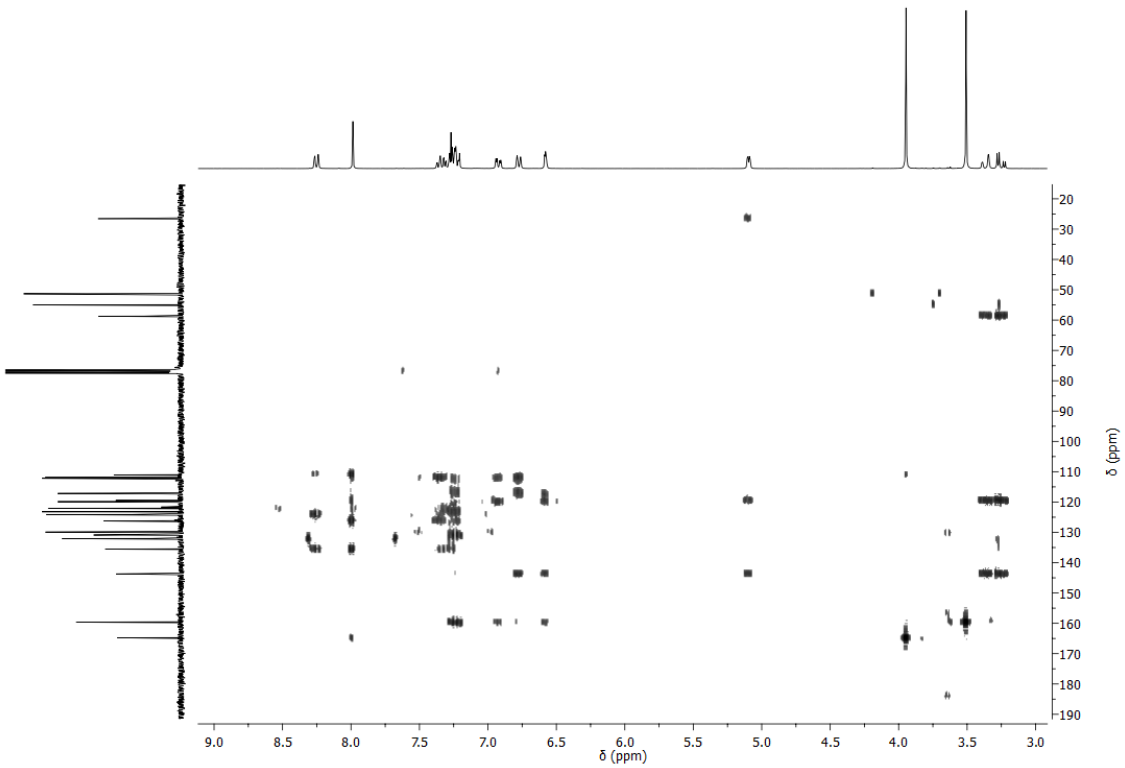
$^{19}$F NMR (282 MHz, $CDCl_3$)



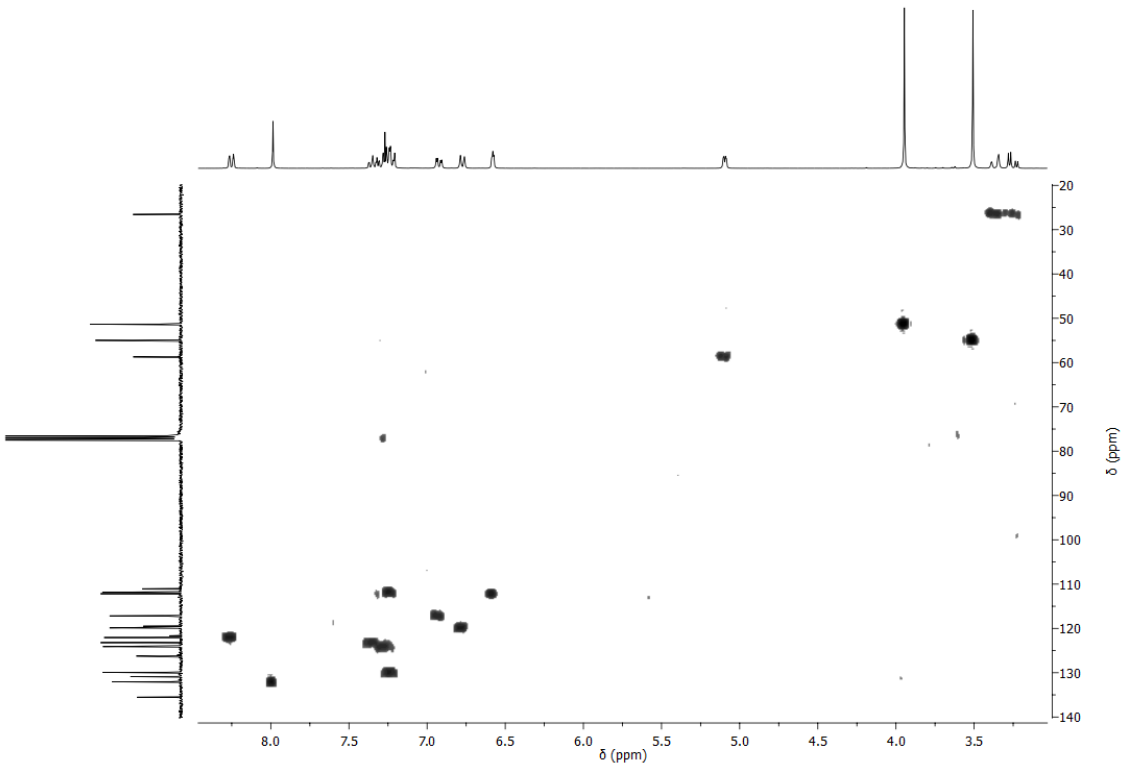

2D-COSY NMR ($CDCl_3$)

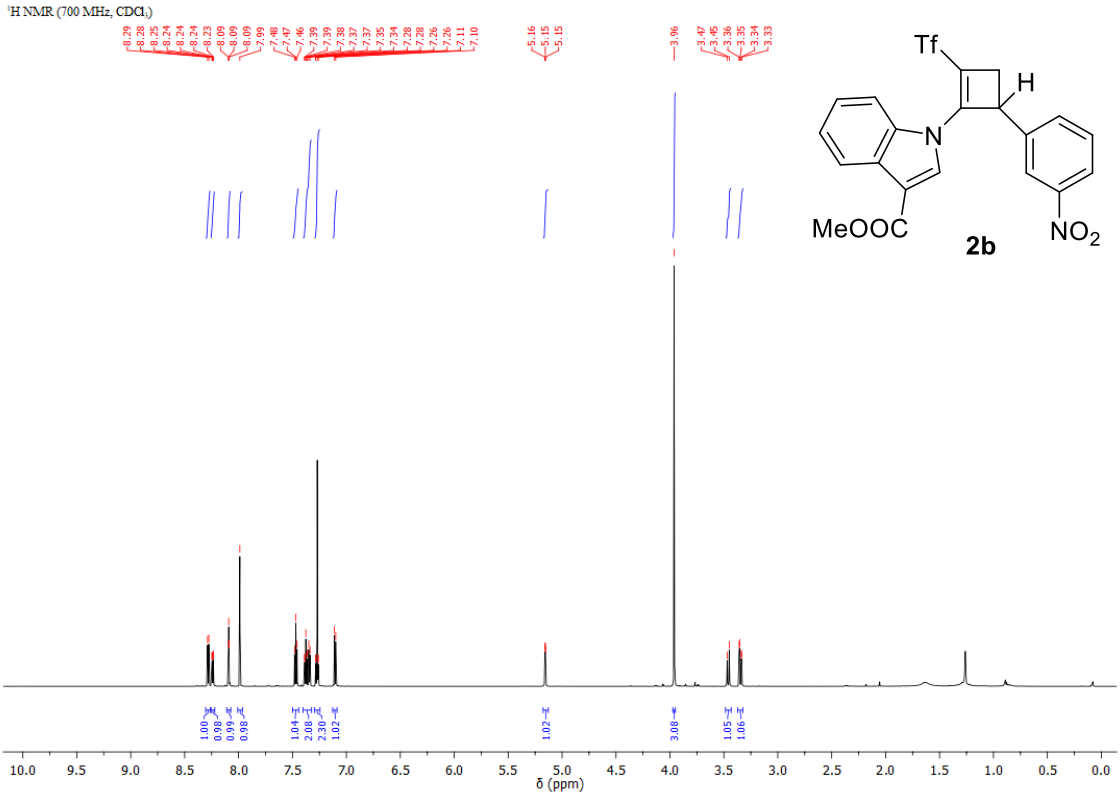


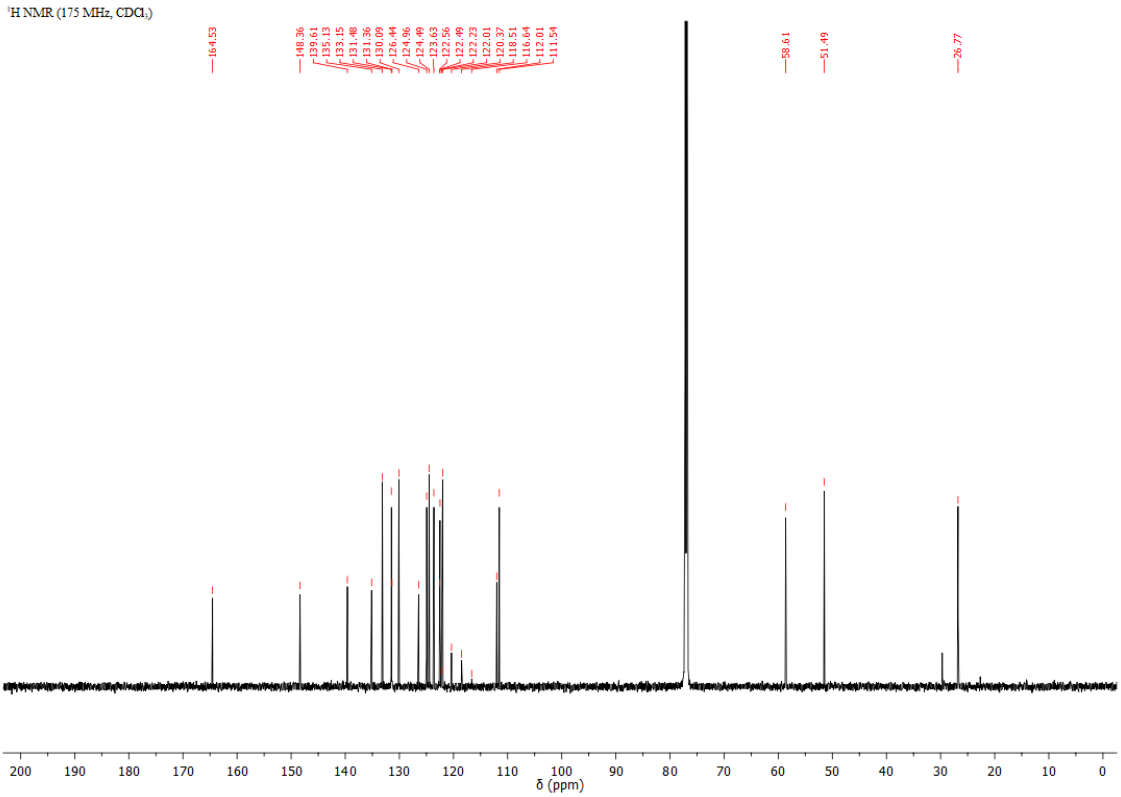
2D-HMBC NMR ($CDCl_3$)



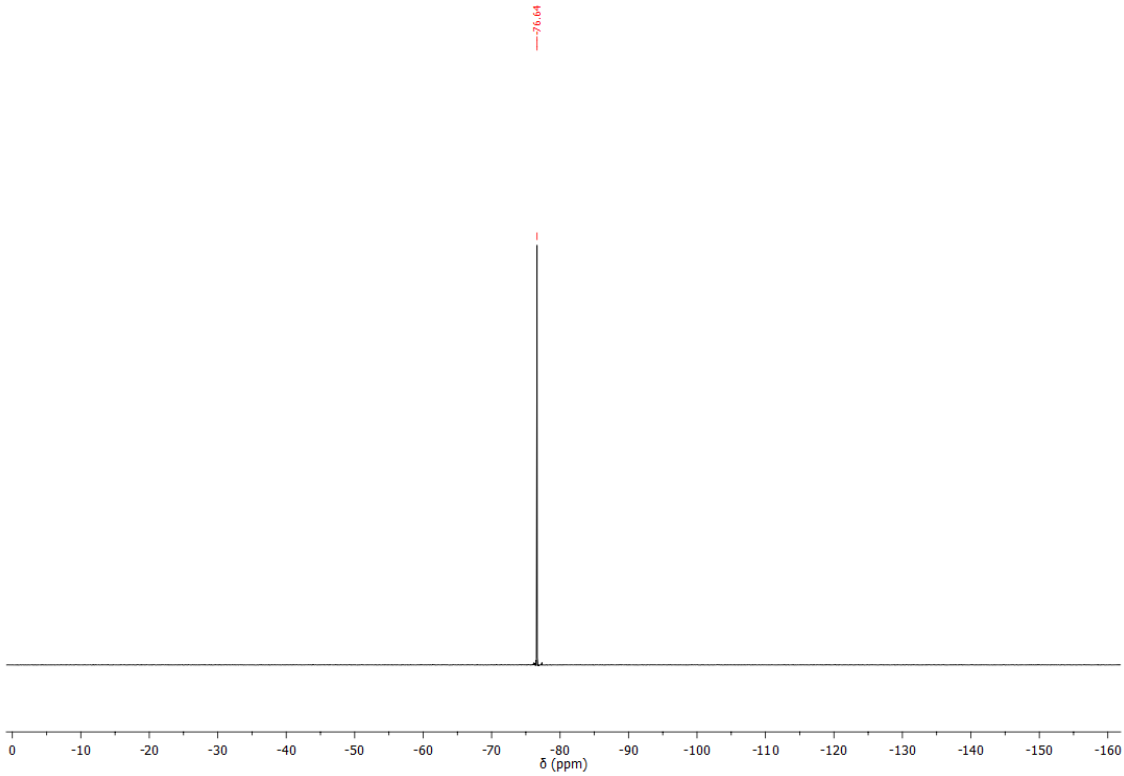

2D-HMQC NMR ($CDCl_3$)



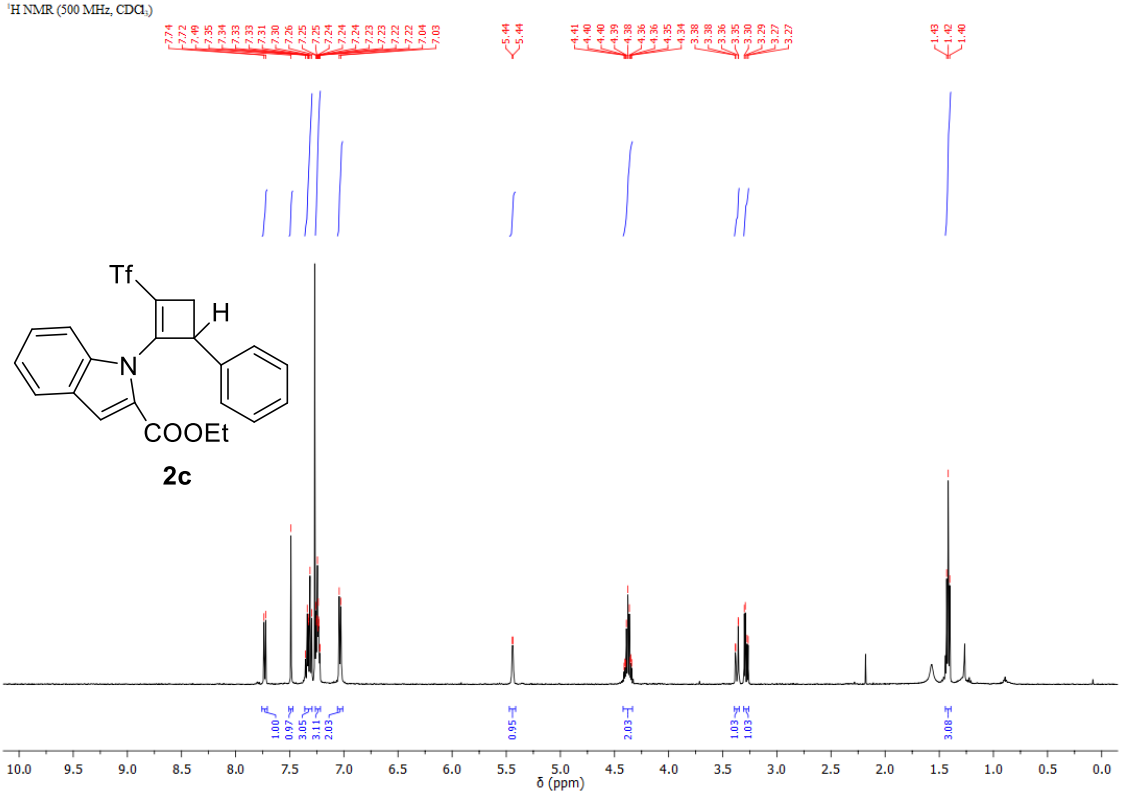

$^1$H NMR (700 MHz, CDCl$_3$)
Tf
H
N
MeOOC
NO$_2$
2b
δ (ppm)


$^1$H NMR (175 MHz, CDCl$_3$)
δ (ppm)

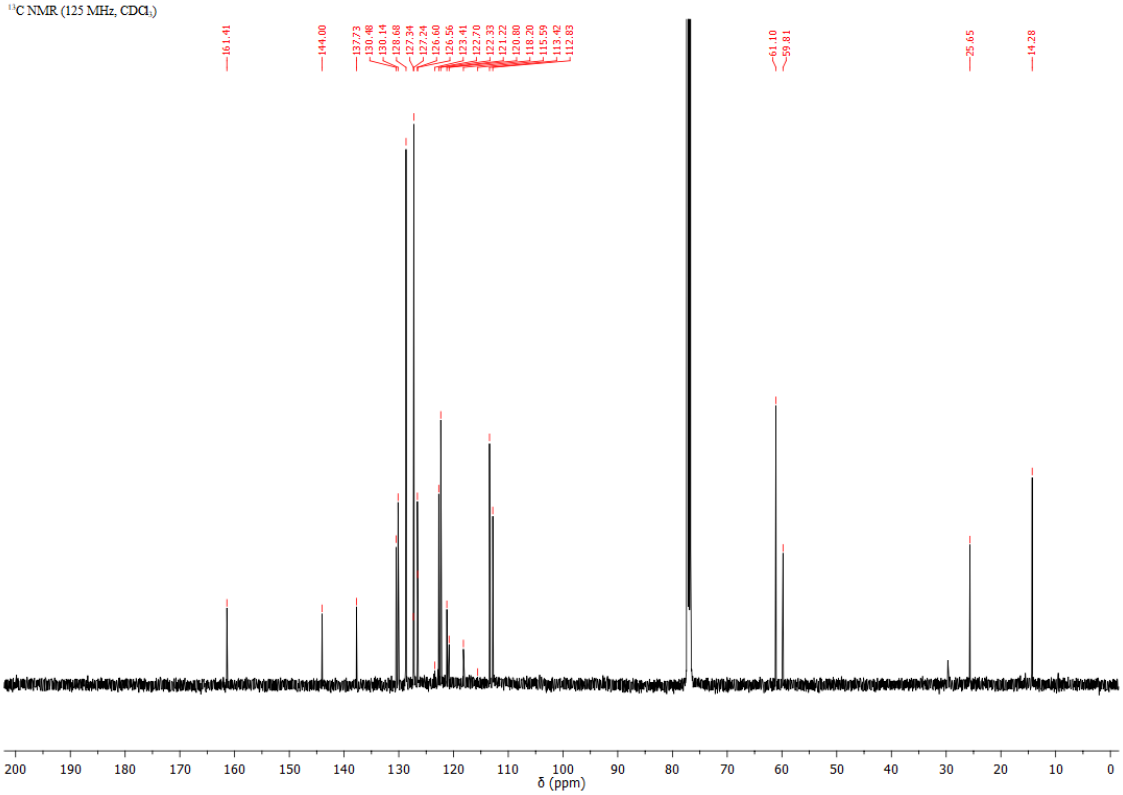
$^{19}$F NMR (282 MHz, $CDCl_3$)



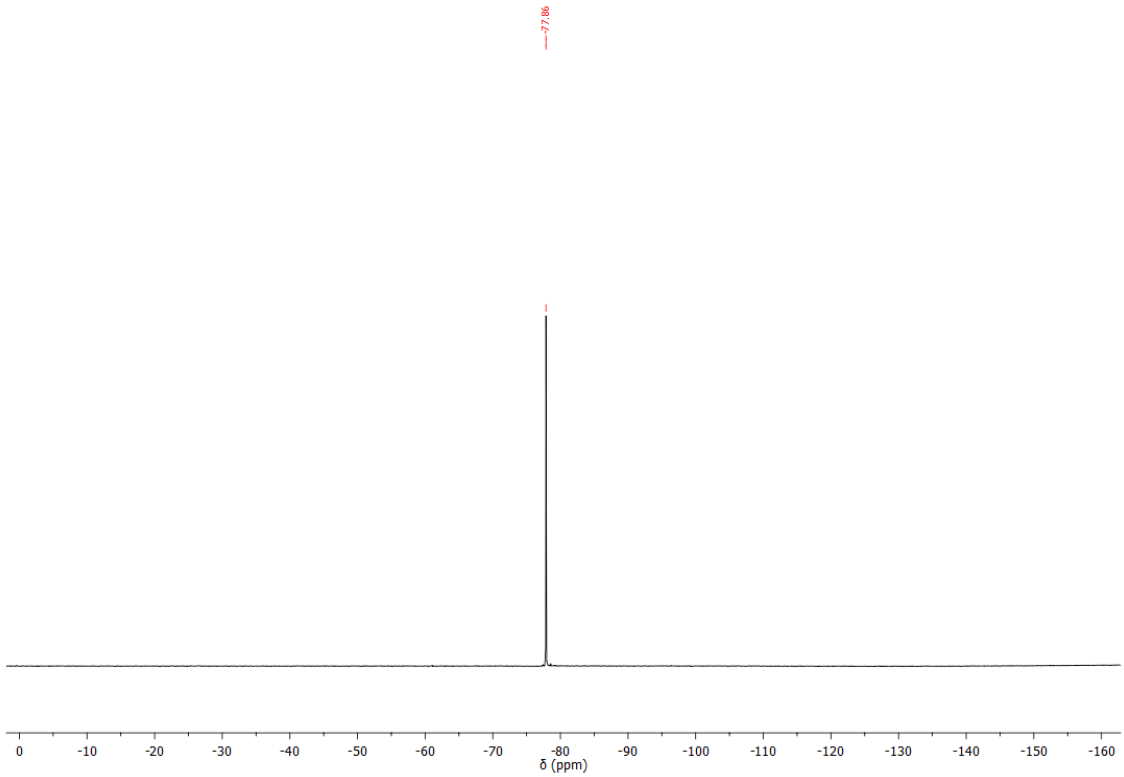
$^1$H NMR (500 MHz, $CDCl_3$)



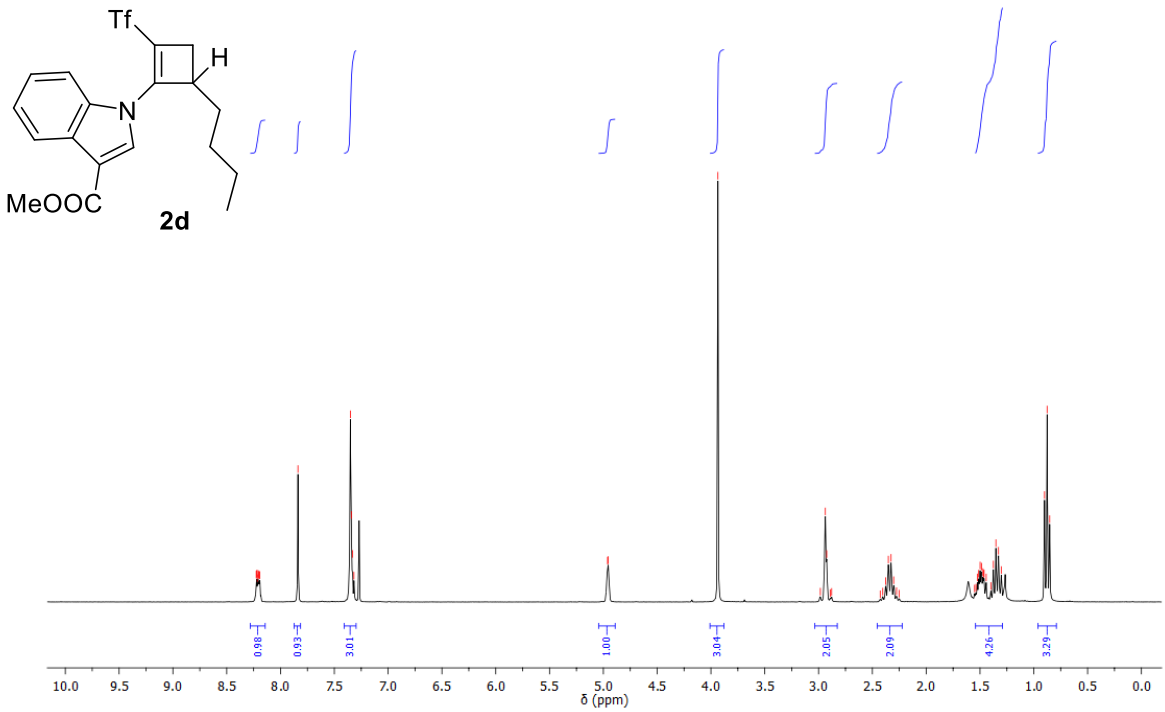

$^{13}$C NMR (125 MHz, $CDCl_3$)



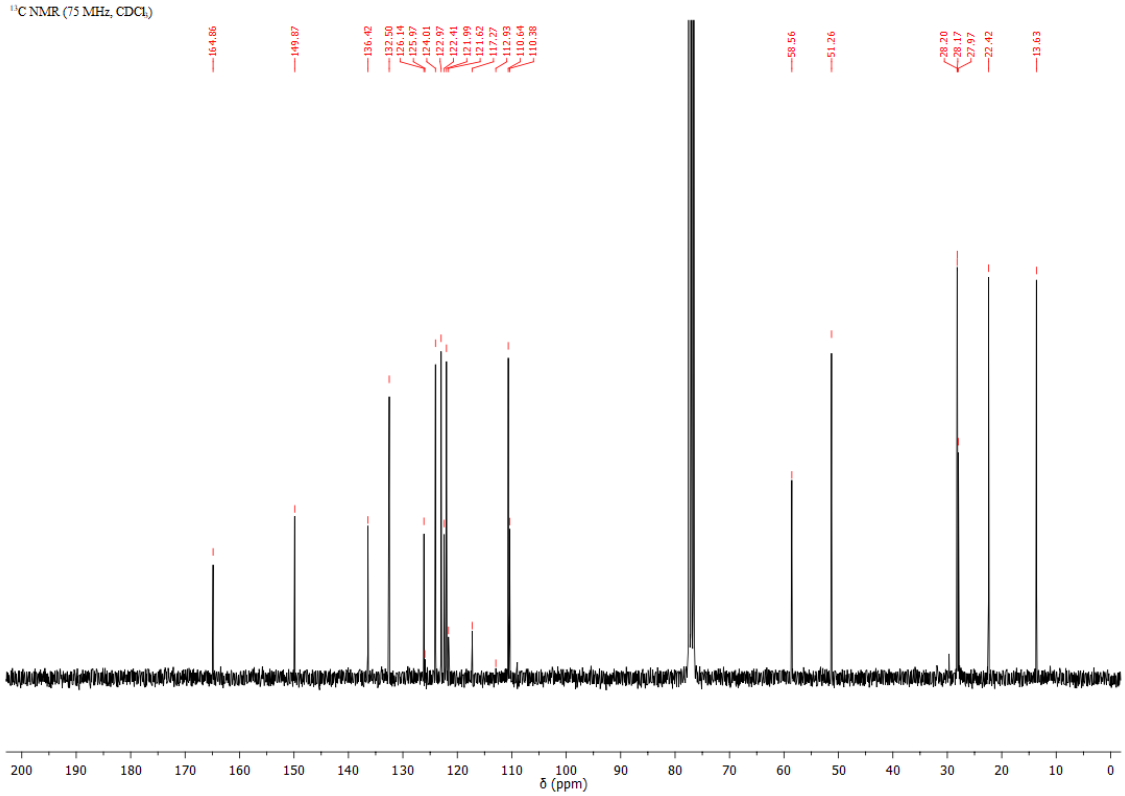
$^{19}$F NMR (282 MHz, $CDCl_3$)



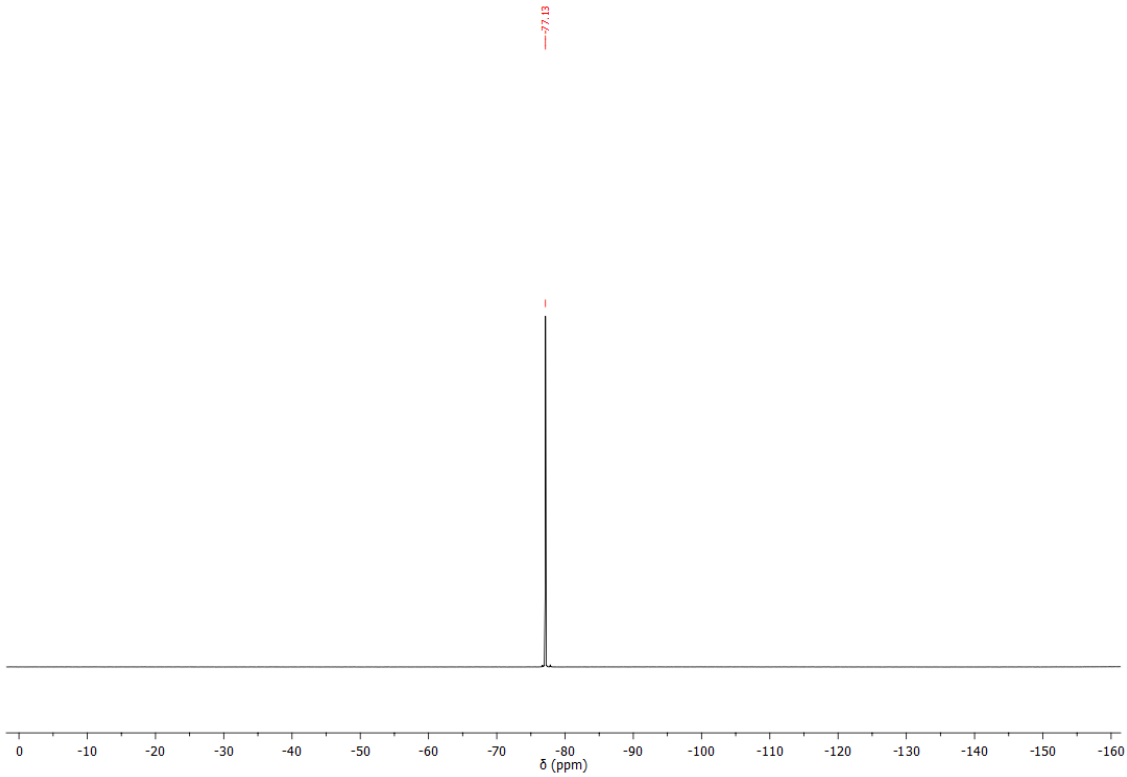
$^1$H NMR (300 MHz, $CDCl_3$)



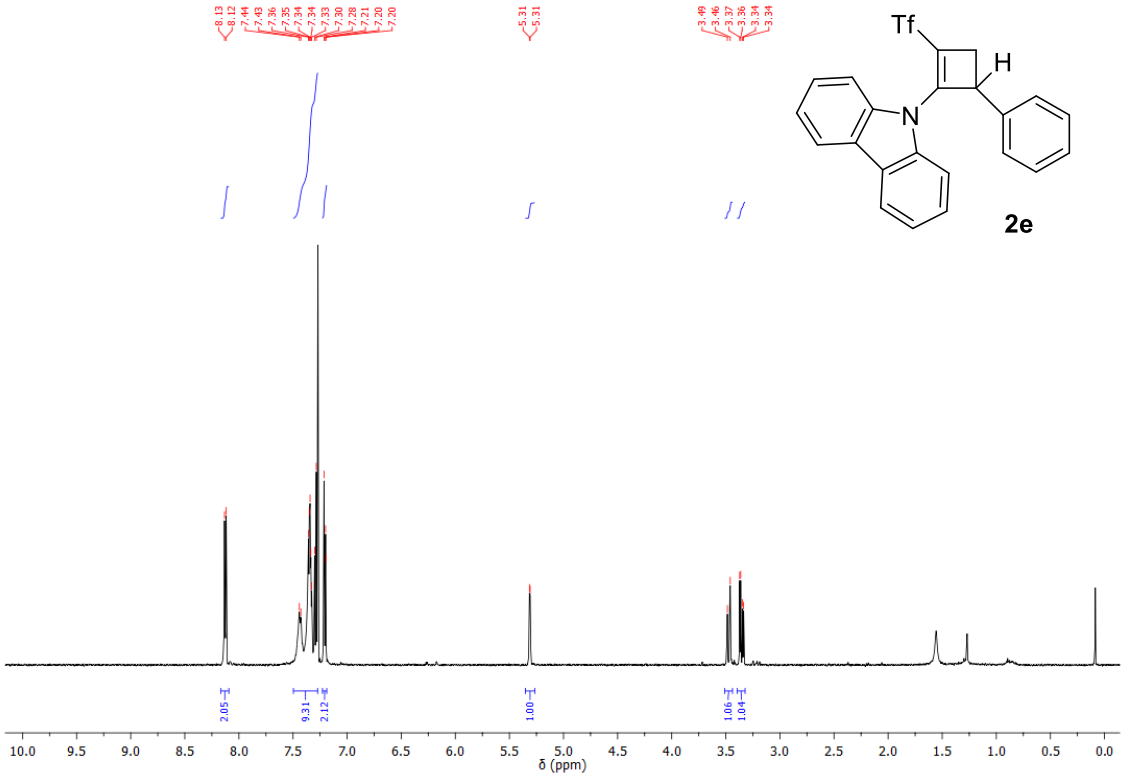

$^{13}$C NMR (75 MHz, $CDCl_3$)



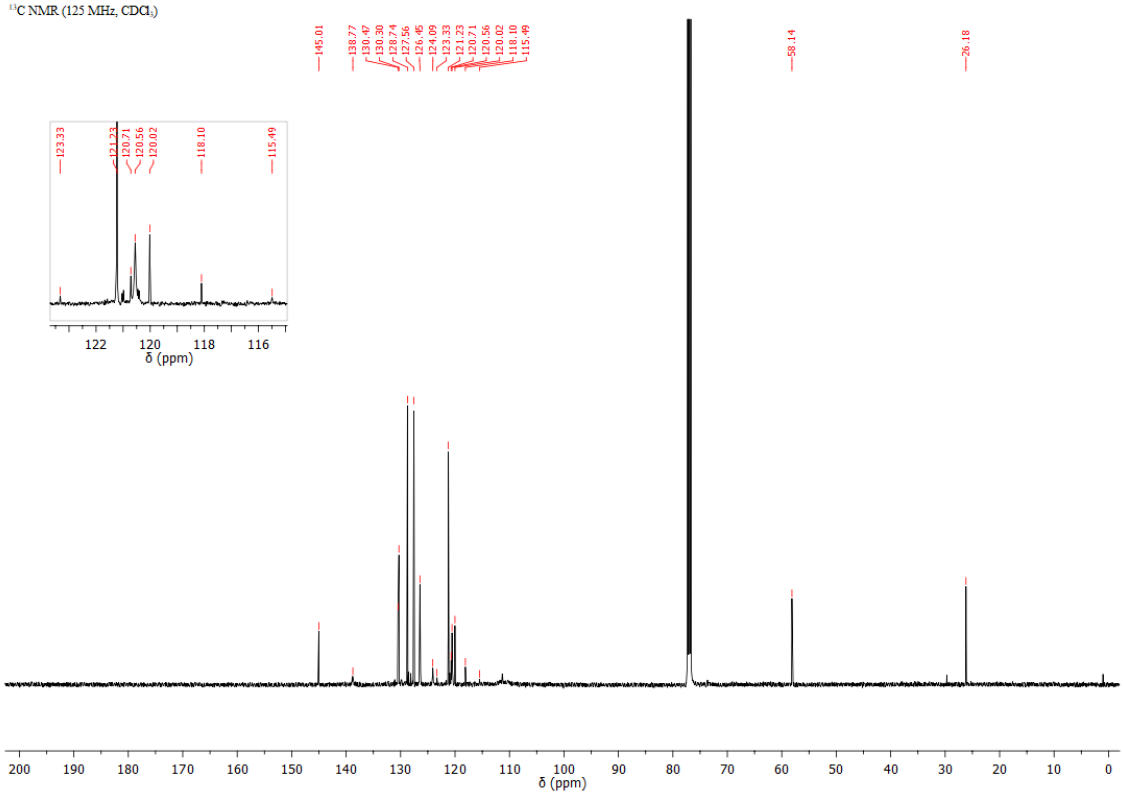
$^{19}$F NMR (282 MHz, $CDCl_3$)



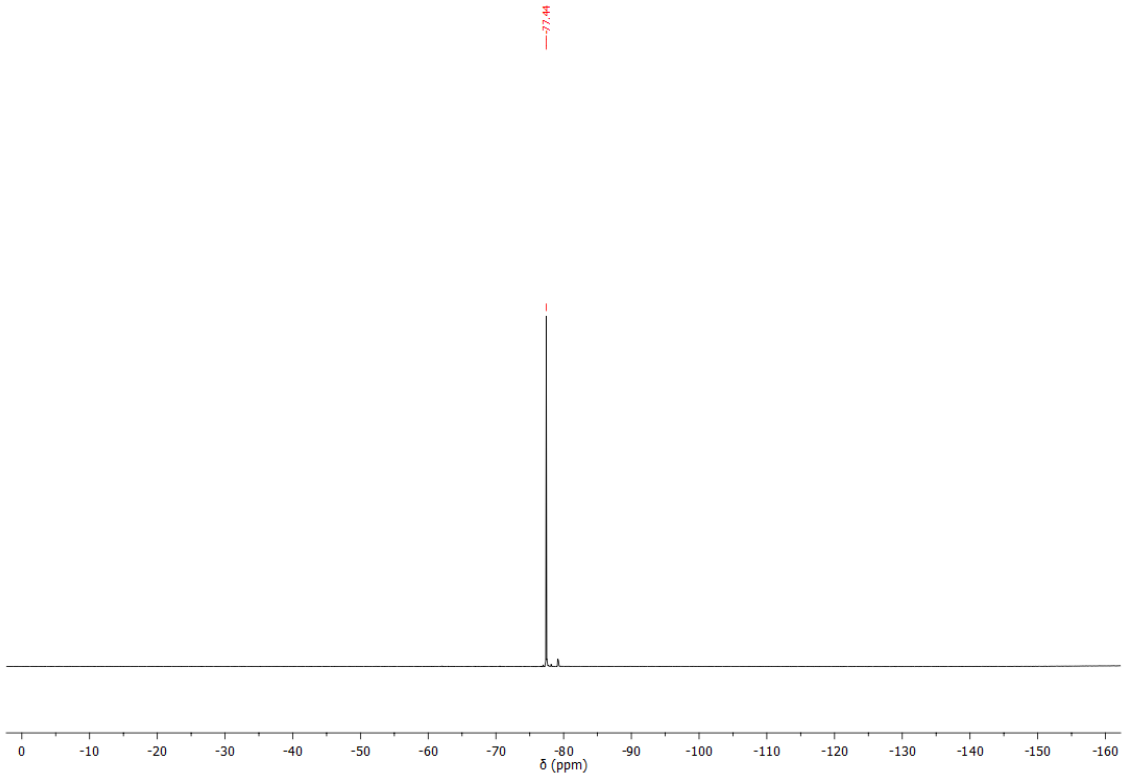
$^1$H NMR (500 MHz, $CDCl_3$)



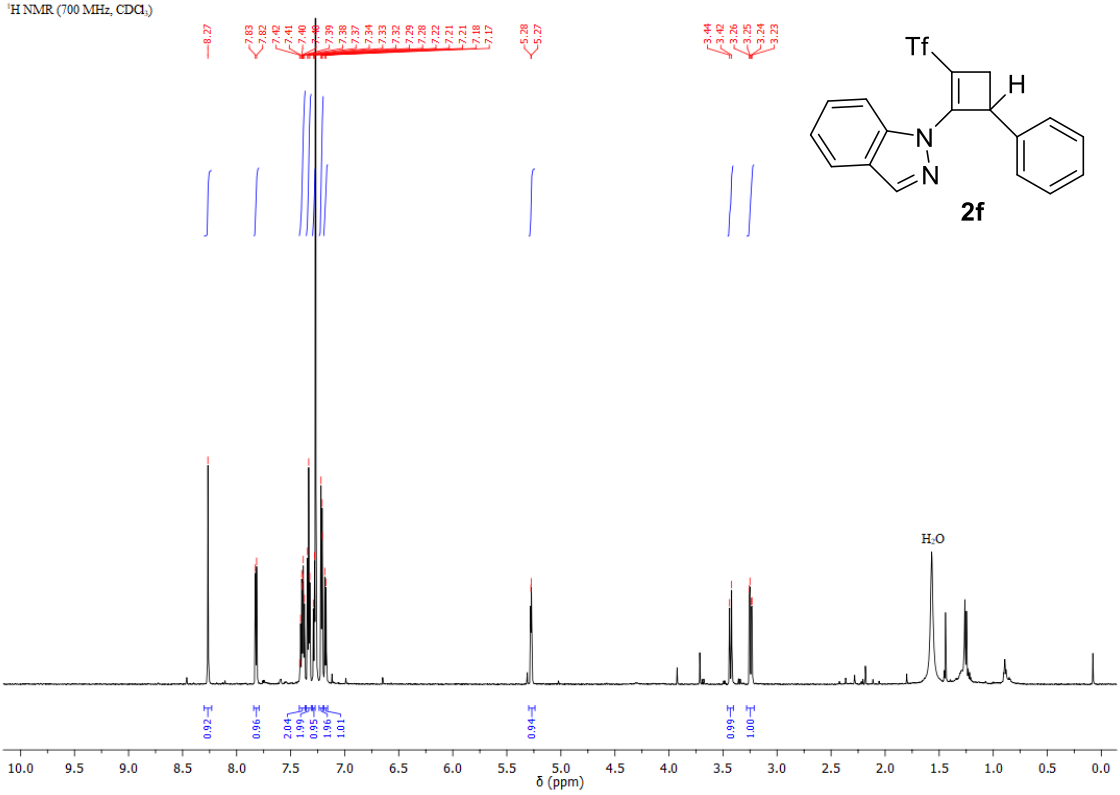

$^{13}$C NMR (125 MHz, $CDCl_3$)



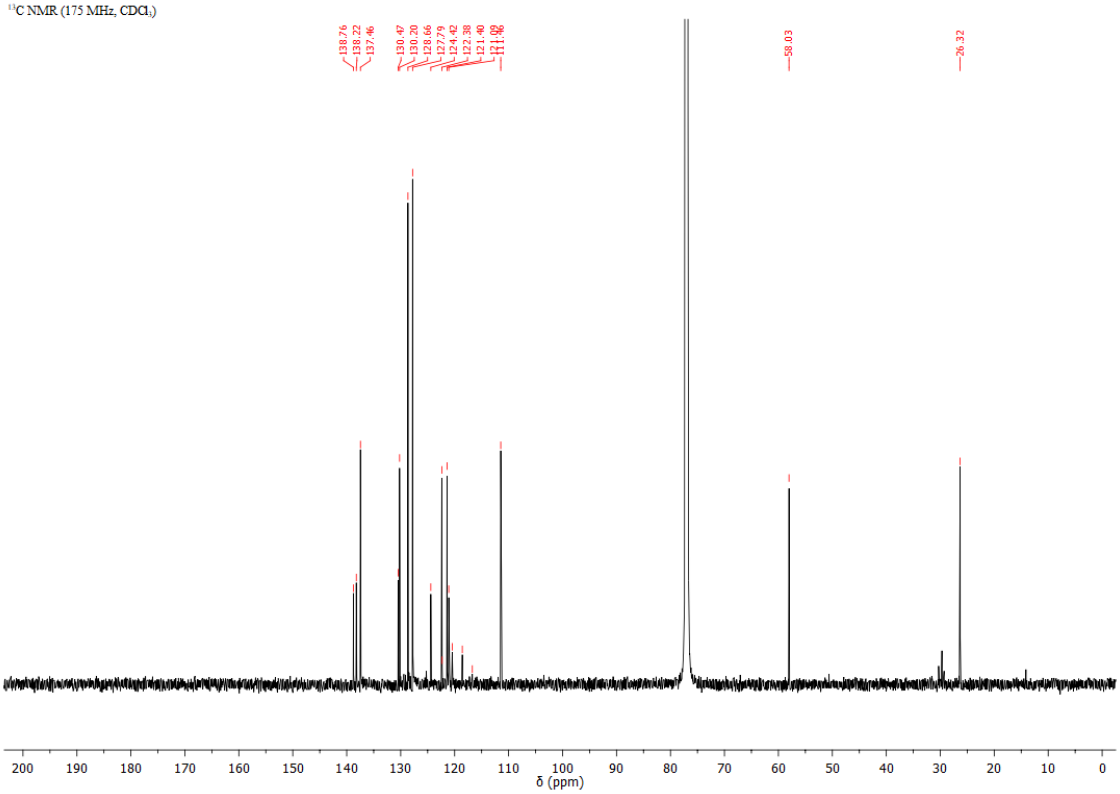
$^{19}$F NMR (282 MHz, $CDCl_3$)



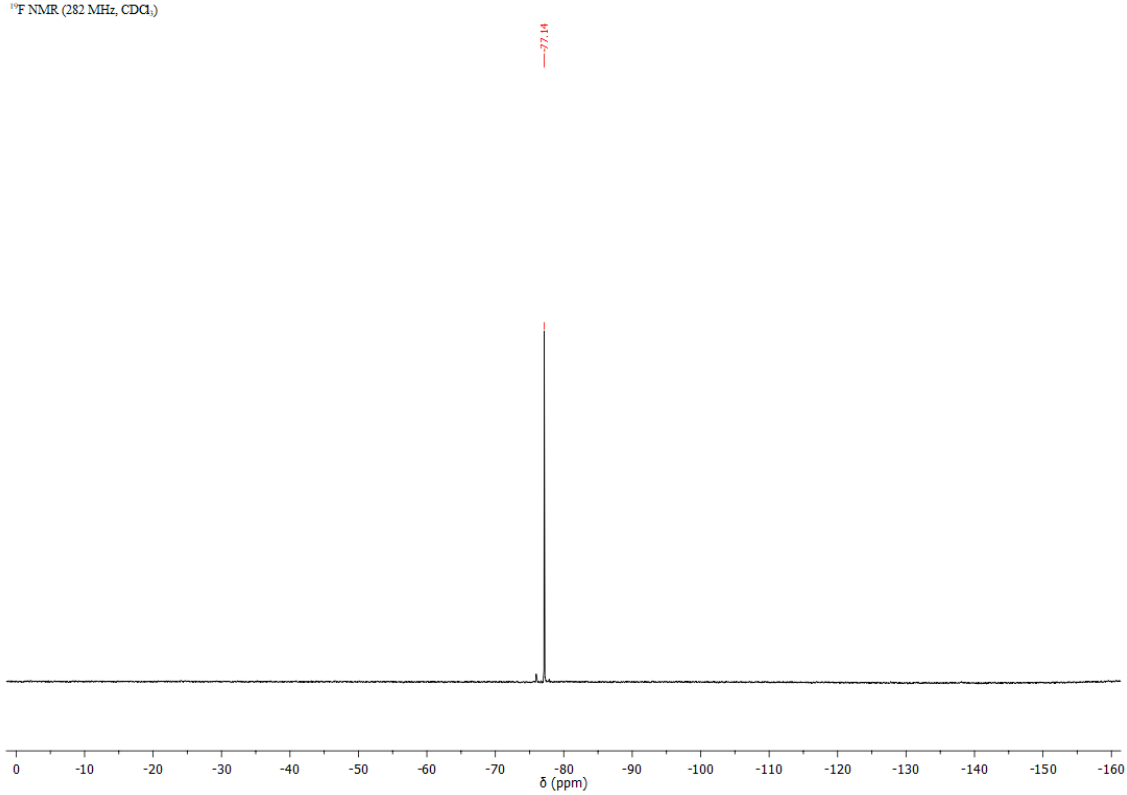
$^1$H NMR (700 MHz, $CDCl_3$)



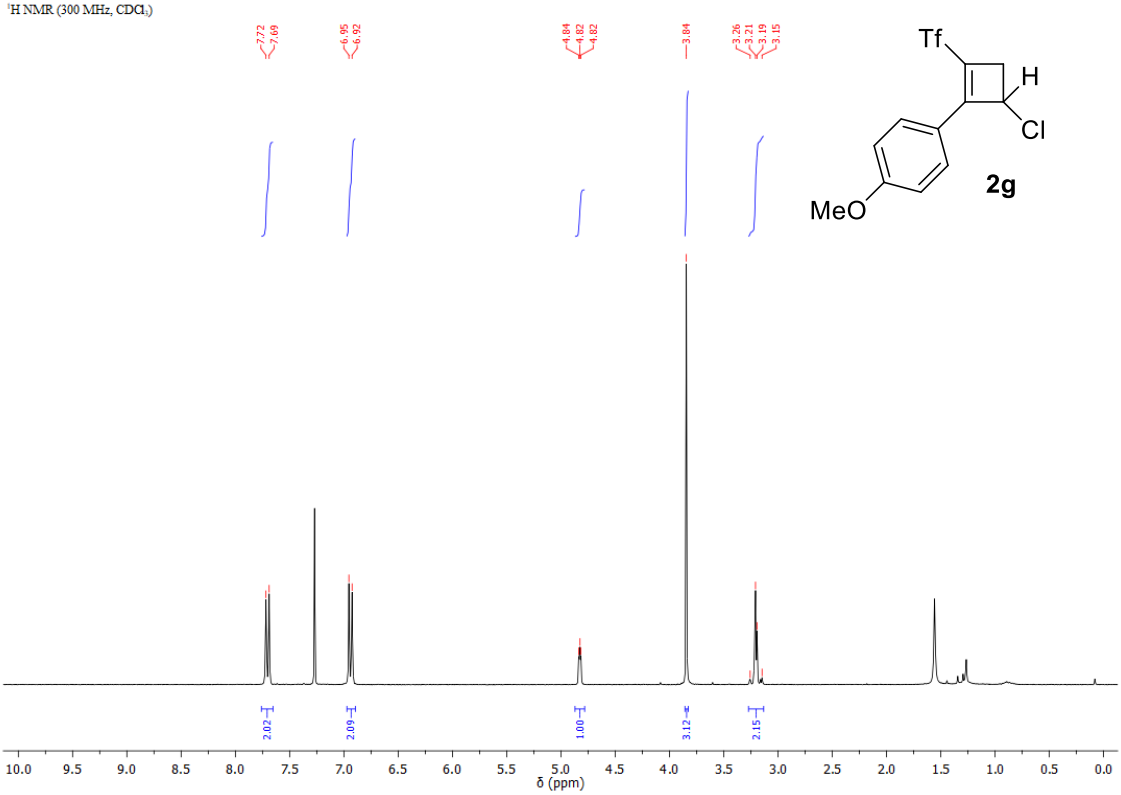

$^{13}$C NMR (175 MHz, $CDCl_3$)



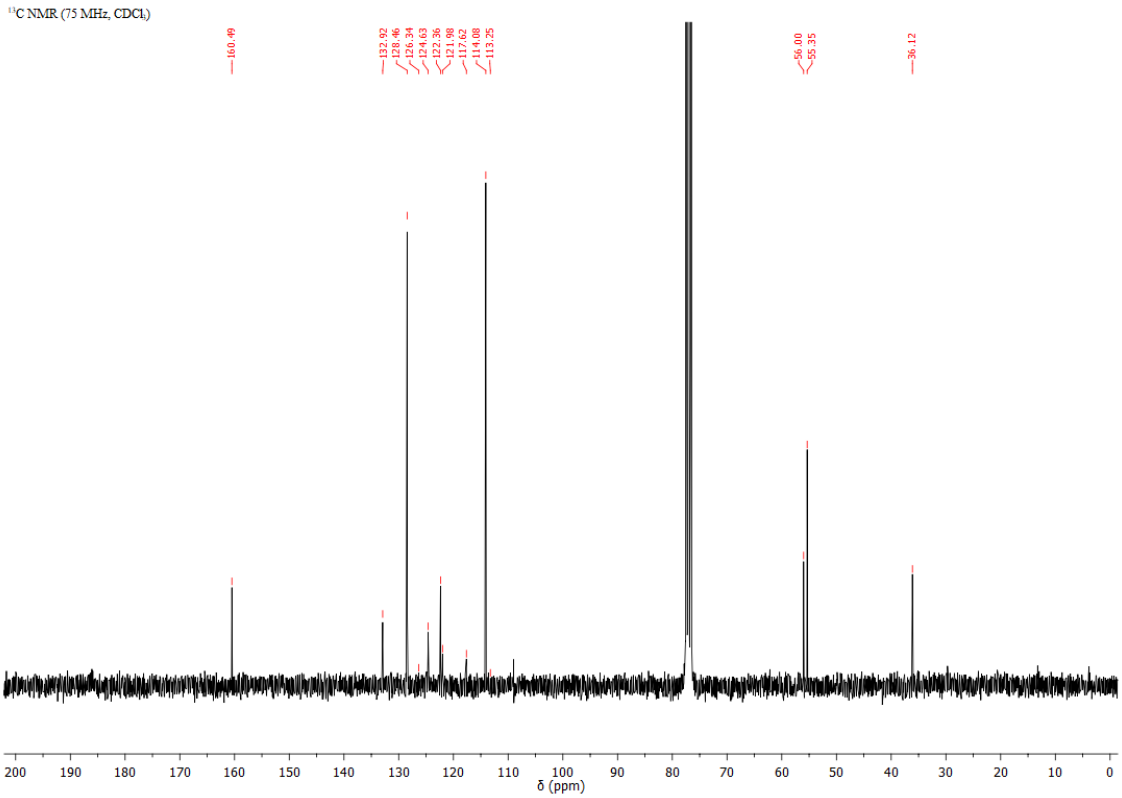
$^{19}$F NMR (282 MHz, $CDCl_3$)



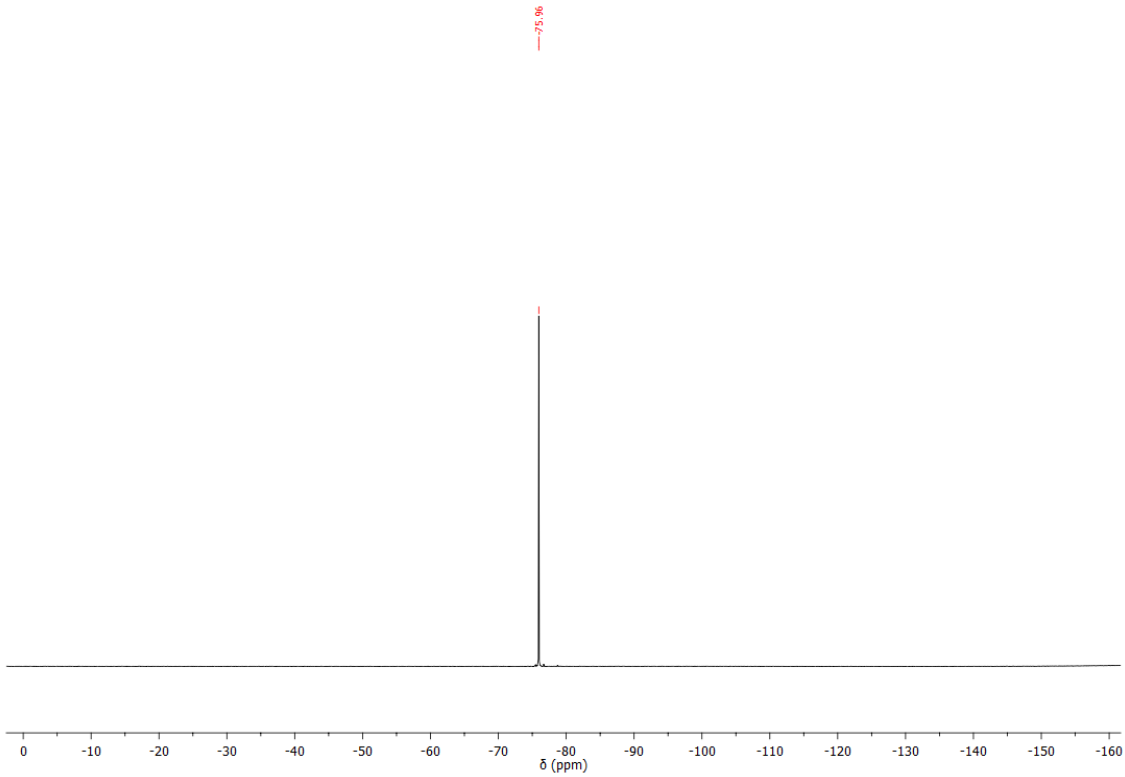
$^1$H NMR (300 MHz, $CDCl_3$)



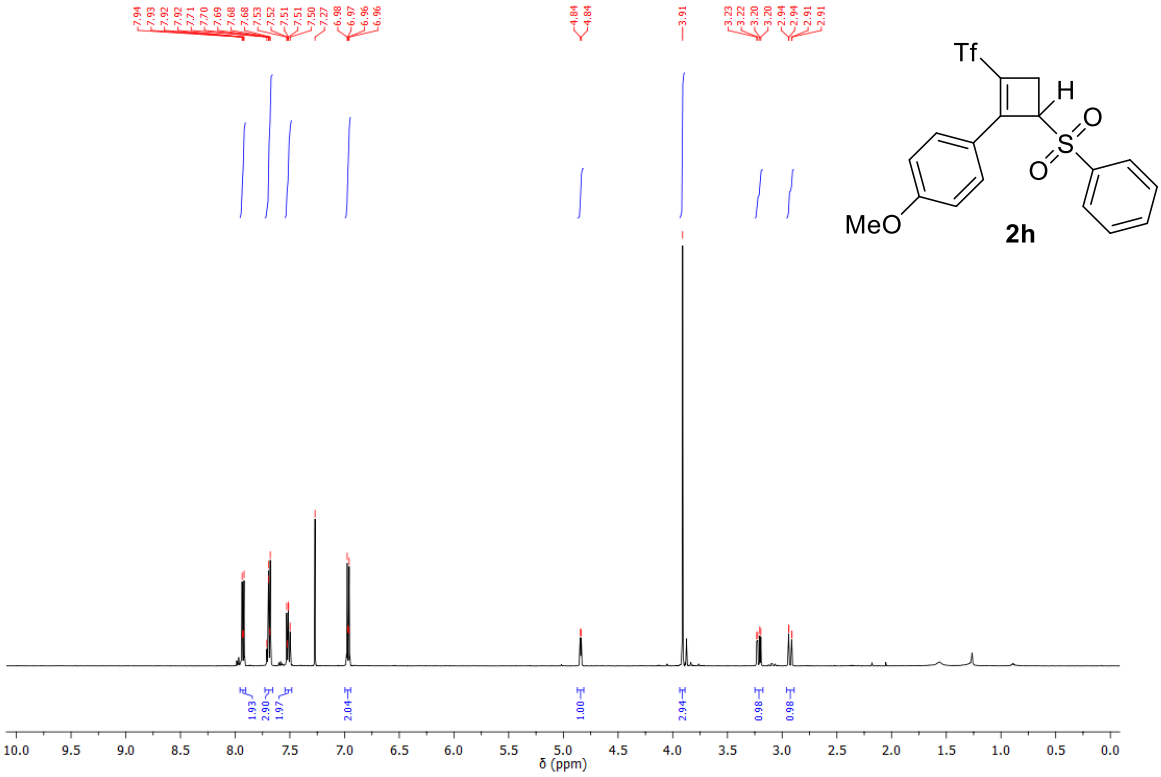

$^{13}$C NMR (75 MHz, $CDCl_3$)



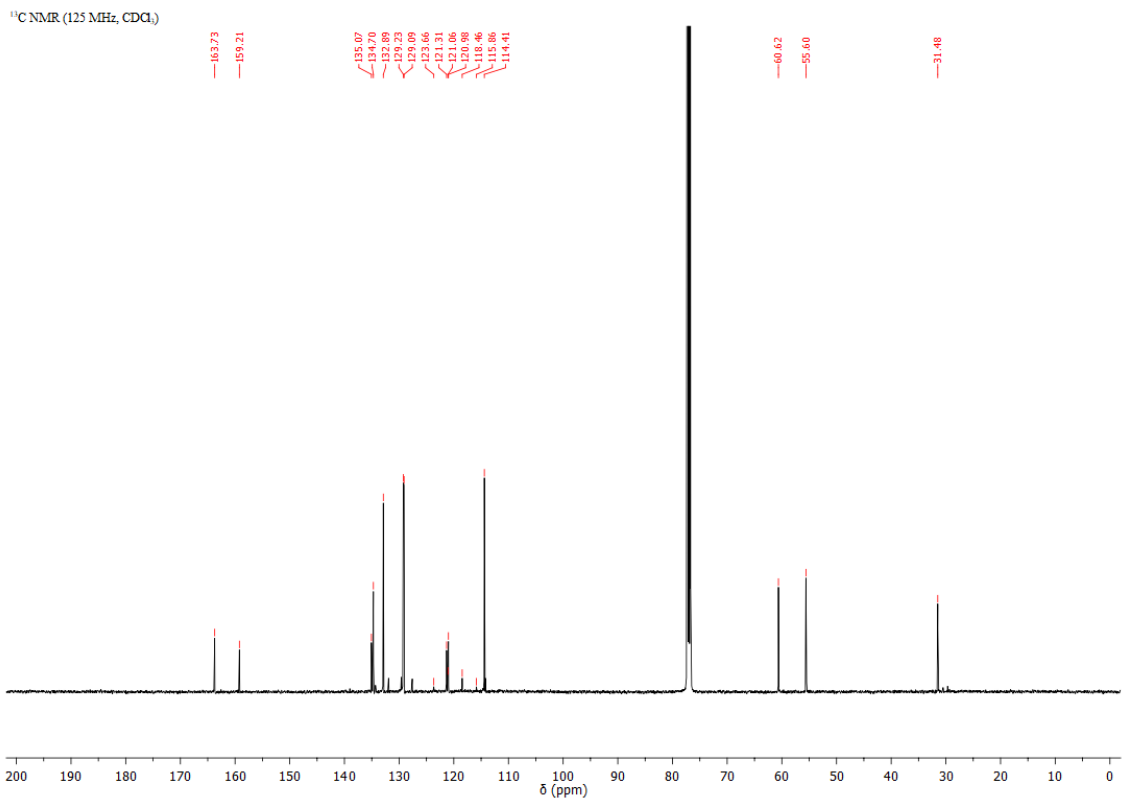
$^{19}$F NMR (282 MHz, $CDCl_3$)



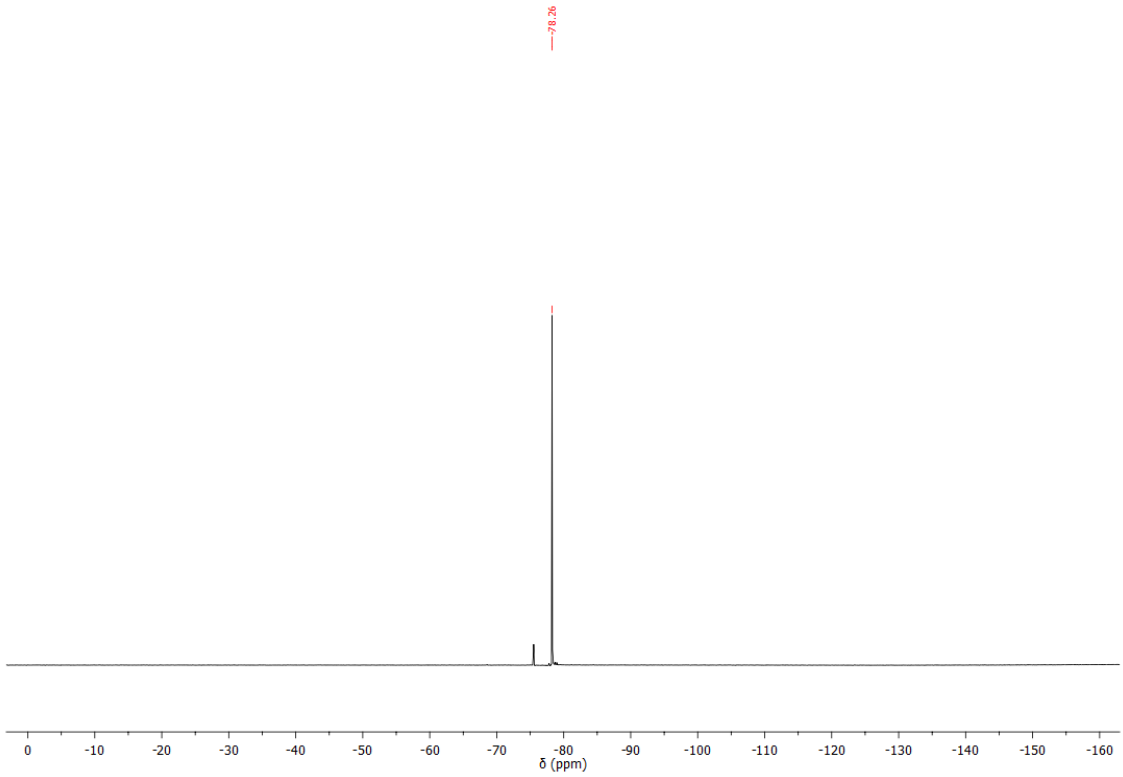
$^1$H NMR (500 MHz, $CDCl_3$)

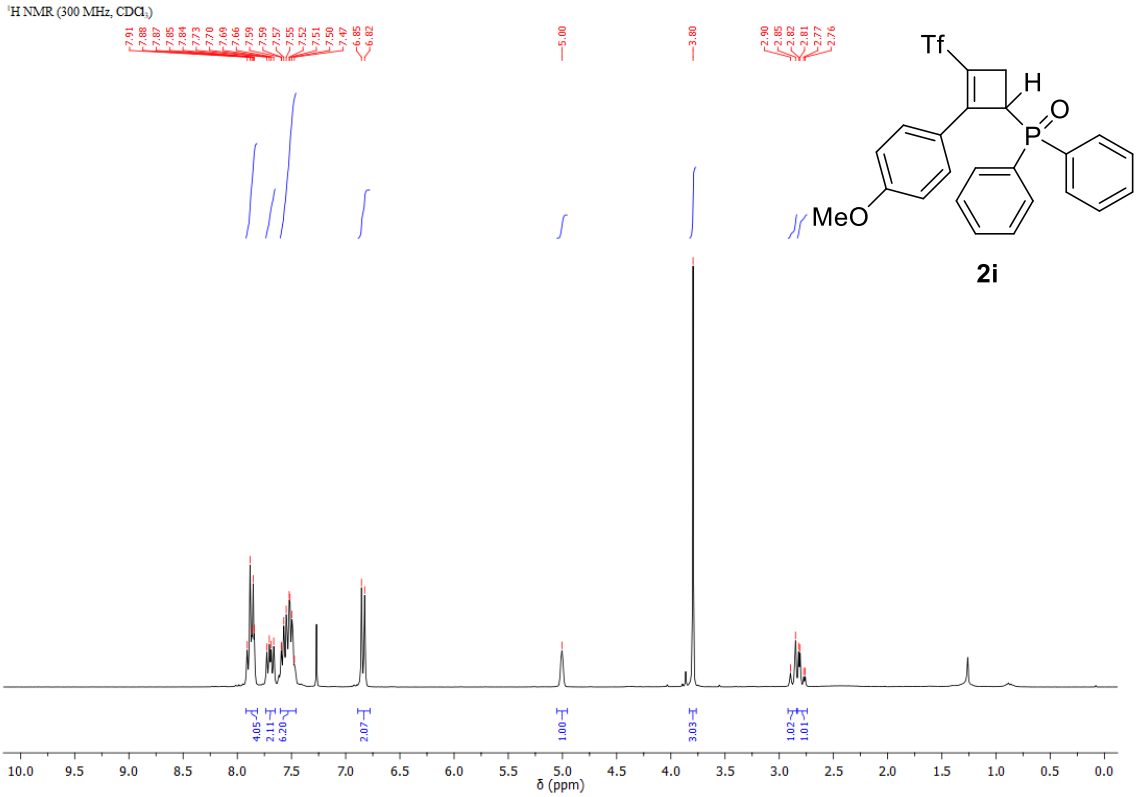


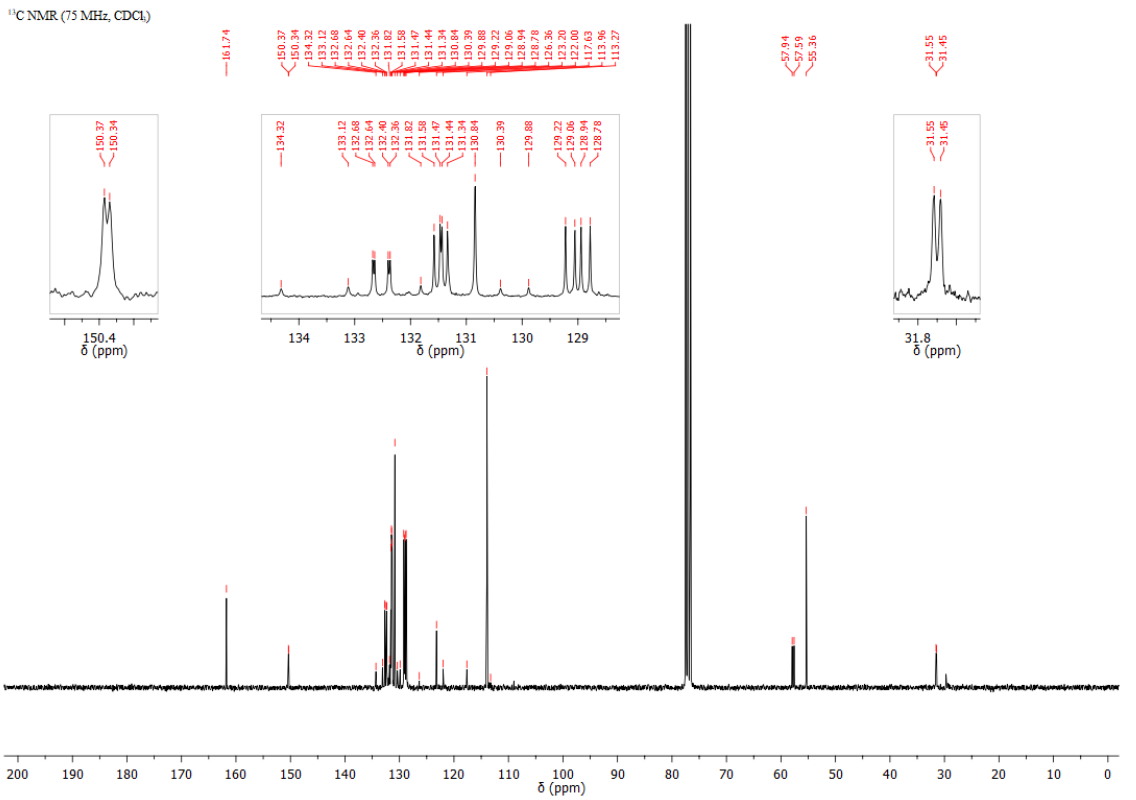

$^{13}$C NMR (125 MHz, $CDCl_3$)



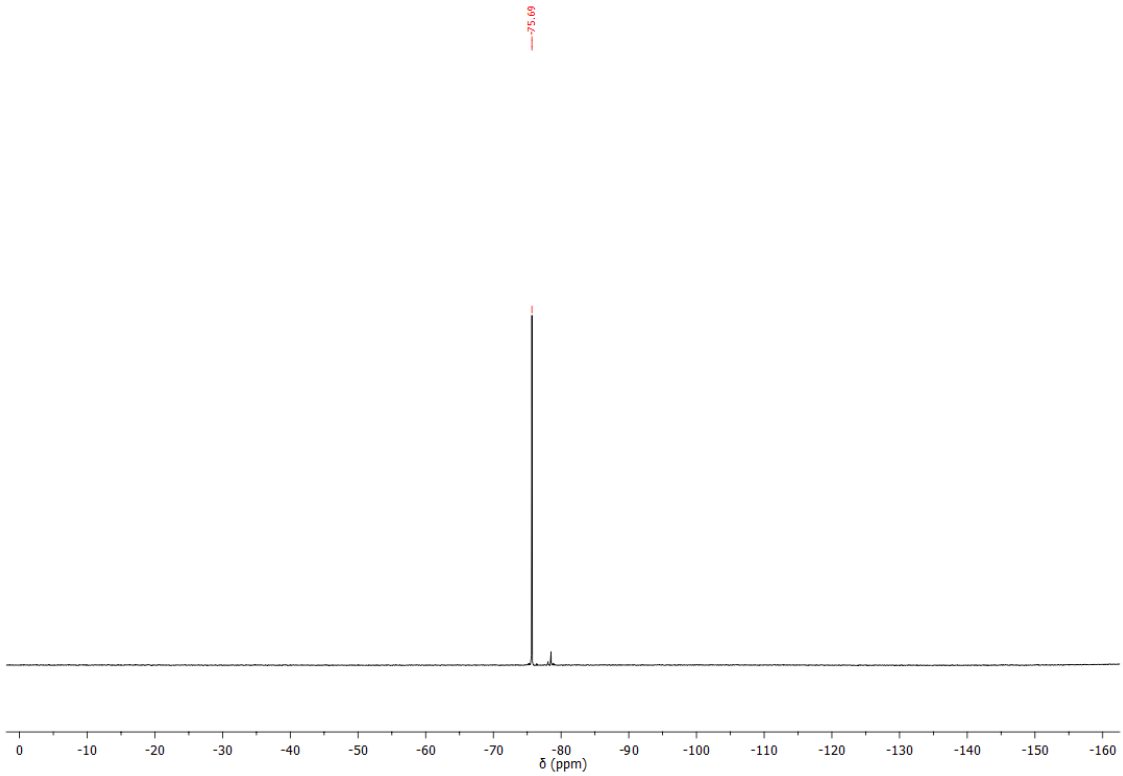
$^{19}$F NMR (282 MHz, $CDCl_3$)



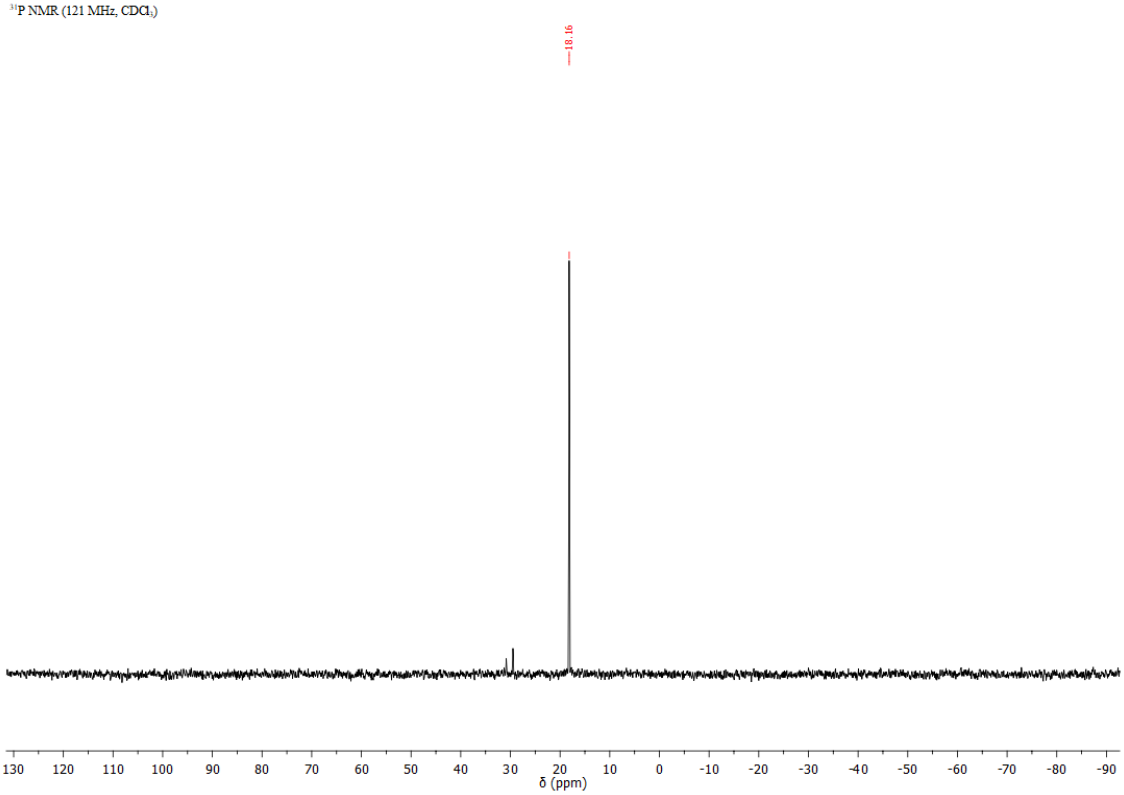

$^1$H NMR (300 MHz, CDCl$_3$)
Tf
H
O
P
MeO
2i
δ (ppm)


$^{13}$C NMR (75 MHz, CDCl$_3$)
δ (ppm)

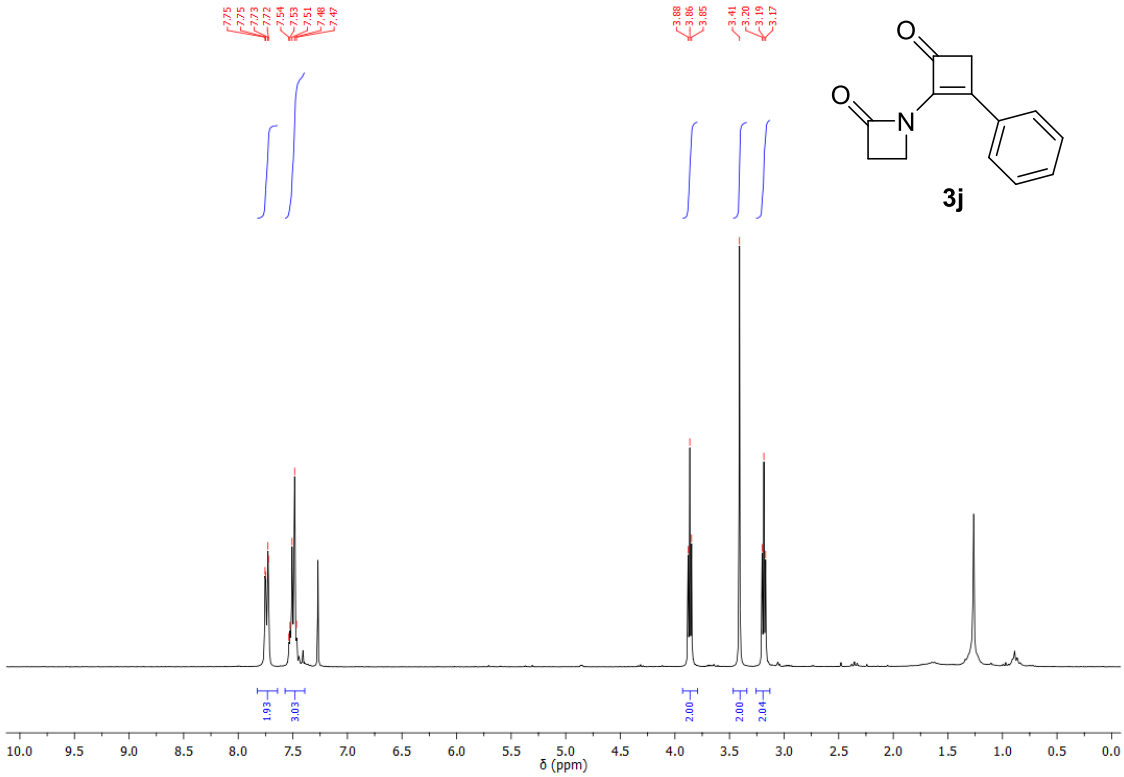
$^{19}$F NMR (282 MHz, $CDCl_3$)



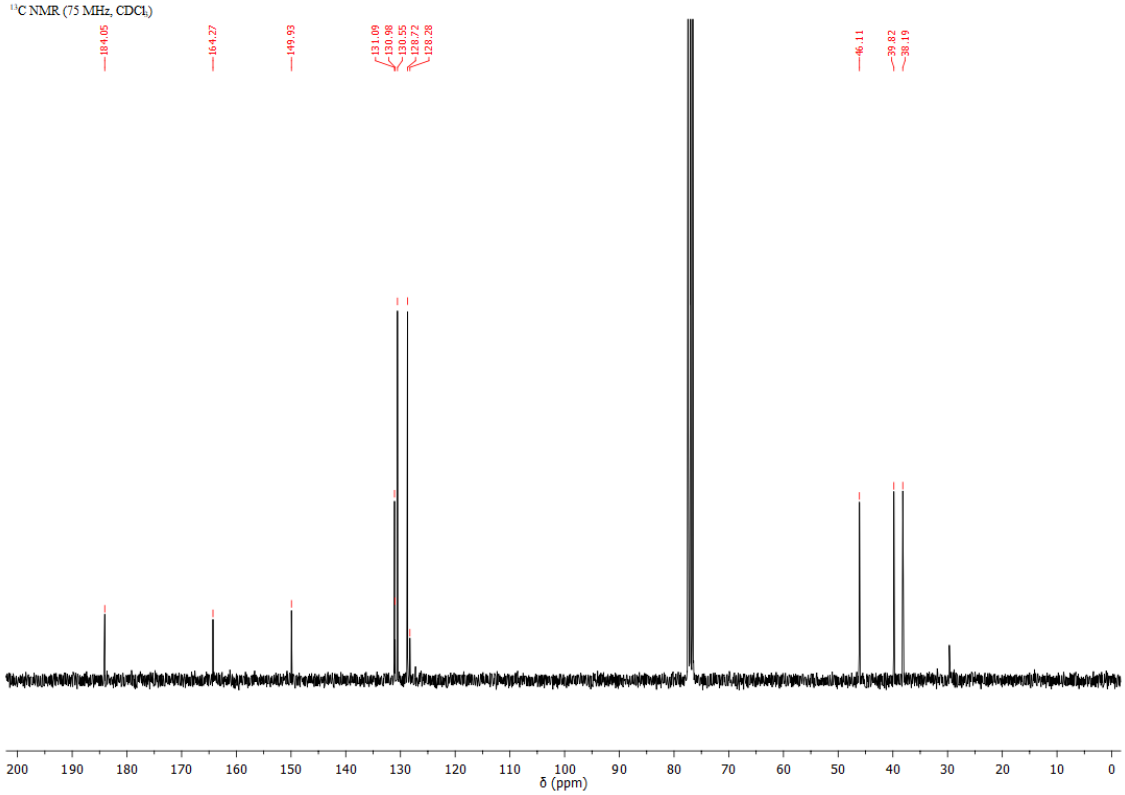

$^{31}$P NMR (121 MHz, $CDCl_3$)



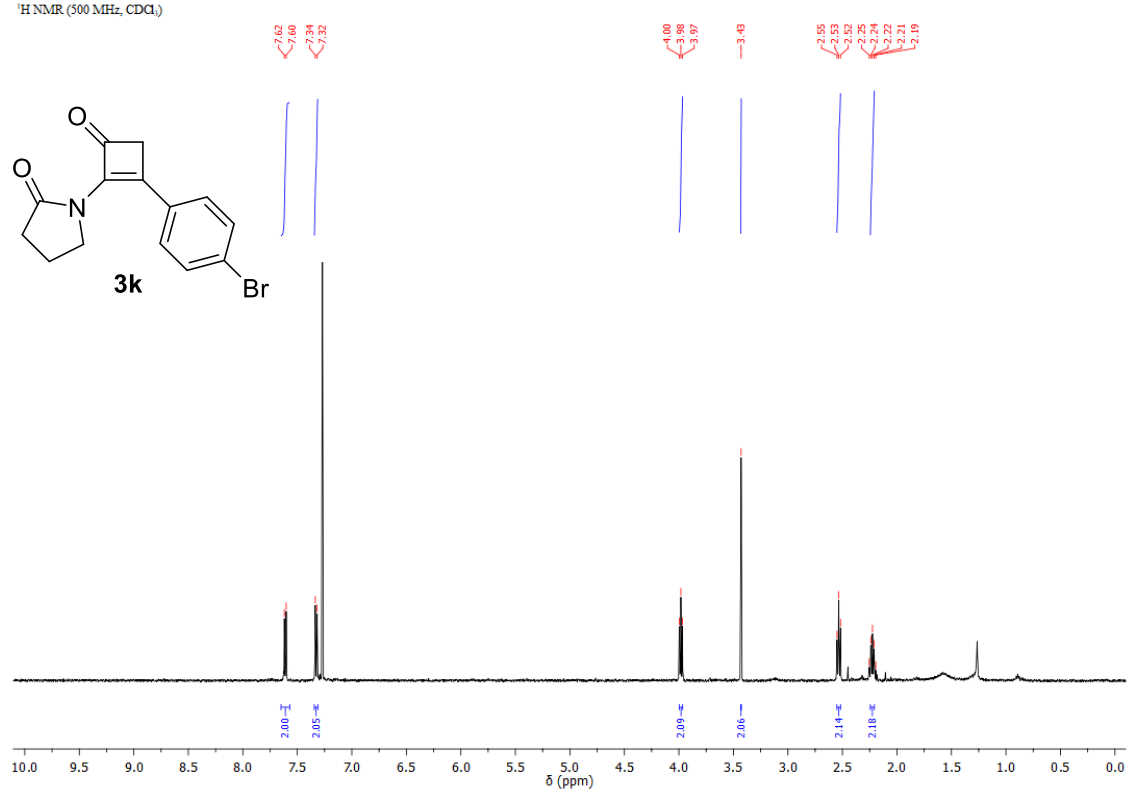
$^1$H NMR (300 MHz, $CDCl_3$)



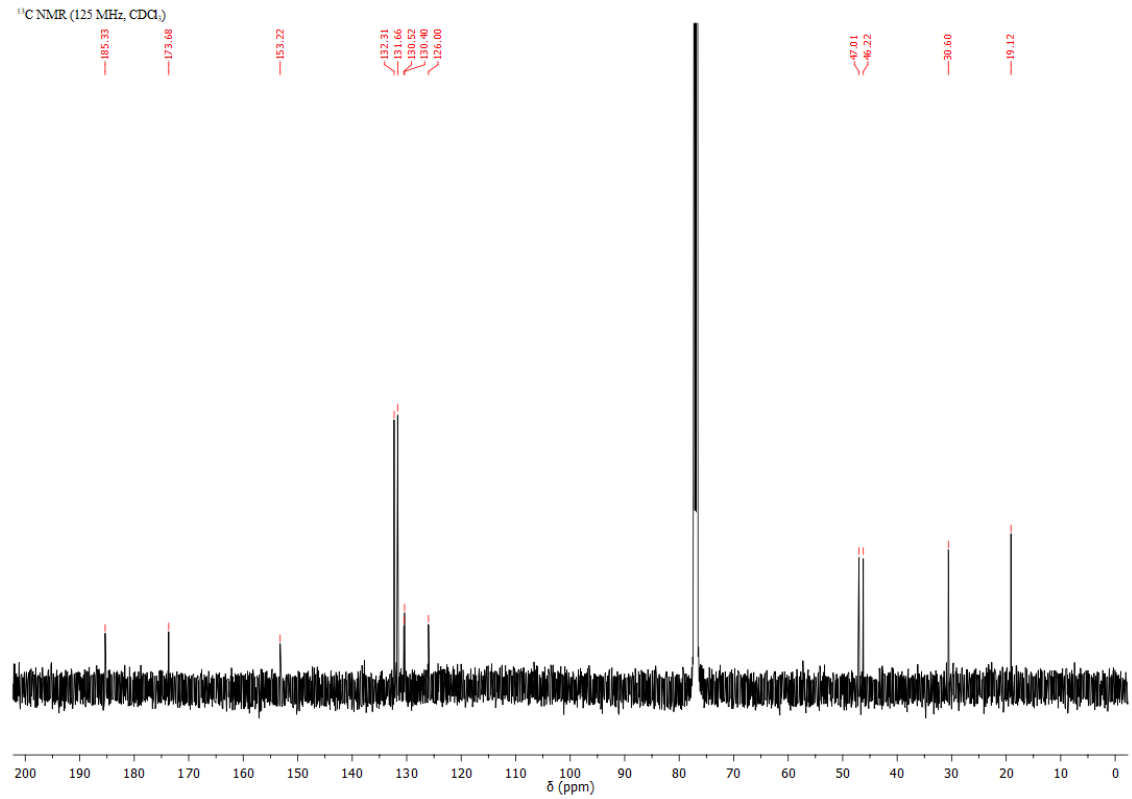

$^{13}$C NMR (75 MHz, $CDCl_3$)



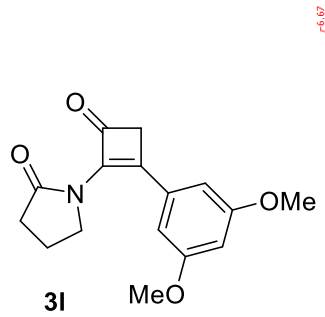
$^1$H NMR (500 MHz, $CDCl_3$)




$^{13}$C NMR (125 MHz, $CDCl_3$)



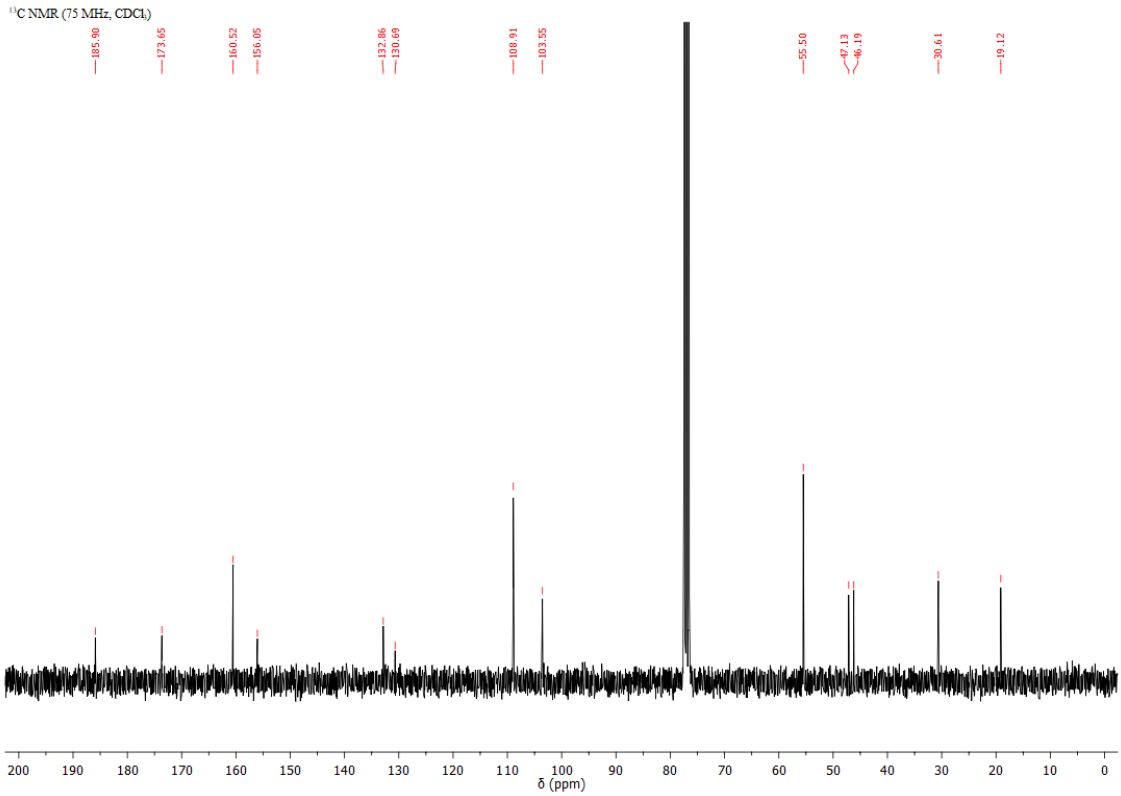
$^1$H NMR (300 MHz, $CDCl_3$)



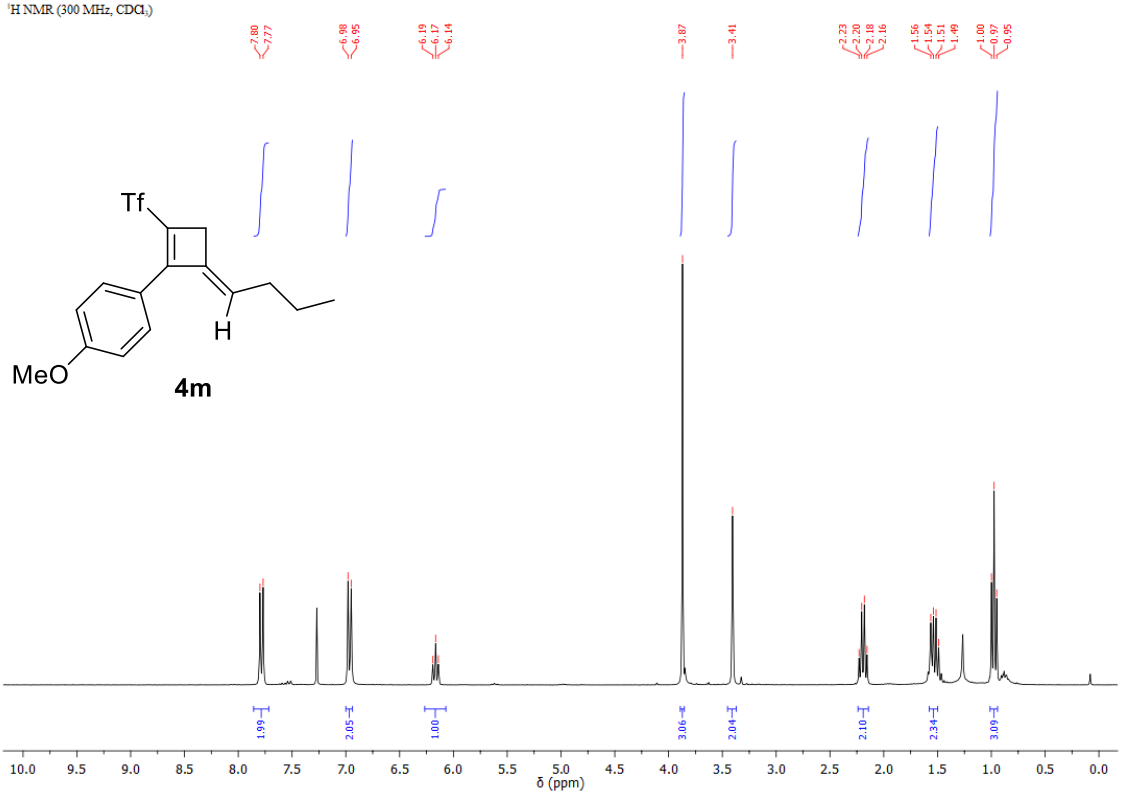

**3l**



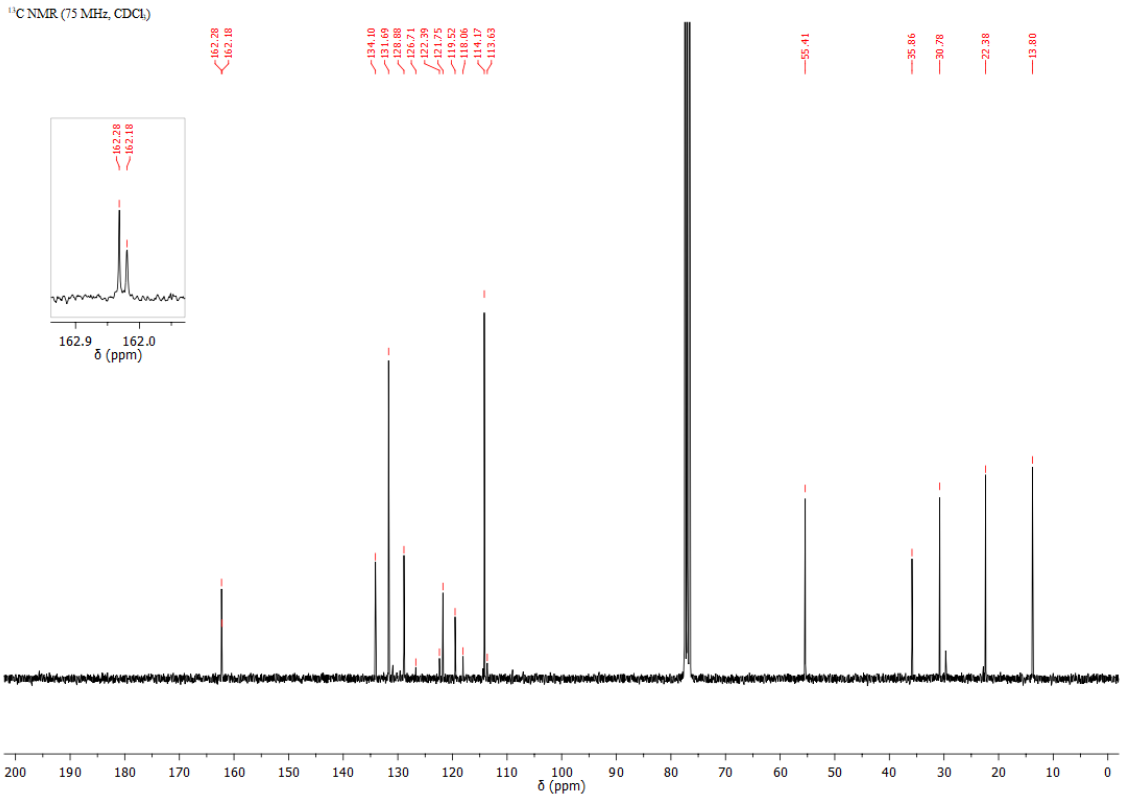

$^{13}$C NMR (75 MHz, $CDCl_3$)



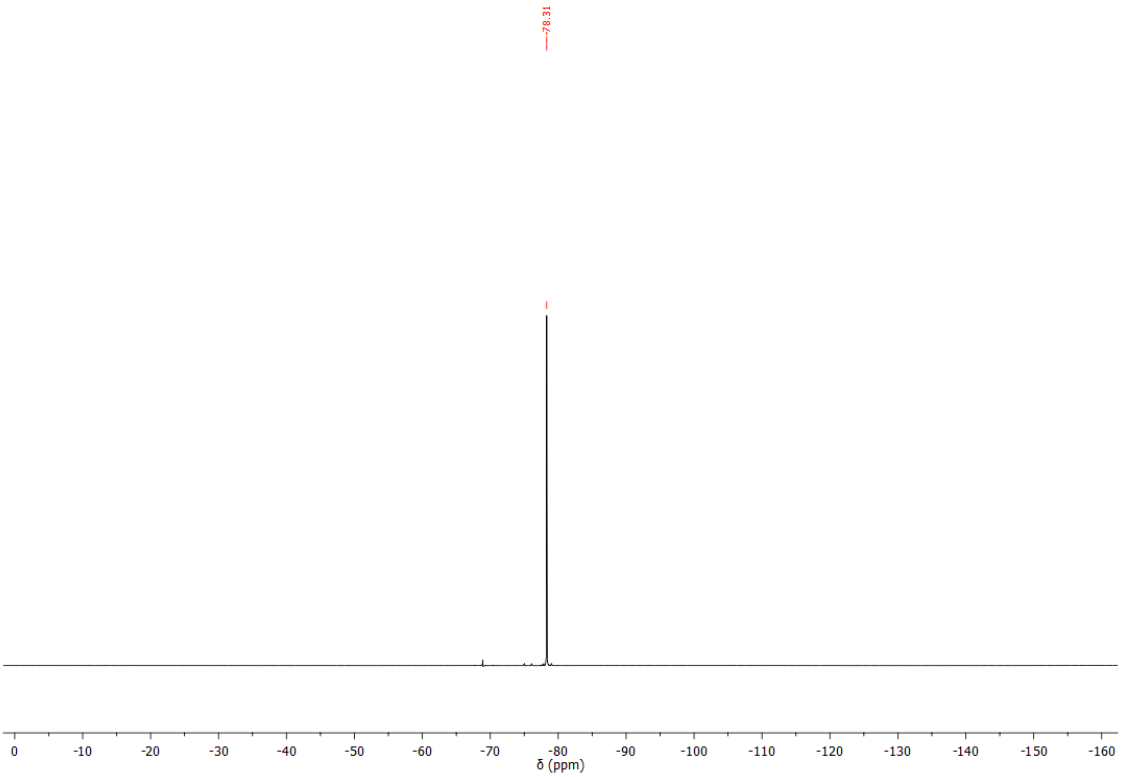
$^1$H NMR (300 MHz, $CDCl_3$)



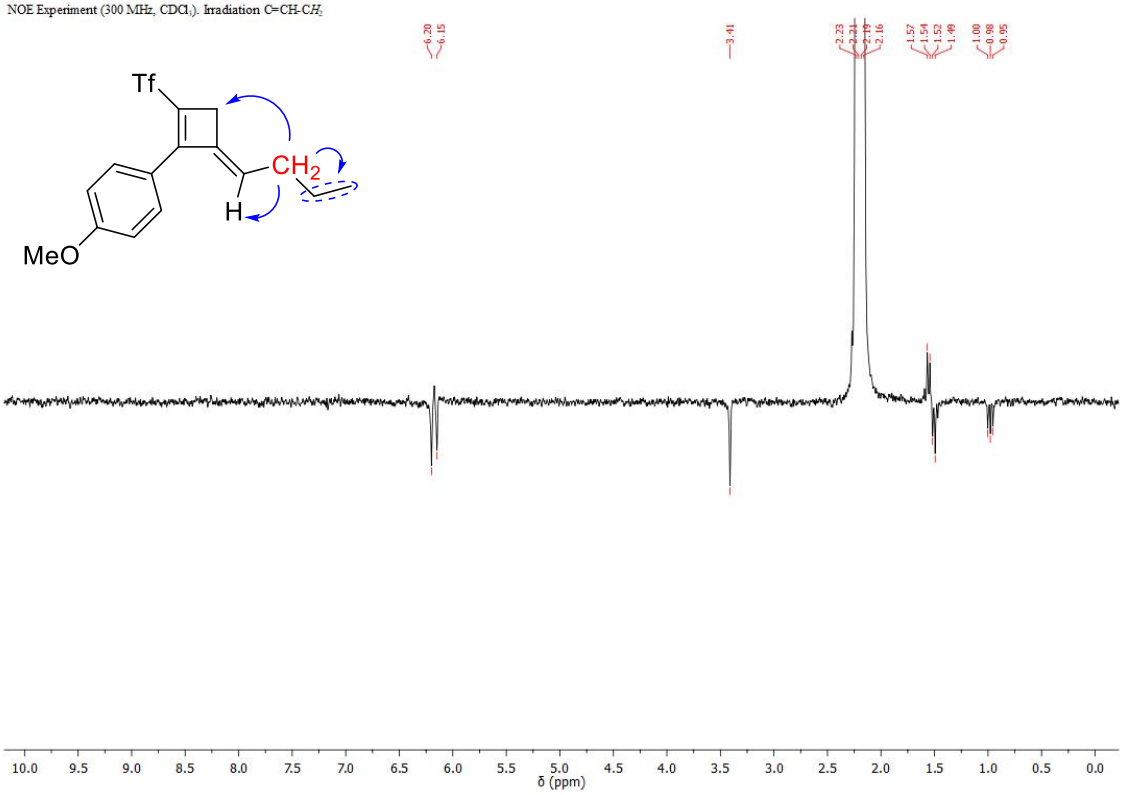

$^{13}$C NMR (75 MHz, $CDCl_3$)



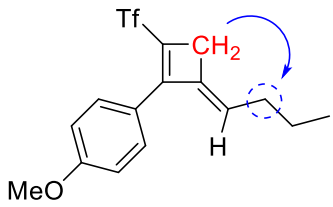
$^{19}$F NMR (282 MHz, $CDCl_3$)




NOE Experiment (300 MHz, $CDCl_3$). Irradiation C=CH-C*H*$_2$



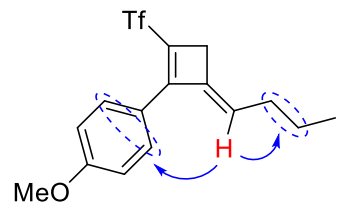
NOE Experiment (300 MHz, $CDCl_3$). Irradiation $CH_2$-cyclobutene



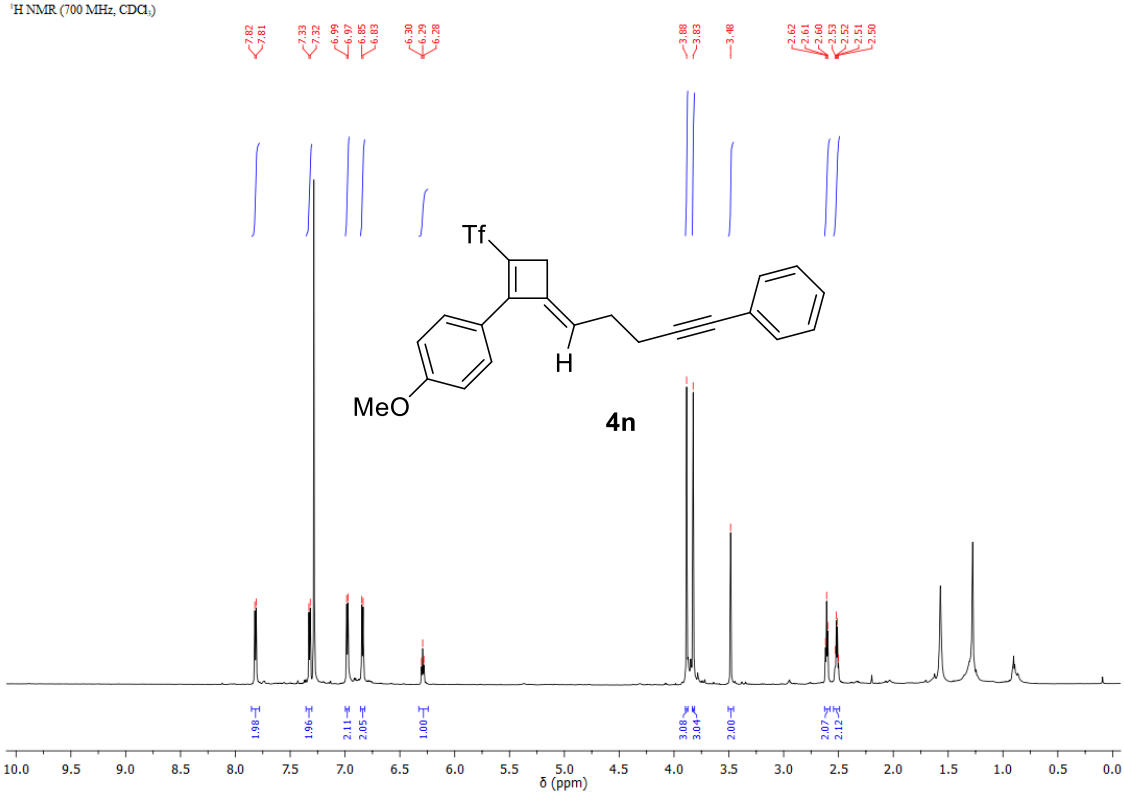




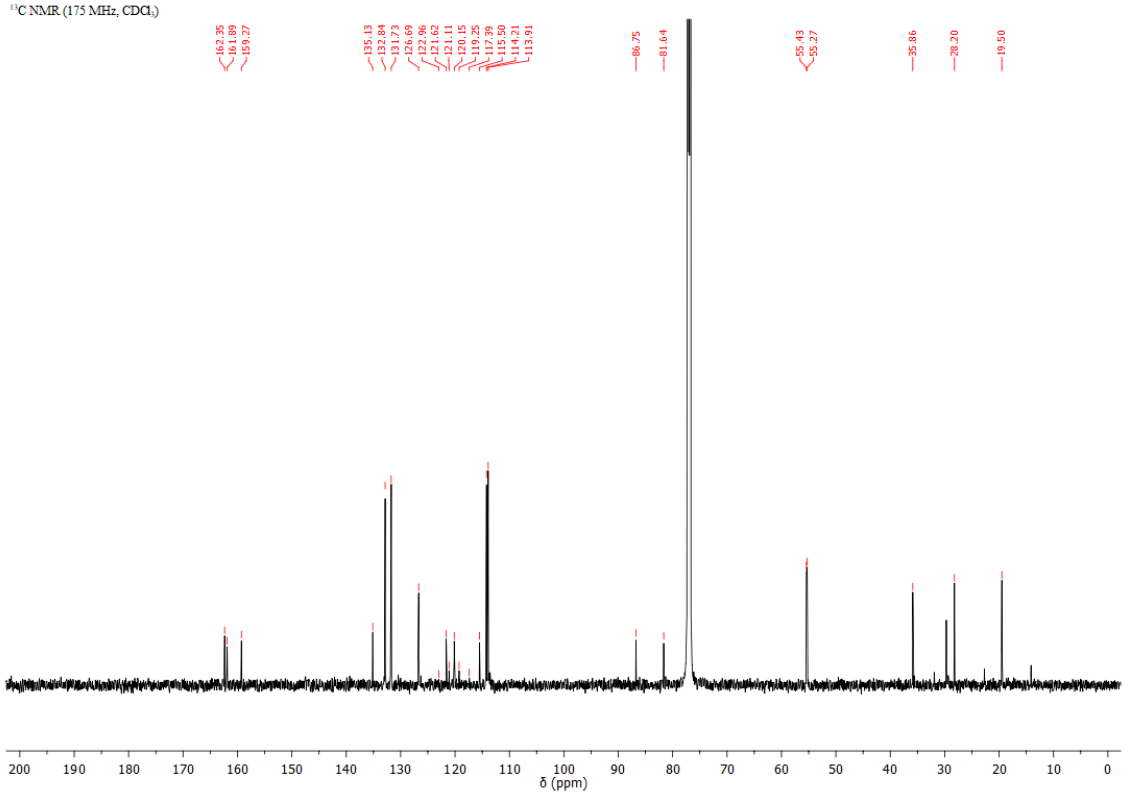
NOE Experiment (300 MHz, $CDCl_3$). Irradiation =CH



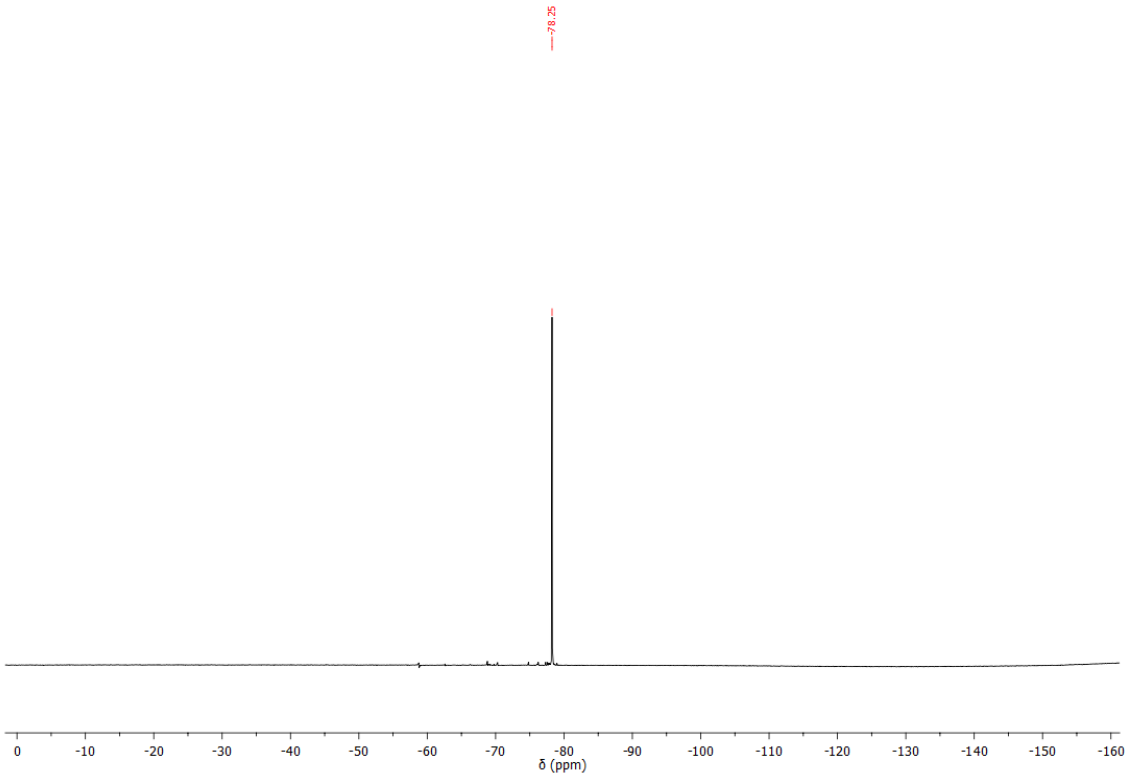
$^1$H NMR (700 MHz, $CDCl_3$)



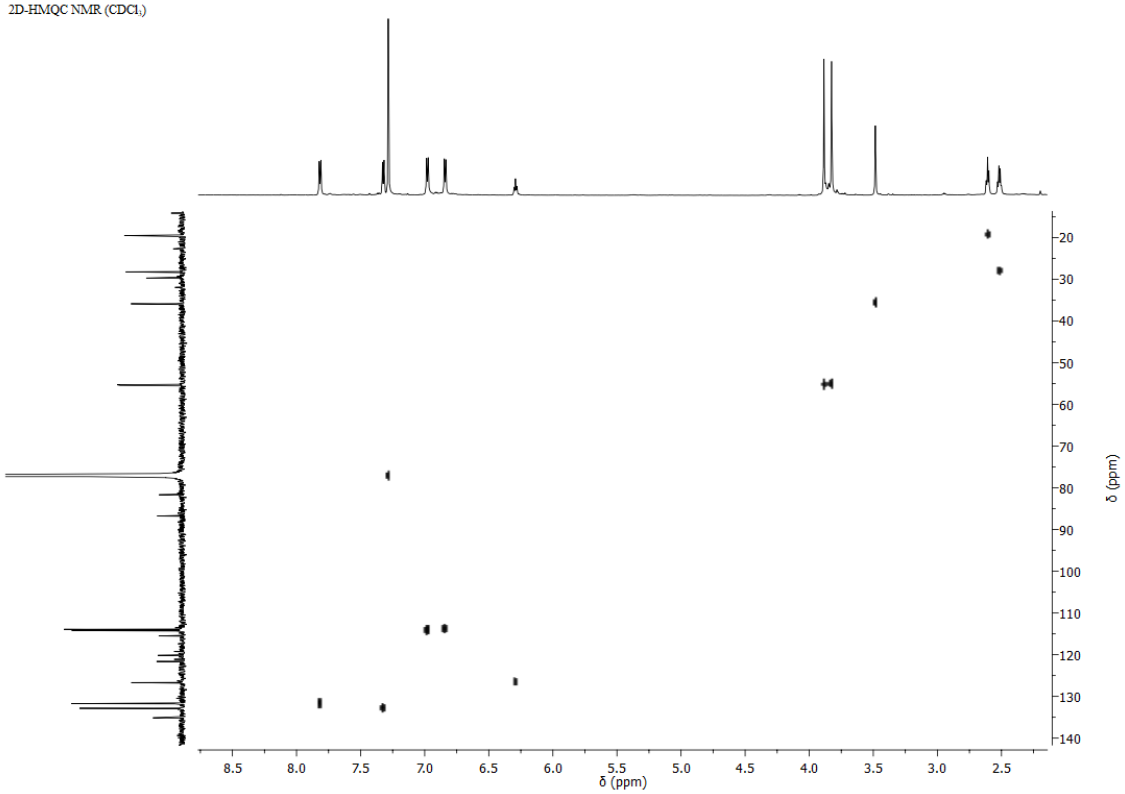

$^{13}$C NMR (175 MHz, $CDCl_3$)



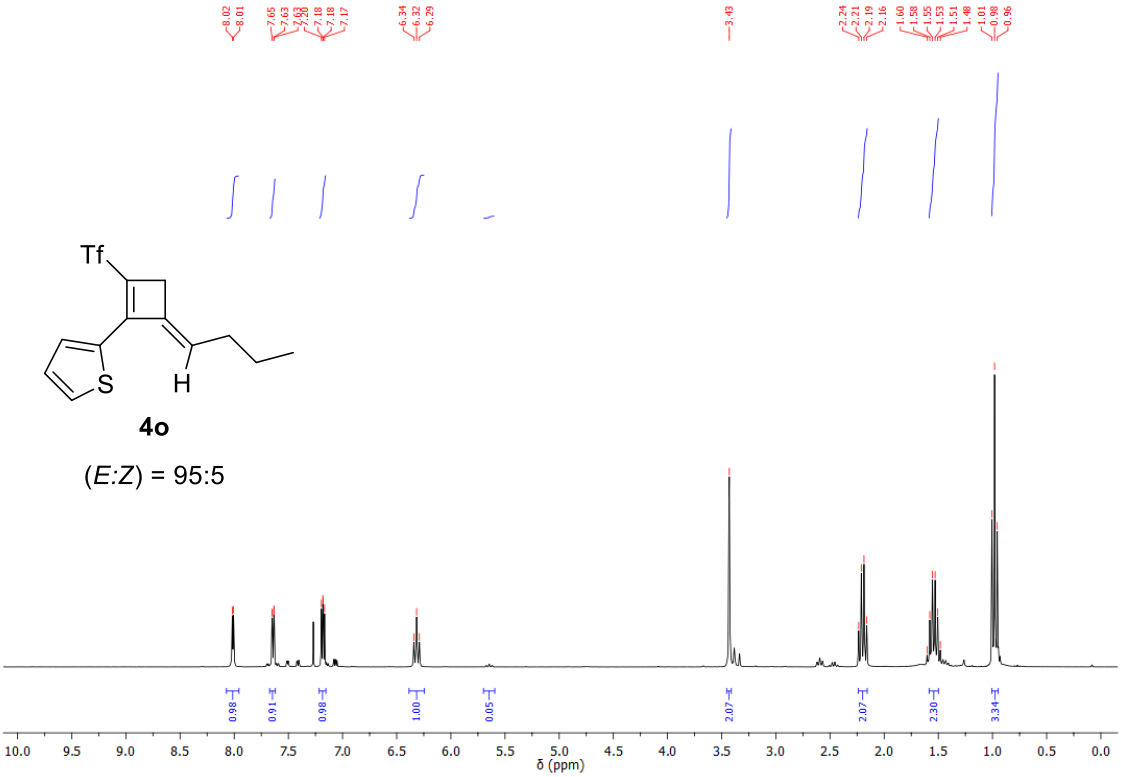
$^{19}$F NMR (282 MHz, $CDCl_3$)




2D-HMQC NMR ($CDCl_3$)



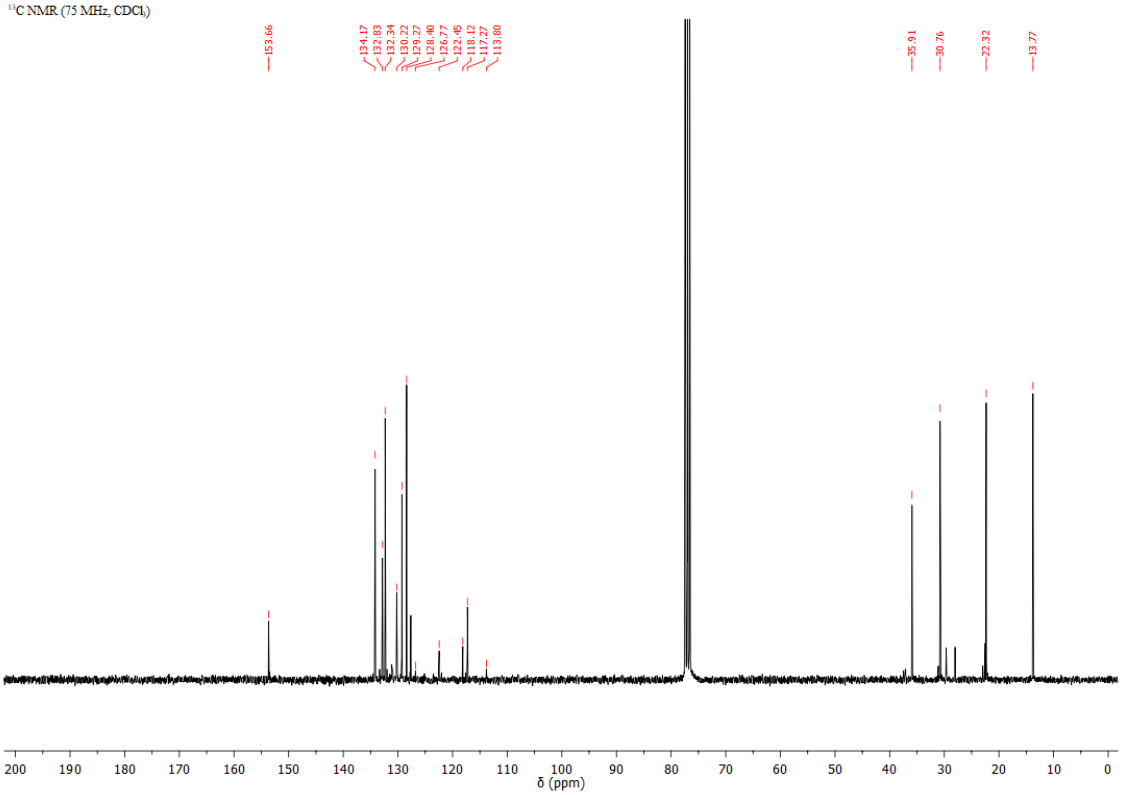
$^1$H NMR (300 MHz, $CDCl_3$)



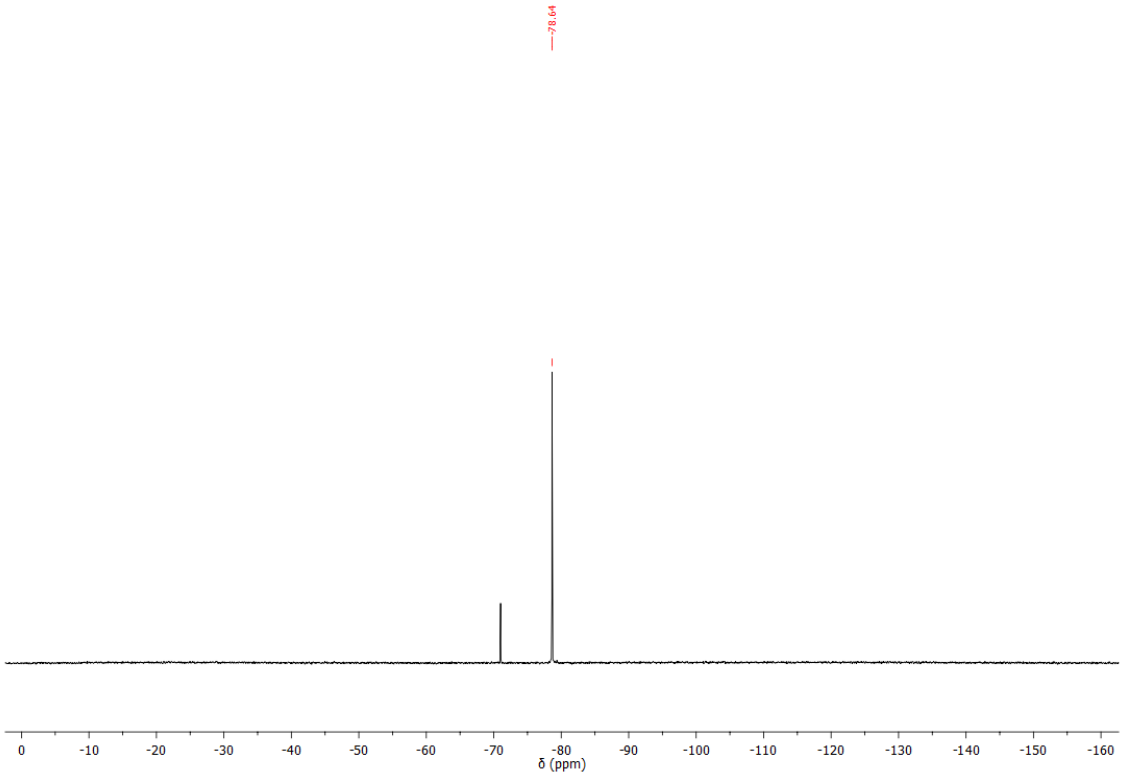

**4o**

(*E*:*Z*) = 95:5

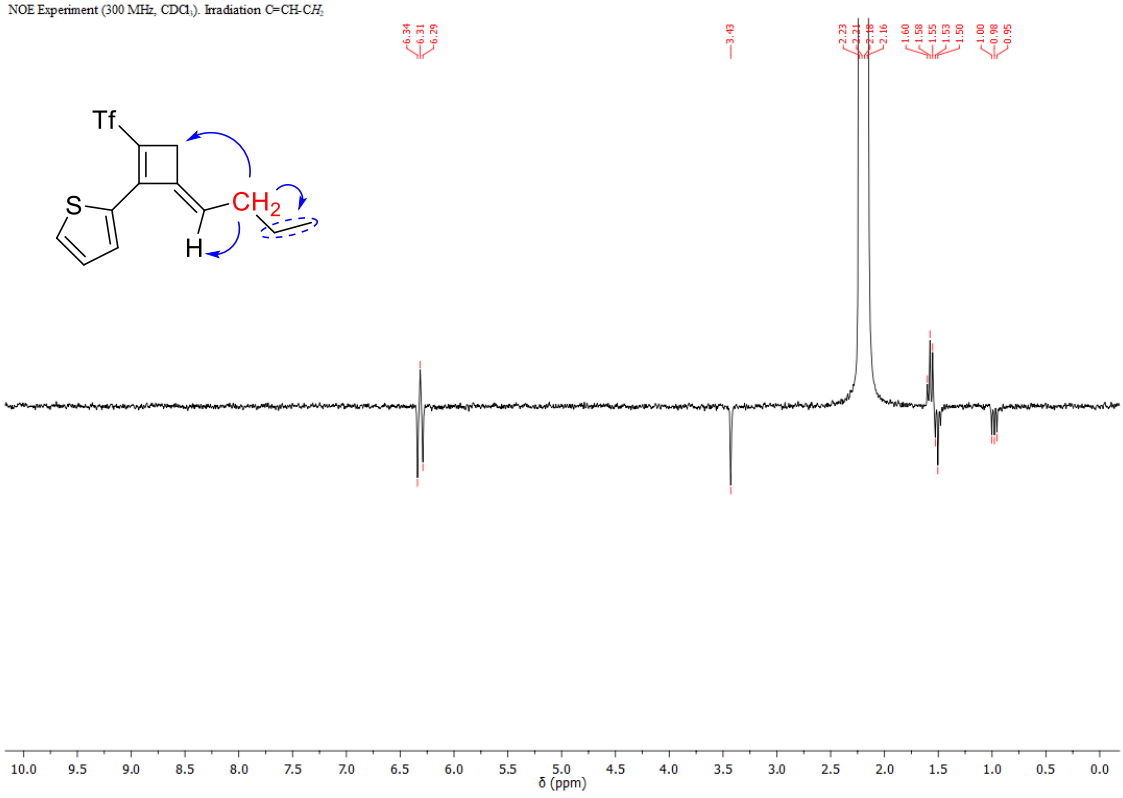
$^{13}$C NMR (75 MHz, $CDCl_3$)



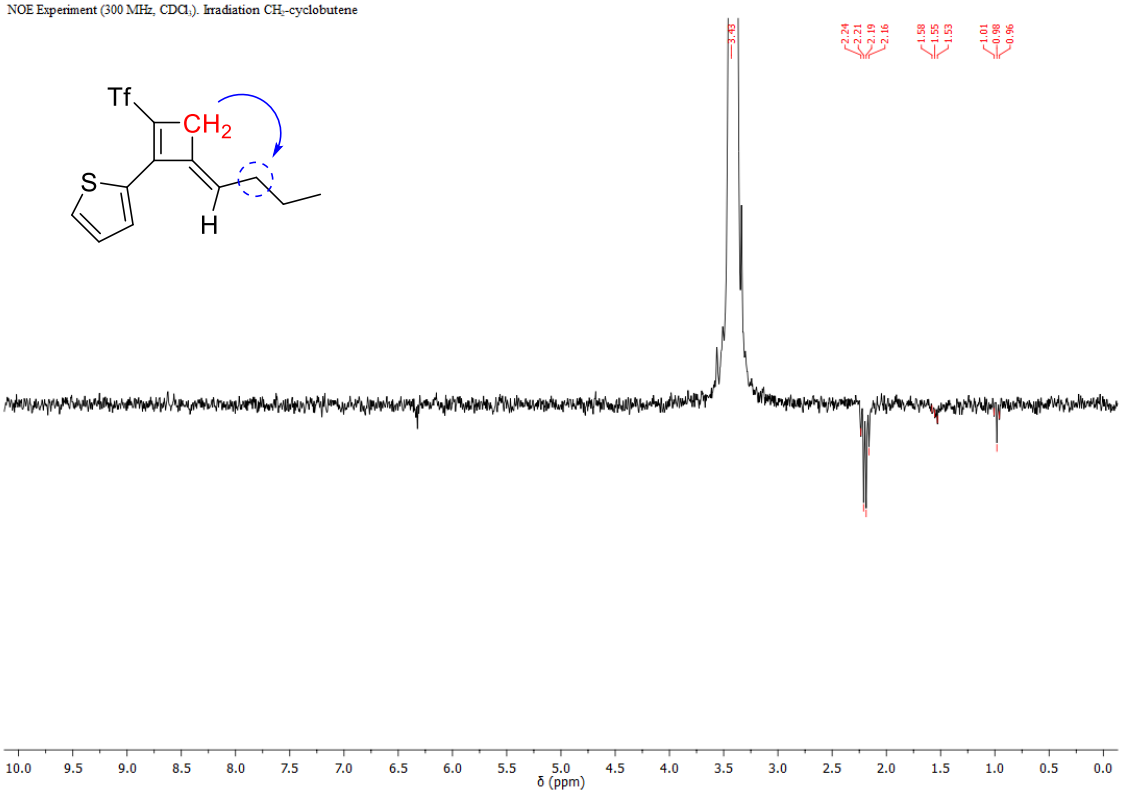
$^{19}$F NMR (282 MHz, $CDCl_3$)



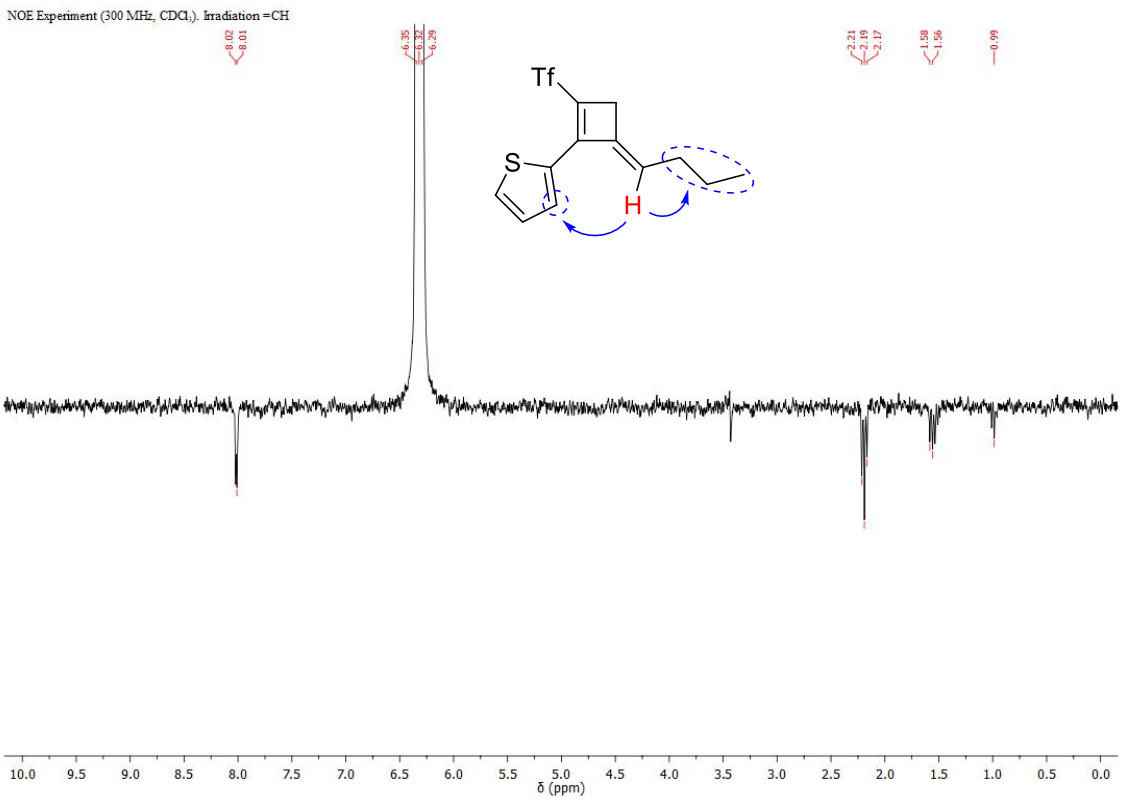

NOE Experiment (300 MHz, $CDCl_3$). Irradiation C=CH-C*H*$_2$



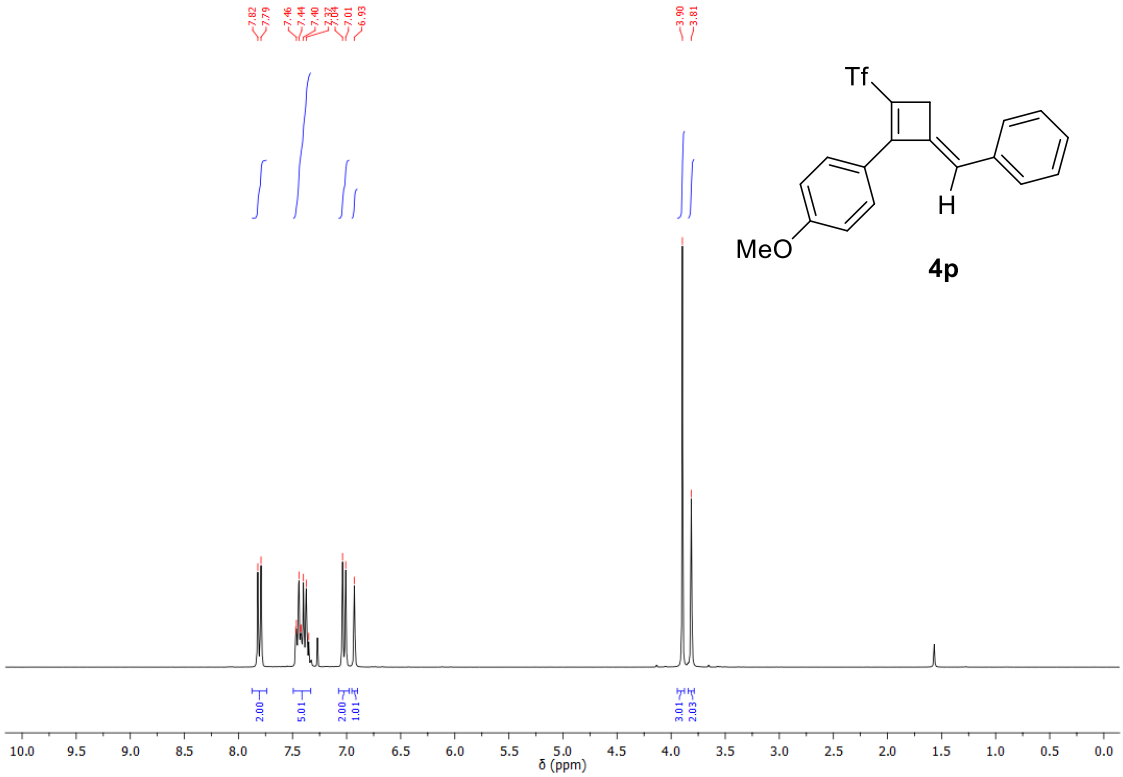
NOE Experiment (300 MHz, $CDCl_3$). Irradiation $CH_2$-cyclobutene



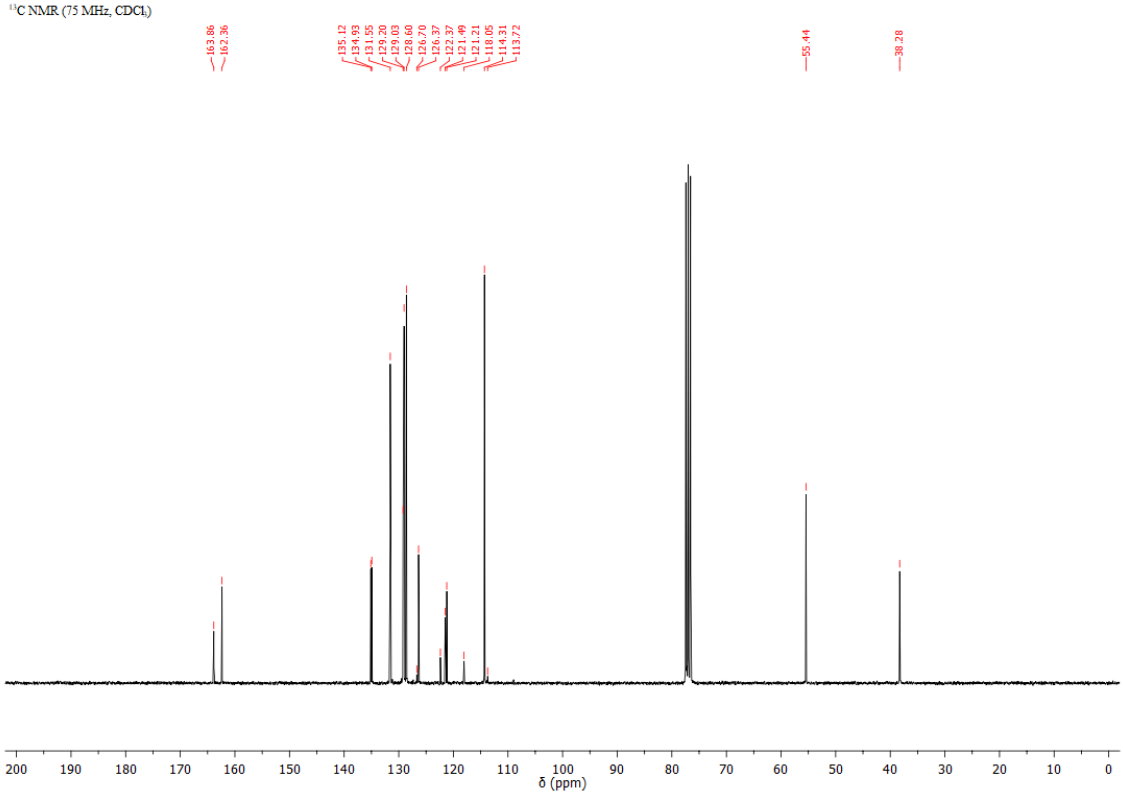

NOE Experiment (300 MHz, $CDCl_3$). Irradiation =CH



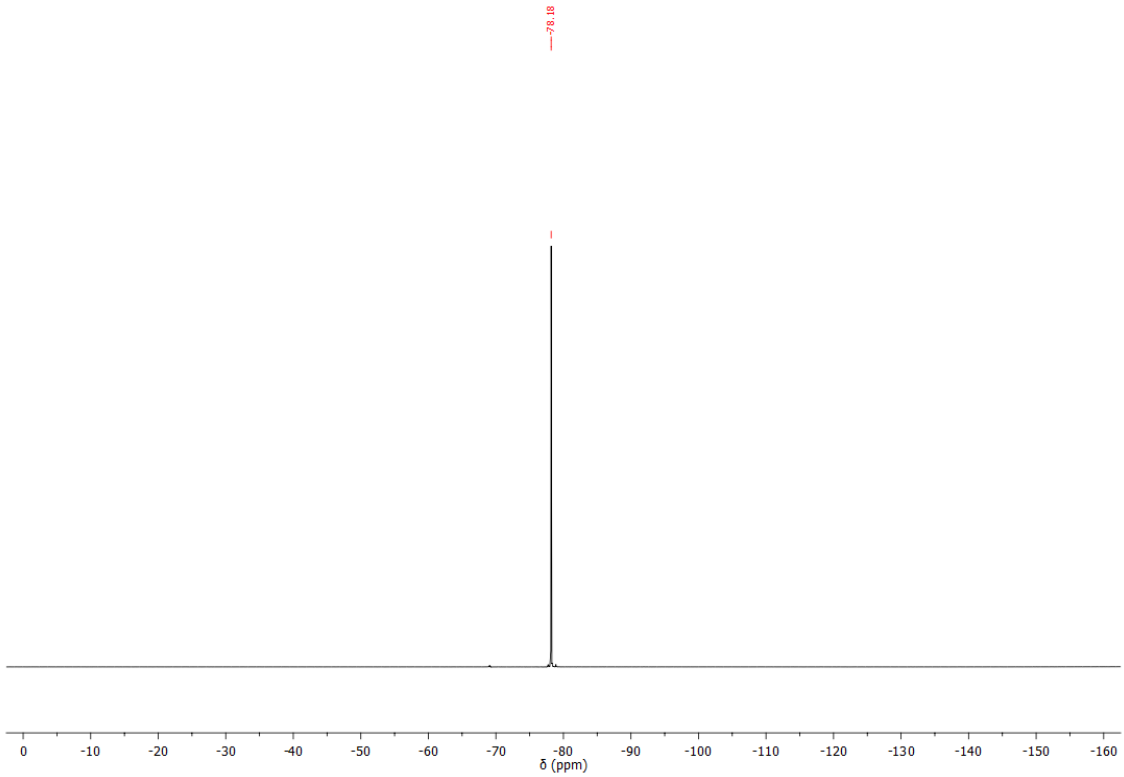
$^1$H NMR (300 MHz, $CDCl_3$)



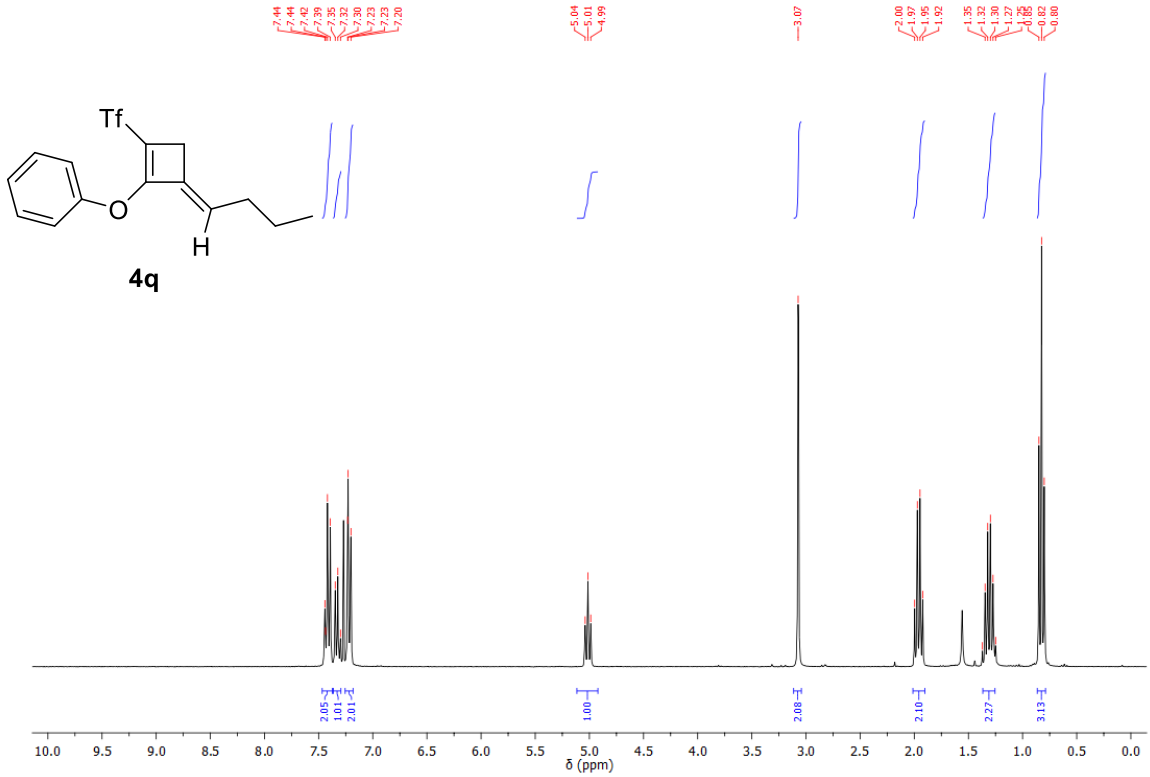

$^{13}$C NMR (75 MHz, $CDCl_3$)



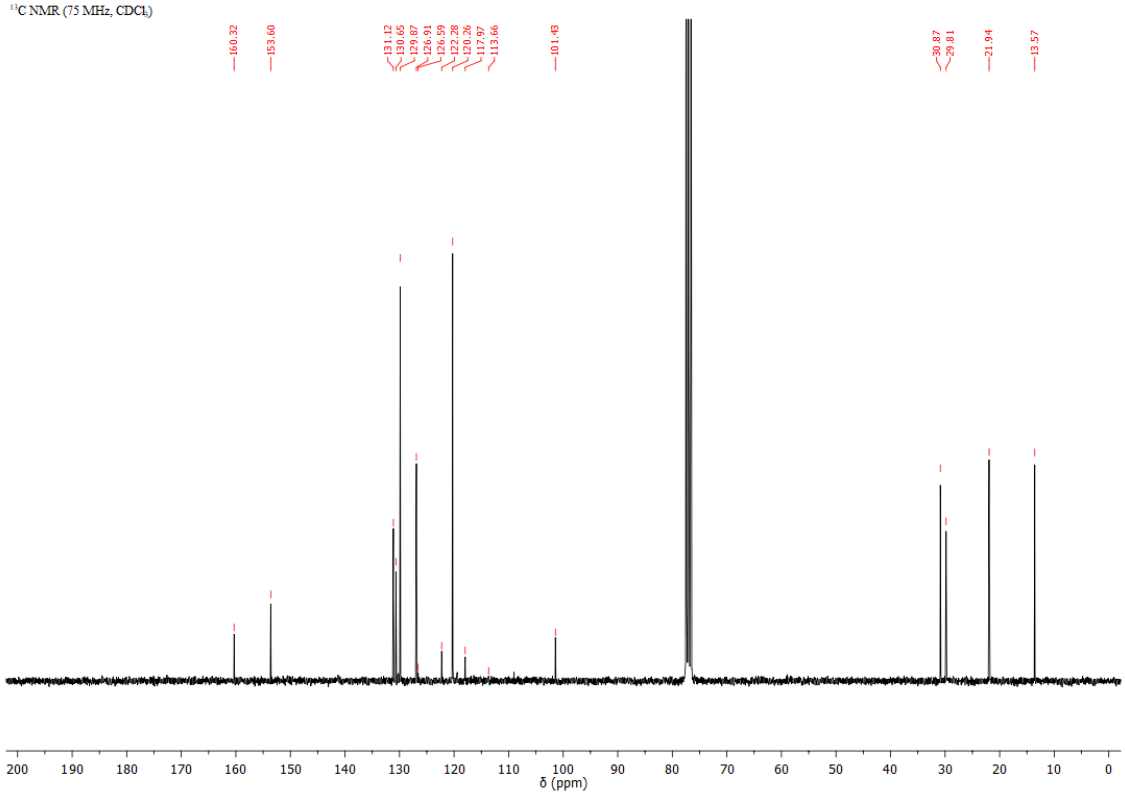
$^{19}$F NMR (282 MHz, $CDCl_3$)



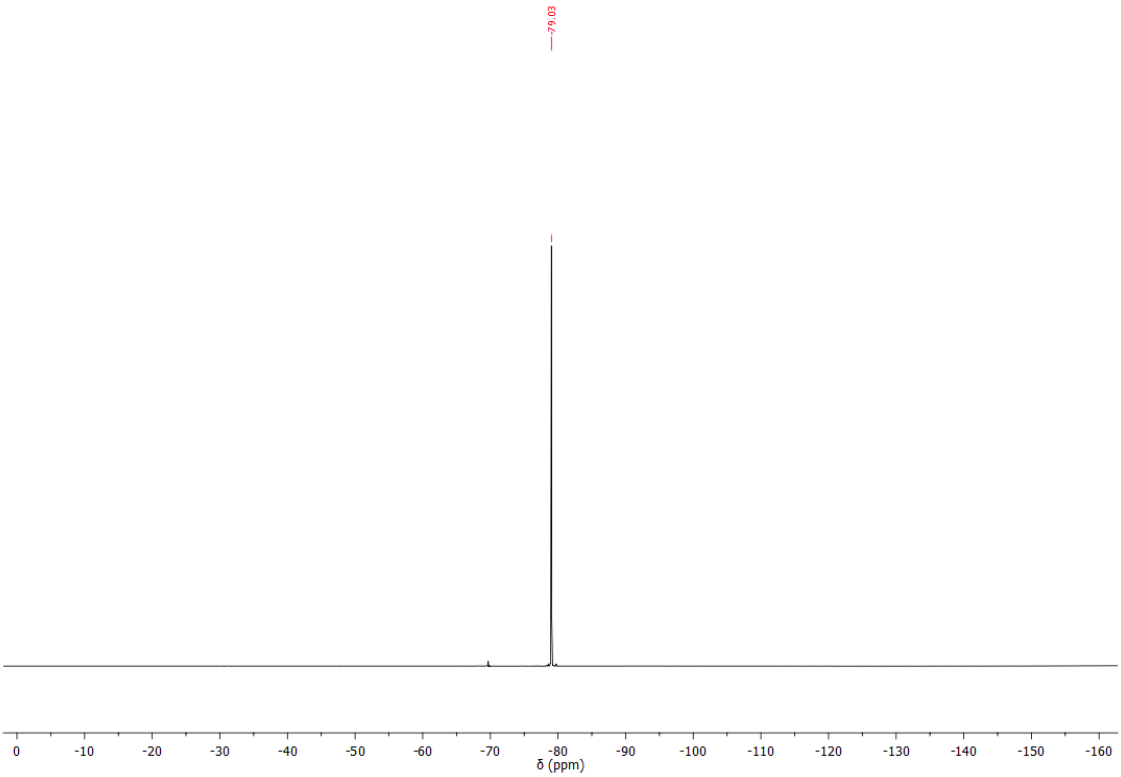
$^1$H NMR (300 MHz, $CDCl_3$)



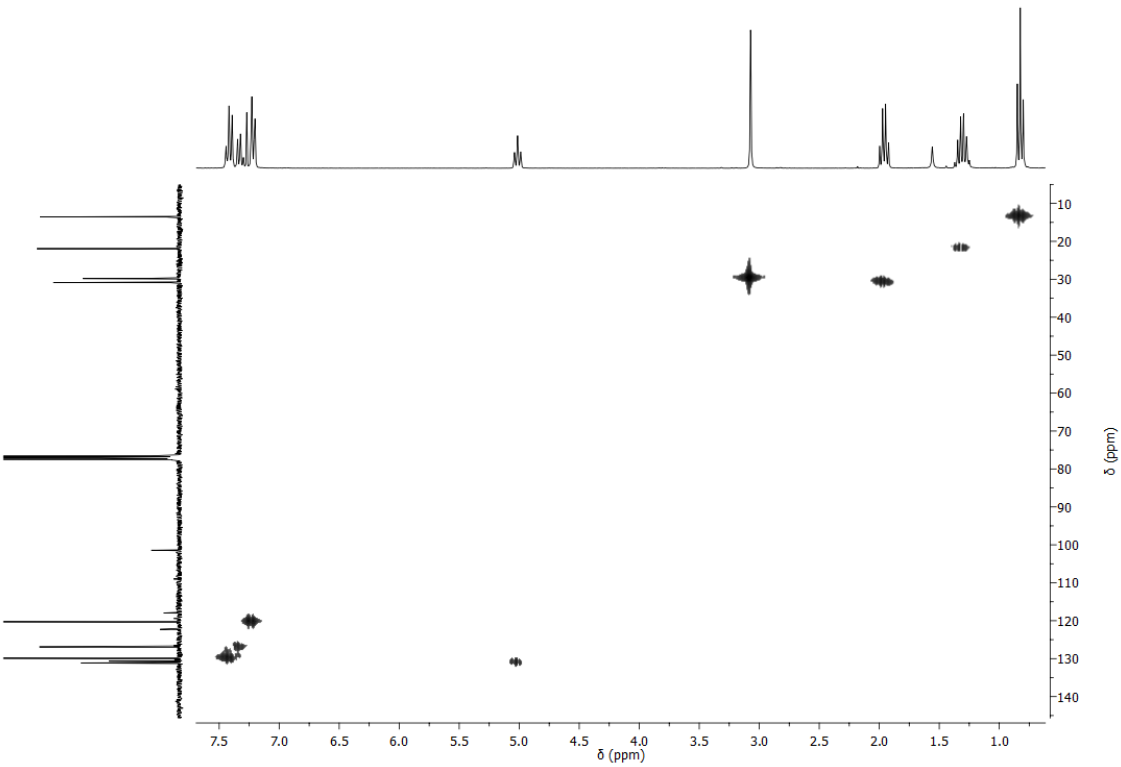

$^{13}$C NMR (75 MHz, $CDCl_3$)



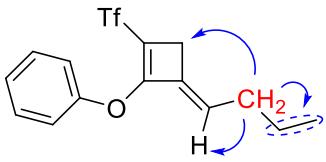
$^{19}$F NMR (282 MHz, $CDCl_3$)




2D-HMQC NMR ($CDCl_3$)



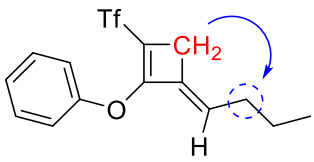
NOE Experiment (300 MHz, $CDCl_3$). Irradiation C=CH-C*H*$_2$

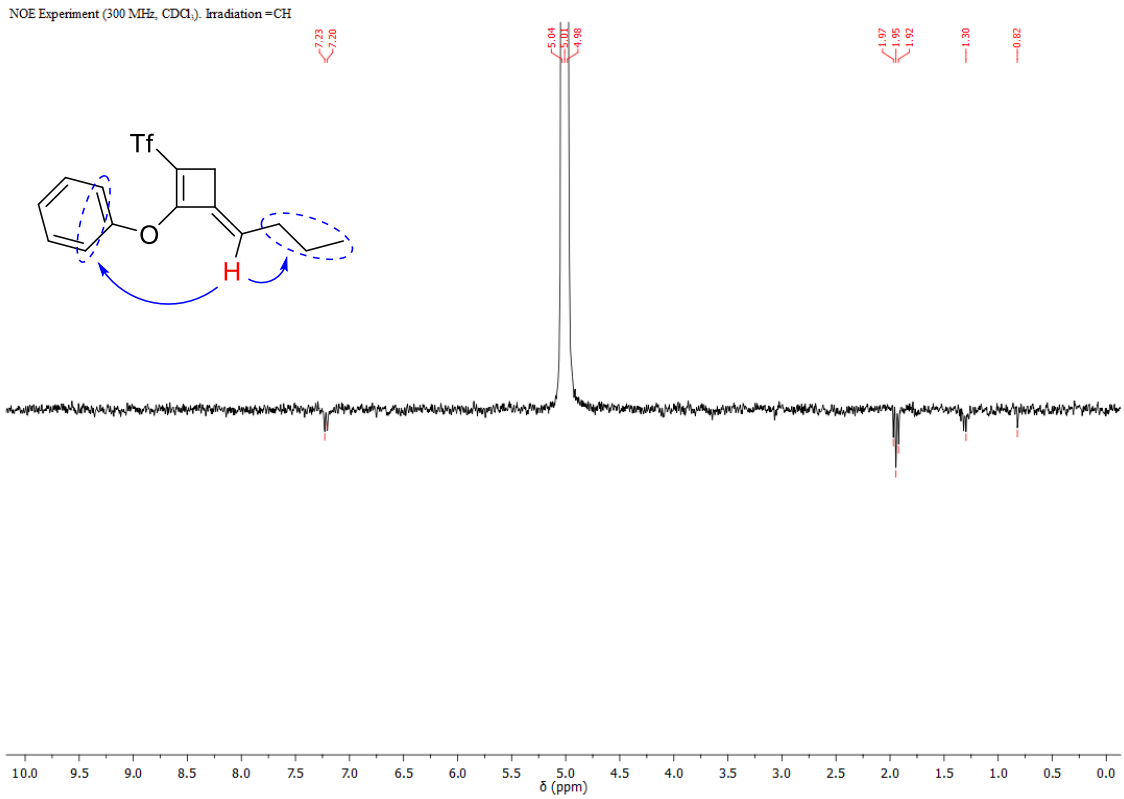




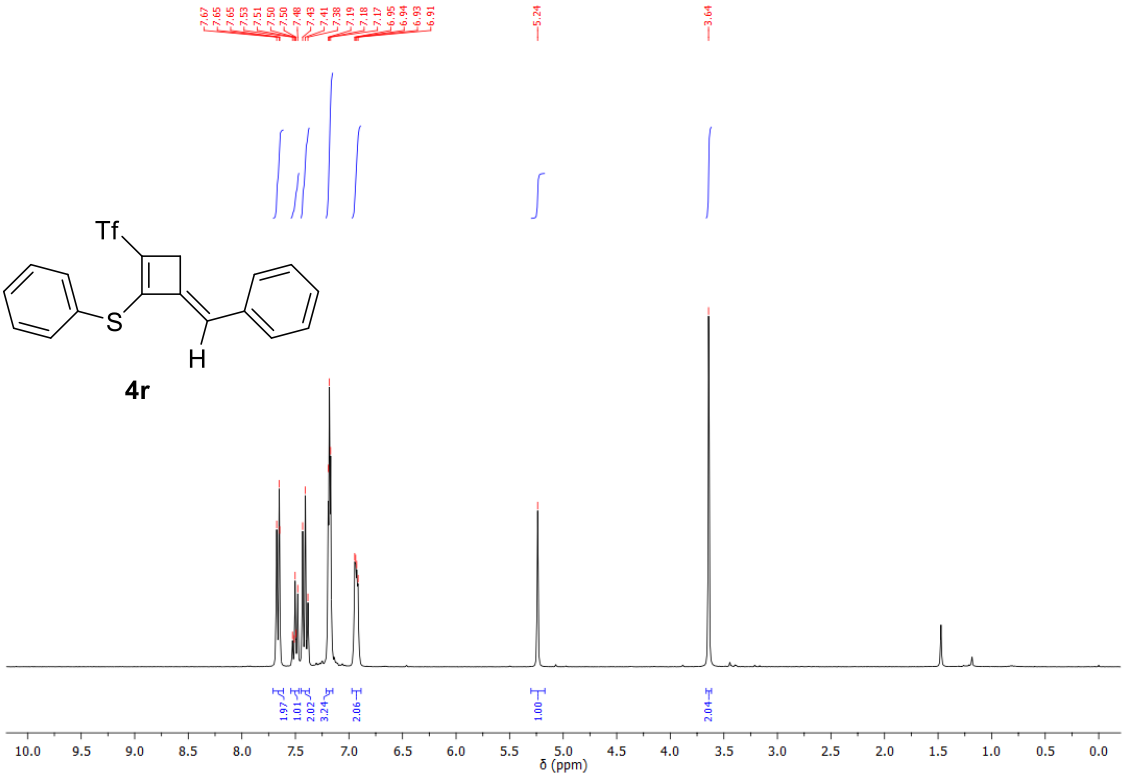


NOE Experiment (300 MHz, $CDCl_3$). Irradiation $CH_2$-cyclobutene



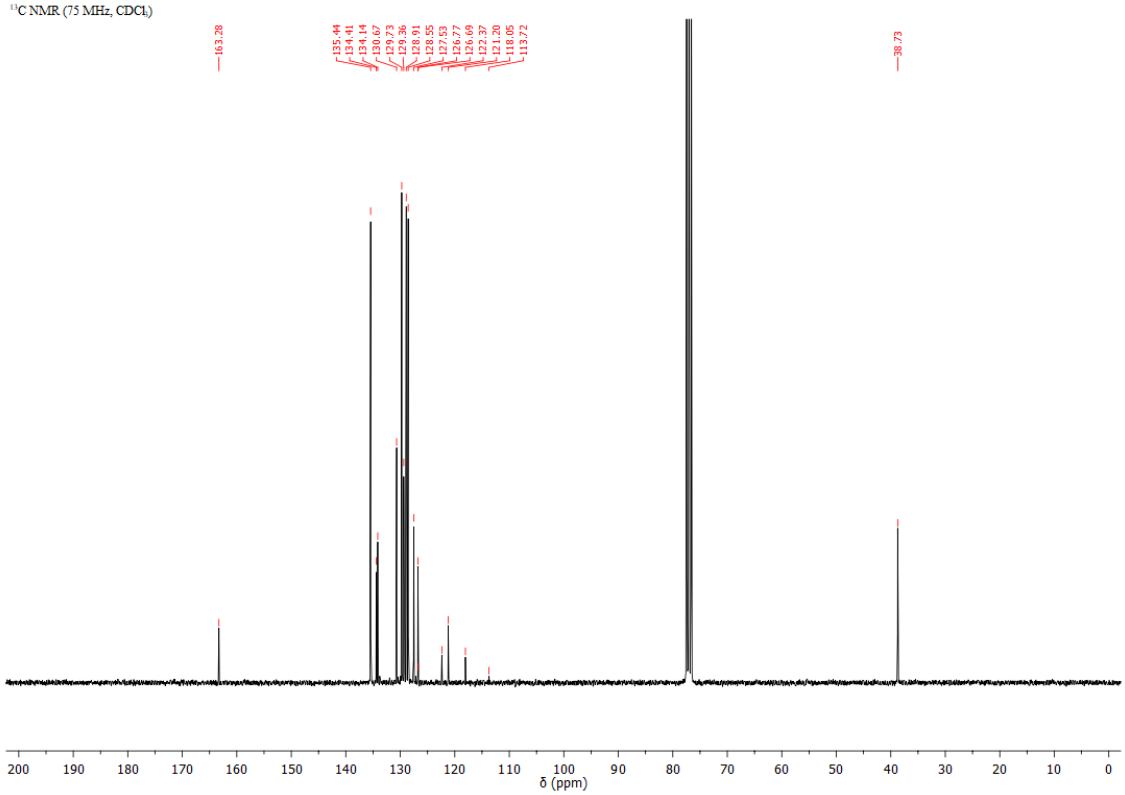

NOE Experiment (300 MHz, CDCl3). Irradiation =CH
7.23
7.20
5.04
5.00
4.98
1.97
1.95
1.92
1.30
0.82
Tf
O
H
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

$^1$H NMR (300 MHz, $CDCl_3$)

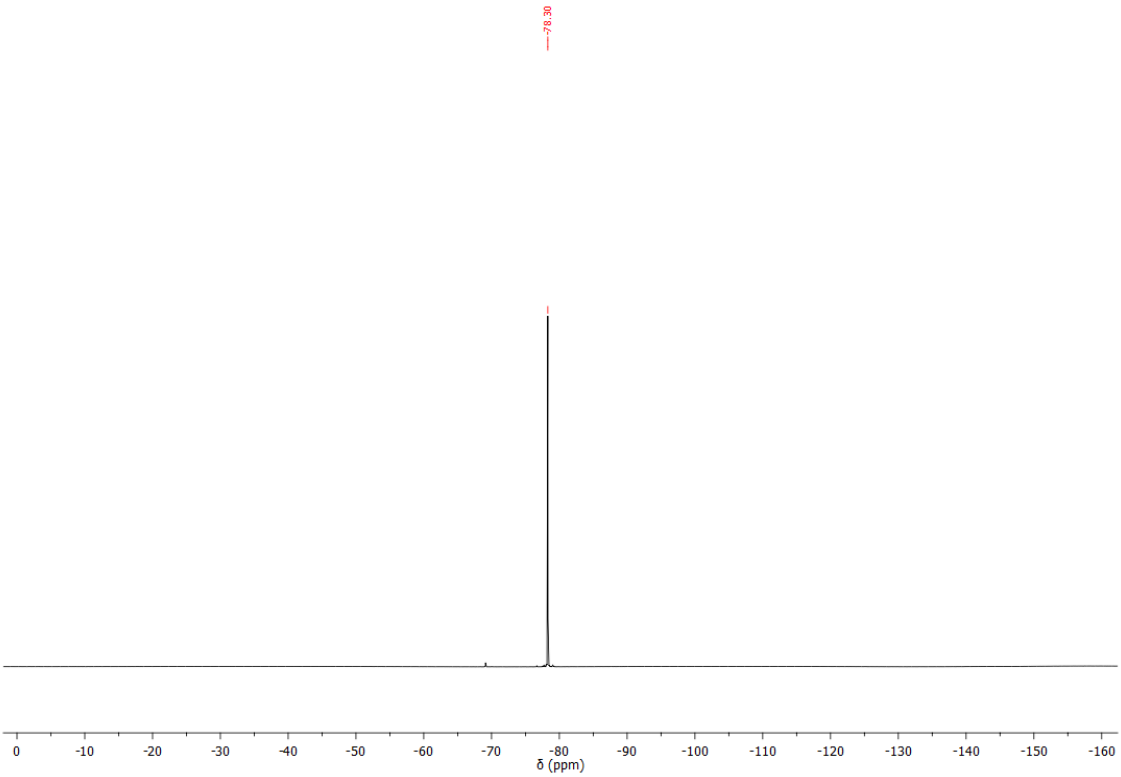



**4r**

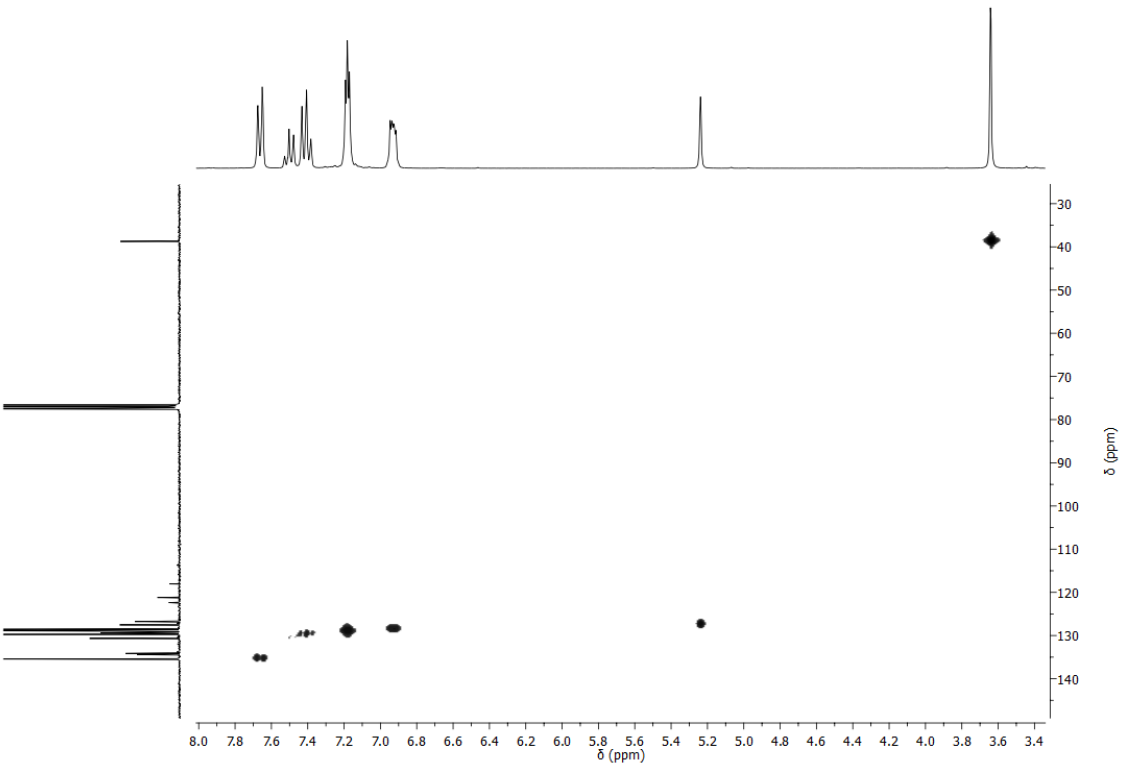
$^{13}$C NMR (75 MHz, $CDCl_3$)



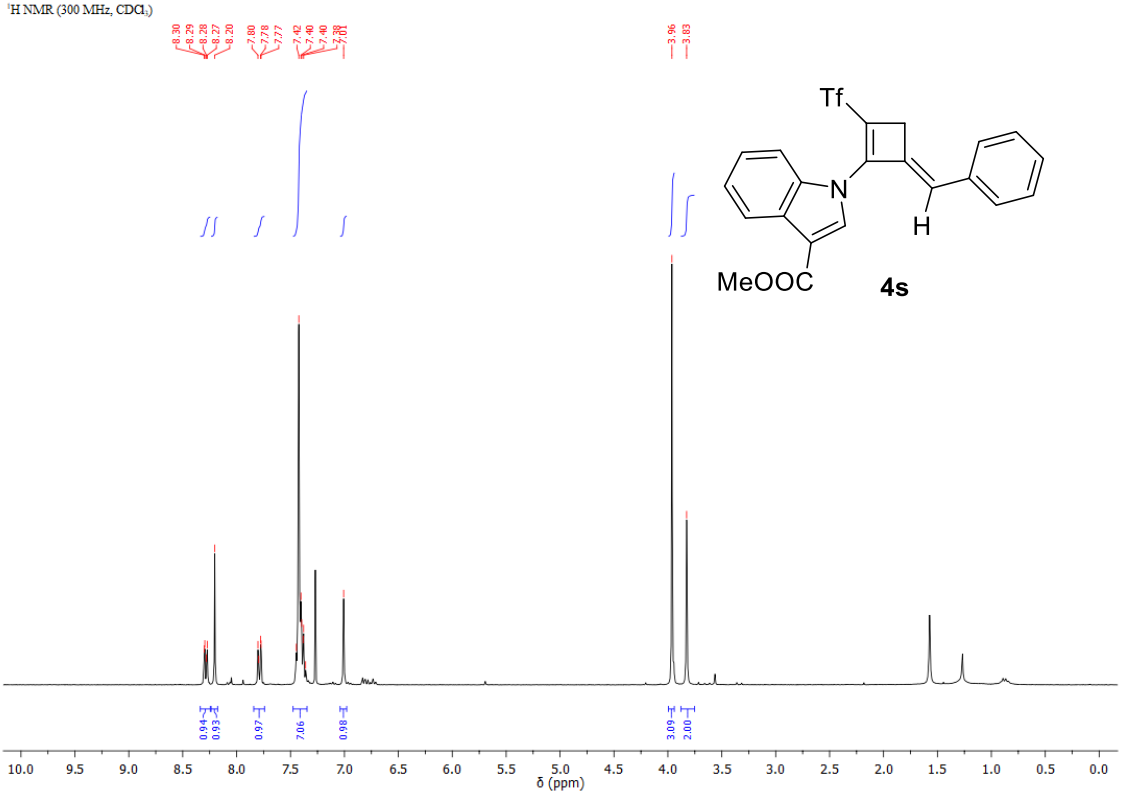
$^{19}$F NMR (282 MHz, $CDCl_3$)



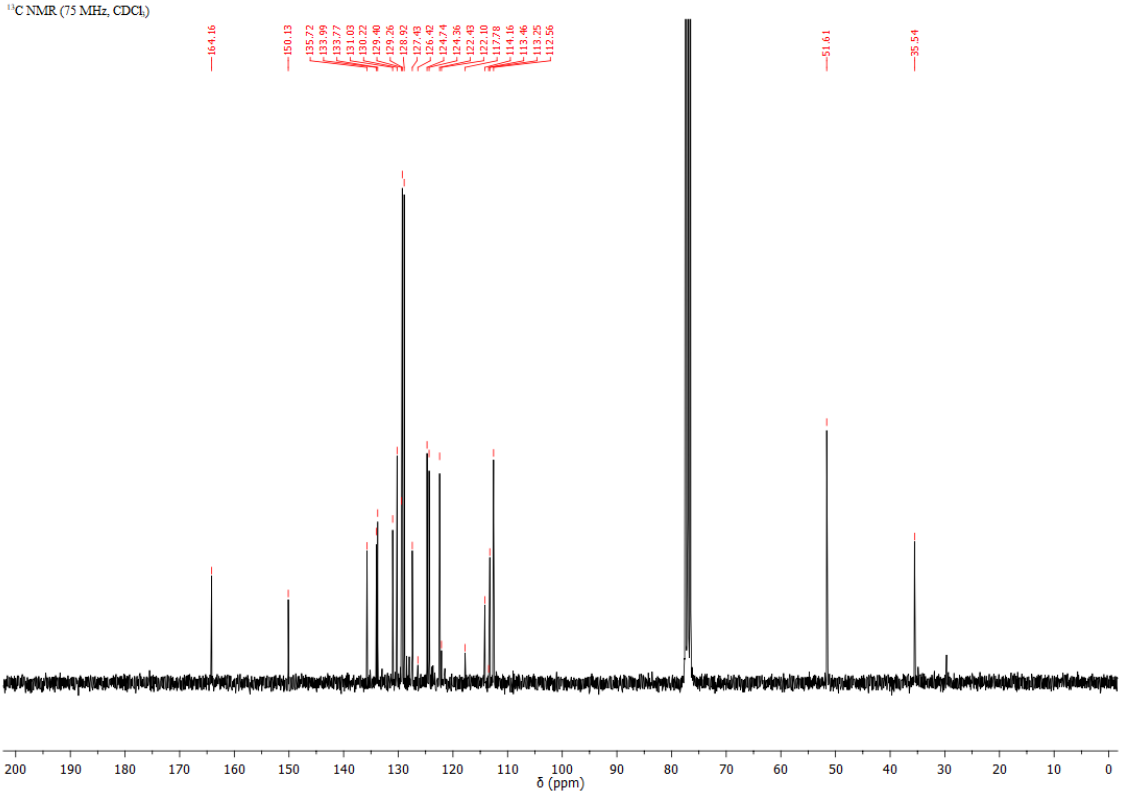

2D-HMQC NMR ($CDCl_3$)



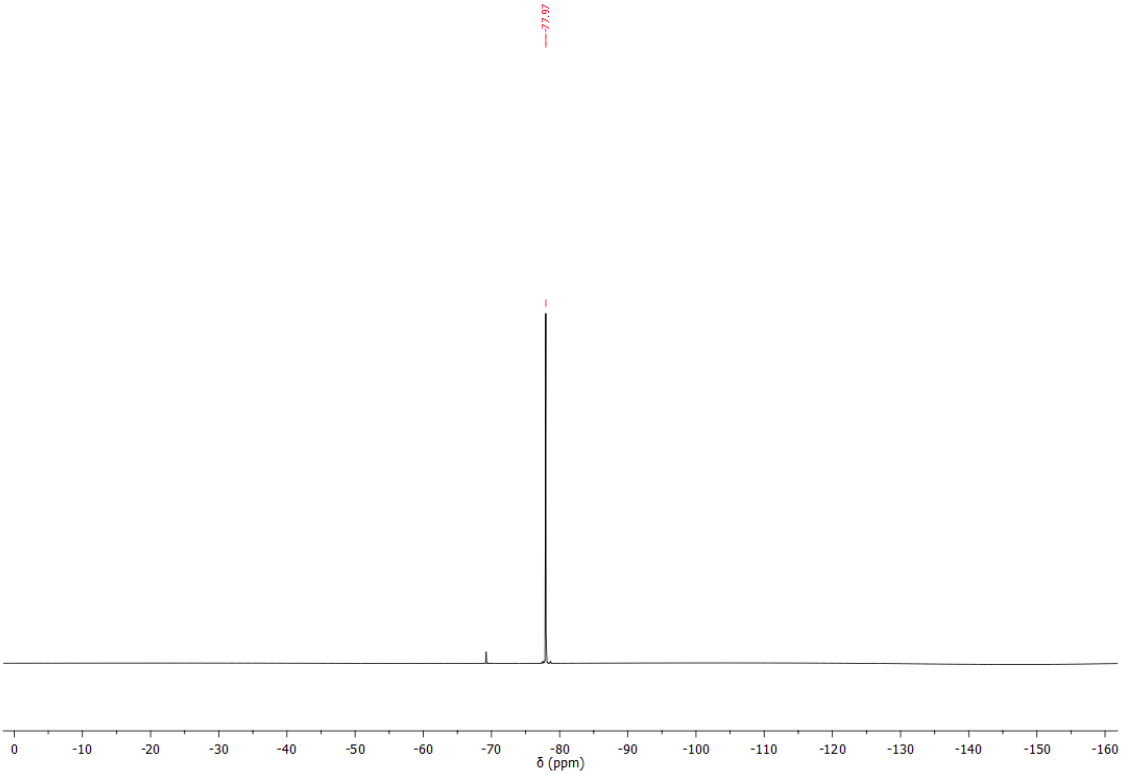
$^1$H NMR (300 MHz, CDCl$_3$)



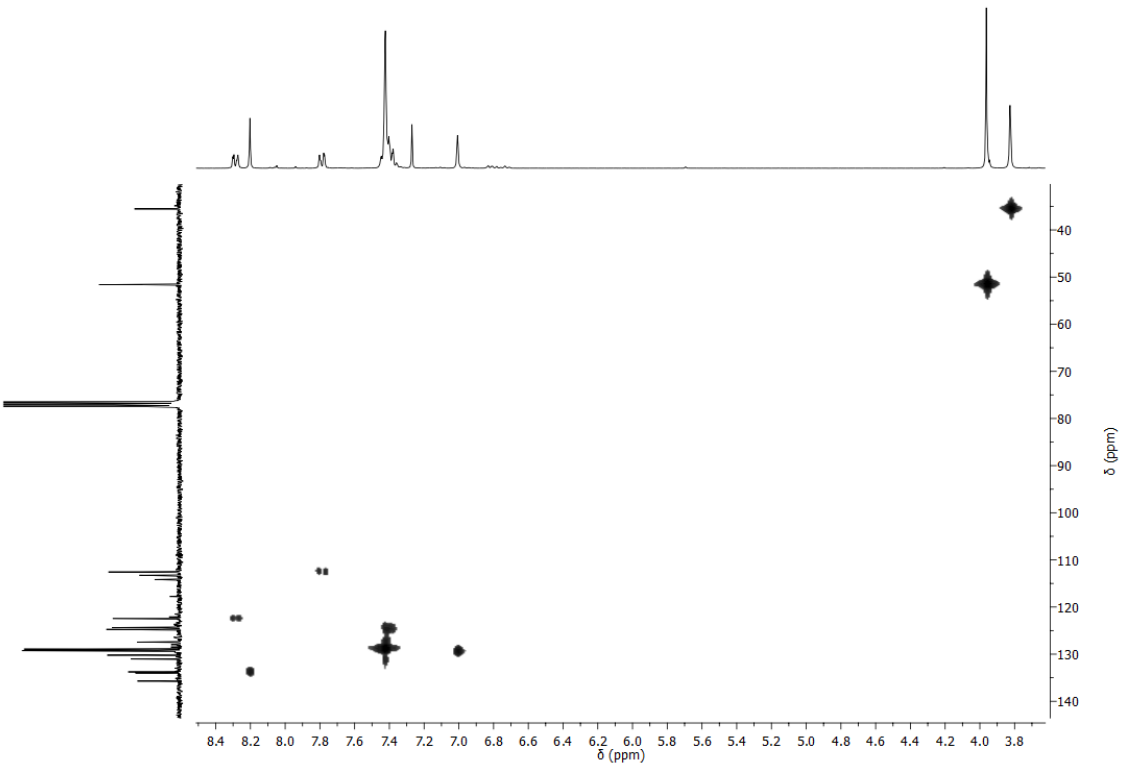

$^{13}$C NMR (75 MHz, CDCl$_3$)

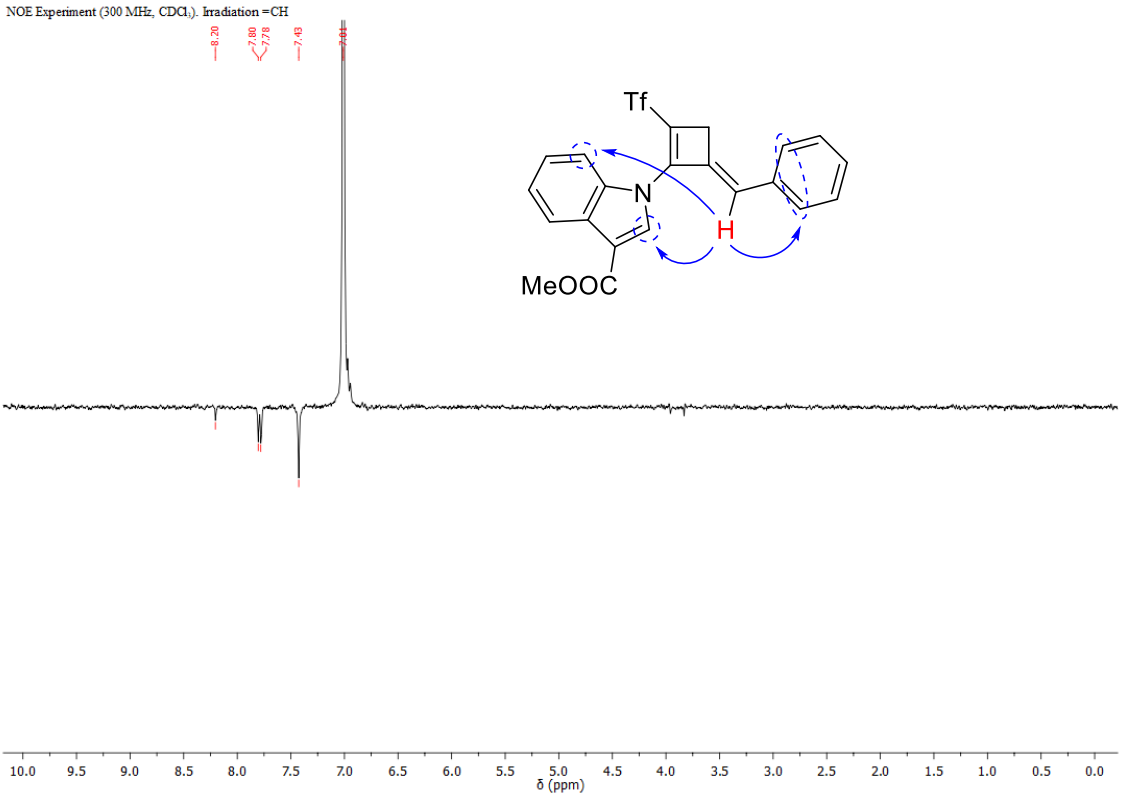


$^{19}$F NMR (282 MHz, $CDCl_3$)

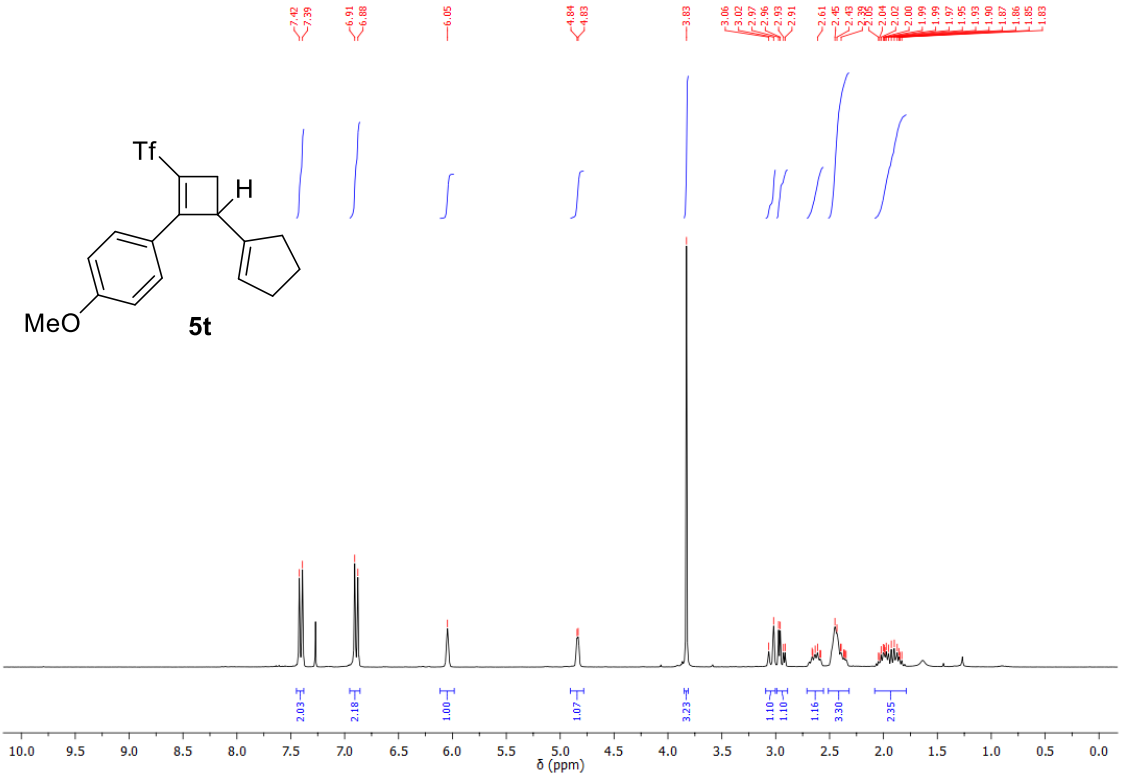



2D-HMQC NMR ($CDCl_3$)

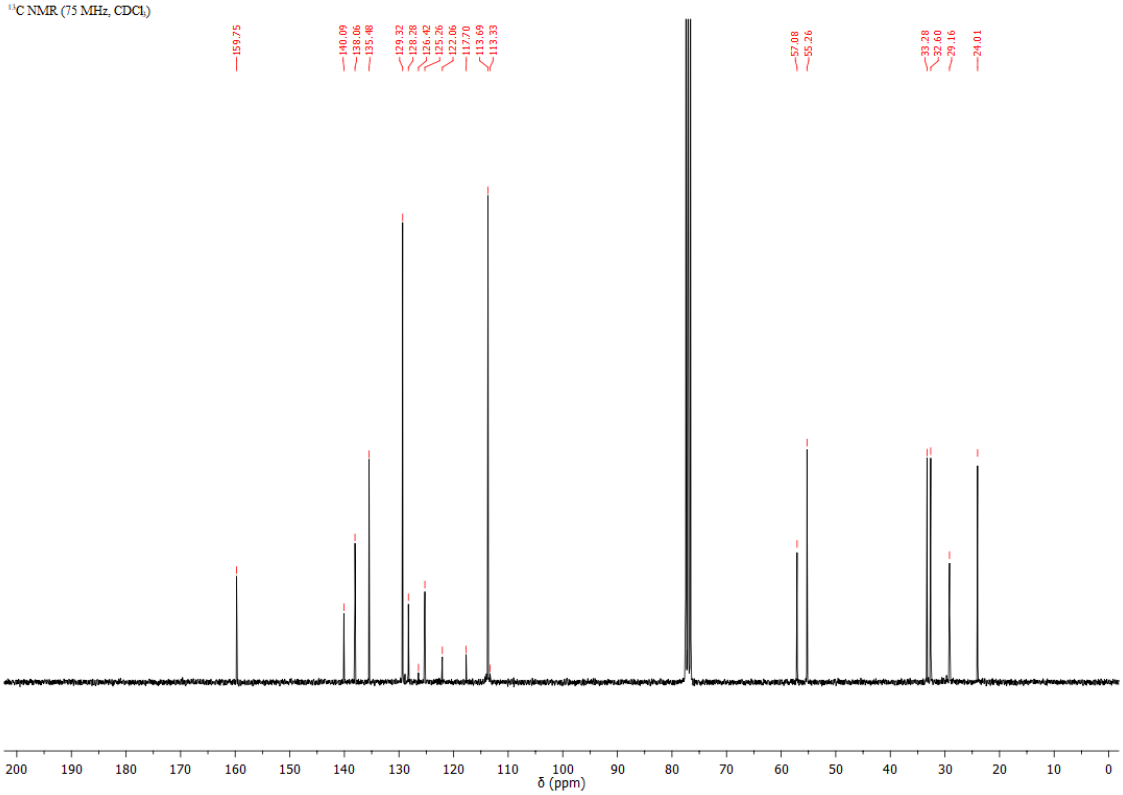



NOE Experiment (300 MHz, CDCl3). Irradiation =CH
8.20
7.80
7.78
7.43
7.01
Tf
N
H
MeOOC
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ (ppm)

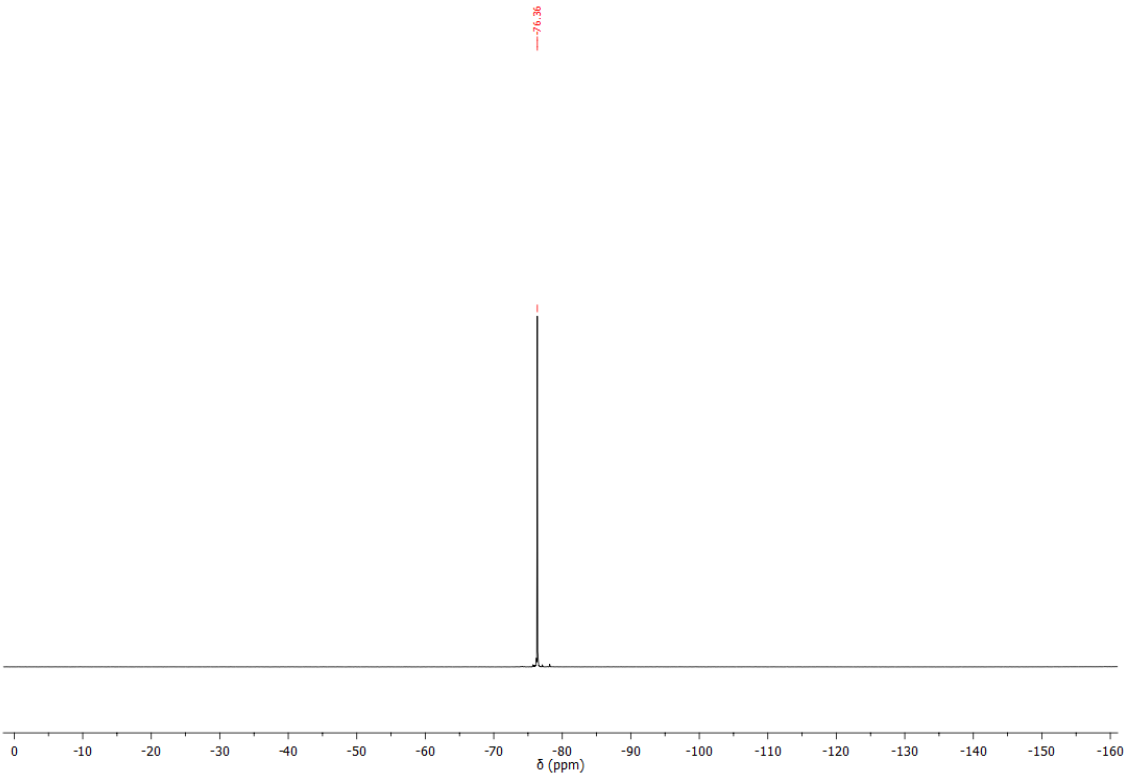
$^1$H NMR (300 MHz, $CDCl_3$)



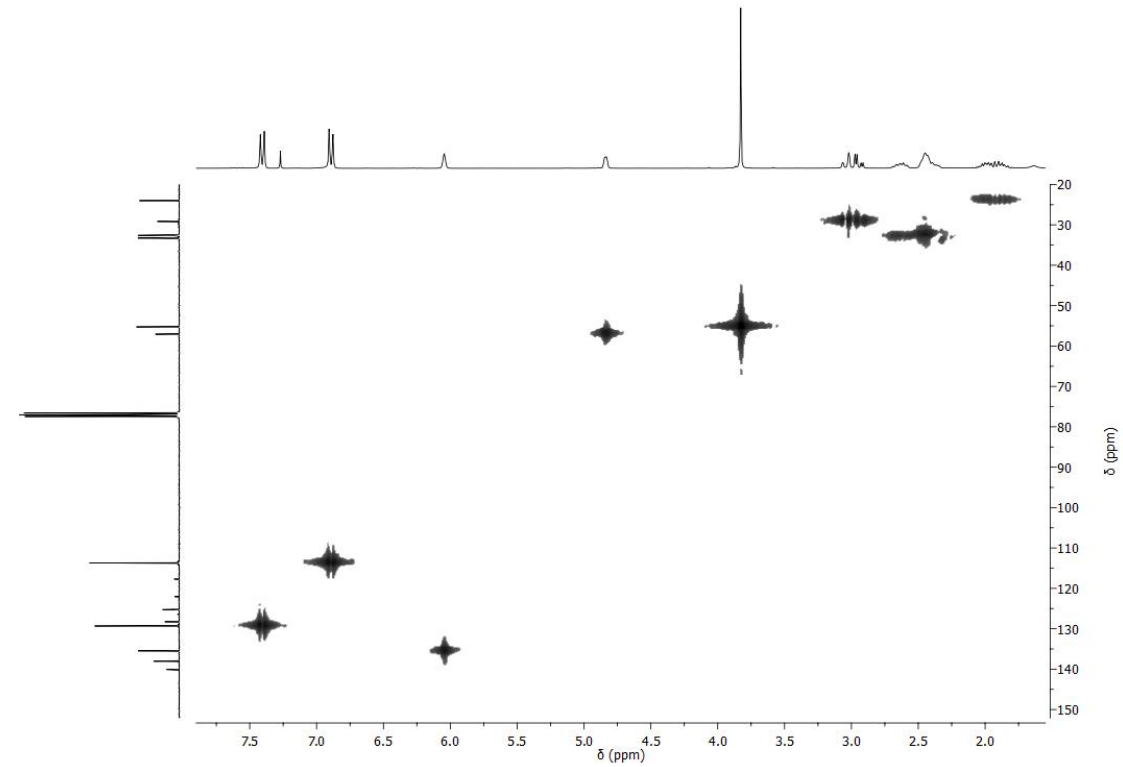

$^{13}$C NMR (75 MHz, $CDCl_3$)



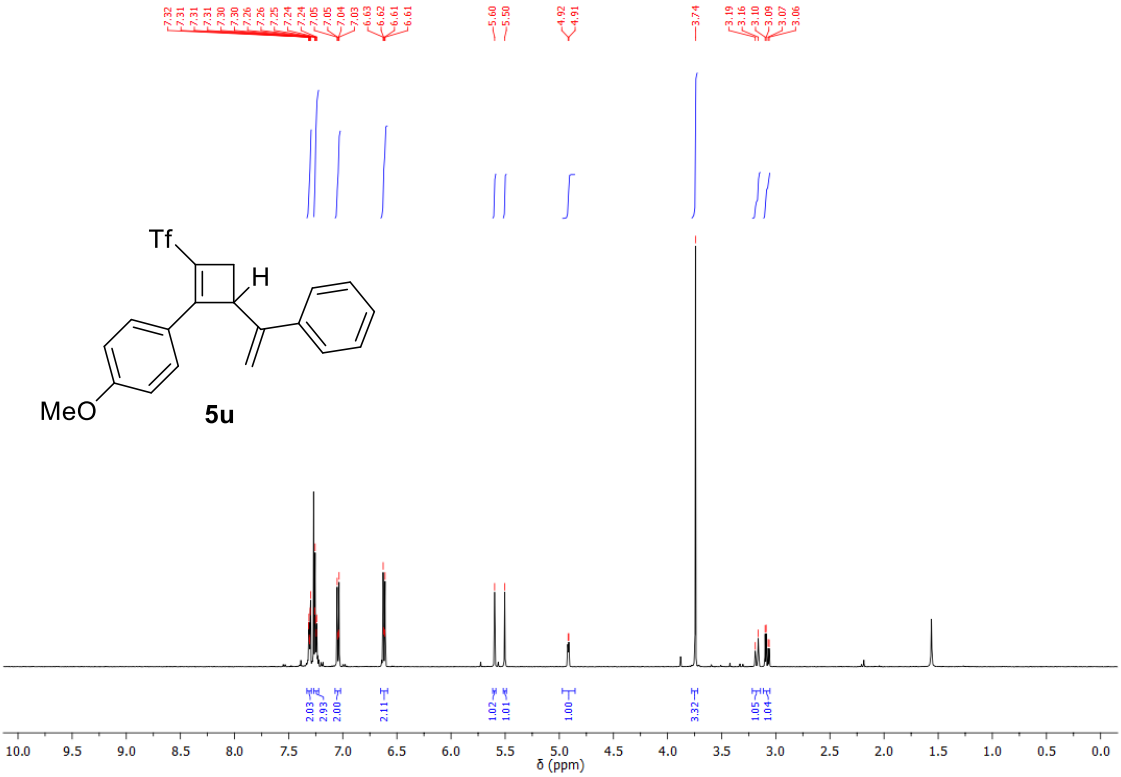
$^{19}$F NMR (282 MHz, $CDCl_3$)



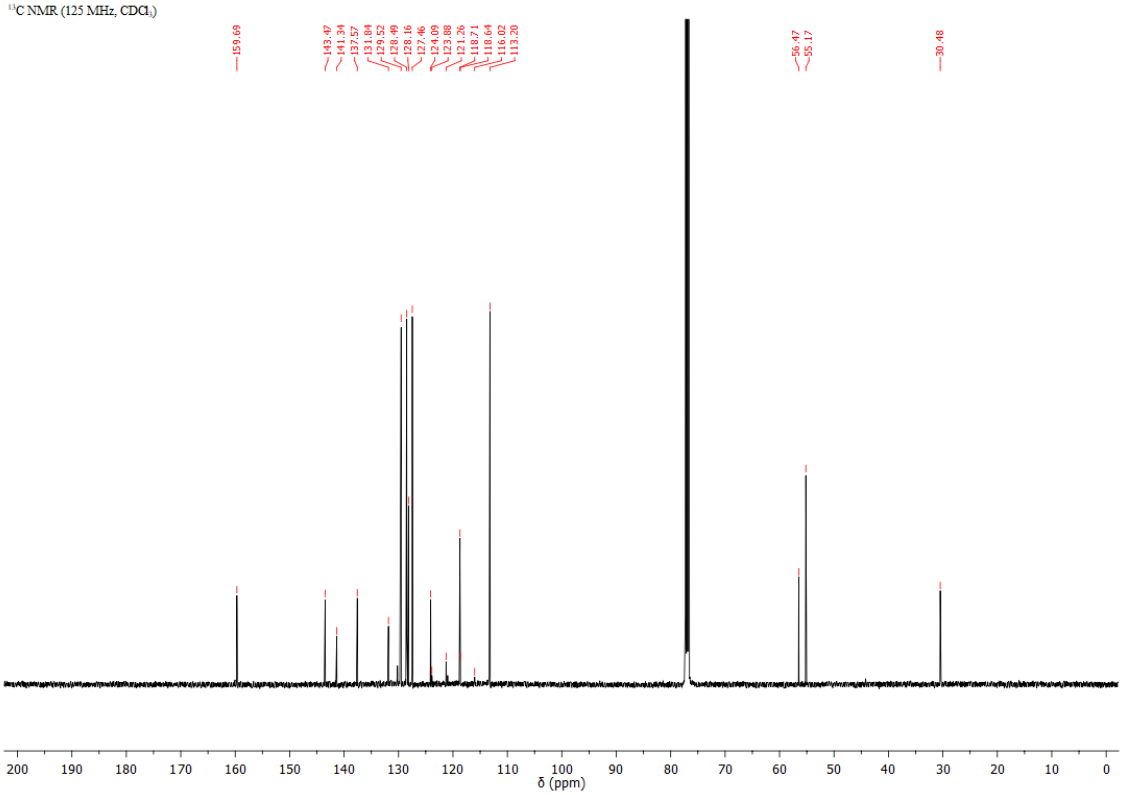

2D-HMQC NMR ($CDCl_3$)



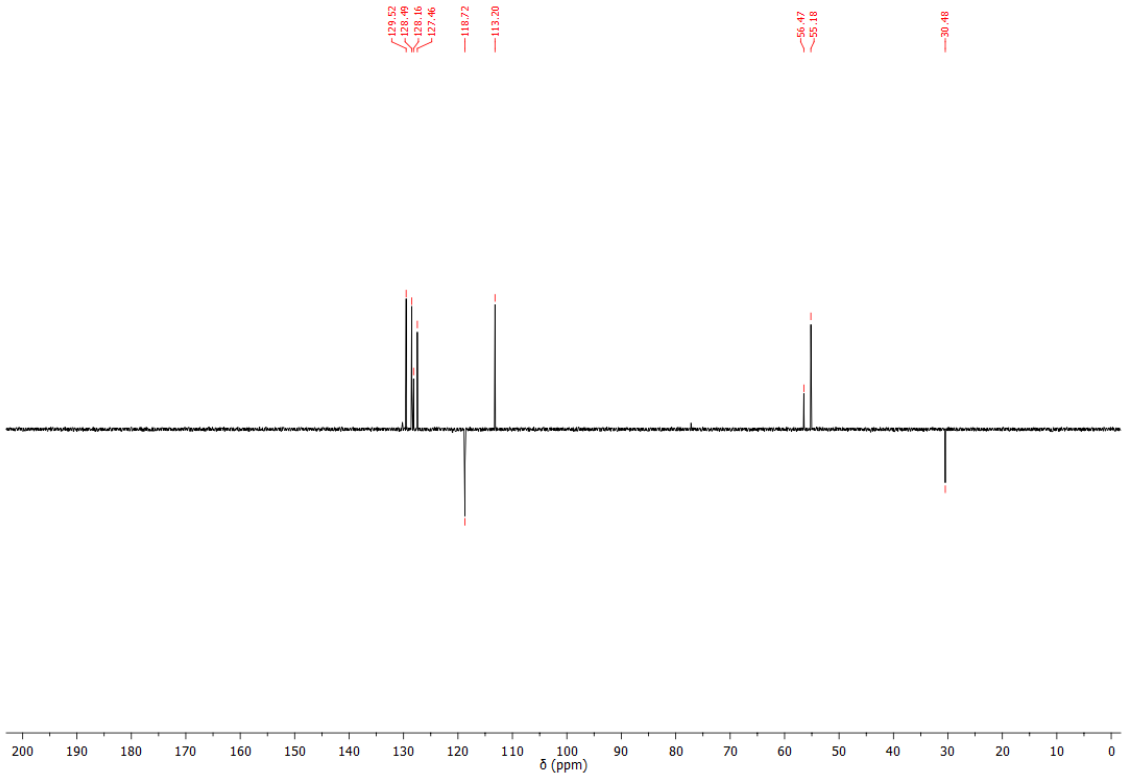
$^1$H NMR (500 MHz, $CDCl_3$)



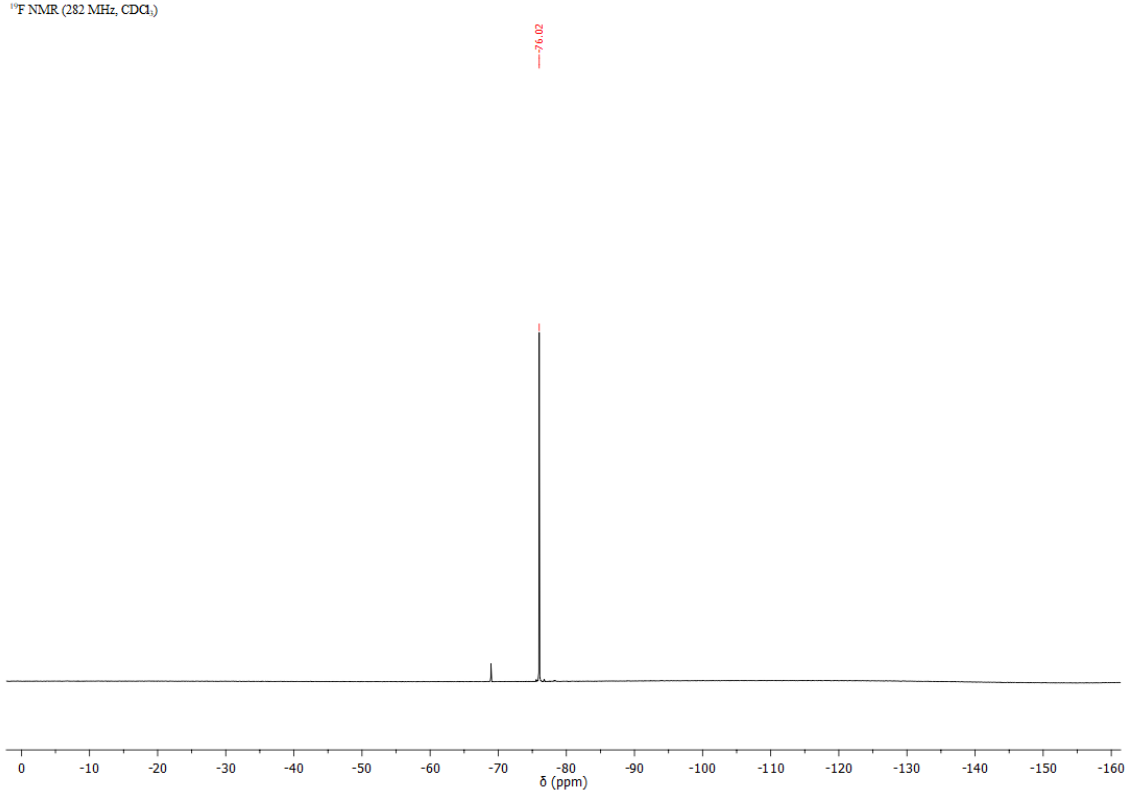

$^{13}$C NMR (125 MHz, $CDCl_3$)



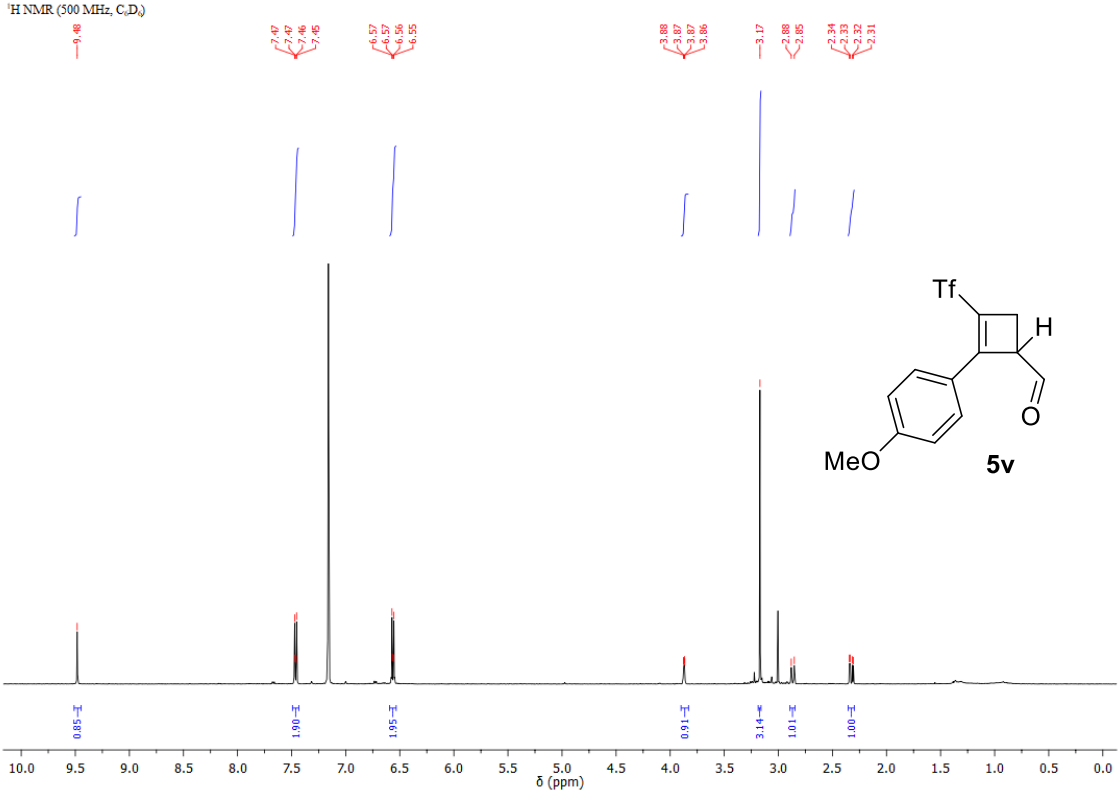
$^{13}$C-DEPT-135 NMR (125 MHz, $CDCl_3$)




$^{19}$F NMR (282 MHz, $CDCl_3$)



$^1$H NMR (500 MHz, $C_5D_5N$)

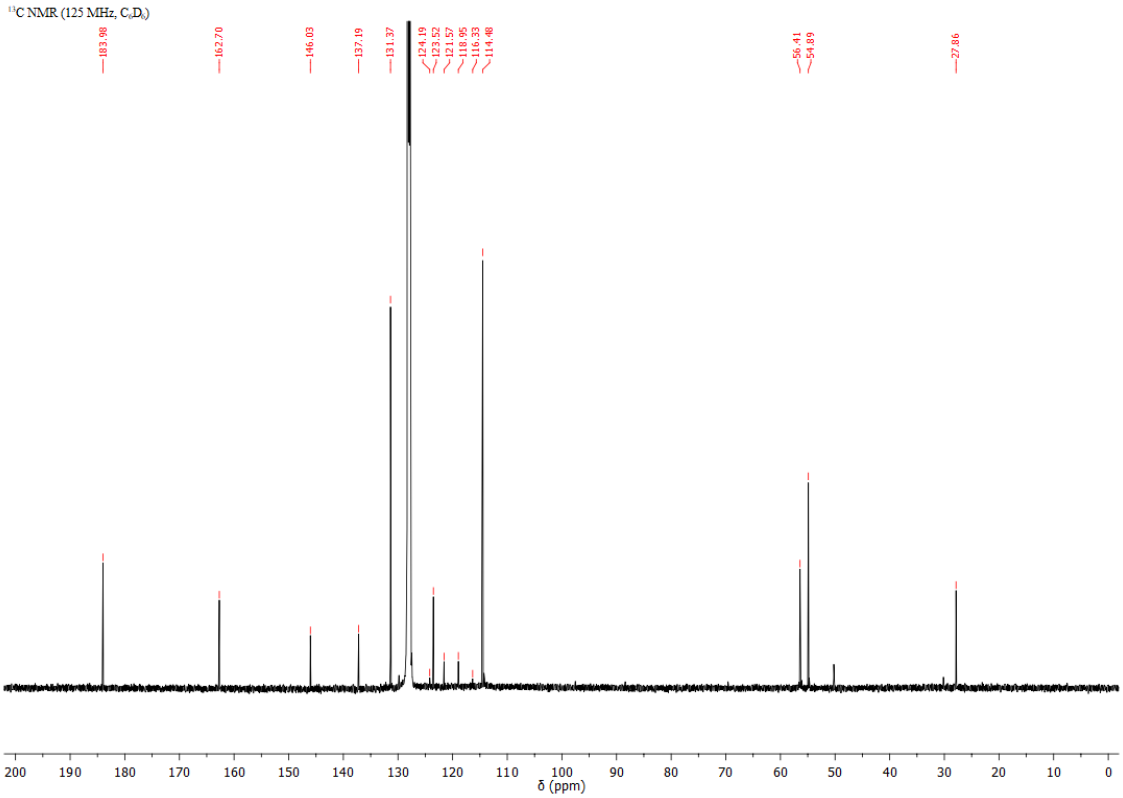




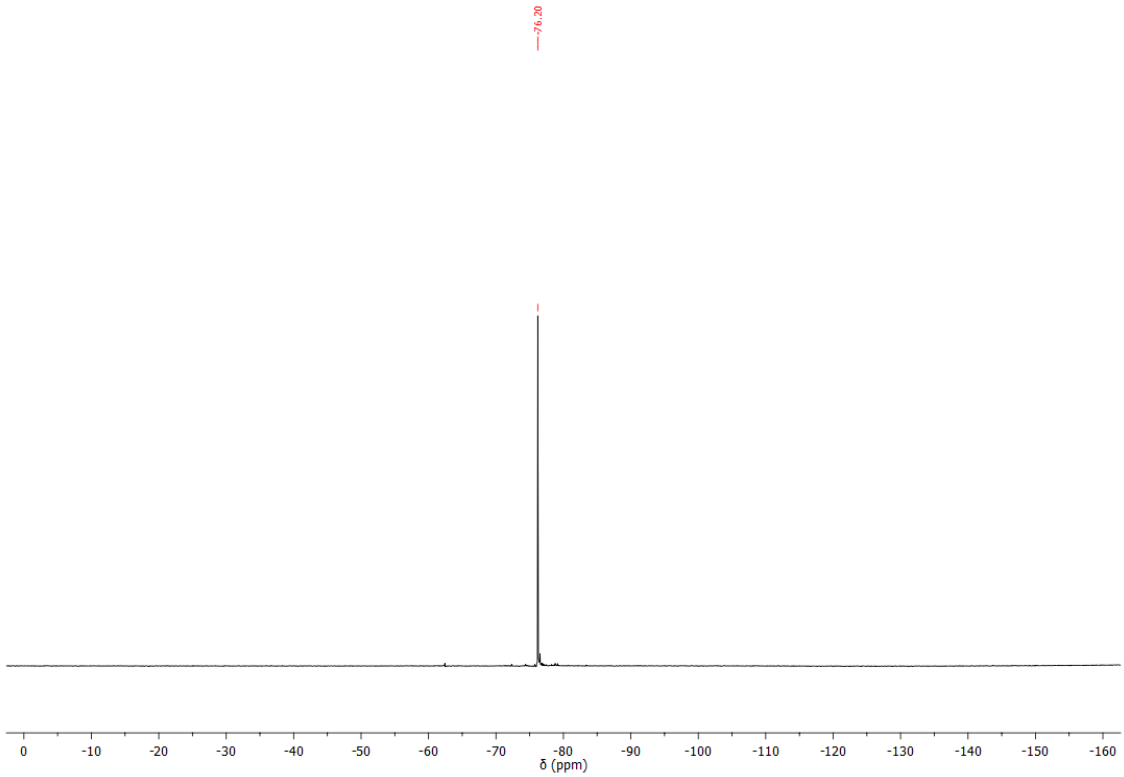


**5v**

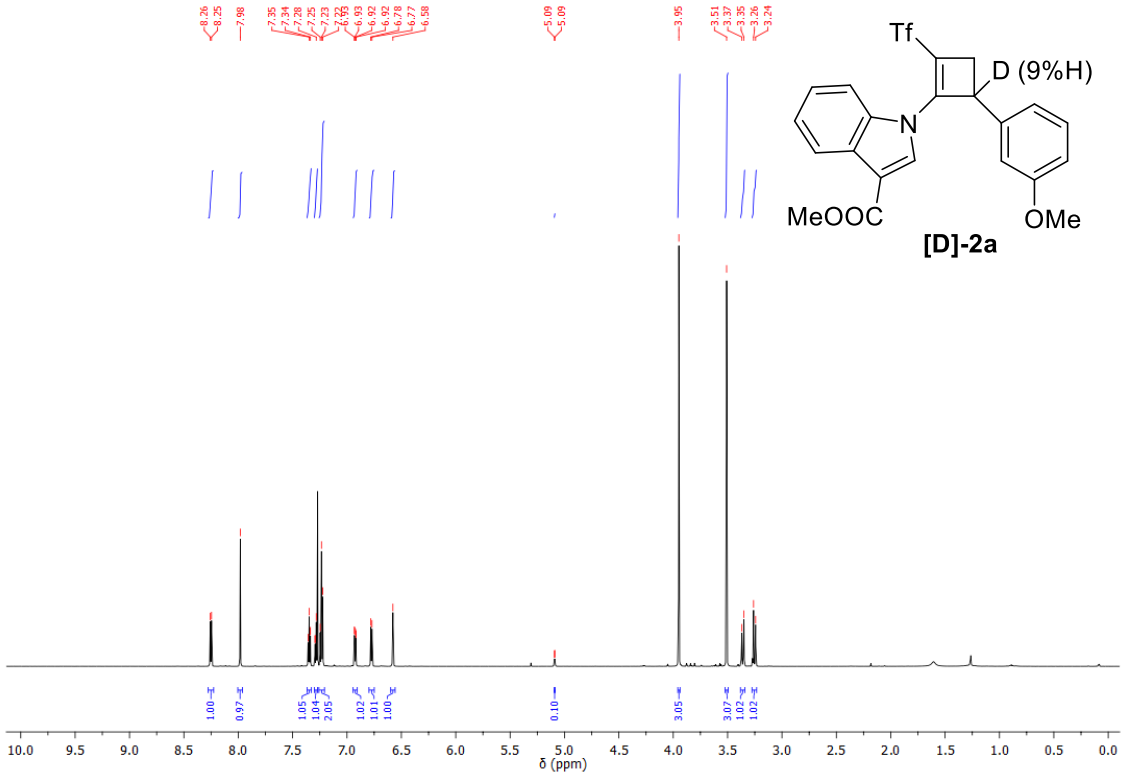
$^{13}$C NMR (125 MHz, $C_5D_5N$)



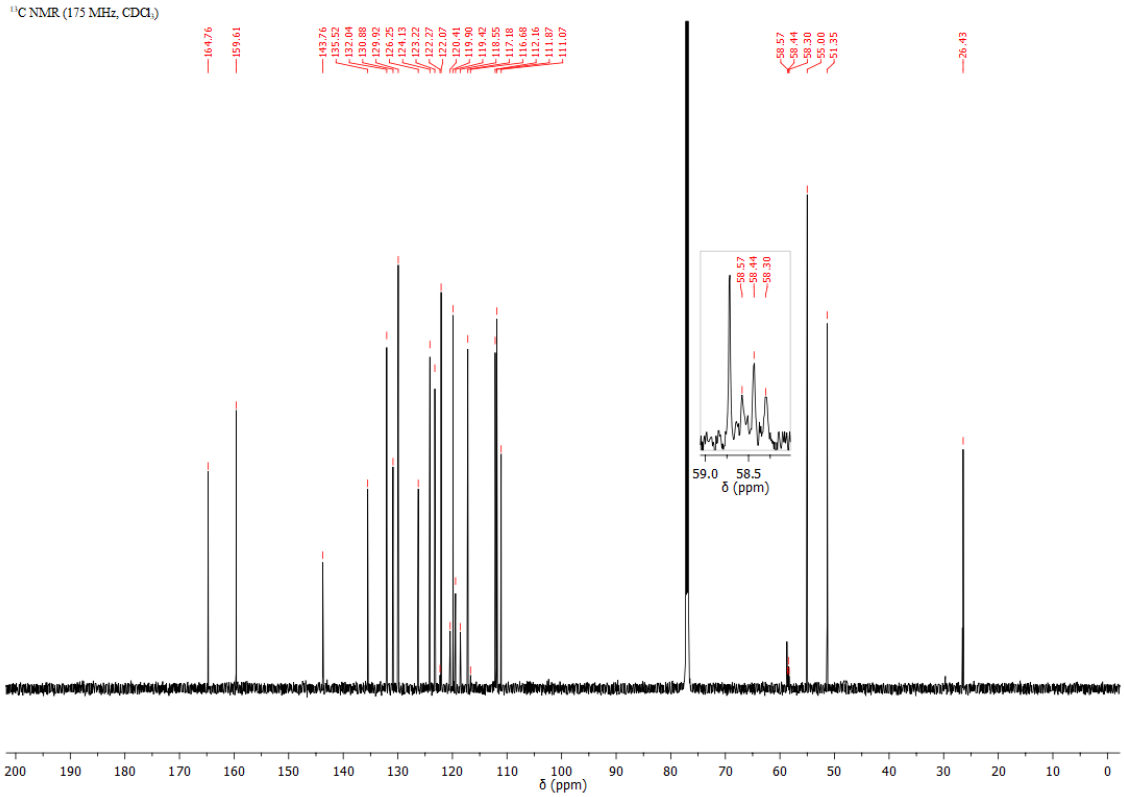
$^{19}$F NMR (282 MHz, $C_6D_6$)



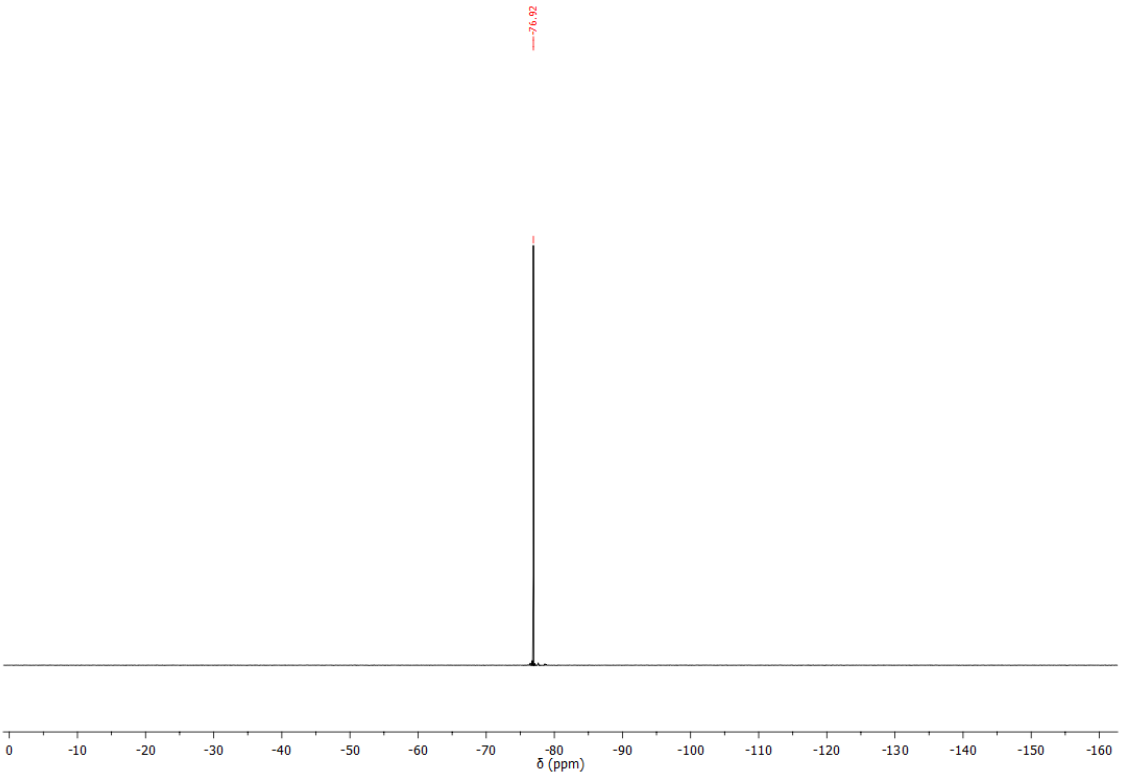
$^1$H NMR (700 MHz, $CDCl_3$)



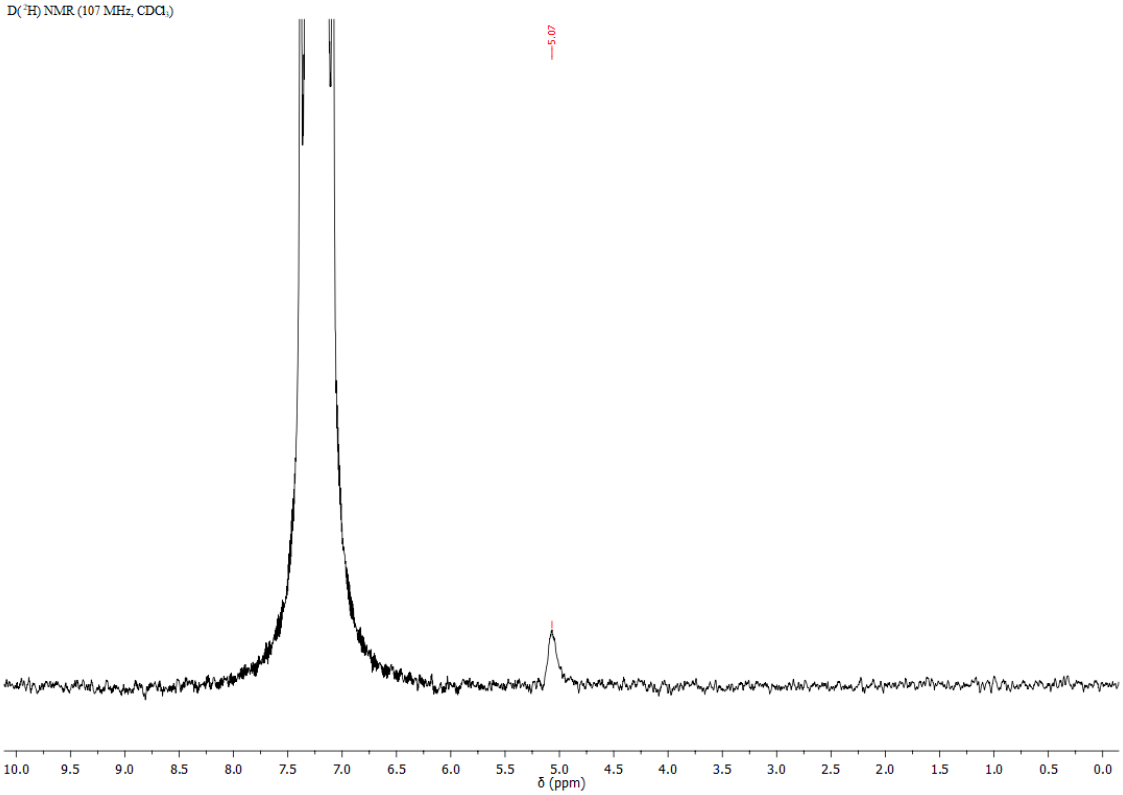

$^{13}$C NMR (175 MHz, $CDCl_3$)



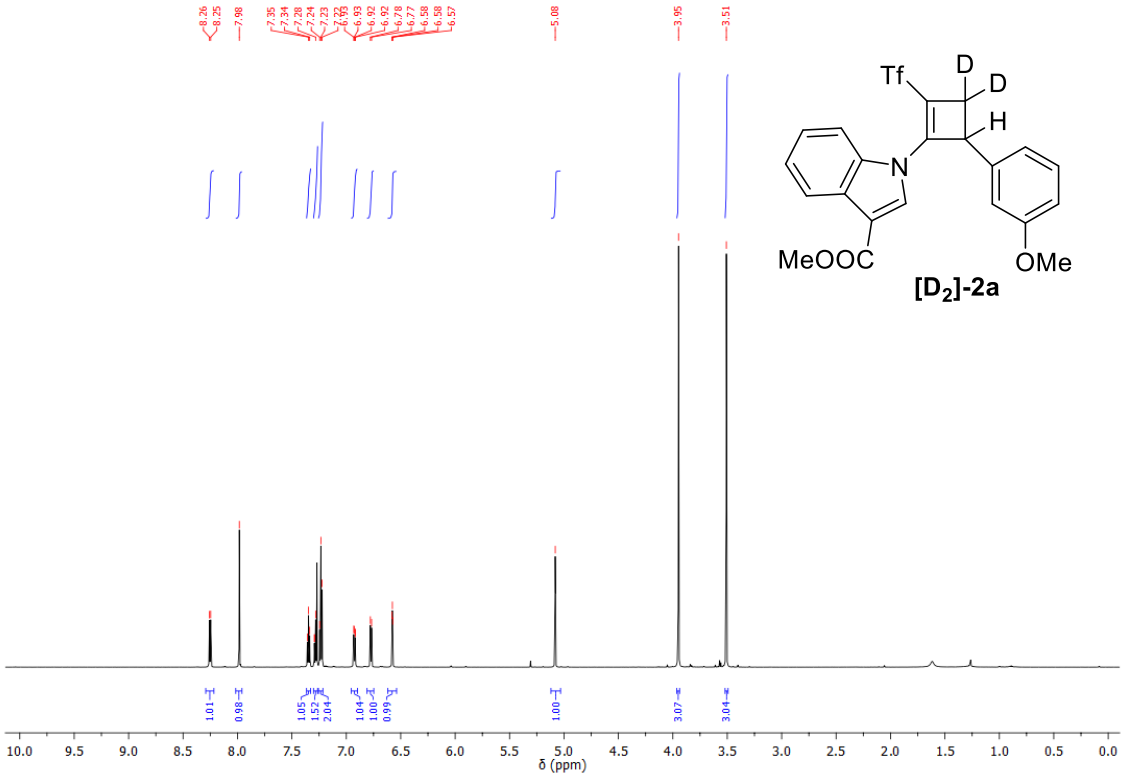
$^{19}$F NMR (282 MHz, $CDCl_3$)




D($^2$H) NMR (107 MHz, $CDCl_3$)



$^1$H NMR (700 MHz, $CDCl_3$)

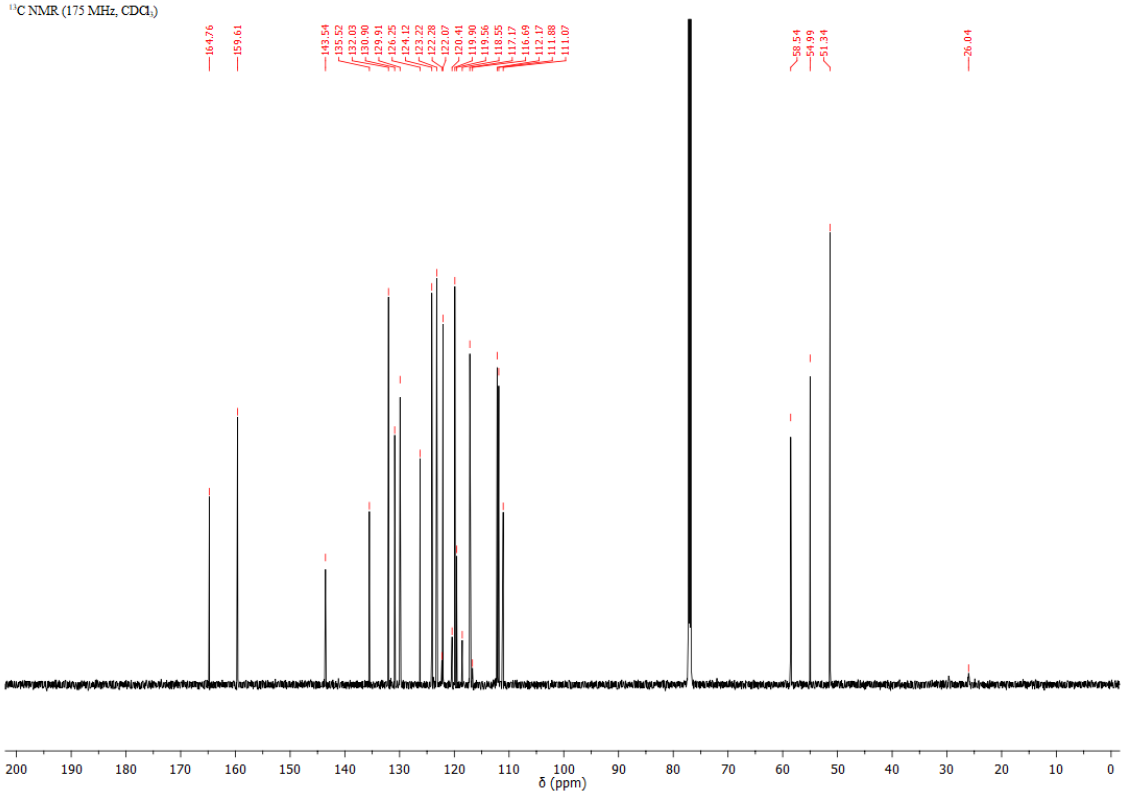




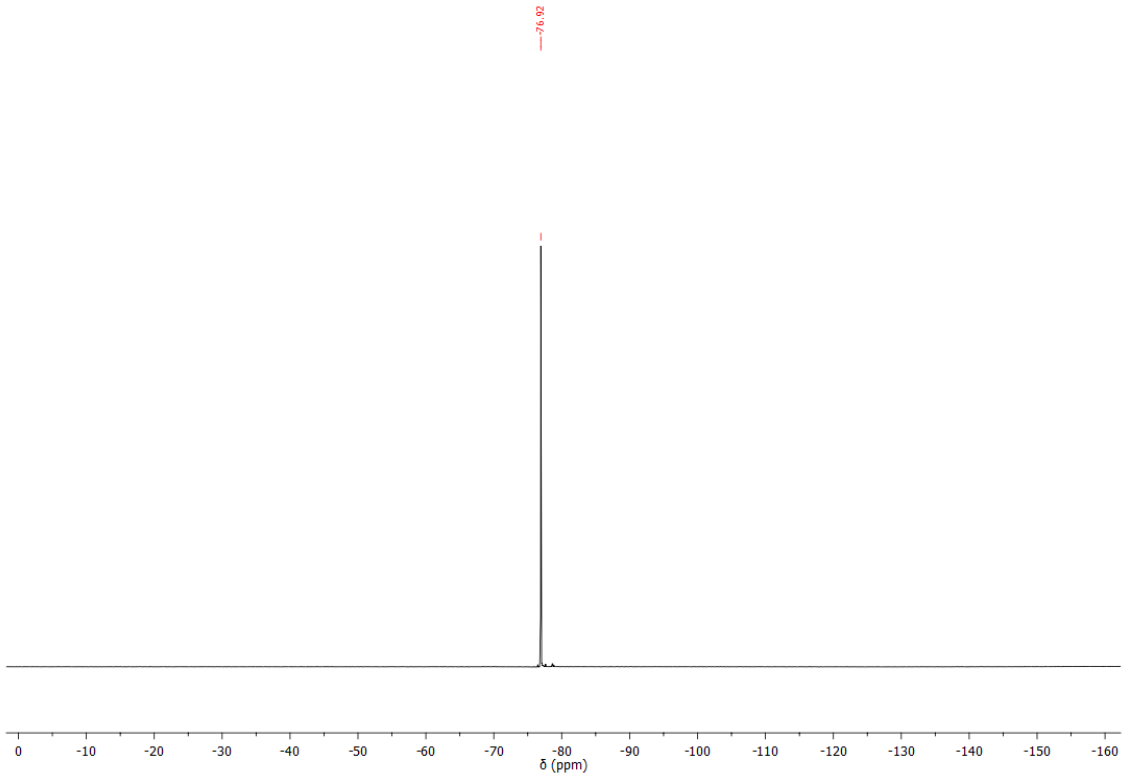


**[$D_2$]-2a**

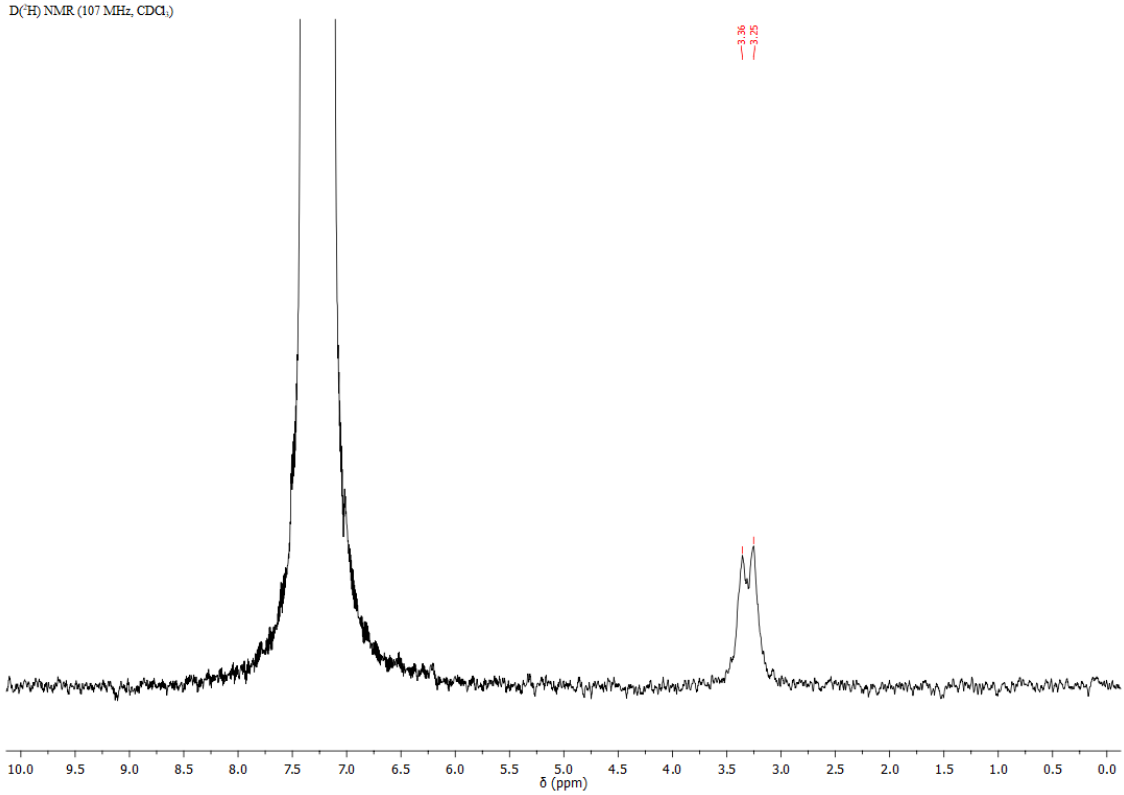
$^{13}$C NMR (175 MHz, $CDCl_3$)



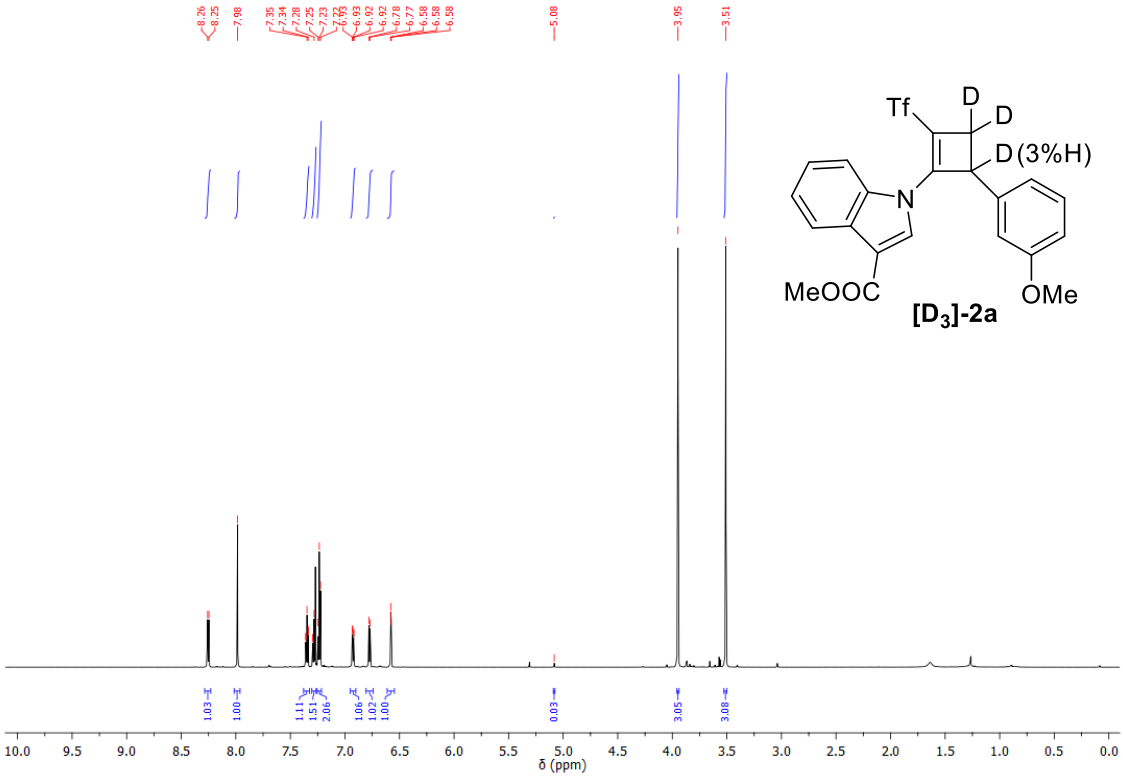
$^{19}$F NMR (282 MHz, $CDCl_3$)




D($^2$H) NMR (107 MHz, $CDCl_3$)



$^1$H NMR (700 MHz, $CDCl_3$)

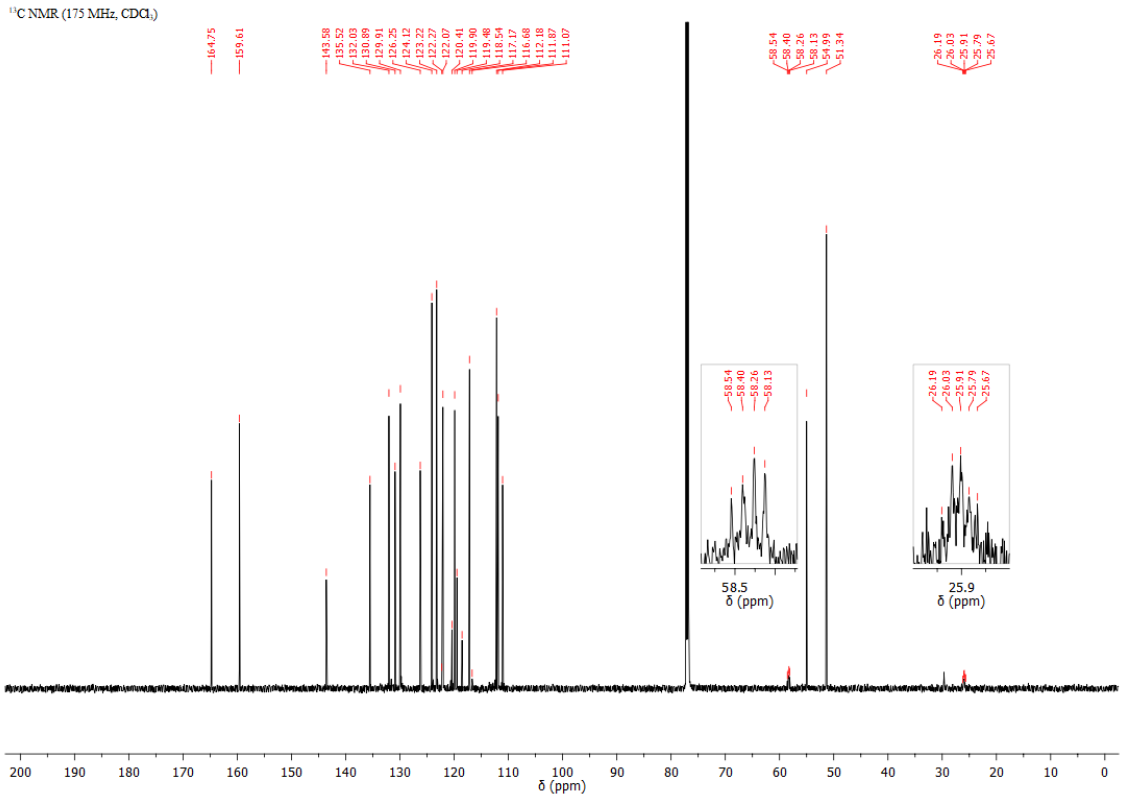




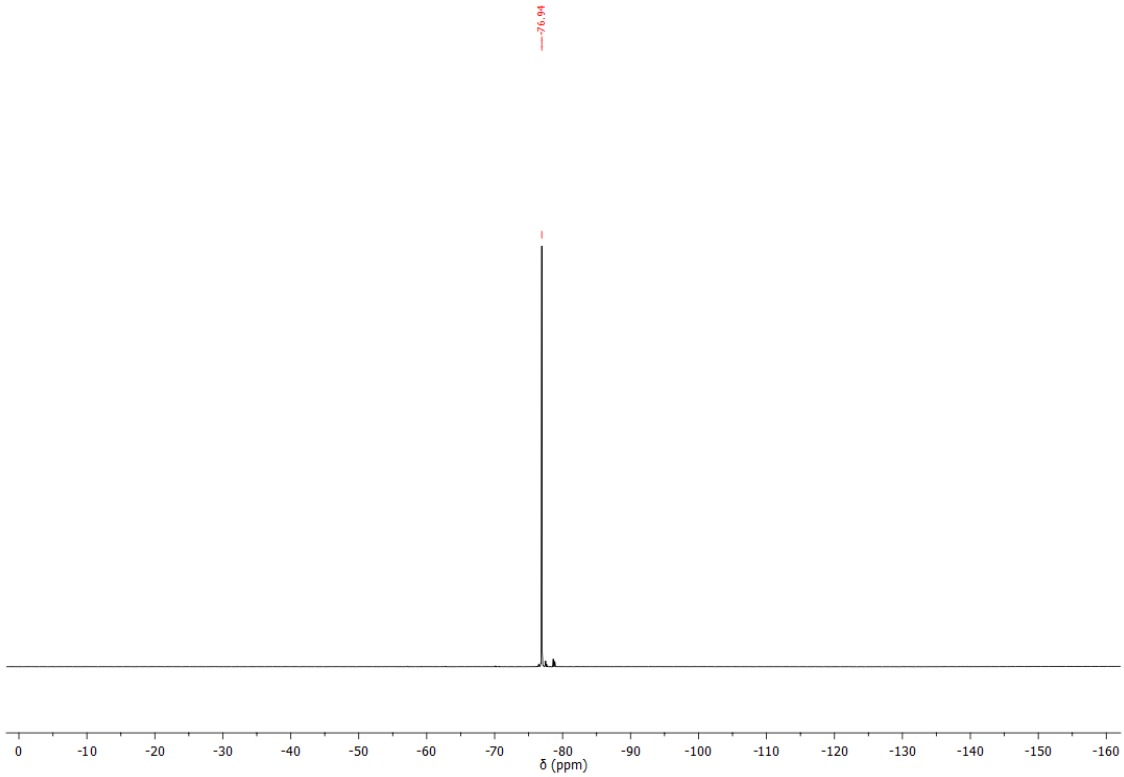


**[$D_3$]-2a**

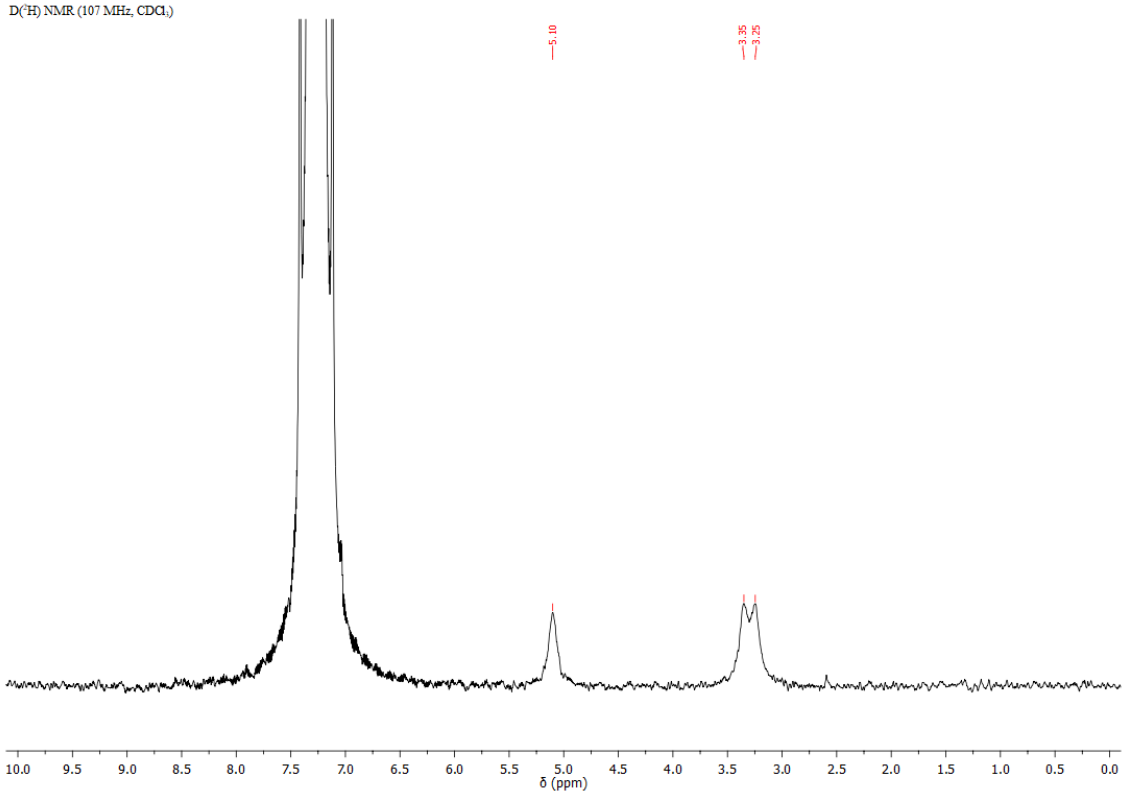
$^{13}$C NMR (175 MHz, $CDCl_3$)



$^{19}$F NMR (282 MHz, $CDCl_3$)




D($^2$H) NMR (107 MHz, $CDCl_3$)



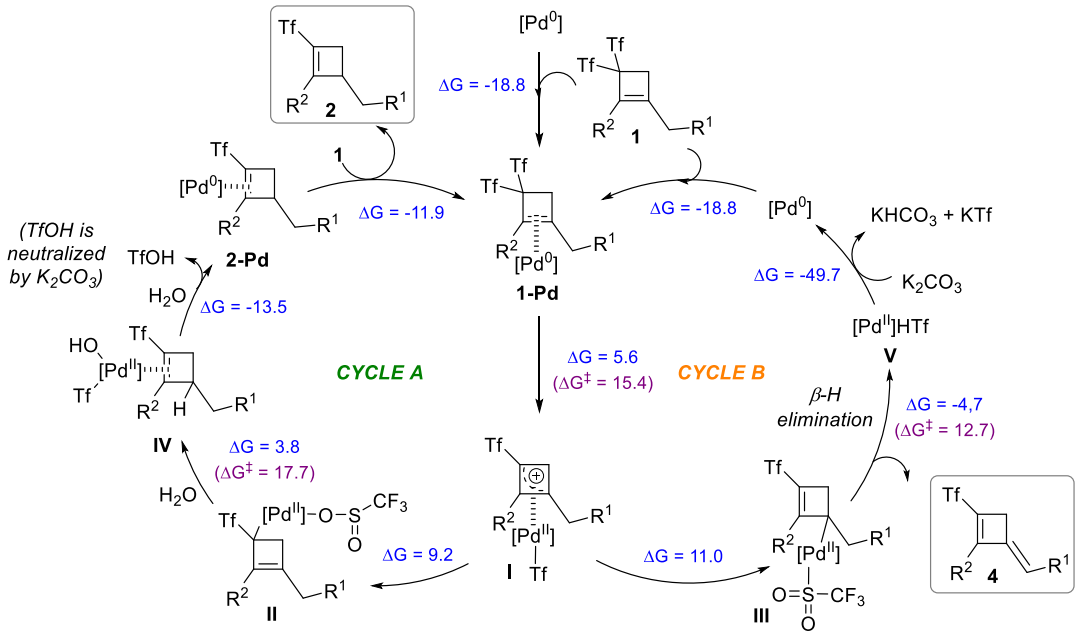
## COMPUTATIONAL METHODS

Calculations were performed with Gaussian 09 at DFT level.[1] The geometries of all complexes here reported were optimized using the B3LYP hybrid functional.[2] Optimizations were carried out using the standard 6-31G(d) basis set for C, H, and N. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double-ζ) basis set, was used for Ni and I.[3] Harmonic frequencies were calculated at the same level to characterize the stationary points and to determine the zero-point energies (ZPE). The starting approximate geometries for the transition states (TS) were graphically located. Intrinsic reaction coordinate (IRC) studies were performed to confirm the relation of the transition states with the corresponding minima.

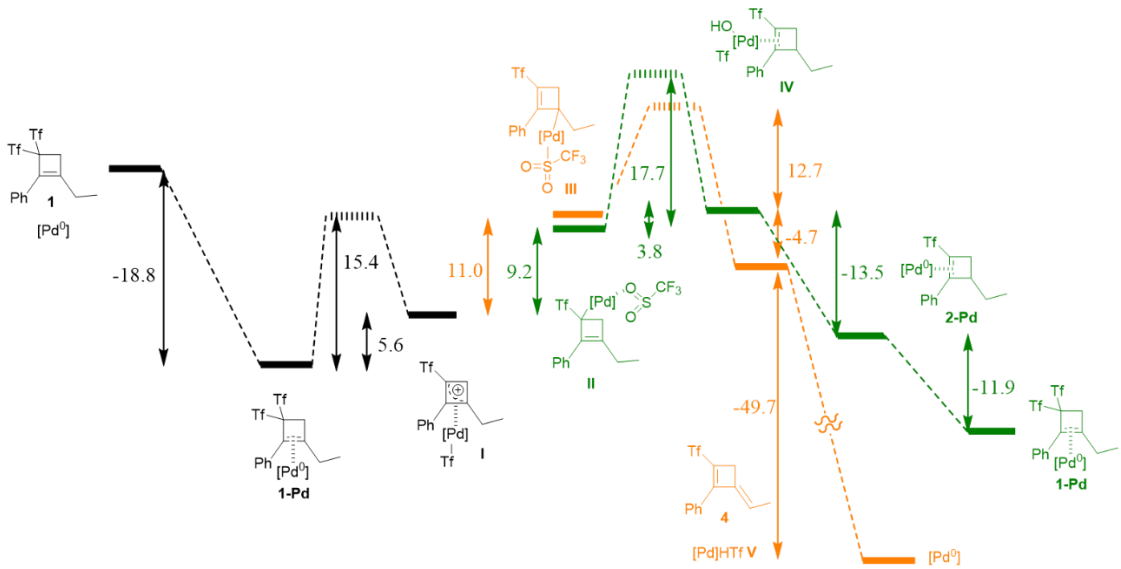
[1] Gaussian 09, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

[2] (a) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627. (b) Kohn, W.; Becke, A. D.; Parr, R. G. *J. Phys. Chem.* **1996**, *100*, 12974-12980. (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 270-283. (d) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 284-298. (e) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299-310.

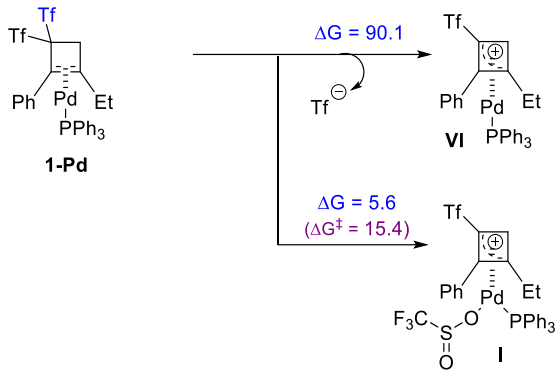
[3] (a) Becke, A. D. *J. Chem. Phys*. **1993**, *98*, 5648- 5653. (b) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098-3100. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789.



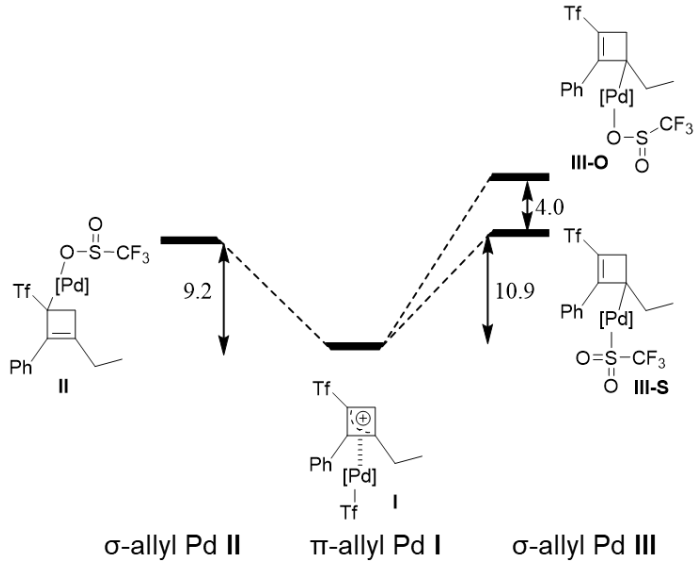

**Supplementary Scheme 1**. Plausible pathways for the formation of (triflyl)cyclobutenes **2** (Cycle A) and **4** (Cycle B). Values of reaction free energies and activation energies (kcal/mol) are calculated at B3LYP/6-31G(d) (C,H,O,S,F,P,K), LANL2DZ (Pd) level in gas phase with $R^1$ = Me, $R^2$ = Ph, [Pd] = $(PPh_3)Pd$.



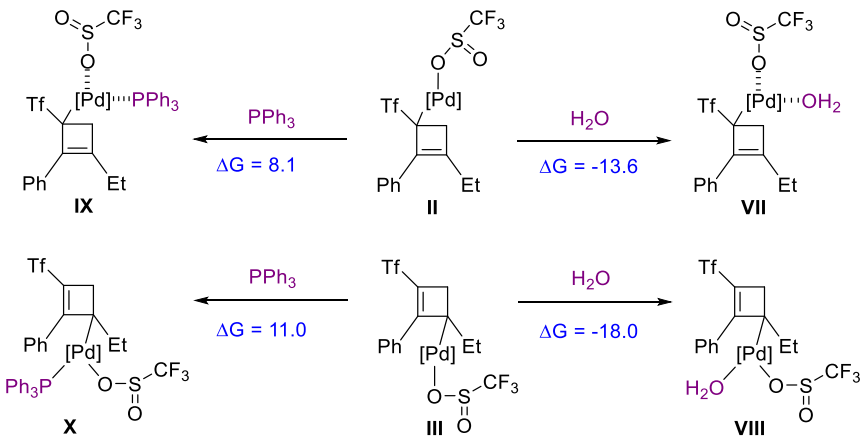

**Supplementary Scheme 2**. Energy profile for the formation of (triflyl)cyclobutenes **2** (Steps for Cycle A depicted in green) and **4** (Steps for Cycle B depicted in orange). Values of reaction free energies and activation energies (kcal/mol) are calculated at B3LYP/6-31G(d) (C,H,O,S,F,P,K), LANL2DZ (Pd) level in gas phase. [Pd] = $(PPh_3)Pd$.



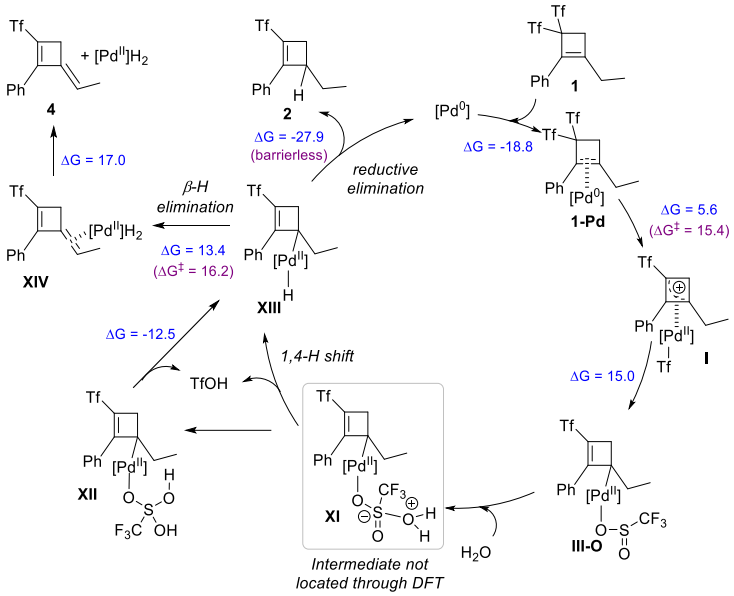

**Supplementary Scheme 3:** Comparison between intra- and intermolecular pathway for the oxidative addition to form π-allyl Pd species **I** and **VI**. Values of reaction free energies and activation energies (kcal/mol) are calculated at B3LYP/6-31G(d) (C,H,O,S,F,P,K), LANL2DZ (Pd) level in gas phase. [Pd] = $(PPh_3)Pd$.



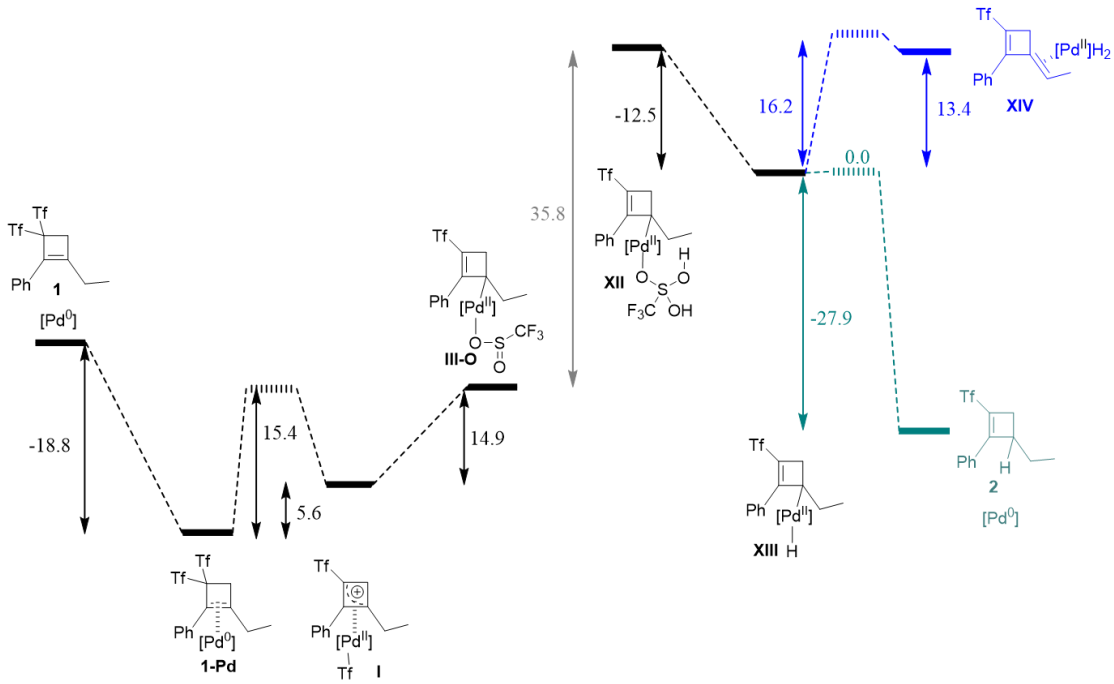

**Supplementary Scheme 4:** Energy scheme for the formation of σ-allyl Pd(II) complexes **II** and **III** from **I**. Sulfur coordinated species **II-S** was not found. Values of reaction free energies (kcal/mol) are calculated at B3LYP/6-31G(d) (C,H,O,S,F,P,K), LANL2DZ (Pd) level in gas phase. [Pd] = $(PPh_3)Pd$.



**Supplementary Scheme 5:** Comparison of coordination to water and $PPh_3$ of σ-allyl Pd(II) complexes **II** and **III.** Values of reaction free energies (kcal/mol) are calculated at B3LYP/6-31G(d) (C,H,O,S,F,P,K), LANL2DZ (Pd) level in gas phase. [$Pd^0$] = ($PPh_3$)Pd.

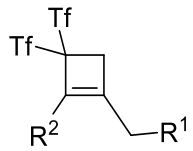



**Supplementary Scheme 6:** Alternative mechanistic proposal for the formation of (triflyl)cyclobutenes **2** (Cycle A) and **4** (Cycle B). Values of reaction free energies and activation energies (kcal/mol) are calculated at B3LYP/6-31G(d) (C,H,O,S,F,P,K), LANL2DZ (Pd) level in gas phase. [$Pd^0$] = ($PPh_3$)Pd.




**Supplementary Scheme 7**. Energy profile for the formation of (triflyl)cyclobutenes **2** and **4**. Values of reaction free energies and activation energies (kcal/mol) are calculated at B3LYP/6-31G(d) (C,H,O,S,F,P,K), LANL2DZ (Pd) level in gas phase. [$Pd^0$] = ($PPh_3$)Pd.

**1**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.709365 | 2.543884 | -0.272232 |
| 2 | 6 | 0 | 0.959186 | 2.118283 | 0.401025 |
| 3 | 6 | 0 | 0.537531 | 0.659254 | 0.038076 |
| 4 | 1 | 0 | 1.280972 | 2.246450 | 1.439510 |
| 5 | 6 | 0 | -0.842087 | 1.211726 | -0.288523 |
| 6 | 6 | 0 | -0.482707 | 2.466163 | 0.065485 |
| 7 | 6 | 0 | -2.067184 | 0.617567 | -0.844877 |
| 8 | 6 | 0 | -4.426720 | -0.425557 | -1.958487 |
| 9 | 6 | 0 | -2.019792 | -0.177230 | -2.003496 |
| 10 | 6 | 0 | -3.313344 | 0.873545 | -0.248171 |
| 11 | 6 | 0 | -4.483533 | 0.358055 | -0.804034 |
| 12 | 6 | 0 | -3.191819 | -0.693464 | -2.553862 |
| 13 | 1 | 0 | -1.061723 | -0.378614 | -2.470965 |
| 14 | 1 | 0 | -3.352118 | 1.447028 | 0.672328 |
| 15 | 1 | 0 | -5.439445 | 0.558795 | -0.327689 |
| 16 | 1 | 0 | -3.140785 | -1.304235 | -3.451357 |
| 17 | 1 | 0 | -5.338966 | -0.830221 | -2.388678 |
| 18 | 6 | 0 | -1.190948 | 3.778629 | 0.109288 |
| 19 | 1 | 0 | -2.184358 | 3.671525 | -0.341297 |
| 20 | 1 | 0 | -0.635067 | 4.500727 | -0.507000 |
| 21 | 6 | 0 | -1.317868 | 4.338487 | 1.539838 |
| 22 | 1 | 0 | -0.333474 | 4.488236 | 1.997208 |
| 23 | 1 | 0 | -1.884904 | 3.654835 | 2.180494 |
| 24 | 1 | 0 | -1.833089 | 5.304808 | 1.527771 |
| 25 | 8 | 0 | 0.744447 | -0.231664 | 1.143355 |
| 26 | 8 | 0 | 1.165637 | 0.091208 | -1.129583 |
| 27 | 16 | 0 | 2.538706 | -0.888001 | -1.201773 |
| 28 | 8 | 0 | 2.531310 | -2.033420 | -0.265535 |
| 29 | 6 | 0 | 3.776057 | 0.333189 | -0.432917 |
| 30 | 9 | 0 | 3.530109 | 0.609874 | 0.847654 |
| 31 | 9 | 0 | 4.982774 | -0.236873 | -0.533008 |
| 32 | 9 | 0 | 3.777967 | 1.471855 | -1.143220 |
| 33 | 16 | 0 | -0.398706 | -1.009108 | 2.091197 |
| 34 | 8 | 0 | -1.596260 | -0.175413 | 2.349780 |
| 35 | 6 | 0 | -1.005809 | -2.334272 | 0.827140 |
| 36 | 9 | 0 | -2.327338 | -2.255627 | 0.705610 |
| 37 | 9 | 0 | -0.680637 | -3.517241 | 1.368426 |
| 38 | 9 | 0 | -0.435459 | -2.238811 | -0.373452 |

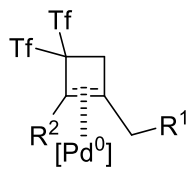
Zero-point correction= 0.252061 (Hartree/Particle)
Thermal correction to Energy= 0.277865
Thermal correction to Enthalpy= 0.278809
Thermal correction to Gibbs Free Energy= 0.193693
Sum of electronic and zero-point Energies= -2236.569080
Sum of electronic and thermal Energies= -2236.543276
Sum of electronic and thermal Enthalpies= -2236.542332
Sum of electronic and thermal Free Energies= -2236.627448

**[$Pd^0$] = $Pd^0$-$PPh_3$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 46 | 0 | -0.019179 | 0.009727 | 2.580038 |
| 2 | 15 | 0 | -0.001488 | 0.000871 | 0.354656 |
| 3 | 6 | 0 | 0.552073 | -1.585635 | -0.424249 |
| 4 | 6 | 0 | 1.313047 | -4.063617 | -1.515358 |
| 5 | 6 | 0 | 0.190918 | -2.787639 | 0.206220 |
| 6 | 6 | 0 | 1.309475 | -1.643392 | -1.604313 |
| 7 | 6 | 0 | 1.688730 | -2.875331 | -2.143510 |
| 8 | 6 | 0 | 0.560728 | -4.016824 | -0.338881 |
| 9 | 1 | 0 | -0.372399 | -2.748890 | 1.135530 |
| 10 | 1 | 0 | 1.611718 | -0.727142 | -2.102145 |
| 11 | 1 | 0 | 2.280343 | -2.903602 | -3.055021 |
| 12 | 1 | 0 | 0.271432 | -4.937612 | 0.160905 |
| 13 | 1 | 0 | 1.611069 | -5.020797 | -1.935153 |
| 14 | 6 | 0 | 1.101381 | 1.265031 | -0.429768 |
| 15 | 6 | 0 | 2.875061 | 3.149733 | -1.529358 |
| 16 | 6 | 0 | 0.785066 | 1.929836 | -1.624543 |
| 17 | 6 | 0 | 2.314827 | 1.565525 | 0.210403 |
| 18 | 6 | 0 | 3.198677 | 2.493995 | -0.338761 |
| 19 | 6 | 0 | 1.666397 | 2.867987 | -2.167906 |
| 20 | 1 | 0 | -0.152730 | 1.721395 | -2.130301 |
| 21 | 1 | 0 | 2.552851 | 1.072747 | 1.150060 |
| 22 | 1 | 0 | 4.134452 | 2.713841 | 0.168474 |
| 23 | 1 | 0 | 1.405087 | 3.379517 | -3.090786 |
| 24 | 1 | 0 | 3.557996 | 3.881728 | -1.952503 |
| 25 | 6 | 0 | -1.642792 | 0.315667 | -0.444295 |
| 26 | 6 | 0 | -4.156071 | 0.897150 | -1.563673 |
| 27 | 6 | 0 | -2.055571 | -0.306546 | -1.632428 |
| 28 | 6 | 0 | -2.511867 | 1.225767 | 0.179444 |
| 29 | 6 | 0 | -3.754793 | 1.521072 | -0.379619 |
| 30 | 6 | 0 | -3.305893 | -0.018412 | -2.185600 |
| 31 | 1 | 0 | -1.404851 | -1.022065 | -2.125683 |
| 32 | 1 | 0 | -2.208500 | 1.689951 | 1.114788 |
| 33 | 1 | 0 | -4.414589 | 2.229068 | 0.115066 |
| 34 | 1 | 0 | -3.614495 | -0.512786 | -3.103215 |
| 35 | 1 | 0 | -5.129190 | 1.117943 | -1.994434 |

| | |
|---|---|
| Zero-point correction= | 0.275503 (Hartree/Particle) |
| Thermal correction to Energy= | 0.293428 |
| Thermal correction to Enthalpy= | 0.294373 |
| Thermal correction to Gibbs Free Energy= | 0.225563 |
| Sum of electronic and zero-point Energies= | -1162.775972 |
| Sum of electronic and thermal Energies= | -1162.758046 |
| Sum of electronic and thermal Enthalpies= | -1162.757102 |
| Sum of electronic and thermal Free Energies= | -1162.825912 |

**1-Pd**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
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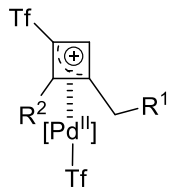
| 5 | 6 | 0 | 1.531758 | -1.146385 | -0.140451 |
| 6 | 6 | 0 | 0.929458 | -1.395397 | -1.397709 |
| 7 | 6 | 0 | 1.808829 | -1.956105 | 1.060814 |
| 8 | 6 | 0 | 2.325570 | -3.500885 | 3.371787 |
| 9 | 6 | 0 | 2.786006 | -1.560445 | 1.994900 |
| 10 | 6 | 0 | 1.101992 | -3.150903 | 1.312057 |
| 11 | 6 | 0 | 1.358432 | -3.910980 | 2.449694 |
| 12 | 6 | 0 | 3.036306 | -2.324347 | 3.135161 |
| 13 | 1 | 0 | 3.376053 | -0.667265 | 1.824224 |
| 14 | 1 | 0 | 0.338504 | -3.478020 | 0.614705 |
| 15 | 1 | 0 | 0.798664 | -4.827493 | 2.617987 |
| 16 | 1 | 0 | 3.796408 | -1.994458 | 3.838139 |
| 17 | 1 | 0 | 2.522789 | -4.093654 | 4.260673 |
| 18 | 6 | 0 | 0.394436 | -2.623916 | -2.087931 |
| 19 | 1 | 0 | -0.217313 | -2.302999 | -2.941012 |
| 20 | 1 | 0 | -0.275462 | -3.182395 | -1.428096 |
| 21 | 6 | 0 | 1.522934 | -3.552083 | -2.585128 |
| 22 | 1 | 0 | 2.124841 | -3.919695 | -1.747428 |
| 23 | 1 | 0 | 2.193042 | -3.034375 | -3.279800 |
| 24 | 1 | 0 | 1.100012 | -4.416607 | -3.108862 |
| 25 | 8 | 0 | 2.068418 | 1.380504 | -0.293812 |
| 26 | 8 | 0 | 3.723517 | -0.223687 | -0.613692 |
| 27 | 16 | 0 | 4.765952 | 0.905457 | -1.350664 |
| 28 | 8 | 0 | 4.990998 | 0.544248 | -2.771874 |
| 29 | 6 | 0 | 6.181597 | 0.108997 | -0.384620 |
| 30 | 9 | 0 | 6.317520 | -1.182628 | -0.667168 |
| 31 | 9 | 0 | 7.299274 | 0.758628 | -0.738022 |
| 32 | 9 | 0 | 5.979944 | 0.272355 | 0.925789 |
| 33 | 16 | 0 | 1.634050 | 1.633935 | 1.323408 |
| 34 | 8 | 0 | 2.813581 | 2.069990 | 2.108670 |
| 35 | 6 | 0 | 0.794035 | 3.246094 | 0.800064 |
| 36 | 9 | 0 | 1.672854 | 4.126202 | 0.333879 |
| 37 | 9 | 0 | 0.207482 | 3.744830 | 1.901881 |
| 38 | 9 | 0 | -0.152745 | 3.019283 | -0.116788 |
| 39 | 46 | 0 | -0.586435 | -0.440473 | -0.060234 |
| 40 | 15 | 0 | -2.888573 | -0.040550 | -0.133389 |
| 41 | 6 | 0 | -3.875923 | -1.591381 | -0.328633 |
| 42 | 6 | 0 | -5.286306 | -4.013711 | -0.536863 |
| 43 | 6 | 0 | -5.044929 | -1.670489 | -1.099653 |
| 44 | 6 | 0 | -3.419642 | -2.744413 | 0.331970 |
| 45 | 6 | 0 | -4.124187 | -3.944242 | 0.235819 |
| 46 | 6 | 0 | -5.742513 | -2.876500 | -1.205055 |
| 47 | 1 | 0 | -5.410376 | -0.792733 | -1.623441 |
| 48 | 1 | 0 | -2.504341 | -2.695204 | 0.917253 |
| 49 | 1 | 0 | -3.760953 | -4.826749 | 0.755864 |
| 50 | 1 | 0 | -6.643338 | -2.924948 | -1.811240 |
| 51 | 1 | 0 | -5.829939 | -4.950868 | -0.621481 |
| 52 | 6 | 0 | -3.616149 | 0.747231 | 1.374735 |
| 53 | 6 | 0 | -4.606765 | 2.014862 | 3.680647 |
| 54 | 6 | 0 | -4.790299 | 0.289607 | 1.990597 |
| 55 | 6 | 0 | -2.942936 | 1.847256 | 1.933008 |
| 56 | 6 | 0 | -3.437805 | 2.479841 | 3.072534 |
| 57 | 6 | 0 | -5.279591 | 0.919689 | 3.137933 |
| 58 | 1 | 0 | -5.323974 | -0.561228 | 1.579250 |
| 59 | 1 | 0 | -2.031836 | 2.213762 | 1.470519 |
| 60 | 1 | 0 | -2.904381 | 3.329997 | 3.489119 |
| 61 | 1 | 0 | -6.188240 | 0.550833 | 3.606563 |

| | | | | | |
|---|---|---|---|---|---|
| 62 | 1 | 0 | -4.987639 | 2.501678 | 4.574387 |
| 63 | 6 | 0 | -3.479762 | 1.041078 | -1.509360 |
| 64 | 6 | 0 | -4.299408 | 2.622738 | -3.682092 |
| 65 | 6 | 0 | -4.603257 | 1.875074 | -1.399128 |
| 66 | 6 | 0 | -2.767347 | 1.018444 | -2.718867 |
| 67 | 6 | 0 | -3.178243 | 1.798137 | -3.800225 |
| 68 | 6 | 0 | -5.008237 | 2.661553 | -2.479866 |
| 69 | 1 | 0 | -5.158897 | 1.917403 | -0.467064 |
| 70 | 1 | 0 | -1.882082 | 0.392949 | -2.801237 |
| 71 | 1 | 0 | -2.616703 | 1.770381 | -4.730234 |
| 72 | 1 | 0 | -5.877010 | 3.306881 | -2.379726 |
| 73 | 1 | 0 | -4.614446 | 3.238180 | -4.520487 |

| | | |
|---|---|---|
| Zero-point correction= | 0.528353 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.574243 | |
| Thermal correction to Enthalpy= | 0.575187 | |
| Thermal correction to Gibbs Free Energy= | 0.437261 | |
| Sum of electronic and zero-point Energies= | -3399.392158 | |
| Sum of electronic and thermal Energies= | -3399.346267 | |
| Sum of electronic and thermal Enthalpies= | -3399.345323 | |
| Sum of electronic and thermal Free Energies= | -3399.483250 | |

**I**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -1.925710 | 2.703827 | -2.624155 |
| 2 | 6 | 0 | -1.336685 | 1.929910 | -2.107742 |
| 3 | 6 | 0 | -1.941105 | 1.555553 | -0.743063 |
| 4 | 1 | 0 | -1.090151 | 1.133668 | -2.811474 |
| 5 | 6 | 0 | -1.083311 | 2.449600 | -0.035373 |
| 6 | 6 | 0 | -0.216945 | 2.514075 | -1.198738 |
| 7 | 6 | 0 | -1.120297 | 3.052379 | 1.296895 |
| 8 | 6 | 0 | -1.231481 | 4.221534 | 3.848036 |
| 9 | 6 | 0 | -2.043332 | 2.590274 | 2.254874 |
| 10 | 6 | 0 | -0.259309 | 4.111416 | 1.635984 |
| 11 | 6 | 0 | -0.316250 | 4.689738 | 2.902666 |
| 12 | 6 | 0 | -2.093309 | 3.171433 | 3.519030 |
| 13 | 1 | 0 | -2.706391 | 1.769645 | 2.002675 |
| 14 | 1 | 0 | 0.449833 | 4.485949 | 0.905215 |
| 15 | 1 | 0 | 0.353045 | 5.509075 | 3.150636 |
| 16 | 1 | 0 | -2.806432 | 2.802089 | 4.250664 |
| 17 | 1 | 0 | -1.274256 | 4.673228 | 4.835312 |
| 18 | 6 | 0 | 0.863654 | 3.470000 | -1.613741 |
| 19 | 1 | 0 | 1.644785 | 3.511578 | -0.846544 |
| 20 | 1 | 0 | 0.425399 | 4.480861 | -1.667168 |
| 21 | 6 | 0 | 1.488984 | 3.124557 | -2.970443 |
| 22 | 1 | 0 | 0.735556 | 3.127285 | -3.766346 |
| 23 | 1 | 0 | 1.957388 | 2.136377 | -2.946831 |
| 24 | 1 | 0 | 2.259220 | 3.856457 | -3.234093 |
| 25 | 8 | 0 | -3.107479 | 1.015430 | -0.370213 |
| 26 | 16 | 0 | -3.486972 | -0.608871 | -1.043028 |
| 27 | 8 | 0 | -2.694591 | -0.823502 | -2.270526 |

| | | | | | |
|---|---|---|---|---|---|
| 28 | 6 | 0 | -5.096293 | 0.136082 | -1.718935 |
| 29 | 9 | 0 | -4.859959 | 1.092713 | -2.617875 |
| 30 | 9 | 0 | -5.775650 | -0.858810 | -2.305051 |
| 31 | 9 | 0 | -5.828222 | 0.630893 | -0.715700 |
| 32 | 46 | 0 | -0.004851 | 0.510609 | -0.309779 |
| 33 | 15 | 0 | 2.227411 | -0.338643 | -0.242808 |
| 34 | 6 | 0 | 2.762333 | -0.747137 | 1.474595 |
| 35 | 6 | 0 | 3.472633 | -1.470184 | 4.092764 |
| 36 | 6 | 0 | 4.113829 | -0.811616 | 1.853319 |
| 37 | 6 | 0 | 1.772190 | -1.033647 | 2.427422 |
| 38 | 6 | 0 | 2.127849 | -1.401386 | 3.726179 |
| 39 | 6 | 0 | 4.464415 | -1.170258 | 3.155489 |
| 40 | 1 | 0 | 4.893914 | -0.568319 | 1.138032 |
| 41 | 1 | 0 | 0.724116 | -0.972344 | 2.155620 |
| 42 | 1 | 0 | 1.346370 | -1.632741 | 4.444206 |
| 43 | 1 | 0 | 5.513199 | -1.214225 | 3.437337 |
| 44 | 1 | 0 | 3.748897 | -1.751731 | 5.105435 |
| 45 | 6 | 0 | 2.384420 | -1.909772 | -1.191983 |
| 46 | 6 | 0 | 2.514176 | -4.298316 | -2.659651 |
| 47 | 6 | 0 | 3.481279 | -2.775844 | -1.045848 |
| 48 | 6 | 0 | 1.352474 | -2.259996 | -2.076404 |
| 49 | 6 | 0 | 1.417440 | -3.449415 | -2.805864 |
| 50 | 6 | 0 | 3.545522 | -3.960187 | -1.778362 |
| 51 | 1 | 0 | 4.279984 | -2.534015 | -0.350996 |
| 52 | 1 | 0 | 0.482056 | -1.616833 | -2.179179 |
| 53 | 1 | 0 | 0.601052 | -3.714182 | -3.471046 |
| 54 | 1 | 0 | 4.396526 | -4.624562 | -1.654110 |
| 55 | 1 | 0 | 2.562212 | -5.227609 | -3.220800 |
| 56 | 6 | 0 | 3.595408 | 0.731420 | -0.865182 |
| 57 | 6 | 0 | 5.585753 | 2.487687 | -1.796787 |
| 58 | 6 | 0 | 4.296041 | 0.452227 | -2.047064 |
| 59 | 6 | 0 | 3.901141 | 1.908463 | -0.158551 |
| 60 | 6 | 0 | 4.892177 | 2.775203 | -0.617343 |
| 61 | 6 | 0 | 5.283386 | 1.327289 | -2.509130 |
| 62 | 1 | 0 | 4.078160 | -0.451845 | -2.606512 |
| 63 | 1 | 0 | 3.370416 | 2.138824 | 0.762051 |
| 64 | 1 | 0 | 5.124036 | 3.674998 | -0.053532 |
| 65 | 1 | 0 | 5.818582 | 1.094656 | -3.425902 |
| 66 | 1 | 0 | 6.356661 | 3.164298 | -2.155290 |
| 67 | 8 | 0 | -1.206128 | -1.082692 | 0.580260 |
| 68 | 16 | 0 | -1.049670 | -2.654054 | 0.624712 |
| 69 | 8 | 0 | -1.967916 | -3.314001 | -0.359084 |
| 70 | 6 | 0 | -1.984407 | -2.831789 | 2.262724 |
| 71 | 9 | 0 | -3.195492 | -2.257975 | 2.222026 |
| 72 | 9 | 0 | -2.138776 | -4.130483 | 2.568718 |
| 73 | 9 | 0 | -1.275857 | -2.253407 | 3.260065 |

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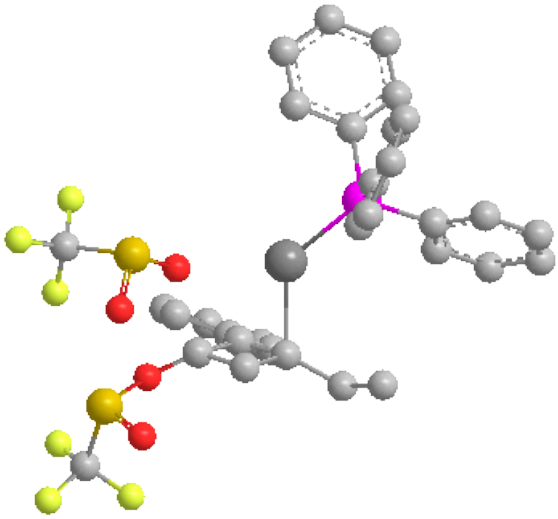
| | |
|---|---|
| Zero-point correction= | 0.527259 (Hartree/Particle) |
| Thermal correction to Energy= | 0.573446 |
| Thermal correction to Enthalpy= | 0.574390 |
| Thermal correction to Gibbs Free Energy= | 0.439463 |
| Sum of electronic and zero-point Energies= | -3399.386511 |
| Sum of electronic and thermal Energies= | -3399.340324 |
| Sum of electronic and thermal Enthalpies= | -3399.339379 |
| Sum of electronic and thermal Free Energies= | -3399.474306 |

**$TS_{1\text{-}I}$**



Imaginary frequency: -187.6530 $cm^{-1}$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.031536 | 0.590094 | -2.765048 |
| 2 | 6 | 0 | -1.418183 | 0.252583 | -1.920894 |
| 3 | 6 | 0 | -2.144605 | 0.386344 | -0.580641 |
| 4 | 1 | 0 | -0.999123 | -0.727798 | -2.143228 |
| 5 | 6 | 0 | -1.224059 | 1.388361 | -0.081781 |
| 6 | 6 | 0 | -0.487866 | 1.338057 | -1.322161 |
| 7 | 6 | 0 | -1.367145 | 2.290824 | 1.065516 |
| 8 | 6 | 0 | -1.681718 | 3.976508 | 3.299620 |
| 9 | 6 | 0 | -2.137612 | 1.881621 | 2.172232 |
| 10 | 6 | 0 | -0.759777 | 3.560050 | 1.100371 |
| 11 | 6 | 0 | -0.916225 | 4.391715 | 2.207403 |
| 12 | 6 | 0 | -2.291256 | 2.719605 | 3.274380 |
| 13 | 1 | 0 | -2.607218 | 0.903388 | 2.162978 |
| 14 | 1 | 0 | -0.172053 | 3.900075 | 0.254046 |
| 15 | 1 | 0 | -0.442792 | 5.370134 | 2.214125 |
| 16 | 1 | 0 | -2.889086 | 2.387287 | 4.118850 |
| 17 | 1 | 0 | -1.803805 | 4.627265 | 4.161114 |
| 18 | 6 | 0 | 0.174878 | 2.409486 | -2.146813 |
| 19 | 1 | 0 | 0.816455 | 3.030172 | -1.513444 |
| 20 | 1 | 0 | -0.620972 | 3.070131 | -2.531439 |
| 21 | 6 | 0 | 0.985419 | 1.867188 | -3.330763 |
| 22 | 1 | 0 | 0.365224 | 1.247404 | -3.988751 |
| 23 | 1 | 0 | 1.828573 | 1.261609 | -2.984896 |
| 24 | 1 | 0 | 1.384623 | 2.692775 | -3.929410 |
| 25 | 8 | 0 | -3.428499 | 0.385801 | -0.325515 |
| 26 | 16 | 0 | -4.594086 | -0.648076 | -1.265736 |
| 27 | 8 | 0 | -4.253368 | -0.635257 | -2.700836 |
| 28 | 6 | 0 | -5.772272 | 0.835627 | -1.112772 |
| 29 | 9 | 0 | -5.307331 | 1.923981 | -1.723393 |
| 30 | 9 | 0 | -6.916333 | 0.456583 | -1.703177 |
| 31 | 9 | 0 | -6.016480 | 1.102067 | 0.172358 |
| 32 | 46 | 0 | 0.725244 | 0.256314 | 0.115938 |
| 33 | 15 | 0 | 2.988466 | -0.208622 | -0.069312 |
| 34 | 6 | 0 | 3.708732 | -0.648537 | 1.575005 |
| 35 | 6 | 0 | 4.676493 | -1.395644 | 4.104070 |
| 36 | 6 | 0 | 4.978942 | -0.232679 | 2.001457 |
| 37 | 6 | 0 | 2.925879 | -1.436298 | 2.436291 |
| 38 | 6 | 0 | 3.409130 | -1.812111 | 3.689285 |
| 39 | 6 | 0 | 5.457846 | -0.604839 | 3.259944 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 1 | 0 | 5.593722 | 0.385625 | 1.354393 |
| 41 | 1 | 0 | 1.933089 | -1.753127 | 2.123736 |
| 42 | 1 | 0 | 2.792075 | -2.421361 | 4.344023 |
| 43 | 1 | 0 | 6.442461 | -0.273926 | 3.579847 |
| 44 | 1 | 0 | 5.050438 | -1.681183 | 5.083611 |
| 45 | 6 | 0 | 3.472791 | -1.629264 | -1.146678 |
| 46 | 6 | 0 | 4.123313 | -3.766309 | -2.850861 |
| 47 | 6 | 0 | 4.603584 | -2.422483 | -0.895223 |
| 48 | 6 | 0 | 2.667765 | -1.928636 | -2.256936 |
| 49 | 6 | 0 | 2.993982 | -2.986098 | -3.107068 |
| 50 | 6 | 0 | 4.925245 | -3.484056 | -1.742978 |
| 51 | 1 | 0 | 5.228496 | -2.218342 | -0.030864 |
| 52 | 1 | 0 | 1.776375 | -1.336086 | -2.444059 |
| 53 | 1 | 0 | 2.359267 | -3.207286 | -3.960845 |
| 54 | 1 | 0 | 5.800163 | -4.093909 | -1.533730 |
| 55 | 1 | 0 | 4.372381 | -4.596390 | -3.506440 |
| 56 | 6 | 0 | 4.047740 | 1.188870 | -0.653788 |
| 57 | 6 | 0 | 5.570924 | 3.408561 | -1.463670 |
| 58 | 6 | 0 | 5.133958 | 1.026922 | -1.526141 |
| 59 | 6 | 0 | 3.729076 | 2.480431 | -0.199823 |
| 60 | 6 | 0 | 4.490481 | 3.580056 | -0.593695 |
| 61 | 6 | 0 | 5.887719 | 2.132423 | -1.930145 |
| 62 | 1 | 0 | 5.391810 | 0.039888 | -1.896746 |
| 63 | 1 | 0 | 2.875220 | 2.617109 | 0.459822 |
| 64 | 1 | 0 | 4.235502 | 4.571705 | -0.229228 |
| 65 | 1 | 0 | 6.723332 | 1.992544 | -2.610916 |
| 66 | 1 | 0 | 6.158429 | 4.266440 | -1.779609 |
| 67 | 8 | 0 | -1.435686 | -1.275052 | 0.465510 |
| 68 | 16 | 0 | -2.084497 | -2.683610 | 0.294234 |
| 69 | 8 | 0 | -3.017539 | -2.682588 | -0.899863 |
| 70 | 6 | 0 | -3.283970 | -2.620159 | 1.762482 |
| 71 | 9 | 0 | -4.076422 | -1.527852 | 1.745293 |
| 72 | 9 | 0 | -4.068768 | -3.708221 | 1.759913 |
| 73 | 9 | 0 | -2.579829 | -2.605480 | 2.906446 |

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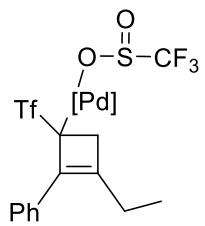
| | |
|---|---|
| Zero-point correction= | 0.525975 (Hartree/Particle) |
| Thermal correction to Energy= | 0.571916 |
| Thermal correction to Enthalpy= | 0.572860 |
| Thermal correction to Gibbs Free Energy= | 0.436176 |
| Sum of electronic and zero-point Energies= | -3399.368847 |
| Sum of electronic and thermal Energies= | -3399.322906 |
| Sum of electronic and thermal Enthalpies= | -3399.321962 |
| Sum of electronic and thermal Free Energies= | -3399.458646 |

**II**

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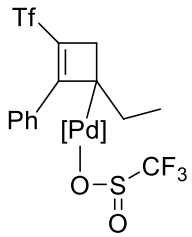
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.640311 | 0.545838 | -1.824833 |
| 2 | 6 | 0 | 2.091371 | -0.135336 | -0.550493 |
| 3 | 1 | 0 | 3.272804 | -0.080503 | -2.458804 |
| 4 | 1 | 0 | 1.882698 | 1.051111 | -2.430029 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | 3.385793 | 1.407650 | -0.804935 |
| 6 | 6 | 0 | 2.970825 | 0.706369 | 0.287610 |
| 7 | 6 | 0 | 3.200819 | 0.780048 | 1.737735 |
| 8 | 6 | 0 | 3.694672 | 0.913081 | 4.498186 |
| 9 | 6 | 0 | 3.069406 | 1.999569 | 2.424148 |
| 10 | 6 | 0 | 3.567513 | -0.373383 | 2.453645 |
| 11 | 6 | 0 | 3.813644 | -0.305153 | 3.824288 |
| 12 | 6 | 0 | 3.319547 | 2.060336 | 3.795794 |
| 13 | 1 | 0 | 2.720270 | 2.875321 | 1.886257 |
| 14 | 1 | 0 | 3.678062 | -1.317319 | 1.927357 |
| 15 | 1 | 0 | 4.103064 | -1.202132 | 4.365838 |
| 16 | 1 | 0 | 3.208961 | 3.006894 | 4.318303 |
| 17 | 1 | 0 | 3.887298 | 0.965412 | 5.566660 |
| 18 | 46 | 0 | 0.099128 | -0.094180 | -0.222080 |
| 19 | 15 | 0 | -2.230992 | -0.795298 | 0.234867 |
| 20 | 6 | 0 | -3.541127 | -0.087114 | -0.843932 |
| 21 | 6 | 0 | -5.474942 | 1.060817 | -2.517367 |
| 22 | 6 | 0 | -4.907896 | -0.328948 | -0.620197 |
| 23 | 6 | 0 | -3.155164 | 0.747003 | -1.903354 |
| 24 | 6 | 0 | -4.121926 | 1.317957 | -2.735649 |
| 25 | 6 | 0 | -5.867744 | 0.238082 | -1.456614 |
| 26 | 1 | 0 | -5.221312 | -0.952698 | 0.212401 |
| 27 | 1 | 0 | -2.105297 | 0.977196 | -2.054821 |
| 28 | 1 | 0 | -3.811479 | 1.975119 | -3.542758 |
| 29 | 1 | 0 | -6.922193 | 0.045812 | -1.276823 |
| 30 | 1 | 0 | -6.225847 | 1.508485 | -3.163041 |
| 31 | 6 | 0 | -2.326293 | -2.624452 | -0.001986 |
| 32 | 6 | 0 | -2.243401 | -5.411316 | -0.381823 |
| 33 | 6 | 0 | -3.107157 | -3.231951 | -0.995132 |
| 34 | 6 | 0 | -1.493557 | -3.434124 | 0.793415 |
| 35 | 6 | 0 | -1.459593 | -4.815763 | 0.611017 |
| 36 | 6 | 0 | -3.062104 | -4.616419 | -1.183675 |
| 37 | 1 | 0 | -3.750872 | -2.627075 | -1.625218 |
| 38 | 1 | 0 | -0.874535 | -2.981505 | 1.565045 |
| 39 | 1 | 0 | -0.819619 | -5.426991 | 1.241954 |
| 40 | 1 | 0 | -3.672293 | -5.070922 | -1.959611 |
| 41 | 1 | 0 | -2.212925 | -6.487459 | -0.528902 |
| 42 | 6 | 0 | -2.863401 | -0.519034 | 1.945247 |
| 43 | 6 | 0 | -3.792881 | 0.059103 | 4.530288 |
| 44 | 6 | 0 | -3.606993 | -1.468957 | 2.661497 |
| 45 | 6 | 0 | -2.586660 | 0.723201 | 2.540749 |
| 46 | 6 | 0 | -3.054458 | 1.010636 | 3.822847 |
| 47 | 6 | 0 | -4.066762 | -1.179664 | 3.948147 |
| 48 | 1 | 0 | -3.821027 | -2.438411 | 2.221890 |
| 49 | 1 | 0 | -2.009864 | 1.468299 | 1.998097 |
| 50 | 1 | 0 | -2.833409 | 1.975394 | 4.271003 |
| 51 | 1 | 0 | -4.638915 | -1.924827 | 4.494711 |
| 52 | 1 | 0 | -4.149778 | 0.280930 | 5.532430 |
| 53 | 8 | 0 | -0.035472 | 1.903084 | -0.944171 |
| 54 | 16 | 0 | -0.377682 | 3.046152 | 0.093741 |
| 55 | 8 | 0 | 0.850713 | 3.719199 | 0.635988 |
| 56 | 6 | 0 | -0.952656 | 4.262963 | -1.234981 |
| 57 | 9 | 0 | -1.287801 | 5.425657 | -0.651538 |
| 58 | 9 | 0 | -0.001904 | 4.499515 | -2.146060 |
| 59 | 9 | 0 | -2.042682 | 3.782767 | -1.864712 |
| 60 | 1 | 0 | 5.100077 | 2.324443 | -1.641854 |
| 61 | 8 | 0 | 1.928932 | -1.534944 | -0.269570 |
| 62 | 16 | 0 | 2.010324 | -2.803726 | -1.438849 |
| 63 | 8 | 0 | 1.875630 | -2.303439 | -2.822782 |
| 64 | 6 | 0 | 3.878253 | -3.035689 | -1.166002 |
| 65 | 9 | 0 | 4.265238 | -4.053643 | -1.941104 |

| | | | | | |
|---|---|---|---|---|---|
| 66 | 9 | 0 | 4.582293 | -1.949209 | -1.476244 |
| 67 | 9 | 0 | 4.085077 | -3.355661 | 0.116105 |
| 68 | 6 | 0 | 4.243764 | 2.608890 | -1.010703 |
| 69 | 1 | 0 | 4.651220 | 2.928714 | -0.044858 |
| 70 | 6 | 0 | 3.488165 | 3.775076 | -1.681313 |
| 71 | 1 | 0 | 3.122527 | 3.489123 | -2.673876 |
| 72 | 1 | 0 | 4.159381 | 4.632432 | -1.804184 |
| 73 | 1 | 0 | 2.629091 | 4.076152 | -1.076252 |

Zero-point correction= 0.527095 (Hartree/Particle)
Thermal correction to Energy= 0.573547
Thermal correction to Enthalpy= 0.574491
Thermal correction to Gibbs Free Energy= 0.437326
Sum of electronic and zero-point Energies= -3399.369915
Sum of electronic and thermal Energies= -3399.323463
Sum of electronic and thermal Enthalpies= -3399.322519
Sum of electronic and thermal Free Energies= -3399.459684

**III-O**



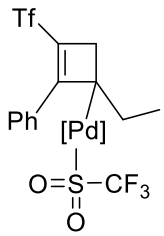

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.446377 | 0.196024 | -1.509325 |
| 2 | 6 | 0 | 1.535339 | -0.910853 | -0.916969 |
| 3 | 1 | 0 | 2.910953 | -0.049658 | -2.470576 |
| 4 | 1 | 0 | 1.991997 | 1.190851 | -1.538285 |
| 5 | 6 | 0 | 3.261459 | -0.082719 | -0.262535 |
| 6 | 6 | 0 | 2.449567 | -1.041534 | 0.254885 |
| 7 | 6 | 0 | 2.416886 | -1.856391 | 1.471425 |
| 8 | 6 | 0 | 2.328699 | -3.421332 | 3.804572 |
| 9 | 6 | 0 | 3.595860 | -2.398008 | 2.012238 |
| 10 | 6 | 0 | 1.194378 | -2.114755 | 2.116070 |
| 11 | 6 | 0 | 1.151206 | -2.890148 | 3.272643 |
| 12 | 6 | 0 | 3.548080 | -3.171884 | 3.171103 |
| 13 | 1 | 0 | 4.542064 | -2.235404 | 1.506106 |
| 14 | 1 | 0 | 0.281663 | -1.671578 | 1.723166 |
| 15 | 1 | 0 | 0.198726 | -3.069854 | 3.763989 |
| 16 | 1 | 0 | 4.467071 | -3.587427 | 3.575923 |
| 17 | 1 | 0 | 2.295661 | -4.025722 | 4.707183 |
| 18 | 6 | 0 | 0.891907 | -2.013330 | -1.692314 |
| 19 | 1 | 0 | 0.966101 | -1.815493 | -2.766460 |
| 20 | 1 | 0 | -0.269591 | -1.974318 | -1.521979 |
| 21 | 6 | 0 | 1.278724 | -3.458468 | -1.347706 |
| 22 | 1 | 0 | 1.115586 | -3.675422 | -0.289803 |
| 23 | 1 | 0 | 2.340544 | -3.616237 | -1.564235 |
| 24 | 1 | 0 | 0.695682 | -4.166634 | -1.945540 |
| 25 | 8 | 0 | 4.353244 | 0.567641 | 0.247857 |
| 26 | 16 | 0 | 5.940610 | 0.085637 | -0.153807 |
| 27 | 8 | 0 | 6.025758 | -1.384872 | -0.328194 |
| 28 | 6 | 0 | 5.928889 | 0.733692 | -1.947502 |
| 29 | 9 | 0 | 7.208328 | 0.953673 | -2.281063 |
| 30 | 9 | 0 | 5.413183 | -0.173208 | -2.779387 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 9 | 0 | 5.248466 | 1.875548 | -2.044250 |
| 32 | 46 | 0 | -0.439938 | -0.343956 | -0.557912 |
| 33 | 15 | 0 | -2.895998 | -0.220834 | -0.422659 |
| 34 | 6 | 0 | -3.676488 | 1.439784 | -0.540405 |
| 35 | 6 | 0 | -4.802411 | 4.000450 | -0.707855 |
| 36 | 6 | 0 | -5.044757 | 1.632128 | -0.279585 |
| 37 | 6 | 0 | -2.876381 | 2.543062 | -0.870400 |
| 38 | 6 | 0 | -3.441392 | 3.819078 | -0.950952 |
| 39 | 6 | 0 | -5.604268 | 2.905278 | -0.369719 |
| 40 | 1 | 0 | -5.668854 | 0.788243 | 0.001573 |
| 41 | 1 | 0 | -1.809777 | 2.410399 | -1.018931 |
| 42 | 1 | 0 | -2.807669 | 4.668972 | -1.186493 |
| 43 | 1 | 0 | -6.662759 | 3.045612 | -0.167195 |
| 44 | 1 | 0 | -5.238915 | 4.993972 | -0.767540 |
| 45 | 6 | 0 | -3.667356 | -1.216769 | -1.774310 |
| 46 | 6 | 0 | -4.668833 | -2.794847 | -3.879040 |
| 47 | 6 | 0 | -4.496664 | -0.655205 | -2.755046 |
| 48 | 6 | 0 | -3.339759 | -2.581775 | -1.869640 |
| 49 | 6 | 0 | -3.843506 | -3.366024 | -2.905806 |
| 50 | 6 | 0 | -4.989236 | -1.440091 | -3.801847 |
| 51 | 1 | 0 | -4.759724 | 0.396070 | -2.706342 |
| 52 | 1 | 0 | -2.693318 | -3.037004 | -1.122302 |
| 53 | 1 | 0 | -3.587986 | -4.421110 | -2.956789 |
| 54 | 1 | 0 | -5.627095 | -0.986674 | -4.555850 |
| 55 | 1 | 0 | -5.055258 | -3.403073 | -4.692216 |
| 56 | 6 | 0 | -3.607083 | -0.913333 | 1.135193 |
| 57 | 6 | 0 | -4.579026 | -1.860353 | 3.594012 |
| 58 | 6 | 0 | -4.643404 | -1.857074 | 1.172767 |
| 59 | 6 | 0 | -3.063581 | -0.446769 | 2.344995 |
| 60 | 6 | 0 | -3.550598 | -0.914534 | 3.564729 |
| 61 | 6 | 0 | -5.123093 | -2.328727 | 2.397689 |
| 62 | 1 | 0 | -5.076213 | -2.230678 | 0.250124 |
| 63 | 1 | 0 | -2.266452 | 0.292685 | 2.331718 |
| 64 | 1 | 0 | -3.122336 | -0.542376 | 4.491360 |
| 65 | 1 | 0 | -5.925236 | -3.061997 | 2.413110 |
| 66 | 1 | 0 | -4.953458 | -2.229647 | 4.544939 |
| 67 | 8 | 0 | 0.154261 | 1.589265 | 0.068916 |
| 68 | 16 | 0 | 0.027186 | 1.917019 | 1.618433 |
| 69 | 8 | 0 | 1.196810 | 1.423981 | 2.408359 |
| 70 | 6 | 0 | 0.398956 | 3.755540 | 1.365844 |
| 71 | 9 | 0 | 0.433831 | 4.365168 | 2.562934 |
| 72 | 9 | 0 | 1.566517 | 3.958328 | 0.747750 |
| 73 | 9 | 0 | -0.579276 | 4.331234 | 0.635396 |

---

Zero-point correction= 0.525629 (Hartree/Particle)
Thermal correction to Energy= 0.571959
Thermal correction to Enthalpy= 0.572904
Thermal correction to Gibbs Free Energy= 0.434192
Sum of electronic and zero-point Energies= -3399.359007
Sum of electronic and thermal Energies= -3399.312676
Sum of electronic and thermal Enthalpies= -3399.311732
Sum of electronic and thermal Free Energies= -3399.450444

**III-S**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.735935 | -1.001925 | 0.772191 |
| 2 | 6 | 0 | 1.608217 | 0.068540 | 0.885421 |
| 3 | 1 | 0 | 3.276299 | -1.182037 | 1.708595 |
| 4 | 1 | 0 | 2.462407 | -1.954309 | 0.315186 |
| 5 | 6 | 0 | 3.349509 | 0.008720 | -0.166294 |
| 6 | 6 | 0 | 2.372057 | 0.944822 | -0.061715 |
| 7 | 6 | 0 | 2.128464 | 2.271601 | -0.636133 |
| 8 | 6 | 0 | 1.658311 | 4.817443 | -1.741033 |
| 9 | 6 | 0 | 3.184068 | 3.187886 | -0.799855 |
| 10 | 6 | 0 | 0.835261 | 2.657680 | -1.031658 |
| 11 | 6 | 0 | 0.602289 | 3.917850 | -1.580787 |
| 12 | 6 | 0 | 2.947171 | 4.447144 | -1.348735 |
| 13 | 1 | 0 | 4.181765 | 2.919603 | -0.467313 |
| 14 | 1 | 0 | 0.014750 | 1.947736 | -0.943730 |
| 15 | 1 | 0 | -0.402619 | 4.187373 | -1.894579 |
| 16 | 1 | 0 | 3.772721 | 5.144551 | -1.463849 |
| 17 | 1 | 0 | 1.478811 | 5.799998 | -2.169320 |
| 18 | 6 | 0 | 1.102752 | 0.534129 | 2.241768 |
| 19 | 1 | 0 | 1.157769 | -0.302656 | 2.946522 |
| 20 | 1 | 0 | 0.003510 | 0.787937 | 2.191912 |
| 21 | 6 | 0 | 1.797461 | 1.782368 | 2.817570 |
| 22 | 1 | 0 | 1.659022 | 2.649329 | 2.166132 |
| 23 | 1 | 0 | 2.873967 | 1.603833 | 2.912890 |
| 24 | 1 | 0 | 1.396093 | 2.022336 | 3.807800 |
| 25 | 8 | 0 | 4.454729 | -0.075630 | -0.975695 |
| 26 | 16 | 0 | 6.002803 | 0.332674 | -0.390511 |
| 27 | 8 | 0 | 5.926834 | 1.449289 | 0.583636 |
| 28 | 6 | 0 | 6.250880 | -1.197705 | 0.723880 |
| 29 | 9 | 0 | 7.575021 | -1.388679 | 0.810851 |
| 30 | 9 | 0 | 5.763123 | -0.980839 | 1.946389 |
| 31 | 9 | 0 | 5.685836 | -2.282519 | 0.195672 |
| 32 | 46 | 0 | -0.378298 | -0.255477 | 0.348248 |
| 33 | 15 | 0 | -2.838493 | 0.092562 | 0.224434 |
| 34 | 6 | 0 | -4.000136 | -1.308593 | -0.034510 |
| 35 | 6 | 0 | -5.739676 | -3.484122 | -0.355617 |
| 36 | 6 | 0 | -5.299206 | -1.111220 | -0.529179 |
| 37 | 6 | 0 | -3.579187 | -2.606665 | 0.287172 |
| 38 | 6 | 0 | -4.448033 | -3.688151 | 0.131641 |
| 39 | 6 | 0 | -6.162954 | -2.194729 | -0.687794 |
| 40 | 1 | 0 | -5.633012 | -0.113676 | -0.798759 |
| 41 | 1 | 0 | -2.568737 | -2.775413 | 0.643331 |
| 42 | 1 | 0 | -4.108077 | -4.690268 | 0.377559 |
| 43 | 1 | 0 | -7.164805 | -2.032284 | -1.076195 |
| 44 | 1 | 0 | -6.412478 | -4.327556 | -0.485443 |
| 45 | 6 | 0 | -3.392386 | 0.859240 | 1.813822 |
| 46 | 6 | 0 | -4.051022 | 2.028604 | 4.287466 |
| 47 | 6 | 0 | -4.361867 | 0.277145 | 2.641952 |
| 48 | 6 | 0 | -2.755362 | 2.037681 | 2.245047 |
| 49 | 6 | 0 | -3.086581 | 2.621054 | 3.466760 |

| | | | | | |
|---|---|---|---|---|---|
| 50 | 6 | 0 | -4.684355 | 0.857732 | 3.872233 |
| 51 | 1 | 0 | -4.867541 | -0.630891 | 2.330306 |
| 52 | 1 | 0 | -2.004125 | 2.510203 | 1.615582 |
| 53 | 1 | 0 | -2.590227 | 3.535976 | 3.779115 |
| 54 | 1 | 0 | -5.435981 | 0.391098 | 4.503363 |
| 55 | 1 | 0 | -4.304914 | 2.478467 | 5.243335 |
| 56 | 6 | 0 | -3.305741 | 1.332754 | -1.059387 |
| 57 | 6 | 0 | -3.927164 | 3.167338 | -3.090603 |
| 58 | 6 | 0 | -4.191148 | 2.393700 | -0.811969 |
| 59 | 6 | 0 | -2.736588 | 1.195678 | -2.338055 |
| 60 | 6 | 0 | -3.051144 | 2.109224 | -3.345318 |
| 61 | 6 | 0 | -4.497577 | 3.306172 | -1.823916 |
| 62 | 1 | 0 | -4.637587 | 2.515068 | 0.169955 |
| 63 | 1 | 0 | -2.063103 | 0.368140 | -2.545568 |
| 64 | 1 | 0 | -2.606453 | 1.992340 | -4.329742 |
| 65 | 1 | 0 | -5.182420 | 4.125110 | -1.619739 |
| 66 | 1 | 0 | -4.165326 | 3.879848 | -3.875969 |
| 67 | 8 | 0 | 1.373250 | -1.505239 | -2.152524 |
| 68 | 16 | 0 | 0.055426 | -1.647451 | -1.485641 |
| 69 | 8 | 0 | -1.165033 | -1.724794 | -2.337779 |
| 70 | 6 | 0 | 0.140116 | -3.414593 | -0.724713 |
| 71 | 9 | 0 | -0.269396 | -3.377997 | 0.567378 |
| 72 | 9 | 0 | -0.645721 | -4.260095 | -1.387950 |
| 73 | 9 | 0 | 1.396171 | -3.876506 | -0.739883 |

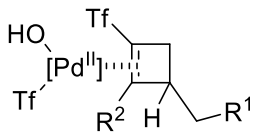
| | | |
|---|---|---|
| Zero-point correction= | 0.527666 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.573614 | |
| Thermal correction to Enthalpy= | 0.574558 | |
| Thermal correction to Gibbs Free Energy= | 0.438156 | |
| Sum of electronic and zero-point Energies= | -3399.367299 | |
| Sum of electronic and thermal Energies= | -3399.321351 | |
| Sum of electronic and thermal Enthalpies= | -3399.320407 | |
| Sum of electronic and thermal Free Energies= | -3399.456809 | |

**$H_2O$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -0.000000 | 0.762208 | -0.478067 |
| 2 | 8 | 0 | -0.000000 | 0.000000 | 0.119517 |
| 3 | 1 | 0 | -0.000000 | -0.762208 | -0.478067 |

| | | |
|---|---|---|
| Zero-point correction= | 0.021144 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.023979 | |
| Thermal correction to Enthalpy= | 0.024923 | |
| Thermal correction to Gibbs Free Energy= | 0.003478 | |
| Sum of electronic and zero-point Energies= | -76.385879 | |
| Sum of electronic and thermal Energies= | -76.383045 | |
| Sum of electronic and thermal Enthalpies= | -76.382101 | |
| Sum of electronic and thermal Free Energies= | -76.403546 | |

**IV**

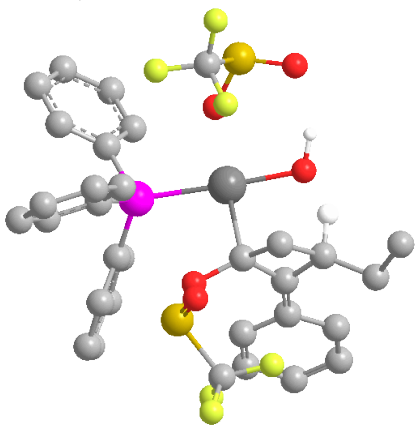



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 2.394821 | 3.724422 | -0.915762 |
| 2 | 6 | 0 | 1.573123 | 3.067925 | -1.223380 |
| 3 | 6 | 0 | 1.554664 | 1.779370 | -0.423544 |
| 4 | 1 | 0 | 0.630587 | 3.612091 | -1.296159 |
| 5 | 6 | 0 | 1.866414 | 0.943470 | -1.499612 |
| 6 | 6 | 0 | 1.921499 | 2.168273 | -2.453311 |
| 7 | 6 | 0 | 2.595893 | -0.317891 | -1.696978 |
| 8 | 6 | 0 | 4.184481 | -2.566518 | -2.258102 |
| 9 | 6 | 0 | 3.532835 | -0.780690 | -0.758997 |
| 10 | 6 | 0 | 2.472352 | -0.995020 | -2.925176 |
| 11 | 6 | 0 | 3.254459 | -2.114760 | -3.199366 |
| 12 | 6 | 0 | 4.322325 | -1.895437 | -1.041947 |
| 13 | 1 | 0 | 3.651781 | -0.255868 | 0.182803 |
| 14 | 1 | 0 | 1.760961 | -0.630431 | -3.661800 |
| 15 | 1 | 0 | 3.147121 | -2.628424 | -4.150923 |
| 16 | 1 | 0 | 5.044226 | -2.239816 | -0.307543 |
| 17 | 1 | 0 | 4.801752 | -3.433978 | -2.475405 |
| 18 | 6 | 0 | 3.304905 | 2.420521 | -3.062215 |
| 19 | 1 | 0 | 3.557235 | 1.587556 | -3.730943 |
| 20 | 1 | 0 | 4.070608 | 2.420390 | -2.273059 |
| 21 | 6 | 0 | 3.360123 | 3.738817 | -3.843598 |
| 22 | 1 | 0 | 3.144835 | 4.598699 | -3.198408 |
| 23 | 1 | 0 | 2.626219 | 3.744527 | -4.657979 |
| 24 | 1 | 0 | 4.352067 | 3.892792 | -4.282935 |
| 25 | 8 | 0 | 1.750217 | 1.616049 | 0.930868 |
| 26 | 16 | 0 | 1.314735 | 3.029680 | 1.838759 |
| 27 | 8 | 0 | 2.458324 | 3.964509 | 1.891366 |
| 28 | 6 | 0 | 1.448280 | 2.013147 | 3.427003 |
| 29 | 9 | 0 | 2.617985 | 1.384291 | 3.526449 |
| 30 | 9 | 0 | 1.321039 | 2.876320 | 4.438004 |
| 31 | 9 | 0 | 0.450928 | 1.125956 | 3.476692 |
| 32 | 46 | 0 | -0.417938 | 0.599015 | -1.030973 |
| 33 | 15 | 0 | -0.348588 | -1.431228 | 0.404160 |
| 34 | 6 | 0 | -1.358416 | -1.213640 | 1.933834 |
| 35 | 6 | 0 | -2.931056 | -0.869349 | 4.236402 |
| 36 | 6 | 0 | -1.345756 | -2.176800 | 2.958316 |
| 37 | 6 | 0 | -2.162503 | -0.074621 | 2.083651 |
| 38 | 6 | 0 | -2.945467 | 0.093645 | 3.227003 |
| 39 | 6 | 0 | -2.128926 | -2.005074 | 4.099975 |
| 40 | 1 | 0 | -0.720633 | -3.059807 | 2.868470 |
| 41 | 1 | 0 | -2.186220 | 0.674428 | 1.303238 |
| 42 | 1 | 0 | -3.571380 | 0.976843 | 3.317483 |
| 43 | 1 | 0 | -2.110218 | -2.758458 | 4.882981 |
| 44 | 1 | 0 | -3.540851 | -0.737291 | 5.126235 |
| 45 | 6 | 0 | -1.206427 | -2.719261 | -0.596170 |
| 46 | 6 | 0 | -2.445758 | -4.640609 | -2.224950 |
| 47 | 6 | 0 | -2.300699 | -3.452324 | -0.119619 |
| 48 | 6 | 0 | -0.743981 | -2.952414 | -1.901577 |
| 49 | 6 | 0 | -1.355777 | -3.912418 | -2.707295 |
| 50 | 6 | 0 | -2.916185 | -4.406781 | -0.932230 |
| 51 | 1 | 0 | -2.685539 | -3.272808 | 0.878509 |
| 52 | 1 | 0 | 0.094184 | -2.380626 | -2.290132 |
| 53 | 1 | 0 | -0.988367 | -4.082148 | -3.715760 |

| | | | | | |
|---|---|---|---|---|---|
| 54 | 1 | 0 | -3.769483 | -4.962901 | -0.553378 |
| 55 | 1 | 0 | -2.929341 | -5.381051 | -2.856326 |
| 56 | 6 | 0 | 1.132033 | -2.323718 | 1.067211 |
| 57 | 6 | 0 | 3.347443 | -3.641322 | 2.196753 |
| 58 | 6 | 0 | 1.494851 | -3.607388 | 0.635365 |
| 59 | 6 | 0 | 1.899477 | -1.707731 | 2.069963 |
| 60 | 6 | 0 | 2.995213 | -2.360753 | 2.631476 |
| 61 | 6 | 0 | 2.595623 | -4.259193 | 1.197459 |
| 62 | 1 | 0 | 0.917401 | -4.107847 | -0.133689 |
| 63 | 1 | 0 | 1.633035 | -0.720876 | 2.424557 |
| 64 | 1 | 0 | 3.569979 | -1.868443 | 3.411504 |
| 65 | 1 | 0 | 2.857862 | -5.256573 | 0.854629 |
| 66 | 1 | 0 | 4.198128 | -4.154033 | 2.637892 |
| 67 | 8 | 0 | -2.427475 | -0.078859 | -1.033376 |
| 68 | 16 | 0 | -3.685494 | 0.511675 | -1.771081 |
| 69 | 8 | 0 | -3.325056 | 1.216283 | -3.047282 |
| 70 | 6 | 0 | -4.074170 | 1.937243 | -0.560232 |
| 71 | 9 | 0 | -2.991752 | 2.595141 | -0.114683 |
| 72 | 9 | 0 | -4.899502 | 2.814194 | -1.143629 |
| 73 | 9 | 0 | -4.702102 | 1.410729 | 0.514549 |
| 74 | 1 | 0 | -1.653873 | 1.940627 | -2.643205 |
| 75 | 1 | 0 | 1.133261 | 2.183669 | -3.205761 |
| 76 | 8 | 0 | -0.813340 | 2.151455 | -2.185666 |

| | |
|---|---|
| Zero-point correction= | 0.554631 (Hartree/Particle) |
| Thermal correction to Energy= | 0.602202 |
| Thermal correction to Enthalpy= | 0.603146 |
| Thermal correction to Gibbs Free Energy= | 0.465803 |
| Sum of electronic and zero-point Energies= | -3475.768355 |
| Sum of electronic and thermal Energies= | -3475.720784 |
| Sum of electronic and thermal Enthalpies= | -3475.719840 |
| Sum of electronic and thermal Free Energies= | -3475.857183 |

**TS$_{II\text{-}IV}$**



Imaginary frequency: -498.6151 $cm^{-1}$

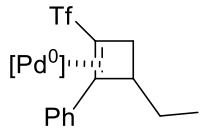
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 2.335323 | 2.129862 | 1.854808 |
| 2 | 6 | 0 | 1.640961 | 2.189531 | 1.015345 |
| 3 | 6 | 0 | 1.420178 | 0.815672 | 0.335693 |
| 4 | 1 | 0 | 0.754337 | 2.756014 | 1.309091 |
| 5 | 6 | 0 | 2.380863 | 1.166410 | -0.692544 |
| 6 | 6 | 0 | 2.338930 | 2.579794 | -0.320155 |
| 7 | 6 | 0 | 3.088614 | 0.413297 | -1.704776 |
| 8 | 6 | 0 | 4.482988 | -1.043992 | -3.665094 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 6 | 0 | 2.949274 | -0.989630 | -1.796408 |
| 10 | 6 | 0 | 3.939667 | 1.066605 | -2.623399 |
| 11 | 6 | 0 | 4.628426 | 0.344262 | -3.591911 |
| 12 | 6 | 0 | 3.641510 | -1.706342 | -2.765828 |
| 13 | 1 | 0 | 2.296064 | -1.509897 | -1.107764 |
| 14 | 1 | 0 | 4.048723 | 2.143089 | -2.580964 |
| 15 | 1 | 0 | 5.275247 | 0.863151 | -4.293550 |
| 16 | 1 | 0 | 3.517311 | -2.783477 | -2.822645 |
| 17 | 1 | 0 | 5.020006 | -1.607177 | -4.423677 |
| 18 | 6 | 0 | 3.490214 | 3.584780 | -0.371576 |
| 19 | 1 | 0 | 3.752861 | 3.804968 | -1.412889 |
| 20 | 1 | 0 | 4.386297 | 3.151654 | 0.095490 |
| 21 | 6 | 0 | 3.126340 | 4.899484 | 0.329146 |
| 22 | 1 | 0 | 2.899243 | 4.737654 | 1.388744 |
| 23 | 1 | 0 | 2.248213 | 5.363256 | -0.134189 |
| 24 | 1 | 0 | 3.956777 | 5.611870 | 0.270764 |
| 25 | 8 | 0 | 1.435205 | -0.441741 | 1.023288 |
| 26 | 16 | 0 | 2.175558 | -0.733245 | 2.509261 |
| 27 | 8 | 0 | 2.005910 | 0.373507 | 3.481297 |
| 28 | 6 | 0 | 3.990008 | -0.585901 | 1.953009 |
| 29 | 9 | 0 | 4.318913 | 0.633428 | 1.511898 |
| 30 | 9 | 0 | 4.745214 | -0.877903 | 3.018775 |
| 31 | 9 | 0 | 4.229606 | -1.484758 | 0.992027 |
| 32 | 46 | 0 | -0.514743 | 0.965894 | -0.715057 |
| 33 | 15 | 0 | -1.314379 | -1.213419 | -0.093651 |
| 34 | 6 | 0 | -1.564707 | -1.484694 | 1.708825 |
| 35 | 6 | 0 | -1.970523 | -1.797790 | 4.471486 |
| 36 | 6 | 0 | -1.805982 | -2.757850 | 2.256595 |
| 37 | 6 | 0 | -1.532735 | -0.373681 | 2.564571 |
| 38 | 6 | 0 | -1.733290 | -0.530918 | 3.937737 |
| 39 | 6 | 0 | -2.008592 | -2.911231 | 3.628273 |
| 40 | 1 | 0 | -1.829437 | -3.632635 | 1.613818 |
| 41 | 1 | 0 | -1.353594 | 0.614988 | 2.157243 |
| 42 | 1 | 0 | -1.695977 | 0.338758 | 4.587021 |
| 43 | 1 | 0 | -2.193011 | -3.900879 | 4.037576 |
| 44 | 1 | 0 | -2.122432 | -1.919469 | 5.540519 |
| 45 | 6 | 0 | -2.946801 | -1.579971 | -0.881616 |
| 46 | 6 | 0 | -5.362980 | -2.177801 | -2.190136 |
| 47 | 6 | 0 | -3.999517 | -2.195517 | -0.189718 |
| 48 | 6 | 0 | -3.132956 | -1.241077 | -2.233064 |
| 49 | 6 | 0 | -4.326510 | -1.550204 | -2.883866 |
| 50 | 6 | 0 | -5.199035 | -2.491064 | -0.841027 |
| 51 | 1 | 0 | -3.897510 | -2.438731 | 0.861576 |
| 52 | 1 | 0 | -2.359883 | -0.701476 | -2.769086 |
| 53 | 1 | 0 | -4.452748 | -1.278641 | -3.928296 |
| 54 | 1 | 0 | -6.005515 | -2.964556 | -0.287486 |
| 55 | 1 | 0 | -6.297179 | -2.408433 | -2.695136 |
| 56 | 6 | 0 | -0.281687 | -2.659454 | -0.643901 |
| 57 | 6 | 0 | 1.323190 | -4.795635 | -1.551016 |
| 58 | 6 | 0 | -0.341253 | -3.089830 | -1.979538 |
| 59 | 6 | 0 | 0.604300 | -3.315376 | 0.226472 |
| 60 | 6 | 0 | 1.396514 | -4.374225 | -0.222382 |
| 61 | 6 | 0 | 0.451847 | -4.146701 | -2.427860 |
| 62 | 1 | 0 | -1.019932 | -2.613268 | -2.677689 |
| 63 | 1 | 0 | 0.673934 | -3.008464 | 1.262780 |
| 64 | 1 | 0 | 2.068083 | -4.871603 | 0.472456 |
| 65 | 1 | 0 | 0.380252 | -4.465632 | -3.464170 |
| 66 | 1 | 0 | 1.933560 | -5.625275 | -1.897600 |
| 67 | 8 | 0 | -2.495280 | 1.398271 | -1.414164 |
| 68 | 16 | 0 | -3.266061 | 2.727669 | -1.125531 |
| 69 | 8 | 0 | -2.406734 | 3.956206 | -1.278945 |

| | | | | | |
|---|---|---|---|---|---|
| 70 | 6 | 0 | -3.386277 | 2.609803 | 0.767795 |
| 71 | 9 | 0 | -2.190022 | 2.792078 | 1.366243 |
| 72 | 9 | 0 | -4.224078 | 3.557274 | 1.214947 |
| 73 | 9 | 0 | -3.863482 | 1.410113 | 1.144850 |
| 74 | 1 | 0 | -0.676676 | 3.384694 | -1.404771 |
| 75 | 1 | 0 | 1.409229 | 2.972227 | -0.967653 |
| 76 | 8 | 0 | 0.065787 | 2.741282 | -1.483982 |

| | | |
|---|---|---|
| Zero-point correction= | 0.551060 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.597523 | |
| Thermal correction to Enthalpy= | 0.598467 | |
| Thermal correction to Gibbs Free Energy= | 0.466508 | |
| Sum of electronic and zero-point Energies= | -3475.750467 | |
| Sum of electronic and thermal Energies= | -3475.704004 | |
| Sum of electronic and thermal Enthalpies= | -3475.703060 | |
| Sum of electronic and thermal Free Energies= | -3475.835019 | |

**2-Pd**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -3.422533 | -0.207363 | 3.020918 |
| 2 | 6 | 0 | -2.468567 | -0.473853 | 2.548219 |
| 3 | 6 | 0 | -2.369749 | 0.005542 | 1.111780 |
| 4 | 1 | 0 | -1.647701 | -0.217079 | 3.222489 |
| 5 | 6 | 0 | -2.416894 | -1.263993 | 0.537524 |
| 6 | 6 | 0 | -2.485492 | -1.924202 | 1.938695 |
| 7 | 6 | 0 | -2.751889 | -1.797309 | -0.786633 |
| 8 | 6 | 0 | -3.412787 | -2.866940 | -3.308402 |
| 9 | 6 | 0 | -3.242924 | -0.966040 | -1.814837 |
| 10 | 6 | 0 | -2.600482 | -3.172125 | -1.050627 |
| 11 | 6 | 0 | -2.927554 | -3.700334 | -2.298385 |
| 12 | 6 | 0 | -3.567921 | -1.499495 | -3.059188 |
| 13 | 1 | 0 | -3.371268 | 0.095017 | -1.628975 |
| 14 | 1 | 0 | -2.212514 | -3.823461 | -0.272511 |
| 15 | 1 | 0 | -2.802399 | -4.764278 | -2.481881 |
| 16 | 1 | 0 | -3.949522 | -0.845195 | -3.838776 |
| 17 | 1 | 0 | -3.669943 | -3.278338 | -4.280746 |
| 18 | 6 | 0 | -3.772350 | -2.710453 | 2.221298 |
| 19 | 1 | 0 | -3.825994 | -3.574257 | 1.546312 |
| 20 | 1 | 0 | -4.638733 | -2.080082 | 1.975955 |
| 21 | 6 | 0 | -3.868013 | -3.190282 | 3.674260 |
| 22 | 1 | 0 | -3.853125 | -2.349120 | 4.377300 |
| 23 | 1 | 0 | -3.029229 | -3.850018 | 3.928602 |
| 24 | 1 | 0 | -4.794945 | -3.749510 | 3.844076 |
| 25 | 8 | 0 | -2.819258 | 1.226458 | 0.614697 |
| 26 | 16 | 0 | -1.605346 | 2.383418 | 0.307474 |
| 27 | 8 | 0 | -1.225745 | 3.098447 | 1.550752 |
| 28 | 6 | 0 | -2.951137 | 3.468660 | -0.471782 |
| 29 | 9 | 0 | -3.940726 | 3.754169 | 0.369481 |
| 30 | 9 | 0 | -2.356063 | 4.608087 | -0.853650 |
| 31 | 9 | 0 | -3.445854 | 2.859343 | -1.560866 |
| 32 | 46 | 0 | -0.287742 | -0.514714 | 0.379276 |
| 33 | 15 | 0 | 1.989082 | -0.133279 | 0.009234 |
| 34 | 6 | 0 | 2.629069 | -1.094383 | -1.435126 |
| 35 | 6 | 0 | 3.482692 | -2.533077 | -3.693277 |

| | | | | | |
|---|---|---|---|---|---|
| 36 | 6 | 0 | 3.941920 | -1.584940 | -1.513002 |
| 37 | 6 | 0 | 1.747384 | -1.343218 | -2.499987 |
| 38 | 6 | 0 | 2.173580 | -2.051646 | -3.624008 |
| 39 | 6 | 0 | 4.363930 | -2.300763 | -2.635351 |
| 40 | 1 | 0 | 4.634922 | -1.415256 | -0.694435 |
| 41 | 1 | 0 | 0.721508 | -0.988048 | -2.436751 |
| 42 | 1 | 0 | 1.478947 | -2.236666 | -4.438937 |
| 43 | 1 | 0 | 5.381926 | -2.678981 | -2.680547 |
| 44 | 1 | 0 | 3.812694 | -3.093231 | -4.564205 |
| 45 | 6 | 0 | 2.492262 | 1.607944 | -0.347210 |
| 46 | 6 | 0 | 3.162995 | 4.299526 | -0.796681 |
| 47 | 6 | 0 | 3.353236 | 1.960553 | -1.397010 |
| 48 | 6 | 0 | 1.966015 | 2.621893 | 0.471400 |
| 49 | 6 | 0 | 2.303577 | 3.956964 | 0.250503 |
| 50 | 6 | 0 | 3.684144 | 3.300004 | -1.619355 |
| 51 | 1 | 0 | 3.764038 | 1.193252 | -2.045528 |
| 52 | 1 | 0 | 1.278934 | 2.372495 | 1.274775 |
| 53 | 1 | 0 | 1.881529 | 4.726977 | 0.890251 |
| 54 | 1 | 0 | 4.349382 | 3.559376 | -2.438952 |
| 55 | 1 | 0 | 3.418808 | 5.340722 | -0.974538 |
| 56 | 6 | 0 | 3.109007 | -0.627170 | 1.394046 |
| 57 | 6 | 0 | 4.743212 | -1.491364 | 3.510189 |
| 58 | 6 | 0 | 4.317053 | 0.029241 | 1.674828 |
| 59 | 6 | 0 | 2.726149 | -1.715006 | 2.194651 |
| 60 | 6 | 0 | 3.540805 | -2.149337 | 3.240221 |
| 61 | 6 | 0 | 5.127388 | -0.400636 | 2.728185 |
| 62 | 1 | 0 | 4.622291 | 0.882356 | 1.076387 |
| 63 | 1 | 0 | 1.778553 | -2.210922 | 1.998078 |
| 64 | 1 | 0 | 3.231294 | -2.993214 | 3.851157 |
| 65 | 1 | 0 | 6.057953 | 0.120182 | 2.938275 |
| 66 | 1 | 0 | 5.373588 | -1.822399 | 4.331234 |
| 67 | 1 | 0 | -1.611211 | -2.527833 | 2.208275 |

| | | |
|---|---|---|
| Zero-point correction= | 0.515565 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.553880 | |
| Thermal correction to Enthalpy= | 0.554824 | |
| Thermal correction to Gibbs Free Energy= | 0.436811 | |
| Sum of electronic and zero-point Energies= | -2513.816343 | |
| Sum of electronic and thermal Energies= | -2513.778028 | |
| Sum of electronic and thermal Enthalpies= | -2513.777084 | |
| Sum of electronic and thermal Free Energies= | -2513.895097 | |

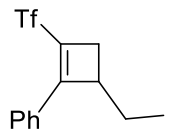
**TfOH**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.006152 | 0.009054 | -0.000946 |
| 2 | 16 | 0 | 0.851617 | -0.148460 | 0.076550 |
| 3 | 8 | 0 | 1.262868 | 0.181691 | 1.433371 |
| 4 | 8 | 0 | 1.247785 | 1.094409 | -0.904411 |
| 5 | 1 | 0 | 1.496888 | 1.853360 | -0.341262 |
| 6 | 8 | 0 | 1.213879 | -1.374870 | -0.600903 |
| 7 | 9 | 0 | -1.421912 | -0.158377 | -1.251393 |
| 8 | 9 | 0 | -1.358119 | 1.220645 | 0.433792 |
| 9 | 9 | 0 | -1.540203 | -0.922509 | 0.784010 |

| | | |
|---|---|---|
| Zero-point correction= | 0.038547 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.046416 | |
| Thermal correction to Enthalpy= | 0.047360 | |
| Thermal correction to Gibbs Free Energy= | 0.005376 | |

| | |
|---|---|
| Sum of electronic and zero-point Energies= | -961.950482 |
| Sum of electronic and thermal Energies= | -961.942613 |
| Sum of electronic and thermal Enthalpies= | -961.941669 |
| Sum of electronic and thermal Free Energies= | -961.983653 |

**2**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.374866 | 2.163154 | -0.076211 |
| 2 | 6 | 0 | -1.097440 | 1.944420 | 0.440886 |
| 3 | 1 | 0 | -1.161643 | 1.978905 | 1.537790 |
| 4 | 1 | 0 | 0.483688 | 2.924978 | -0.857149 |
| 5 | 1 | 0 | 1.126668 | 2.340195 | 0.698623 |
| 6 | 6 | 0 | 0.251854 | 0.744679 | -0.559911 |
| 7 | 6 | 0 | -0.999162 | 0.514470 | -0.113088 |
| 8 | 6 | 0 | -1.930309 | -0.605146 | -0.114065 |
| 9 | 6 | 0 | -3.735456 | -2.767810 | -0.070498 |
| 10 | 6 | 0 | -1.652573 | -1.790135 | -0.825534 |
| 11 | 6 | 0 | -3.128740 | -0.530451 | 0.619501 |
| 12 | 6 | 0 | -4.021229 | -1.601134 | 0.641013 |
| 13 | 6 | 0 | -2.546790 | -2.856562 | -0.801831 |
| 14 | 1 | 0 | -0.732240 | -1.864813 | -1.395650 |
| 15 | 1 | 0 | -3.354898 | 0.370073 | 1.183160 |
| 16 | 1 | 0 | -4.940844 | -1.523956 | 1.215104 |
| 17 | 1 | 0 | -2.317295 | -3.762028 | -1.357604 |
| 18 | 1 | 0 | -4.431711 | -3.601912 | -0.055590 |
| 19 | 6 | 0 | -2.153270 | 2.866166 | -0.178746 |
| 20 | 1 | 0 | -3.154003 | 2.461942 | 0.022583 |
| 21 | 1 | 0 | -2.035231 | 2.853878 | -1.271165 |
| 22 | 6 | 0 | -2.071065 | 4.305776 | 0.342199 |
| 23 | 1 | 0 | -1.093121 | 4.753589 | 0.128903 |
| 24 | 1 | 0 | -2.222887 | 4.343777 | 1.428022 |
| 25 | 1 | 0 | -2.835121 | 4.938600 | -0.123057 |
| 26 | 8 | 0 | 1.090418 | -0.060117 | -1.316180 |
| 27 | 16 | 0 | 2.748010 | -0.143759 | -0.981445 |
| 28 | 8 | 0 | 3.322444 | 1.187573 | -0.677174 |
| 29 | 6 | 0 | 2.551851 | -0.961002 | 0.725793 |
| 30 | 9 | 0 | 3.755338 | -1.444905 | 1.062780 |
| 31 | 9 | 0 | 2.157884 | -0.085117 | 1.649946 |
| 32 | 9 | 0 | 1.680373 | -1.969010 | 0.656046 |

| | |
|---|---|
| Zero-point correction= | 0.239352 (Hartree/Particle) |
| Thermal correction to Energy= | 0.257763 |
| Thermal correction to Enthalpy= | 0.258708 |
| Thermal correction to Gibbs Free Energy= | 0.189818 |
| Sum of electronic and zero-point Energies= | -1351.008622 |
| Sum of electronic and thermal Energies= | -1350.990211 |
| Sum of electronic and thermal Enthalpies= | -1350.989267 |
| Sum of electronic and thermal Free Energies= | -1351.058157 |

**V = [Pd$^{II}$]HTf**

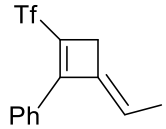
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 15 | 0 | 1.148674 | -0.084607 | 0.051069 |
| 2 | 6 | 0 | 2.181138 | 0.391951 | 1.492057 |
| 3 | 6 | 0 | 3.769134 | 1.039318 | 3.710114 |
| 4 | 6 | 0 | 3.168066 | 1.386813 | 1.391986 |
| 5 | 6 | 0 | 1.989549 | -0.264814 | 2.717776 |
| 6 | 6 | 0 | 2.784051 | 0.055805 | 3.818950 |
| 7 | 6 | 0 | 3.958080 | 1.705462 | 2.497188 |
| 8 | 1 | 0 | 3.311578 | 1.920454 | 0.457120 |
| 9 | 1 | 0 | 1.210135 | -1.015118 | 2.811244 |
| 10 | 1 | 0 | 2.624455 | -0.456168 | 4.763568 |
| 11 | 1 | 0 | 4.716861 | 2.478376 | 2.411318 |
| 12 | 1 | 0 | 4.381880 | 1.293148 | 4.570674 |
| 13 | 6 | 0 | 2.120276 | -1.319747 | -0.896963 |
| 14 | 6 | 0 | 3.526196 | -3.207587 | -2.418349 |
| 15 | 6 | 0 | 1.429305 | -2.299463 | -1.626747 |
| 16 | 6 | 0 | 3.523652 | -1.300085 | -0.928697 |
| 17 | 6 | 0 | 4.220898 | -2.241558 | -1.686530 |
| 18 | 6 | 0 | 2.130631 | -3.235367 | -2.387838 |
| 19 | 1 | 0 | 0.344007 | -2.334196 | -1.585216 |
| 20 | 1 | 0 | 4.072968 | -0.560287 | -0.354402 |
| 21 | 1 | 0 | 5.307136 | -2.223315 | -1.700202 |
| 22 | 1 | 0 | 1.585937 | -3.990720 | -2.947015 |
| 23 | 1 | 0 | 4.072187 | -3.941869 | -3.004210 |
| 24 | 6 | 0 | 1.071403 | 1.419050 | -1.001821 |
| 25 | 6 | 0 | 0.830476 | 3.743235 | -2.551577 |
| 26 | 6 | 0 | 0.337608 | 2.519812 | -0.524955 |
| 27 | 6 | 0 | 1.674476 | 1.491893 | -2.265843 |
| 28 | 6 | 0 | 1.553185 | 2.651667 | -3.034587 |
| 29 | 6 | 0 | 0.223385 | 3.675762 | -1.294676 |
| 30 | 1 | 0 | -0.147379 | 2.472415 | 0.446470 |
| 31 | 1 | 0 | 2.236292 | 0.647800 | -2.652305 |
| 32 | 1 | 0 | 2.023691 | 2.698237 | -4.012796 |
| 33 | 1 | 0 | -0.346168 | 4.519775 | -0.916371 |
| 34 | 1 | 0 | 0.735115 | 4.642503 | -3.153672 |
| 35 | 46 | 0 | -0.972179 | -0.735594 | 0.589122 |
| 36 | 1 | 0 | -0.278993 | -1.980800 | 1.125858 |
| 37 | 8 | 0 | -2.868413 | -1.313293 | 1.221170 |
| 38 | 16 | 0 | -3.964412 | -1.230911 | 0.081534 |
| 39 | 8 | 0 | -5.329767 | -1.319761 | 0.666707 |
| 40 | 6 | 0 | -3.784230 | 0.651663 | -0.236700 |
| 41 | 9 | 0 | -2.434451 | 0.981181 | -0.372078 |
| 42 | 9 | 0 | -4.266533 | 1.408118 | 0.744127 |
| 43 | 9 | 0 | -4.364265 | 1.000961 | -1.390942 |

---

Zero-point correction= 0.306495 (Hartree/Particle)
Thermal correction to Energy= 0.333111
Thermal correction to Enthalpy= 0.334055
Thermal correction to Gibbs Free Energy= 0.243898
Sum of electronic and zero-point Energies= -2049.547677
Sum of electronic and thermal Energies= -2049.521061
Sum of electronic and thermal Enthalpies= -2049.520117
Sum of electronic and thermal Free Energies= -2049.610274

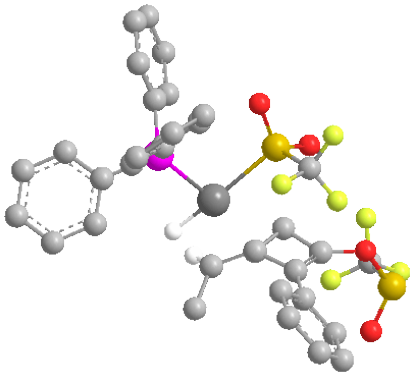
**4**



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.109256 | 0.804536 | -0.011420 |
| 2 | 6 | 0 | -1.425749 | 0.467873 | -0.019870 |
| 3 | 6 | 0 | -0.305347 | 2.301681 | -0.113087 |
| 4 | 1 | 0 | 0.030854 | 2.896727 | 0.746316 |
| 5 | 1 | 0 | 0.050524 | 2.772298 | -1.038728 |
| 6 | 6 | 0 | -1.798026 | 1.902531 | -0.101362 |
| 7 | 6 | 0 | -2.913588 | 2.637973 | -0.111878 |
| 8 | 1 | 0 | -3.878446 | 2.137328 | -0.059773 |
| 9 | 6 | 0 | -2.946909 | 4.139358 | -0.173494 |
| 10 | 1 | 0 | -3.459150 | 4.563234 | 0.701169 |
| 11 | 1 | 0 | -3.495477 | 4.490777 | -1.058359 |
| 12 | 1 | 0 | -1.939846 | 4.567710 | -0.212475 |
| 13 | 6 | 0 | -2.157587 | -0.794107 | 0.030143 |
| 14 | 6 | 0 | -3.558615 | -3.235429 | 0.133470 |
| 15 | 6 | 0 | -1.493393 | -1.992630 | 0.359283 |
| 16 | 6 | 0 | -3.533743 | -0.846913 | -0.253099 |
| 17 | 6 | 0 | -4.225959 | -2.056073 | -0.201365 |
| 18 | 6 | 0 | -2.188965 | -3.197414 | 0.410886 |
| 19 | 1 | 0 | -0.429886 | -1.971616 | 0.576096 |
| 20 | 1 | 0 | -4.058910 | 0.059430 | -0.534432 |
| 21 | 1 | 0 | -5.289272 | -2.076040 | -0.425478 |
| 22 | 1 | 0 | -1.660643 | -4.111213 | 0.669827 |
| 23 | 1 | 0 | -4.099370 | -4.176997 | 0.175727 |
| 24 | 8 | 0 | 1.010720 | 0.018788 | 0.038544 |
| 25 | 16 | 0 | 2.485568 | 0.849851 | 0.293677 |
| 26 | 8 | 0 | 2.825253 | 0.893521 | 1.731907 |
| 27 | 6 | 0 | 3.377055 | -0.661658 | -0.406730 |
| 28 | 9 | 0 | 3.080949 | -0.780927 | -1.703231 |
| 29 | 9 | 0 | 3.059796 | -1.778012 | 0.239065 |
| 30 | 9 | 0 | 4.687394 | -0.426183 | -0.274855 |

| | | |
|---|---|---|
| Zero-point correction= | 0.215415 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.233722 | |
| Thermal correction to Enthalpy= | 0.234666 | |
| Thermal correction to Gibbs Free Energy= | 0.165298 | |
| Sum of electronic and zero-point Energies= | -1349.803923 | |
| Sum of electronic and thermal Energies= | -1349.785616 | |
| Sum of electronic and thermal Enthalpies= | -1349.784672 | |
| Sum of electronic and thermal Free Energies= | -1349.854040 | |

**$TS_{III\text{-}V}$**



Imaginary frequency: -248.6702 $cm^{-1}$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.493797 | -1.430841 | 0.570887 |
| 2 | 6 | 0 | 1.708933 | -0.242957 | 1.174666 |
| 3 | 1 | 0 | 2.936399 | -2.100834 | 1.315406 |
| 4 | 1 | 0 | 1.986140 | -1.989426 | -0.219735 |
| 5 | 6 | 0 | 3.378071 | -0.314643 | 0.048793 |
| 6 | 6 | 0 | 2.655894 | 0.723252 | 0.548214 |
| 7 | 6 | 0 | 2.751391 | 2.185982 | 0.520141 |
| 8 | 6 | 0 | 2.927291 | 4.990891 | 0.449002 |
| 9 | 6 | 0 | 3.997755 | 2.826219 | 0.635817 |
| 10 | 6 | 0 | 1.595547 | 2.973485 | 0.372757 |
| 11 | 6 | 0 | 1.684045 | 4.363701 | 0.336425 |
| 12 | 6 | 0 | 4.080665 | 4.217711 | 0.597829 |
| 13 | 1 | 0 | 4.893544 | 2.232165 | 0.785604 |
| 14 | 1 | 0 | 0.630483 | 2.489211 | 0.250556 |
| 15 | 1 | 0 | 0.782030 | 4.956559 | 0.211031 |
| 16 | 1 | 0 | 5.050289 | 4.698975 | 0.693991 |
| 17 | 1 | 0 | 2.995967 | 6.075079 | 0.421881 |
| 18 | 6 | 0 | 0.982921 | -0.205526 | 2.368530 |
| 19 | 1 | 0 | 0.800719 | -1.173482 | 2.833471 |
| 20 | 1 | 0 | -0.826695 | -0.105088 | 2.053095 |
| 21 | 6 | 0 | 0.967457 | 0.980689 | 3.309890 |
| 22 | 1 | 0 | 0.929618 | 1.932617 | 2.777913 |
| 23 | 1 | 0 | 1.894104 | 0.967377 | 3.900094 |
| 24 | 1 | 0 | 0.125522 | 0.929796 | 4.006179 |
| 25 | 8 | 0 | 4.457990 | -0.355981 | -0.790204 |
| 26 | 16 | 0 | 6.048595 | -0.538237 | -0.194406 |
| 27 | 8 | 0 | 6.225666 | 0.182543 | 1.089931 |
| 28 | 6 | 0 | 5.888794 | -2.360186 | 0.348793 |
| 29 | 9 | 0 | 7.128093 | -2.870230 | 0.325024 |
| 30 | 9 | 0 | 5.407473 | -2.445401 | 1.590222 |
| 31 | 9 | 0 | 5.114278 | -3.049212 | -0.487026 |
| 32 | 46 | 0 | -0.520011 | -0.231262 | 0.509649 |
| 33 | 15 | 0 | -2.899212 | -0.290761 | 0.310031 |
| 34 | 6 | 0 | -3.743328 | -0.248182 | 1.959568 |
| 35 | 6 | 0 | -5.013106 | -0.099413 | 4.466326 |
| 36 | 6 | 0 | -4.825345 | -1.086765 | 2.262106 |
| 37 | 6 | 0 | -3.309071 | 0.668714 | 2.931451 |
| 38 | 6 | 0 | -3.943078 | 0.749275 | 4.170793 |
| 39 | 6 | 0 | -5.449290 | -1.016608 | 3.510854 |
| 40 | 1 | 0 | -5.180522 | -1.803592 | 1.529574 |
| 41 | 1 | 0 | -2.470148 | 1.325647 | 2.717014 |
| 42 | 1 | 0 | -3.596472 | 1.469001 | 4.907562 |
| 43 | 1 | 0 | -6.278025 | -1.683510 | 3.732724 |
| 44 | 1 | 0 | -5.500016 | -0.046432 | 5.436232 |

| | | | | | |
|---|---|---|---|---|---|
| 45 | 6 | 0 | -3.716673 | 1.072442 | -0.629318 |
| 46 | 6 | 0 | -4.898860 | 3.150469 | -2.100245 |
| 47 | 6 | 0 | -4.551588 | 2.006622 | 0.004027 |
| 48 | 6 | 0 | -3.475736 | 1.189860 | -2.010066 |
| 49 | 6 | 0 | -4.071212 | 2.221574 | -2.735206 |
| 50 | 6 | 0 | -5.136596 | 3.040463 | -0.730089 |
| 51 | 1 | 0 | -4.756093 | 1.930603 | 1.066118 |
| 52 | 1 | 0 | -2.828503 | 0.474949 | -2.508888 |
| 53 | 1 | 0 | -3.880355 | 2.299633 | -3.802028 |
| 54 | 1 | 0 | -5.782265 | 3.755243 | -0.226741 |
| 55 | 1 | 0 | -5.355776 | 3.955016 | -2.670438 |
| 56 | 6 | 0 | -3.489338 | -1.848663 | -0.456339 |
| 57 | 6 | 0 | -4.368352 | -4.285085 | -1.526818 |
| 58 | 6 | 0 | -4.715825 | -1.922679 | -1.133119 |
| 59 | 6 | 0 | -2.705124 | -3.003874 | -0.328966 |
| 60 | 6 | 0 | -3.144667 | -4.216536 | -0.857992 |
| 61 | 6 | 0 | -5.151325 | -3.137422 | -1.664704 |
| 62 | 1 | 0 | -5.325026 | -1.032472 | -1.255304 |
| 63 | 1 | 0 | -1.740039 | -2.949252 | 0.168071 |
| 64 | 1 | 0 | -2.523129 | -5.102334 | -0.762692 |
| 65 | 1 | 0 | -6.099649 | -3.183633 | -2.193174 |
| 66 | 1 | 0 | -4.706008 | -5.227899 | -1.948449 |
| 67 | 8 | 0 | -1.293187 | -0.998916 | -2.635545 |
| 68 | 16 | 0 | -0.043953 | -0.639246 | -1.890137 |
| 69 | 8 | 0 | 1.162321 | -1.474009 | -2.176839 |
| 70 | 6 | 0 | 0.391731 | 1.033040 | -2.675987 |
| 71 | 9 | 0 | 1.663859 | 1.373352 | -2.426568 |
| 72 | 9 | 0 | 0.201143 | 1.008648 | -3.996974 |
| 73 | 9 | 0 | -0.408030 | 1.990189 | -2.147741 |

| | |
|---|---|
| Zero-point correction= | 0.523603 (Hartree/Particle) |
| Thermal correction to Energy= | 0.569065 |
| Thermal correction to Enthalpy= | 0.570009 |
| Thermal correction to Gibbs Free Energy= | 0.436906 |
| Sum of electronic and zero-point Energies= | -3399.349839 |
| Sum of electronic and thermal Energies= | -3399.304377 |
| Sum of electronic and thermal Enthalpies= | -3399.303433 |
| Sum of electronic and thermal Free Energies= | -3399.436537 |

**$K_2CO_3$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.215838 | 0.000000 |
| 2 | 8 | 0 | 1.131530 | 0.849789 | 0.000000 |
| 3 | 8 | 0 | -0.001991 | -1.087603 | -0.000000 |
| 4 | 8 | 0 | -1.129573 | 0.853263 | -0.000000 |
| 5 | 19 | 0 | 0.004223 | 3.021703 | 0.000000 |
| 6 | 19 | 0 | -0.004209 | -3.348998 | -0.000000 |

| | |
|---|---|
| Zero-point correction= | 0.016202 (Hartree/Particle) |
| Thermal correction to Energy= | 0.021555 |
| Thermal correction to Enthalpy= | 0.022499 |
| Thermal correction to Gibbs Free Energy= | -0.015218 |
| Sum of electronic and zero-point Energies= | -1463.649655 |
| Sum of electronic and thermal Energies= | -1463.644302 |
| Sum of electronic and thermal Enthalpies= | -1463.643358 |
| Sum of electronic and thermal Free Energies= | -1463.681074 |

**$KHCO_3$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.638193 | -0.849623 | -0.000520 |
| 2 | 6 | 0 | -0.993074 | 0.042605 | -0.000120 |
| 3 | 8 | 0 | -0.461565 | -1.110805 | 0.000585 |
| 4 | 8 | 0 | -2.369329 | 0.084285 | -0.000478 |
| 5 | 8 | 0 | -0.405582 | 1.152557 | 0.000545 |
| 6 | 19 | 0 | 1.815182 | -0.021805 | -0.000209 |

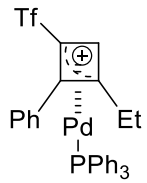
| | |
|---|---|
| Zero-point correction= | 0.028140 (Hartree/Particle) |
| Thermal correction to Energy= | 0.033366 |
| Thermal correction to Enthalpy= | 0.034310 |
| Thermal correction to Gibbs Free Energy= | -0.001523 |
| Sum of electronic and zero-point Energies= | -864.329437 |
| Sum of electronic and thermal Energies= | -864.324212 |
| Sum of electronic and thermal Enthalpies= | -864.323268 |
| Sum of electronic and thermal Free Energies= | -864.359101 |

**KTf**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.638585 | -0.925460 | -1.254148 |
| 2 | 16 | 0 | -0.184979 | -1.237201 | -0.000212 |
| 3 | 8 | 0 | 0.638269 | -0.926262 | 1.254097 |
| 4 | 6 | 0 | -1.291834 | 0.315398 | -0.000004 |
| 5 | 9 | 0 | -2.070295 | 0.376005 | -1.088245 |
| 6 | 9 | 0 | -0.508032 | 1.444990 | 0.000612 |
| 7 | 9 | 0 | -2.071072 | 0.375543 | 1.087808 |
| 8 | 19 | 0 | 2.228444 | 0.681461 | 0.000119 |

| | |
|---|---|
| Zero-point correction= | 0.022742 (Hartree/Particle) |
| Thermal correction to Energy= | 0.031269 |
| Thermal correction to Enthalpy= | 0.032213 |
| Thermal correction to Gibbs Free Energy= | -0.012216 |
| Sum of electronic and zero-point Energies= | -1486.150688 |
| Sum of electronic and thermal Energies= | -1486.142161 |
| Sum of electronic and thermal Enthalpies= | -1486.141217 |
| Sum of electronic and thermal Free Energies= | -1486.185646 |

**VI**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 2.744745 | -0.090841 | 3.128874 |
| 2 | 6 | 0 | 2.087673 | -0.319037 | 2.277583 |
| 3 | 6 | 0 | 2.716539 | 0.039505 | 0.928517 |
| 4 | 1 | 0 | 1.638158 | -1.304011 | 2.419633 |
| 5 | 6 | 0 | 2.119576 | 1.321808 | 0.865449 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | 1.165879 | 0.878841 | 1.888060 |
| 7 | 6 | 0 | 2.397473 | 2.559214 | 0.146124 |
| 8 | 6 | 0 | 2.995779 | 4.948889 | -1.193823 |
| 9 | 6 | 0 | 3.583254 | 2.678915 | -0.605358 |
| 10 | 6 | 0 | 1.519589 | 3.657555 | 0.221241 |
| 11 | 6 | 0 | 1.819059 | 4.841351 | -0.447202 |
| 12 | 6 | 0 | 3.876818 | 3.866651 | -1.268951 |
| 13 | 1 | 0 | 4.278106 | 1.846981 | -0.652473 |
| 14 | 1 | 0 | 0.602455 | 3.582272 | 0.795274 |
| 15 | 1 | 0 | 1.137324 | 5.684130 | -0.382502 |
| 16 | 1 | 0 | 4.795731 | 3.950789 | -1.841162 |
| 17 | 1 | 0 | 3.227700 | 5.874958 | -1.711412 |
| 18 | 6 | 0 | 0.229743 | 1.626422 | 2.789541 |
| 19 | 1 | 0 | -0.488520 | 2.200187 | 2.195238 |
| 20 | 1 | 0 | 0.839661 | 2.366759 | 3.333985 |
| 21 | 6 | 0 | -0.508762 | 0.737348 | 3.796362 |
| 22 | 1 | 0 | 0.191086 | 0.182079 | 4.430523 |
| 23 | 1 | 0 | -1.159508 | 0.016701 | 3.291270 |
| 24 | 1 | 0 | -1.134685 | 1.351719 | 4.449972 |
| 25 | 8 | 0 | 3.796699 | -0.481729 | 0.270661 |
| 26 | 16 | 0 | 3.488321 | -1.560380 | -1.055238 |
| 27 | 8 | 0 | 2.116248 | -1.269911 | -1.568886 |
| 28 | 6 | 0 | 3.252182 | -3.120319 | 0.010701 |
| 29 | 9 | 0 | 2.076792 | -3.084080 | 0.644368 |
| 30 | 9 | 0 | 3.274952 | -4.153289 | -0.827345 |
| 31 | 9 | 0 | 4.242108 | -3.215153 | 0.888064 |
| 32 | 46 | 0 | 0.581354 | -0.159970 | 0.082233 |
| 33 | 15 | 0 | -1.778931 | -0.179334 | -0.211963 |
| 34 | 6 | 0 | -2.178435 | -0.218242 | -2.003925 |
| 35 | 6 | 0 | -2.731093 | -0.386030 | -4.747879 |
| 36 | 6 | 0 | -3.290148 | 0.447768 | -2.544551 |
| 37 | 6 | 0 | -1.344266 | -0.964598 | -2.853429 |
| 38 | 6 | 0 | -1.622304 | -1.049479 | -4.217482 |
| 39 | 6 | 0 | -3.562423 | 0.361006 | -3.910943 |
| 40 | 1 | 0 | -3.939596 | 1.037844 | -1.905575 |
| 41 | 1 | 0 | -0.475694 | -1.482930 | -2.453356 |
| 42 | 1 | 0 | -0.970555 | -1.628522 | -4.865155 |
| 43 | 1 | 0 | -4.424596 | 0.879500 | -4.320408 |
| 44 | 1 | 0 | -2.944672 | -0.448411 | -5.810940 |
| 45 | 6 | 0 | -2.613710 | -1.643453 | 0.515398 |
| 46 | 6 | 0 | -3.858498 | -3.876390 | 1.668375 |
| 47 | 6 | 0 | -3.871339 | -2.070393 | 0.056467 |
| 48 | 6 | 0 | -1.984189 | -2.355109 | 1.548232 |
| 49 | 6 | 0 | -2.605774 | -3.463906 | 2.125228 |
| 50 | 6 | 0 | -4.488486 | -3.180047 | 0.633232 |
| 51 | 1 | 0 | -4.363751 | -1.544030 | -0.755594 |
| 52 | 1 | 0 | -1.002915 | -2.043478 | 1.896058 |
| 53 | 1 | 0 | -2.109671 | -4.007499 | 2.924089 |
| 54 | 1 | 0 | -5.459628 | -3.504106 | 0.270646 |
| 55 | 1 | 0 | -4.340889 | -4.742341 | 2.112253 |
| 56 | 6 | 0 | -2.648412 | 1.297833 | 0.448097 |
| 57 | 6 | 0 | -3.872406 | 3.618910 | 1.444654 |
| 58 | 6 | 0 | -3.642632 | 1.207513 | 1.431911 |
| 59 | 6 | 0 | -2.267612 | 2.565665 | -0.029531 |
| 60 | 6 | 0 | -2.882077 | 3.716788 | 0.461621 |
| 61 | 6 | 0 | -4.248712 | 2.365746 | 1.927741 |
| 62 | 1 | 0 | -3.951674 | 0.237501 | 1.807406 |
| 63 | 1 | 0 | -1.500118 | 2.651322 | -0.795137 |
| 64 | 1 | 0 | -2.592406 | 4.689876 | 0.074923 |
| 65 | 1 | 0 | -5.020292 | 2.283296 | 2.687784 |
| 66 | 1 | 0 | -4.349231 | 4.516437 | 1.827588 |

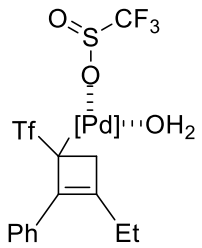
| | |
|---|---|
| Zero-point correction= | 0.504685 (Hartree/Particle) |
| Thermal correction to Energy= | 0.542395 |
| Thermal correction to Enthalpy= | 0.543339 |
| Thermal correction to Gibbs Free Energy= | 0.428555 |
| Sum of electronic and zero-point Energies= | -2513.006823 |
| Sum of electronic and thermal Energies= | -2512.969113 |
| Sum of electronic and thermal Enthalpies= | -2512.968169 |
| Sum of electronic and thermal Free Energies= | -2513.082953 |

**$Tf^-$**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.817798 | 0.000059 | 0.001768 |
| 2 | 9 | 0 | 1.443362 | -1.087623 | -0.532428 |
| 3 | 9 | 0 | 1.100711 | -0.000701 | 1.325318 |
| 4 | 9 | 0 | 1.443349 | 1.088314 | -0.531164 |
| 5 | 16 | 0 | -1.065164 | 0.000005 | -0.422445 |
| 6 | 8 | 0 | -1.484306 | -1.277997 | 0.274590 |
| 7 | 8 | 0 | -1.484564 | 1.277953 | 0.274533 |

| | |
|---|---|
| Zero-point correction= | 0.021275 (Hartree/Particle) |
| Thermal correction to Energy= | 0.028159 |
| Thermal correction to Enthalpy= | 0.029103 |
| Thermal correction to Gibbs Free Energy= | -0.011204 |
| Sum of electronic and zero-point Energies= | -886.224245 |
| Sum of electronic and thermal Energies= | -886.217362 |
| Sum of electronic and thermal Enthalpies= | -886.216418 |
| Sum of electronic and thermal Free Energies= | -886.256725 |

**VII**

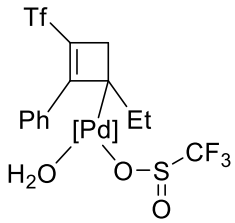



| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | 1.888733 | 1.808924 | 2.136360 |
| 2 | 6 | 0 | 1.559586 | 1.990042 | 1.110714 |
| 3 | 6 | 0 | 1.324558 | 0.684597 | 0.261006 |
| 4 | 1 | 0 | 0.718836 | 2.693110 | 1.140540 |
| 5 | 6 | 0 | 2.503149 | 1.106805 | -0.584955 |
| 6 | 6 | 0 | 2.665648 | 2.273138 | 0.102669 |
| 7 | 6 | 0 | 3.168507 | 0.450307 | -1.710650 |
| 8 | 6 | 0 | 4.430526 | -0.834224 | -3.876424 |
| 9 | 6 | 0 | 2.495278 | -0.535023 | -2.454521 |
| 10 | 6 | 0 | 4.495164 | 0.764372 | -2.061659 |
| 11 | 6 | 0 | 5.116220 | 0.133019 | -3.137289 |
| 12 | 6 | 0 | 3.120304 | -1.168345 | -3.526785 |
| 13 | 1 | 0 | 1.476177 | -0.797211 | -2.188903 |
| 14 | 1 | 0 | 5.050310 | 1.487253 | -1.472062 |
| 15 | 1 | 0 | 6.141311 | 0.388772 | -3.392436 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 1 | 0 | 2.581673 | -1.927914 | -4.086853 |
| 17 | 1 | 0 | 4.917032 | -1.328722 | -4.712975 |
| 18 | 6 | 0 | 3.584535 | 3.453351 | 0.006129 |
| 19 | 1 | 0 | 4.072113 | 3.467841 | -0.976034 |
| 20 | 1 | 0 | 4.389073 | 3.324191 | 0.747326 |
| 21 | 6 | 0 | 2.888092 | 4.800047 | 0.267596 |
| 22 | 1 | 0 | 2.413879 | 4.819152 | 1.254767 |
| 23 | 1 | 0 | 2.112378 | 5.006040 | -0.480209 |
| 24 | 1 | 0 | 3.611259 | 5.621164 | 0.226394 |
| 25 | 8 | 0 | 1.461098 | -0.608348 | 0.922309 |
| 26 | 16 | 0 | 2.170286 | -0.982198 | 2.385017 |
| 27 | 8 | 0 | 1.869827 | -0.008884 | 3.468235 |
| 28 | 6 | 0 | 4.002503 | -0.627661 | 1.990240 |
| 29 | 9 | 0 | 4.315628 | 0.665261 | 2.104888 |
| 30 | 9 | 0 | 4.704866 | -1.319453 | 2.903178 |
| 31 | 9 | 0 | 4.328554 | -1.069112 | 0.774729 |
| 32 | 46 | 0 | -0.516311 | 0.865925 | -0.663801 |
| 33 | 15 | 0 | -1.360254 | -1.232056 | -0.075844 |
| 34 | 6 | 0 | -1.559350 | -1.537922 | 1.723290 |
| 35 | 6 | 0 | -1.958834 | -1.905749 | 4.477250 |
| 36 | 6 | 0 | -1.745418 | -2.828475 | 2.250672 |
| 37 | 6 | 0 | -1.580832 | -0.436918 | 2.592211 |
| 38 | 6 | 0 | -1.779321 | -0.622171 | 3.961484 |
| 39 | 6 | 0 | -1.943491 | -3.008619 | 3.619747 |
| 40 | 1 | 0 | -1.735001 | -3.693086 | 1.594271 |
| 41 | 1 | 0 | -1.446834 | 0.564797 | 2.198563 |
| 42 | 1 | 0 | -1.783276 | 0.238832 | 4.623133 |
| 43 | 1 | 0 | -2.083976 | -4.010848 | 4.015472 |
| 44 | 1 | 0 | -2.106951 | -2.048567 | 5.544133 |
| 45 | 6 | 0 | -3.040141 | -1.494921 | -0.800969 |
| 46 | 6 | 0 | -5.541180 | -1.960507 | -1.997667 |
| 47 | 6 | 0 | -4.078350 | -2.095326 | -0.073436 |
| 48 | 6 | 0 | -3.281062 | -1.107850 | -2.130388 |
| 49 | 6 | 0 | -4.518123 | -1.350533 | -2.725849 |
| 50 | 6 | 0 | -5.319995 | -2.324729 | -0.669550 |
| 51 | 1 | 0 | -3.929581 | -2.381059 | 0.961579 |
| 52 | 1 | 0 | -2.515385 | -0.585676 | -2.692710 |
| 53 | 1 | 0 | -4.686404 | -1.042560 | -3.754068 |
| 54 | 1 | 0 | -6.113934 | -2.787847 | -0.089825 |
| 55 | 1 | 0 | -6.508260 | -2.140024 | -2.459656 |
| 56 | 6 | 0 | -0.397163 | -2.672927 | -0.737749 |
| 57 | 6 | 0 | 1.117552 | -4.785052 | -1.830885 |
| 58 | 6 | 0 | -0.562979 | -3.060343 | -2.078259 |
| 59 | 6 | 0 | 0.542545 | -3.364149 | 0.043608 |
| 60 | 6 | 0 | 1.288422 | -4.412146 | -0.497628 |
| 61 | 6 | 0 | 0.188095 | -4.104510 | -2.618863 |
| 62 | 1 | 0 | -1.290547 | -2.560389 | -2.707288 |
| 63 | 1 | 0 | 0.694237 | -3.091784 | 1.080022 |
| 64 | 1 | 0 | 2.005868 | -4.935621 | 0.128546 |
| 65 | 1 | 0 | 0.036659 | -4.389640 | -3.656508 |
| 66 | 1 | 0 | 1.700060 | -5.600342 | -2.250950 |
| 67 | 8 | 0 | -2.500838 | 1.526118 | -1.430231 |
| 68 | 16 | 0 | -3.086241 | 2.927418 | -1.125057 |
| 69 | 8 | 0 | -2.041295 | 4.025755 | -1.283970 |
| 70 | 6 | 0 | -3.188000 | 2.836399 | 0.772170 |
| 71 | 9 | 0 | -1.965273 | 2.860068 | 1.352394 |
| 72 | 9 | 0 | -3.884110 | 3.885732 | 1.232591 |
| 73 | 9 | 0 | -3.808197 | 1.709442 | 1.160449 |
| 74 | 1 | 0 | -0.588196 | 3.341378 | -1.554868 |
| 75 | 1 | 0 | 0.981051 | 3.042714 | -1.312145 |
| 76 | 8 | 0 | 0.161862 | 2.681686 | -1.688355 |

| | |
|---|---|
| Zero-point correction= | 0.554062 (Hartree/Particle) |
| Thermal correction to Energy= | 0.601502 |
| Thermal correction to Enthalpy= | 0.602446 |
| Thermal correction to Gibbs Free Energy= | 0.467144 |
| Sum of electronic and zero-point Energies= | -3475.797970 |
| Sum of electronic and thermal Energies= | -3475.750530 |
| Sum of electronic and thermal Enthalpies= | -3475.749586 |
| Sum of electronic and thermal Free Energies= | -3475.884888 |

**VIII**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.358765 | -0.209697 | -1.238741 |
| 2 | 6 | 0 | 1.249924 | -1.052784 | -0.503479 |
| 3 | 1 | 0 | 2.684573 | -0.602642 | -2.206967 |
| 4 | 1 | 0 | 2.146594 | 0.858309 | -1.341433 |
| 5 | 6 | 0 | 3.195002 | -0.589117 | -0.047611 |
| 6 | 6 | 0 | 2.243029 | -1.276888 | 0.625012 |
| 7 | 6 | 0 | 2.170306 | -1.985055 | 1.896754 |
| 8 | 6 | 0 | 2.017994 | -3.381398 | 4.340712 |
| 9 | 6 | 0 | 3.287578 | -2.065521 | 2.752503 |
| 10 | 6 | 0 | 0.976145 | -2.613767 | 2.297049 |
| 11 | 6 | 0 | 0.901926 | -3.304754 | 3.505488 |
| 12 | 6 | 0 | 3.209207 | -2.757295 | 3.958167 |
| 13 | 1 | 0 | 4.212655 | -1.576090 | 2.466538 |
| 14 | 1 | 0 | 0.100858 | -2.548506 | 1.658338 |
| 15 | 1 | 0 | -0.031245 | -3.780577 | 3.795859 |
| 16 | 1 | 0 | 4.080536 | -2.806339 | 4.606038 |
| 17 | 1 | 0 | 1.960157 | -3.917640 | 5.284085 |
| 18 | 6 | 0 | 0.772780 | -2.291760 | -1.258678 |
| 19 | 1 | 0 | 0.280008 | -1.972201 | -2.183092 |
| 20 | 1 | 0 | 0.012066 | -2.813281 | -0.669591 |
| 21 | 6 | 0 | 1.880718 | -3.308159 | -1.597768 |
| 22 | 1 | 0 | 2.306622 | -3.748882 | -0.690506 |
| 23 | 1 | 0 | 2.702509 | -2.859904 | -2.166154 |
| 24 | 1 | 0 | 1.460762 | -4.120331 | -2.202493 |
| 25 | 8 | 0 | 4.488646 | -0.288420 | 0.328652 |
| 26 | 16 | 0 | 5.754434 | -0.374136 | -0.808587 |
| 27 | 8 | 0 | 5.406153 | -1.248881 | -1.953576 |
| 28 | 6 | 0 | 5.529871 | 1.394658 | -1.482873 |
| 29 | 9 | 0 | 6.692516 | 1.714674 | -2.070696 |
| 30 | 9 | 0 | 4.553650 | 1.468785 | -2.388142 |
| 31 | 9 | 0 | 5.292663 | 2.250007 | -0.489157 |
| 32 | 46 | 0 | -0.197821 | 0.263274 | 0.240532 |
| 33 | 15 | 0 | -2.225829 | -0.592269 | -0.584522 |
| 34 | 6 | 0 | -3.123865 | 0.876458 | -1.253480 |
| 35 | 6 | 0 | -4.397253 | 3.119155 | -2.365170 |
| 36 | 6 | 0 | -4.497774 | 1.077650 | -1.066020 |
| 37 | 6 | 0 | -2.393006 | 1.819964 | -1.992738 |
| 38 | 6 | 0 | -3.026833 | 2.929859 | -2.551284 |

| | | | | | |
|---|---|---|---|---|---|
| 39 | 6 | 0 | -5.128127 | 2.193945 | -1.618505 |
| 40 | 1 | 0 | -5.078223 | 0.378214 | -0.474553 |
| 41 | 1 | 0 | -1.320069 | 1.694466 | -2.112645 |
| 42 | 1 | 0 | -2.445992 | 3.653414 | -3.116524 |
| 43 | 1 | 0 | -6.192580 | 2.342137 | -1.457577 |
| 44 | 1 | 0 | -4.890504 | 3.989212 | -2.789816 |
| 45 | 6 | 0 | -2.408664 | -1.837313 | -1.941855 |
| 46 | 6 | 0 | -2.552974 | -3.739262 | -4.012328 |
| 47 | 6 | 0 | -2.451579 | -1.431845 | -3.284961 |
| 48 | 6 | 0 | -2.439780 | -3.212465 | -1.653300 |
| 49 | 6 | 0 | -2.513809 | -4.153970 | -2.679623 |
| 50 | 6 | 0 | -2.522084 | -2.376329 | -4.310643 |
| 51 | 1 | 0 | -2.439817 | -0.376312 | -3.535973 |
| 52 | 1 | 0 | -2.413876 | -3.553491 | -0.623042 |
| 53 | 1 | 0 | -2.540824 | -5.212441 | -2.435382 |
| 54 | 1 | 0 | -2.558443 | -2.042433 | -5.344039 |
| 55 | 1 | 0 | -2.609627 | -4.473010 | -4.811620 |
| 56 | 6 | 0 | -3.277551 | -1.291996 | 0.759660 |
| 57 | 6 | 0 | -4.853585 | -2.318870 | 2.847510 |
| 58 | 6 | 0 | -4.485431 | -1.958699 | 0.483602 |
| 59 | 6 | 0 | -2.869836 | -1.152602 | 2.095295 |
| 60 | 6 | 0 | -3.654302 | -1.664508 | 3.130876 |
| 61 | 6 | 0 | -5.268261 | -2.464457 | 1.521591 |
| 62 | 1 | 0 | -4.811169 | -2.096077 | -0.542854 |
| 63 | 1 | 0 | -1.949757 | -0.626243 | 2.321721 |
| 64 | 1 | 0 | -3.324508 | -1.547635 | 4.159400 |
| 65 | 1 | 0 | -6.199312 | -2.975978 | 1.292739 |
| 66 | 1 | 0 | -5.462570 | -2.716687 | 3.654861 |
| 67 | 8 | 0 | -1.661582 | 1.635457 | 1.329855 |
| 68 | 16 | 0 | -1.348283 | 2.802334 | 2.292533 |
| 69 | 8 | 0 | 0.029834 | 2.657919 | 2.923949 |
| 70 | 6 | 0 | -1.037478 | 4.180087 | 1.011706 |
| 71 | 9 | 0 | -0.585614 | 5.283050 | 1.623347 |
| 72 | 9 | 0 | -0.125365 | 3.834137 | 0.060752 |
| 73 | 9 | 0 | -2.181103 | 4.478550 | 0.379802 |
| 74 | 1 | 0 | 1.350791 | 2.390929 | 0.423580 |
| 75 | 1 | 0 | 1.062235 | 1.927062 | 1.854883 |
| 76 | 8 | 0 | 1.453180 | 1.603025 | 0.983880 |

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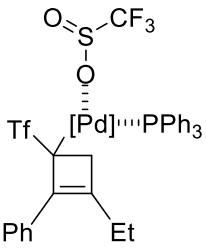
| | |
|---|---|
| Zero-point correction= | 0.554382 (Hartree/Particle) |
| Thermal correction to Energy= | 0.602134 |
| Thermal correction to Enthalpy= | 0.603078 |
| Thermal correction to Gibbs Free Energy= | 0.463414 |
| Sum of electronic and zero-point Energies= | -3475.791668 |
| Sum of electronic and thermal Energies= | -3475.743917 |
| Sum of electronic and thermal Enthalpies= | -3475.742973 |
| Sum of electronic and thermal Free Energies= | -3475.882636 |

**IX**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 46 | 0 | -0.048410 | -0.077946 | -0.350925 |
| 2 | 15 | 0 | -0.084178 | 2.276266 | -0.289889 |
| 3 | 6 | 0 | 0.042756 | 2.877388 | 1.450157 |
| 4 | 6 | 0 | 0.294947 | 3.615824 | 4.155483 |
| 5 | 6 | 0 | -1.076116 | 3.301897 | 2.182881 |
| 6 | 6 | 0 | 1.287562 | 2.800924 | 2.103059 |
| 7 | 6 | 0 | 1.410578 | 3.172950 | 3.440918 |
| 8 | 6 | 0 | -0.946776 | 3.671299 | 3.524111 |
| 9 | 1 | 0 | -2.055703 | 3.336786 | 1.722409 |
| 10 | 1 | 0 | 2.155994 | 2.431462 | 1.573274 |
| 11 | 1 | 0 | 2.381842 | 3.109115 | 3.923918 |
| 12 | 1 | 0 | -1.827565 | 3.995036 | 4.071023 |
| 13 | 1 | 0 | 0.392888 | 3.905618 | 5.198242 |
| 14 | 6 | 0 | 1.143912 | 3.272801 | -1.251004 |
| 15 | 6 | 0 | 2.823137 | 4.829148 | -2.875644 |
| 16 | 6 | 0 | 1.655290 | 4.488925 | -0.781110 |
| 17 | 6 | 0 | 1.476284 | 2.845955 | -2.545929 |
| 18 | 6 | 0 | 2.311719 | 3.618359 | -3.351672 |
| 19 | 6 | 0 | 2.492895 | 5.260979 | -1.591379 |
| 20 | 1 | 0 | 1.410535 | 4.836285 | 0.217539 |
| 21 | 1 | 0 | 1.095908 | 1.898640 | -2.918338 |
| 22 | 1 | 0 | 2.570240 | 3.269598 | -4.347490 |
| 23 | 1 | 0 | 2.887560 | 6.200176 | -1.212787 |
| 24 | 1 | 0 | 3.478001 | 5.428170 | -3.502302 |
| 25 | 6 | 0 | -1.608395 | 3.025032 | -1.022789 |
| 26 | 6 | 0 | -3.774493 | 4.170908 | -2.400463 |
| 27 | 6 | 0 | -2.024706 | 4.335377 | -0.733830 |
| 28 | 6 | 0 | -2.269743 | 2.314391 | -2.033330 |
| 29 | 6 | 0 | -3.347958 | 2.881083 | -2.717543 |
| 30 | 6 | 0 | -3.106638 | 4.897746 | -1.410320 |
| 31 | 1 | 0 | -1.503706 | 4.922006 | 0.015898 |
| 32 | 1 | 0 | -1.940133 | 1.312890 | -2.287767 |
| 33 | 1 | 0 | -3.852766 | 2.307223 | -3.489431 |
| 34 | 1 | 0 | -3.422650 | 5.909492 | -1.170379 |
| 35 | 1 | 0 | -4.615138 | 4.613633 | -2.927856 |
| 36 | 8 | 0 | 0.065660 | -2.221894 | -0.469235 |
| 37 | 16 | 0 | -0.818603 | -2.998452 | -1.514656 |
| 38 | 8 | 0 | -0.380778 | -2.731232 | -2.932503 |
| 39 | 6 | 0 | -0.086188 | -4.701456 | -1.136343 |
| 40 | 9 | 0 | -0.712538 | -5.610879 | -1.906036 |
| 41 | 9 | 0 | 1.229116 | -4.773166 | -1.389030 |
| 42 | 9 | 0 | -0.293730 | -5.026431 | 0.148807 |
| 43 | 15 | 0 | -2.589536 | -0.496284 | 0.354344 |
| 44 | 6 | 0 | -3.836591 | -0.767502 | -0.989544 |
| 45 | 6 | 0 | -5.678119 | -1.234383 | -3.069782 |
| 46 | 6 | 0 | -5.221312 | -0.752388 | -0.742228 |
| 47 | 6 | 0 | -3.393807 | -1.015330 | -2.298958 |
| 48 | 6 | 0 | -4.307399 | -1.249712 | -3.329202 |
| 49 | 6 | 0 | -6.132814 | -0.984331 | -1.773102 |

| | | | | | |
|---|---|---|---|---|---|
| 50 | 1 | 0 | -5.593196 | -0.549949 | 0.257206 |
| 51 | 1 | 0 | -2.333989 | -1.042714 | -2.530892 |
| 52 | 1 | 0 | -3.938691 | -1.450589 | -4.331077 |
| 53 | 1 | 0 | -7.198608 | -0.970308 | -1.560639 |
| 54 | 1 | 0 | -6.388664 | -1.416877 | -3.871579 |
| 55 | 6 | 0 | -2.603415 | -2.054362 | 1.350489 |
| 56 | 6 | 0 | -2.542870 | -4.348246 | 2.970649 |
| 57 | 6 | 0 | -3.677054 | -2.956670 | 1.345919 |
| 58 | 6 | 0 | -1.493338 | -2.324124 | 2.166386 |
| 59 | 6 | 0 | -1.467451 | -3.458869 | 2.977448 |
| 60 | 6 | 0 | -3.644300 | -4.096818 | 2.150466 |
| 61 | 1 | 0 | -4.534639 | -2.783463 | 0.705003 |
| 62 | 1 | 0 | -0.630640 | -1.667206 | 2.148302 |
| 63 | 1 | 0 | -0.592240 | -3.654602 | 3.590457 |
| 64 | 1 | 0 | -4.479604 | -4.791843 | 2.129589 |
| 65 | 1 | 0 | -2.517460 | -5.240338 | 3.590809 |
| 66 | 6 | 0 | -3.484096 | 0.676494 | 1.487168 |
| 67 | 6 | 0 | -4.791671 | 2.488222 | 3.207541 |
| 68 | 6 | 0 | -3.420650 | 0.518294 | 2.880797 |
| 69 | 6 | 0 | -4.205929 | 1.766927 | 0.969888 |
| 70 | 6 | 0 | -4.857097 | 2.659813 | 1.822705 |
| 71 | 6 | 0 | -4.068067 | 1.416203 | 3.731880 |
| 72 | 1 | 0 | -2.878184 | -0.318469 | 3.307900 |
| 73 | 1 | 0 | -4.276518 | 1.915245 | -0.101929 |
| 74 | 1 | 0 | -5.419301 | 3.488135 | 1.399564 |
| 75 | 1 | 0 | -4.013018 | 1.267472 | 4.807038 |
| 76 | 1 | 0 | -5.305788 | 3.179612 | 3.870066 |
| 77 | 1 | 0 | 3.001952 | -0.096203 | -2.757887 |
| 78 | 6 | 0 | 2.356321 | -0.729025 | -2.143760 |
| 79 | 6 | 0 | 2.049803 | -0.200787 | -0.705531 |
| 80 | 1 | 0 | 1.468589 | -1.032777 | -2.709173 |
| 81 | 6 | 0 | 2.708603 | -1.435828 | -0.163882 |
| 82 | 6 | 0 | 3.026315 | -1.879555 | -1.411677 |
| 83 | 6 | 0 | 2.868444 | -1.914294 | 1.206779 |
| 84 | 6 | 0 | 3.127249 | -2.810253 | 3.873615 |
| 85 | 6 | 0 | 2.225752 | -1.243405 | 2.264351 |
| 86 | 6 | 0 | 3.660723 | -3.034751 | 1.521287 |
| 87 | 6 | 0 | 3.782564 | -3.478943 | 2.836295 |
| 88 | 6 | 0 | 2.351368 | -1.686015 | 3.580256 |
| 89 | 1 | 0 | 1.626124 | -0.364342 | 2.044206 |
| 90 | 1 | 0 | 4.190877 | -3.556206 | 0.731639 |
| 91 | 1 | 0 | 4.397185 | -4.349041 | 3.052927 |
| 92 | 1 | 0 | 1.846732 | -1.147533 | 4.378990 |
| 93 | 1 | 0 | 3.227906 | -3.156059 | 4.899079 |
| 94 | 6 | 0 | 3.747706 | -3.060142 | -1.983424 |
| 95 | 1 | 0 | 3.590018 | -3.933195 | -1.339632 |
| 96 | 1 | 0 | 4.829208 | -2.850311 | -1.960512 |
| 97 | 6 | 0 | 3.319503 | -3.386549 | -3.422410 |
| 98 | 1 | 0 | 3.558187 | -2.559443 | -4.100693 |
| 99 | 1 | 0 | 2.242484 | -3.568296 | -3.474369 |
| 100 | 1 | 0 | 3.843087 | -4.278257 | -3.784516 |
| 101 | 8 | 0 | 2.647222 | 1.065377 | -0.298058 |
| 102 | 16 | 0 | 4.199689 | 1.632252 | -0.647139 |
| 103 | 8 | 0 | 4.873513 | 0.947334 | -1.781074 |
| 104 | 6 | 0 | 5.108027 | 0.940437 | 0.875223 |
| 105 | 9 | 0 | 5.479001 | -0.327265 | 0.738530 |
| 106 | 9 | 0 | 6.210829 | 1.701648 | 1.006629 |
| 107 | 9 | 0 | 4.363586 | 1.086972 | 1.980014 |

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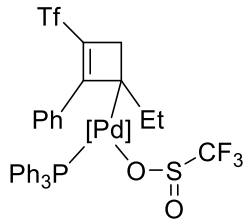
Zero-point correction= 0.804651 (Hartree/Particle)
Thermal correction to Energy= 0.867652

Thermal correction to Enthalpy= 0.868596
Thermal correction to Gibbs Free Energy= 0.697804
Sum of electronic and zero-point Energies= -4435.393585
Sum of electronic and thermal Energies= -4435.330584
Sum of electronic and thermal Enthalpies= -4435.329640
Sum of electronic and thermal Free Energies= -4435.500432

**X**



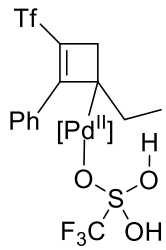

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.725500 | -1.277059 | -0.928946 |
| 2 | 6 | 0 | 1.562853 | -1.663921 | 0.053459 |
| 3 | 1 | 0 | 3.196801 | -2.120966 | -1.443574 |
| 4 | 1 | 0 | 2.491361 | -0.475379 | -1.629985 |
| 5 | 6 | 0 | 3.394717 | -0.806886 | 0.333594 |
| 6 | 6 | 0 | 2.370132 | -1.061942 | 1.183748 |
| 7 | 6 | 0 | 2.184024 | -0.921433 | 2.624321 |
| 8 | 6 | 0 | 1.910220 | -0.720334 | 5.424130 |
| 9 | 6 | 0 | 2.992987 | -0.035219 | 3.364582 |
| 10 | 6 | 0 | 1.222674 | -1.685015 | 3.314239 |
| 11 | 6 | 0 | 1.090052 | -1.587554 | 4.699232 |
| 12 | 6 | 0 | 2.856590 | 0.056803 | 4.748416 |
| 13 | 1 | 0 | 3.694008 | 0.600352 | 2.837531 |
| 14 | 1 | 0 | 0.584302 | -2.368513 | 2.763777 |
| 15 | 1 | 0 | 0.348357 | -2.194768 | 5.212580 |
| 16 | 1 | 0 | 3.490435 | 0.744690 | 5.302471 |
| 17 | 1 | 0 | 1.810547 | -0.646945 | 6.504068 |
| 18 | 6 | 0 | 1.261930 | -3.160265 | 0.124288 |
| 19 | 1 | 0 | 0.960378 | -3.501474 | -0.869848 |
| 20 | 1 | 0 | 0.409335 | -3.346472 | 0.785767 |
| 21 | 6 | 0 | 2.436556 | -4.029625 | 0.616413 |
| 22 | 1 | 0 | 2.678902 | -3.816566 | 1.662693 |
| 23 | 1 | 0 | 3.346500 | -3.875315 | 0.028989 |
| 24 | 1 | 0 | 2.160701 | -5.088358 | 0.541666 |
| 25 | 8 | 0 | 4.634394 | -0.275373 | 0.598212 |
| 26 | 16 | 0 | 6.032326 | -1.155817 | 0.147839 |
| 27 | 8 | 0 | 5.703600 | -2.559166 | -0.206808 |
| 28 | 6 | 0 | 6.260138 | -0.267466 | -1.511728 |
| 29 | 9 | 0 | 7.368758 | -0.782547 | -2.067398 |
| 30 | 9 | 0 | 5.237523 | -0.439068 | -2.346791 |
| 31 | 9 | 0 | 6.451429 | 1.030627 | -1.281672 |
| 32 | 46 | 0 | -0.119554 | -0.349892 | -0.235376 |
| 33 | 15 | 0 | -1.824783 | -1.940842 | -0.572266 |
| 34 | 6 | 0 | -2.896479 | -1.235783 | -1.910471 |
| 35 | 6 | 0 | -4.337688 | -0.285458 | -4.130921 |
| 36 | 6 | 0 | -4.287948 | -1.388646 | -1.974705 |
| 37 | 6 | 0 | -2.240018 | -0.578240 | -2.964997 |
| 38 | 6 | 0 | -2.953930 | -0.114299 | -4.071200 |
| 39 | 6 | 0 | -5.001447 | -0.913933 | -3.076487 |
| 40 | 1 | 0 | -4.828676 | -1.856957 | -1.161403 |
| 41 | 1 | 0 | -1.164054 | -0.427674 | -2.913680 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 1 | 0 | -2.427812 | 0.386340 | -4.879520 |
| 43 | 1 | 0 | -6.080985 | -1.032344 | -3.104745 |
| 44 | 1 | 0 | -4.896607 | 0.078620 | -4.988721 |
| 45 | 6 | 0 | -1.589203 | -3.665466 | -1.230982 |
| 46 | 6 | 0 | -1.117730 | -6.246343 | -2.257701 |
| 47 | 6 | 0 | -1.307058 | -3.856471 | -2.593668 |
| 48 | 6 | 0 | -1.626822 | -4.790372 | -0.391729 |
| 49 | 6 | 0 | -1.396048 | -6.069126 | -0.902241 |
| 50 | 6 | 0 | -1.073245 | -5.134521 | -3.101052 |
| 51 | 1 | 0 | -1.274110 | -3.007853 | -3.268836 |
| 52 | 1 | 0 | -1.833509 | -4.676197 | 0.666867 |
| 53 | 1 | 0 | -1.432069 | -6.925951 | -0.234826 |
| 54 | 1 | 0 | -0.859004 | -5.259366 | -4.158974 |
| 55 | 1 | 0 | -0.936136 | -7.241503 | -2.654044 |
| 56 | 6 | 0 | -2.854242 | -2.225335 | 0.932441 |
| 57 | 6 | 0 | -4.305641 | -2.615258 | 3.312055 |
| 58 | 6 | 0 | -3.986537 | -3.060634 | 0.953510 |
| 59 | 6 | 0 | -2.449240 | -1.613088 | 2.128744 |
| 60 | 6 | 0 | -3.168736 | -1.806761 | 3.310930 |
| 61 | 6 | 0 | -4.710753 | -3.244352 | 2.131325 |
| 62 | 1 | 0 | -4.292377 | -3.590944 | 0.057300 |
| 63 | 1 | 0 | -1.566387 | -0.980424 | 2.133893 |
| 64 | 1 | 0 | -2.835061 | -1.323635 | 4.224868 |
| 65 | 1 | 0 | -5.585936 | -3.888477 | 2.128954 |
| 66 | 1 | 0 | -4.868028 | -2.766294 | 4.229529 |
| 67 | 8 | 0 | 1.292940 | 1.216629 | -0.726457 |
| 68 | 16 | 0 | 1.787469 | 2.521001 | 0.006523 |
| 69 | 8 | 0 | 2.673584 | 2.231387 | 1.183569 |
| 70 | 6 | 0 | 3.029905 | 2.961743 | -1.358425 |
| 71 | 9 | 0 | 3.752995 | 4.029271 | -0.977400 |
| 72 | 9 | 0 | 3.873644 | 1.952631 | -1.625516 |
| 73 | 9 | 0 | 2.386947 | 3.282454 | -2.499572 |
| 74 | 15 | 0 | -1.907891 | 1.739488 | 0.155134 |
| 75 | 6 | 0 | -1.736540 | 2.293878 | 1.912591 |
| 76 | 6 | 0 | -1.352904 | 3.124023 | 4.574345 |
| 77 | 6 | 0 | -2.716100 | 3.056374 | 2.574747 |
| 78 | 6 | 0 | -0.566588 | 1.952030 | 2.609795 |
| 79 | 6 | 0 | -0.374078 | 2.368455 | 3.929232 |
| 80 | 6 | 0 | -2.524381 | 3.466874 | 3.894229 |
| 81 | 1 | 0 | -3.634900 | 3.324824 | 2.063169 |
| 82 | 1 | 0 | 0.213051 | 1.369334 | 2.130572 |
| 83 | 1 | 0 | 0.542800 | 2.092900 | 4.440823 |
| 84 | 1 | 0 | -3.291600 | 4.056257 | 4.390021 |
| 85 | 1 | 0 | -1.205920 | 3.445753 | 5.602138 |
| 86 | 6 | 0 | -1.470848 | 3.232612 | -0.846696 |
| 87 | 6 | 0 | -0.860787 | 5.436064 | -2.479101 |
| 88 | 6 | 0 | -1.638283 | 4.541238 | -0.369066 |
| 89 | 6 | 0 | -0.985373 | 3.043146 | -2.148974 |
| 90 | 6 | 0 | -0.687484 | 4.138407 | -2.961548 |
| 91 | 6 | 0 | -1.333279 | 5.634585 | -1.179883 |
| 92 | 1 | 0 | -1.992418 | 4.710439 | 0.642481 |
| 93 | 1 | 0 | -0.812508 | 2.038592 | -2.518451 |
| 94 | 1 | 0 | -0.298691 | 3.975181 | -3.962715 |
| 95 | 1 | 0 | -1.459074 | 6.642392 | -0.792897 |
| 96 | 1 | 0 | -0.617091 | 6.288818 | -3.107164 |
| 97 | 6 | 0 | -3.753634 | 1.688422 | -0.061576 |
| 98 | 6 | 0 | -6.549839 | 1.536004 | -0.400743 |
| 99 | 6 | 0 | -4.380959 | 2.310209 | -1.152286 |
| 100 | 6 | 0 | -4.554142 | 0.980478 | 0.852642 |
| 101 | 6 | 0 | -5.937360 | 0.909039 | 0.686793 |
| 102 | 6 | 0 | -5.765361 | 2.233418 | -1.319338 |

| | | | | | |
|---|---|---|---|---|---|
| 103 | 1 | 0 | -3.790550 | 2.865940 | -1.872301 |
| 104 | 1 | 0 | -4.101569 | 0.497809 | 1.712154 |
| 105 | 1 | 0 | -6.535492 | 0.365527 | 1.413730 |
| 106 | 1 | 0 | -6.229067 | 2.729817 | -2.167923 |
| 107 | 1 | 0 | -7.628223 | 1.485041 | -0.526925 |

Zero-point correction= 0.804571 (Hartree/Particle)
Thermal correction to Energy= 0.867781
Thermal correction to Enthalpy= 0.868725
Thermal correction to Gibbs Free Energy= 0.697151
Sum of electronic and zero-point Energies= -4435.379066
Sum of electronic and thermal Energies= -4435.315856
Sum of electronic and thermal Enthalpies= -4435.314912
Sum of electronic and thermal Free Energies= -4435.486486

**XII**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.323477 | -0.111646 | -1.643571 |
| 2 | 6 | 0 | 1.401919 | -1.078560 | -0.854633 |
| 3 | 1 | 0 | 2.739747 | -0.525447 | -2.568515 |
| 4 | 1 | 0 | 1.903509 | 0.882736 | -1.819791 |
| 5 | 6 | 0 | 3.183889 | -0.224570 | -0.402746 |
| 6 | 6 | 0 | 2.376598 | -1.082119 | 0.278138 |
| 7 | 6 | 0 | 2.388693 | -1.705763 | 1.602074 |
| 8 | 6 | 0 | 2.396184 | -2.877237 | 4.160900 |
| 9 | 6 | 0 | 3.601727 | -2.010315 | 2.247300 |
| 10 | 6 | 0 | 1.181000 | -2.009276 | 2.258904 |
| 11 | 6 | 0 | 1.186127 | -2.587189 | 3.527885 |
| 12 | 6 | 0 | 3.601207 | -2.588906 | 3.514561 |
| 13 | 1 | 0 | 4.541377 | -1.823233 | 1.738945 |
| 14 | 1 | 0 | 0.234427 | -1.764749 | 1.781641 |
| 15 | 1 | 0 | 0.243094 | -2.802767 | 4.022402 |
| 16 | 1 | 0 | 4.546600 | -2.822233 | 3.996822 |
| 17 | 1 | 0 | 2.400998 | -3.327225 | 5.149865 |
| 18 | 6 | 0 | 0.675262 | -2.243029 | -1.443558 |
| 19 | 1 | 0 | 0.682697 | -2.178784 | -2.536187 |
| 20 | 1 | 0 | -0.465795 | -2.135893 | -1.199221 |
| 21 | 6 | 0 | 1.042996 | -3.652782 | -0.958188 |
| 22 | 1 | 0 | 0.937702 | -3.748889 | 0.124549 |
| 23 | 1 | 0 | 2.084960 | -3.870018 | -1.216219 |
| 24 | 1 | 0 | 0.405741 | -4.402388 | -1.438334 |
| 25 | 8 | 0 | 4.299259 | 0.477809 | -0.026902 |
| 26 | 16 | 0 | 5.870880 | -0.045628 | -0.457439 |
| 27 | 8 | 0 | 5.966695 | -1.524397 | -0.420732 |
| 28 | 6 | 0 | 5.741376 | 0.339406 | -2.321930 |
| 29 | 9 | 0 | 6.993590 | 0.540255 | -2.754261 |
| 30 | 9 | 0 | 5.211529 | -0.689306 | -2.984219 |
| 31 | 9 | 0 | 5.020853 | 1.439762 | -2.540753 |
| 32 | 46 | 0 | -0.517557 | -0.361208 | -0.486238 |

| | | | | | |
|---|---|---|---|---|---|
| 33 | 15 | 0 | -2.980575 | -0.171092 | -0.386580 |
| 34 | 6 | 0 | -3.743692 | 1.487062 | -0.614778 |
| 35 | 6 | 0 | -4.829803 | 4.046070 | -0.977691 |
| 36 | 6 | 0 | -5.089983 | 1.737883 | -0.298501 |
| 37 | 6 | 0 | -2.948784 | 2.531411 | -1.108093 |
| 38 | 6 | 0 | -3.490406 | 3.807478 | -1.282142 |
| 39 | 6 | 0 | -5.629475 | 3.009214 | -0.485695 |
| 40 | 1 | 0 | -5.712151 | 0.944543 | 0.105108 |
| 41 | 1 | 0 | -1.898618 | 2.365534 | -1.322629 |
| 42 | 1 | 0 | -2.848468 | 4.611792 | -1.627669 |
| 43 | 1 | 0 | -6.670973 | 3.194562 | -0.236188 |
| 44 | 1 | 0 | -5.249720 | 5.040159 | -1.107100 |
| 45 | 6 | 0 | -3.711438 | -1.199885 | -1.740076 |
| 46 | 6 | 0 | -4.642138 | -2.816555 | -3.848582 |
| 47 | 6 | 0 | -4.364501 | -0.630252 | -2.841896 |
| 48 | 6 | 0 | -3.527360 | -2.594188 | -1.712944 |
| 49 | 6 | 0 | -3.994337 | -3.395708 | -2.753332 |
| 50 | 6 | 0 | -4.823081 | -1.434482 | -3.889396 |
| 51 | 1 | 0 | -4.518610 | 0.443070 | -2.884036 |
| 52 | 1 | 0 | -3.030047 | -3.058748 | -0.864386 |
| 53 | 1 | 0 | -3.852992 | -4.472524 | -2.709407 |
| 54 | 1 | 0 | -5.326592 | -0.975009 | -4.735841 |
| 55 | 1 | 0 | -5.002411 | -3.440228 | -4.662155 |
| 56 | 6 | 0 | -3.749847 | -0.835451 | 1.152243 |
| 57 | 6 | 0 | -4.849815 | -1.744068 | 3.567689 |
| 58 | 6 | 0 | -4.953509 | -1.559168 | 1.157207 |
| 59 | 6 | 0 | -3.096651 | -0.572274 | 2.369271 |
| 60 | 6 | 0 | -3.653501 | -1.023801 | 3.568030 |
| 61 | 6 | 0 | -5.498266 | -2.011859 | 2.360231 |
| 62 | 1 | 0 | -5.462704 | -1.778919 | 0.223603 |
| 63 | 1 | 0 | -2.161817 | -0.011775 | 2.380604 |
| 64 | 1 | 0 | -3.145340 | -0.810123 | 4.504733 |
| 65 | 1 | 0 | -6.429068 | -2.573203 | 2.352213 |
| 66 | 1 | 0 | -5.275529 | -2.097035 | 4.503496 |
| 67 | 8 | 0 | 0.276187 | 1.602367 | -0.212523 |
| 68 | 16 | 0 | -0.200933 | 2.500973 | 1.001392 |
| 69 | 8 | 0 | -0.293205 | 1.078304 | 2.201732 |
| 70 | 6 | 0 | 1.472162 | 2.941351 | 1.784939 |
| 71 | 9 | 0 | 1.260724 | 3.638929 | 2.904904 |
| 72 | 9 | 0 | 2.192560 | 1.845651 | 2.089646 |
| 73 | 9 | 0 | 2.235637 | 3.675196 | 0.959705 |
| 74 | 8 | 0 | -0.136979 | 3.992287 | 0.029531 |
| 75 | 1 | 0 | 0.516453 | 0.539957 | 2.209381 |
| 76 | 1 | 0 | 0.624728 | 3.963157 | -0.577041 |

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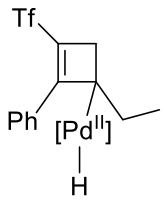
Zero-point correction= 0.550760 (Hartree/Particle)
Thermal correction to Energy= 0.598790
Thermal correction to Enthalpy= 0.599734
Thermal correction to Gibbs Free Energy= 0.459632
Sum of electronic and zero-point Energies= -3475.712165
Sum of electronic and thermal Energies= -3475.664135
Sum of electronic and thermal Enthalpies= -3475.663191
Sum of electronic and thermal Free Energies= -3475.803294

**XIII**




| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.542910 | -1.484231 | -0.055939 |
| 2 | 6 | 0 | -1.581002 | -0.385619 | -0.632215 |
| 3 | 1 | 0 | -3.046747 | -2.097387 | -0.811827 |
| 4 | 1 | 0 | -2.098627 | -2.138003 | 0.700847 |
| 5 | 6 | 0 | -3.310089 | -0.304526 | 0.477577 |
| 6 | 6 | 0 | -2.482727 | 0.656228 | 0.003792 |
| 7 | 6 | 0 | -2.419974 | 2.117906 | 0.062995 |
| 8 | 6 | 0 | -2.271145 | 4.930102 | 0.175430 |
| 9 | 6 | 0 | -3.589843 | 2.897718 | 0.146231 |
| 10 | 6 | 0 | -1.177535 | 2.777737 | 0.024001 |
| 11 | 6 | 0 | -1.104125 | 4.168562 | 0.082470 |
| 12 | 6 | 0 | -3.511832 | 4.287921 | 0.205173 |
| 13 | 1 | 0 | -4.559123 | 2.410943 | 0.130426 |
| 14 | 1 | 0 | -0.267496 | 2.182230 | -0.022148 |
| 15 | 1 | 0 | -0.133545 | 4.657957 | 0.059811 |
| 16 | 1 | 0 | -4.426047 | 4.873024 | 0.264476 |
| 17 | 1 | 0 | -2.214929 | 6.014738 | 0.219172 |
| 18 | 6 | 0 | -1.403578 | -0.368567 | -2.161558 |
| 19 | 1 | 0 | -1.122519 | -1.378079 | -2.489737 |
| 20 | 1 | 0 | -0.557379 | 0.290761 | -2.447118 |
| 21 | 6 | 0 | -2.636520 | 0.103949 | -2.959557 |
| 22 | 1 | 0 | -2.864855 | 1.152506 | -2.746899 |
| 23 | 1 | 0 | -3.522136 | -0.486159 | -2.699503 |
| 24 | 1 | 0 | -2.461297 | 0.001588 | -4.036686 |
| 25 | 8 | 0 | -4.353310 | -0.265218 | 1.399033 |
| 26 | 16 | 0 | -5.966628 | -0.262194 | 0.893340 |
| 27 | 8 | 0 | -6.166922 | 0.607296 | -0.292928 |
| 28 | 6 | 0 | -6.001001 | -2.014097 | 0.145236 |
| 29 | 9 | 0 | -7.283538 | -2.410063 | 0.159943 |
| 30 | 9 | 0 | -5.564689 | -2.014073 | -1.115508 |
| 31 | 9 | 0 | -5.278305 | -2.868303 | 0.874256 |
| 32 | 46 | 0 | 0.449463 | -0.353827 | -0.215700 |
| 33 | 1 | 0 | 0.070467 | -0.731549 | 1.245911 |
| 34 | 15 | 0 | 2.856032 | -0.286875 | 0.070874 |
| 35 | 6 | 0 | 3.555225 | -1.799678 | 0.857288 |
| 36 | 6 | 0 | 4.536553 | -4.178112 | 1.980382 |
| 37 | 6 | 0 | 4.732279 | -1.792055 | 1.621871 |
| 38 | 6 | 0 | 2.868920 | -3.010524 | 0.674383 |
| 39 | 6 | 0 | 3.360847 | -4.193605 | 1.227249 |
| 40 | 6 | 0 | 5.218771 | -2.975782 | 2.179493 |
| 41 | 1 | 0 | 5.265005 | -0.860926 | 1.790856 |
| 42 | 1 | 0 | 1.938957 | -3.016698 | 0.111734 |
| 43 | 1 | 0 | 2.818908 | -5.123780 | 1.079428 |
| 44 | 1 | 0 | 6.128772 | -2.956893 | 2.773370 |
| 45 | 1 | 0 | 4.915232 | -5.097716 | 2.418497 |
| 46 | 6 | 0 | 3.802549 | -0.106231 | -1.506042 |
| 47 | 6 | 0 | 5.101857 | 0.240350 | -3.975839 |
| 48 | 6 | 0 | 4.898338 | -0.909510 | -1.853263 |
| 49 | 6 | 0 | 3.362779 | 0.869284 | -2.418323 |
| 50 | 6 | 0 | 4.010993 | 1.046670 | -3.639522 |
| 51 | 6 | 0 | 5.541115 | -0.736830 | -3.082200 |

| | | | | | |
|---|---|---|---|---|---|
| 52 | 1 | 0 | 5.250862 | -1.672802 | -1.166818 |
| 53 | 1 | 0 | 2.509622 | 1.497102 | -2.169119 |
| 54 | 1 | 0 | 3.660074 | 1.807805 | -4.331171 |
| 55 | 1 | 0 | 6.386809 | -1.369472 | -3.338674 |
| 56 | 1 | 0 | 5.602568 | 0.371308 | -4.931265 |
| 57 | 6 | 0 | 3.471097 | 1.104161 | 1.113567 |
| 58 | 6 | 0 | 4.309991 | 3.199325 | 2.783690 |
| 59 | 6 | 0 | 4.705376 | 1.736556 | 0.895862 |
| 60 | 6 | 0 | 2.656823 | 1.541892 | 2.171167 |
| 61 | 6 | 0 | 3.077995 | 2.579336 | 3.003869 |
| 62 | 6 | 0 | 5.120740 | 2.778482 | 1.727517 |
| 63 | 1 | 0 | 5.339623 | 1.421294 | 0.072487 |
| 64 | 1 | 0 | 1.689647 | 1.073269 | 2.330327 |
| 65 | 1 | 0 | 2.438173 | 2.909068 | 3.817864 |
| 66 | 1 | 0 | 6.077193 | 3.262328 | 1.547546 |
| 67 | 1 | 0 | 4.633909 | 4.012243 | 3.428098 |

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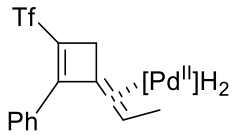
Zero-point correction= 0.509695 (Hartree/Particle)
Thermal correction to Energy= 0.548348
Thermal correction to Enthalpy= 0.549292
Thermal correction to Gibbs Free Energy= 0.429787
Sum of electronic and zero-point Energies= -2513.759589
Sum of electronic and thermal Energies= -2513.720936
Sum of electronic and thermal Enthalpies= -2513.719992
Sum of electronic and thermal Free Energies= -2513.839497

**XIV**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.407409 | -1.357986 | 0.568281 |
| 2 | 6 | 0 | 1.686802 | -0.122325 | 1.166462 |
| 3 | 1 | 0 | 2.960592 | -1.965406 | 1.292441 |
| 4 | 1 | 0 | 1.781014 | -1.997955 | -0.060200 |
| 5 | 6 | 0 | 3.183130 | -0.298860 | -0.183493 |
| 6 | 6 | 0 | 2.502527 | 0.774773 | 0.290673 |
| 7 | 6 | 0 | 2.516673 | 2.217247 | 0.030869 |
| 8 | 6 | 0 | 2.522942 | 4.974585 | -0.519045 |
| 9 | 6 | 0 | 3.728434 | 2.904091 | -0.162251 |
| 10 | 6 | 0 | 1.308920 | 2.934235 | -0.050528 |
| 11 | 6 | 0 | 1.314451 | 4.300907 | -0.324986 |
| 12 | 6 | 0 | 3.726987 | 4.271567 | -0.435839 |
| 13 | 1 | 0 | 4.668030 | 2.369422 | -0.065936 |
| 14 | 1 | 0 | 0.369217 | 2.403719 | 0.079439 |
| 15 | 1 | 0 | 0.372312 | 4.838933 | -0.390388 |
| 16 | 1 | 0 | 4.671630 | 4.790873 | -0.574931 |
| 17 | 1 | 0 | 2.526359 | 6.040973 | -0.729146 |
| 18 | 6 | 0 | 1.119203 | 0.024581 | 2.423259 |
| 19 | 1 | 0 | 1.010783 | -0.886369 | 3.008133 |
| 20 | 1 | 0 | -1.286562 | -0.170515 | 2.427085 |
| 21 | 6 | 0 | 1.099555 | 1.312097 | 3.216178 |
| 22 | 1 | 0 | 1.012433 | 2.194276 | 2.578938 |
| 23 | 1 | 0 | 2.039630 | 1.403187 | 3.780364 |
| 24 | 1 | 0 | 0.273557 | 1.319258 | 3.931338 |
| 25 | 8 | 0 | 4.104212 | -0.429044 | -1.199590 |
| 26 | 16 | 0 | 5.777614 | -0.488363 | -0.876173 |
| 27 | 8 | 0 | 6.147946 | 0.423529 | 0.233381 |
| 28 | 6 | 0 | 5.792067 | -2.206294 | -0.051032 |
| 29 | 9 | 0 | 7.035460 | -2.687743 | -0.193681 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 9 | 0 | 5.505049 | -2.119324 | 1.247357 |
| 31 | 9 | 0 | 4.934106 | -3.035318 | -0.649937 |
| 32 | 46 | 0 | -0.603239 | -0.162726 | 0.938993 |
| 33 | 1 | 0 | -0.073923 | -0.208322 | -0.627057 |
| 34 | 15 | 0 | -2.702334 | -0.292019 | 0.002572 |
| 35 | 6 | 0 | -4.168927 | -0.334939 | 1.130596 |
| 36 | 6 | 0 | -6.400801 | -0.281852 | 2.836773 |
| 37 | 6 | 0 | -5.325632 | -1.064984 | 0.814484 |
| 38 | 6 | 0 | -4.142735 | 0.415441 | 2.315404 |
| 39 | 6 | 0 | -5.253987 | 0.448077 | 3.157709 |
| 40 | 6 | 0 | -6.432556 | -1.040849 | 1.666165 |
| 41 | 1 | 0 | -5.364700 | -1.659427 | -0.092843 |
| 42 | 1 | 0 | -3.238405 | 0.951862 | 2.585688 |
| 43 | 1 | 0 | -5.218015 | 1.034044 | 4.072233 |
| 44 | 1 | 0 | -7.317318 | -1.619279 | 1.413536 |
| 45 | 1 | 0 | -7.261801 | -0.265244 | 3.499771 |
| 46 | 6 | 0 | -3.091746 | 1.100781 | -1.151496 |
| 47 | 6 | 0 | -3.622599 | 3.194503 | -2.951731 |
| 48 | 6 | 0 | -4.365946 | 1.688014 | -1.207866 |
| 49 | 6 | 0 | -2.084564 | 1.582549 | -2.004902 |
| 50 | 6 | 0 | -2.351786 | 2.616896 | -2.901587 |
| 51 | 6 | 0 | -4.626718 | 2.728893 | -2.102190 |
| 52 | 1 | 0 | -5.157406 | 1.339163 | -0.553265 |
| 53 | 1 | 0 | -1.091412 | 1.147212 | -1.952540 |
| 54 | 1 | 0 | -1.561313 | 2.976729 | -3.554720 |
| 55 | 1 | 0 | -5.617138 | 3.175542 | -2.130453 |
| 56 | 1 | 0 | -3.827038 | 4.006151 | -3.645006 |
| 57 | 6 | 0 | -2.897971 | -1.816578 | -1.014972 |
| 58 | 6 | 0 | -3.161851 | -4.202136 | -2.468823 |
| 59 | 6 | 0 | -3.598909 | -1.833001 | -2.228979 |
| 60 | 6 | 0 | -2.324010 | -3.006392 | -0.540149 |
| 61 | 6 | 0 | -2.460741 | -4.192585 | -1.260081 |
| 62 | 6 | 0 | -3.727256 | -3.021575 | -2.952320 |
| 63 | 1 | 0 | -4.038543 | -0.918478 | -2.615060 |
| 64 | 1 | 0 | -1.760643 | -2.994868 | 0.389359 |
| 65 | 1 | 0 | -2.011805 | -5.107275 | -0.882323 |
| 66 | 1 | 0 | -4.267445 | -3.021374 | -3.895376 |
| 67 | 1 | 0 | -3.260909 | -5.125040 | -3.034009 |

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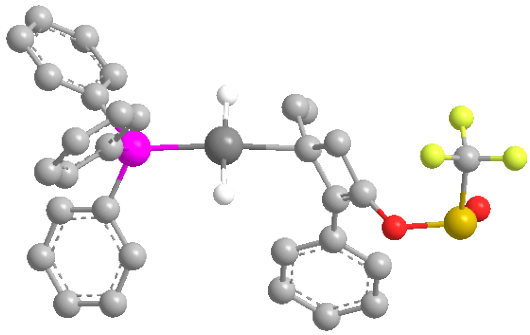
Zero-point correction= 0.506714 (Hartree/Particle)
Thermal correction to Energy= 0.545008
Thermal correction to Enthalpy= 0.545952
Thermal correction to Gibbs Free Energy= 0.428696
Sum of electronic and zero-point Energies= -2513.740191
Sum of electronic and thermal Energies= -2513.701897
Sum of electronic and thermal Enthalpies= -2513.700952
Sum of electronic and thermal Free Energies= -2513.818209

**TS$_{XIII-XIV}$**



Imaginary frequency: -577.4634 $cm^{-1}$

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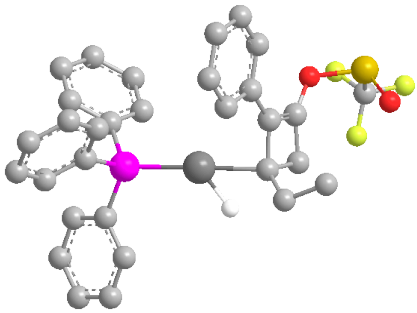
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.500980 | -1.430446 | 0.355361 |
| 2 | 6 | 0 | 1.654583 | -0.247849 | 0.905684 |
| 3 | 1 | 0 | 3.008582 | -2.031089 | 1.118308 |
| 4 | 1 | 0 | 1.981268 | -2.084516 | -0.351030 |
| 5 | 6 | 0 | 3.301004 | -0.317006 | -0.282819 |
| 6 | 6 | 0 | 2.536135 | 0.711283 | 0.161641 |
| 7 | 6 | 0 | 2.522031 | 2.162715 | -0.040787 |
| 8 | 6 | 0 | 2.481750 | 4.943676 | -0.465319 |
| 9 | 6 | 0 | 3.722370 | 2.892018 | -0.118896 |
| 10 | 6 | 0 | 1.301918 | 2.851090 | -0.172604 |
| 11 | 6 | 0 | 1.284174 | 4.228770 | -0.384709 |
| 12 | 6 | 0 | 3.698031 | 4.269980 | -0.331243 |
| 13 | 1 | 0 | 4.669334 | 2.379946 | 0.018857 |
| 14 | 1 | 0 | 0.371408 | 2.290189 | -0.131928 |
| 15 | 1 | 0 | 0.332363 | 4.742896 | -0.491046 |
| 16 | 1 | 0 | 4.633895 | 4.820468 | -0.382250 |
| 17 | 1 | 0 | 2.467105 | 6.018376 | -0.627184 |
| 18 | 6 | 0 | 1.083103 | -0.154380 | 2.203048 |
| 19 | 1 | 0 | 1.074792 | -1.085585 | 2.766888 |
| 20 | 1 | 0 | -0.699294 | -0.221636 | 2.189304 |
| 21 | 6 | 0 | 1.177059 | 1.099860 | 3.049882 |
| 22 | 1 | 0 | 0.983526 | 2.003104 | 2.468299 |
| 23 | 1 | 0 | 2.195060 | 1.178027 | 3.456220 |
| 24 | 1 | 0 | 0.475238 | 1.068960 | 3.888239 |
| 25 | 8 | 0 | 4.301995 | -0.376719 | -1.231873 |
| 26 | 16 | 0 | 5.941720 | -0.409460 | -0.775000 |
| 27 | 8 | 0 | 6.195591 | 0.465626 | 0.396010 |
| 28 | 6 | 0 | 5.939538 | -2.157668 | -0.015557 |
| 29 | 9 | 0 | 7.202356 | -2.605480 | -0.081884 |
| 30 | 9 | 0 | 5.555749 | -2.127996 | 1.260703 |
| 31 | 9 | 0 | 5.150382 | -2.984197 | -0.705942 |
| 32 | 46 | 0 | -0.490443 | -0.291527 | 0.543658 |
| 33 | 1 | 0 | -0.183103 | -0.399199 | -1.062255 |
| 34 | 15 | 0 | -2.753499 | -0.316329 | -0.019618 |
| 35 | 6 | 0 | -4.003683 | -0.420082 | 1.342490 |
| 36 | 6 | 0 | -5.870116 | -0.463448 | 3.444787 |
| 37 | 6 | 0 | -5.214116 | -1.117904 | 1.207825 |
| 38 | 6 | 0 | -3.738759 | 0.247340 | 2.548055 |
| 39 | 6 | 0 | -4.667935 | 0.233479 | 3.587944 |
| 40 | 6 | 0 | -6.138416 | -1.141553 | 2.255093 |
| 41 | 1 | 0 | -5.436672 | -1.650543 | 0.288876 |
| 42 | 1 | 0 | -2.791489 | 0.764131 | 2.673271 |
| 43 | 1 | 0 | -4.447360 | 0.757186 | 4.514315 |
| 44 | 1 | 0 | -7.067260 | -1.693786 | 2.138781 |
| 45 | 1 | 0 | -6.589575 | -0.484147 | 4.259032 |
| 46 | 6 | 0 | -3.260358 | 1.192141 | -0.960144 |
| 47 | 6 | 0 | -3.951117 | 3.473889 | -2.447854 |
| 48 | 6 | 0 | -4.487793 | 1.837725 | -0.745726 |
| 49 | 6 | 0 | -2.379147 | 1.708090 | -1.926221 |
| 50 | 6 | 0 | -2.726813 | 2.837537 | -2.667080 |
| 51 | 6 | 0 | -4.828645 | 2.972699 | -1.485713 |
| 52 | 1 | 0 | -5.178852 | 1.459426 | 0.000361 |
| 53 | 1 | 0 | -1.420590 | 1.223269 | -2.084717 |
| 54 | 1 | 0 | -2.035475 | 3.224230 | -3.411070 |
| 55 | 1 | 0 | -5.781316 | 3.464156 | -1.306291 |
| 56 | 1 | 0 | -4.217314 | 4.358056 | -3.021105 |
| 57 | 6 | 0 | -3.197304 | -1.719832 | -1.128775 |
| 58 | 6 | 0 | -3.820801 | -3.933513 | -2.737321 |
| 59 | 6 | 0 | -4.171613 | -1.615925 | -2.132459 |
| 60 | 6 | 0 | -2.530562 | -2.941186 | -0.948313 |
| 61 | 6 | 0 | -2.845527 | -4.043028 | -1.743147 |

| | | | | | |
|---|---|---|---|---|---|
| 62 | 6 | 0 | -4.479735 | -2.718551 | -2.932766 |
| 63 | 1 | 0 | -4.683907 | -0.672676 | -2.297260 |
| 64 | 1 | 0 | -1.751405 | -3.017441 | -0.194458 |
| 65 | 1 | 0 | -2.320783 | -4.982921 | -1.594405 |
| 66 | 1 | 0 | -5.231781 | -2.624767 | -3.711762 |
| 67 | 1 | 0 | -4.059502 | -4.789327 | -3.363144 |

Zero-point correction= 0.505648 (Hartree/Particle)
Thermal correction to Energy= 0.543490
Thermal correction to Enthalpy= 0.544434
Thermal correction to Gibbs Free Energy= 0.428073
Sum of electronic and zero-point Energies= -2513.736066
Sum of electronic and thermal Energies= -2513.698224
Sum of electronic and thermal Enthalpies= -2513.697279
Sum of electronic and thermal Free Energies= -2513.813640

**TS$_{XII-2}$**



Imaginary frequency: -639.8789 $cm^{-1}$

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.651680 | -0.722728 | 1.436360 |
| 2 | 6 | 0 | 1.619021 | 0.422544 | 1.750242 |
| 3 | 1 | 0 | 3.466635 | -0.815596 | 2.162717 |
| 4 | 1 | 0 | 2.214446 | -1.709551 | 1.255238 |
| 5 | 6 | 0 | 2.970411 | 0.096947 | 0.217820 |
| 6 | 6 | 0 | 2.102688 | 1.111410 | 0.472617 |
| 7 | 6 | 0 | 1.767080 | 2.376044 | -0.181672 |
| 8 | 6 | 0 | 1.142380 | 4.836256 | -1.412116 |
| 9 | 6 | 0 | 2.378252 | 2.753053 | -1.394914 |
| 10 | 6 | 0 | 0.834531 | 3.258644 | 0.397907 |
| 11 | 6 | 0 | 0.527336 | 4.475218 | -0.211540 |
| 12 | 6 | 0 | 2.067959 | 3.968371 | -1.999542 |
| 13 | 1 | 0 | 3.090359 | 2.080770 | -1.861646 |
| 14 | 1 | 0 | 0.349278 | 2.982512 | 1.329123 |
| 15 | 1 | 0 | -0.191589 | 5.142998 | 0.256212 |
| 16 | 1 | 0 | 2.548282 | 4.239379 | -2.936169 |
| 17 | 1 | 0 | 0.903449 | 5.784126 | -1.886744 |
| 18 | 6 | 0 | 1.774951 | 1.146255 | 3.094906 |
| 19 | 1 | 0 | 1.671199 | 0.396853 | 3.891007 |
| 20 | 1 | 0 | 0.940257 | 1.843041 | 3.237589 |
| 21 | 6 | 0 | 3.100414 | 1.906893 | 3.269375 |
| 22 | 1 | 0 | 3.172321 | 2.749095 | 2.572516 |
| 23 | 1 | 0 | 3.971142 | 1.263914 | 3.098967 |
| 24 | 1 | 0 | 3.176452 | 2.307980 | 4.286945 |
| 25 | 8 | 0 | 3.760105 | -0.135973 | -0.888509 |
| 26 | 16 | 0 | 5.457313 | -0.346709 | -0.649193 |
| 27 | 8 | 0 | 5.860423 | 0.069336 | 0.715054 |
| 28 | 6 | 0 | 5.353149 | -2.239417 | -0.576836 |
| 29 | 9 | 0 | 6.613885 | -2.695288 | -0.579367 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 9 | 0 | 4.732928 | -2.680889 | 0.516594 |
| 31 | 9 | 0 | 4.724607 | -2.689394 | -1.665730 |
| 32 | 46 | 0 | -0.336412 | 0.087028 | 0.921915 |
| 33 | 1 | 0 | 0.221678 | -0.575244 | 2.247335 |
| 34 | 15 | 0 | -2.476792 | -0.404488 | 0.014984 |
| 35 | 6 | 0 | -3.440289 | -1.656235 | 0.972512 |
| 36 | 6 | 0 | -4.878757 | -3.491295 | 2.539271 |
| 37 | 6 | 0 | -4.325381 | -2.564849 | 0.372052 |
| 38 | 6 | 0 | -3.276554 | -1.686501 | 2.366596 |
| 39 | 6 | 0 | -3.997127 | -2.592978 | 3.144709 |
| 40 | 6 | 0 | -5.038581 | -3.477614 | 1.152425 |
| 41 | 1 | 0 | -4.453697 | -2.567339 | -0.706218 |
| 42 | 1 | 0 | -2.568760 | -1.006831 | 2.833482 |
| 43 | 1 | 0 | -3.860062 | -2.605302 | 4.222753 |
| 44 | 1 | 0 | -5.716711 | -4.179718 | 0.674302 |
| 45 | 1 | 0 | -5.432271 | -4.204291 | 3.144618 |
| 46 | 6 | 0 | -3.632581 | 1.031908 | -0.125519 |
| 47 | 6 | 0 | -5.274860 | 3.297805 | -0.393761 |
| 48 | 6 | 0 | -5.012137 | 0.944683 | 0.114510 |
| 49 | 6 | 0 | -3.085482 | 2.273543 | -0.490168 |
| 50 | 6 | 0 | -3.901623 | 3.395722 | -0.630986 |
| 51 | 6 | 0 | -5.826523 | 2.072165 | -0.017695 |
| 52 | 1 | 0 | -5.452446 | -0.002404 | 0.410649 |
| 53 | 1 | 0 | -2.015000 | 2.364872 | -0.658301 |
| 54 | 1 | 0 | -3.462480 | 4.347894 | -0.916631 |
| 55 | 1 | 0 | -6.892992 | 1.990498 | 0.175672 |
| 56 | 1 | 0 | -5.910004 | 4.173874 | -0.494774 |
| 57 | 6 | 0 | -2.435537 | -1.095458 | -1.699495 |
| 58 | 6 | 0 | -2.244567 | -2.219157 | -4.268302 |
| 59 | 6 | 0 | -3.421538 | -0.838459 | -2.664358 |
| 60 | 6 | 0 | -1.346383 | -1.913308 | -2.043503 |
| 61 | 6 | 0 | -1.255289 | -2.476722 | -3.316387 |
| 62 | 6 | 0 | -3.324549 | -1.397375 | -3.940838 |
| 63 | 1 | 0 | -4.262584 | -0.195142 | -2.423456 |
| 64 | 1 | 0 | -0.566678 | -2.098878 | -1.308629 |
| 65 | 1 | 0 | -0.406790 | -3.107677 | -3.567226 |
| 66 | 1 | 0 | -4.093212 | -1.186828 | -4.679947 |
| 67 | 1 | 0 | -2.169960 | -2.650611 | -5.262972 |

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Zero-point correction= 0.508789 (Hartree/Particle)
Thermal correction to Energy= 0.547259
Thermal correction to Enthalpy= 0.548203
Thermal correction to Gibbs Free Energy= 0.427654
Sum of electronic and zero-point Energies= -2513.759485
Sum of electronic and thermal Energies= -2513.721016
Sum of electronic and thermal Enthalpies= -2513.720072
Sum of electronic and thermal Free Energies= -2513.840620

**$[Pd^{II}]H_2$**

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 46 | 0 | -0.434927 | 0.363616 | 2.468981 |
| 2 | 1 | 0 | 0.787764 | -0.620641 | 2.988704 |
| 3 | 1 | 0 | -1.660352 | 1.337904 | 1.900719 |
| 4 | 15 | 0 | -0.029550 | 0.015563 | 0.316600 |
| 5 | 6 | 0 | 0.593690 | 1.538123 | -0.515531 |
| 6 | 6 | 0 | 1.479773 | 3.878435 | -1.788282 |
| 7 | 6 | 0 | 1.688827 | 1.499339 | -1.392820 |
| 8 | 6 | 0 | -0.048485 | 2.765235 | -0.276224 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 6 | 0 | 0.389927 | 3.924130 | -0.914908 |
| 10 | 6 | 0 | 2.127988 | 2.665834 | -2.023250 |
| 11 | 1 | 0 | 2.203169 | 0.564117 | -1.584810 |
| 12 | 1 | 0 | -0.880031 | 2.802258 | 0.420681 |
| 13 | 1 | 0 | -0.115681 | 4.866318 | -0.721637 |
| 14 | 1 | 0 | 2.979858 | 2.622514 | -2.696547 |
| 15 | 1 | 0 | 1.824933 | 4.785140 | -2.277946 |
| 16 | 6 | 0 | -1.543862 | -0.471490 | -0.608025 |
| 17 | 6 | 0 | -3.843842 | -1.308553 | -1.975237 |
| 18 | 6 | 0 | -2.429503 | -1.383587 | -0.014212 |
| 19 | 6 | 0 | -1.823791 | 0.022747 | -1.889765 |
| 20 | 6 | 0 | -2.971787 | -0.395080 | -2.568058 |
| 21 | 6 | 0 | -3.569867 | -1.802789 | -0.696886 |
| 22 | 1 | 0 | -2.230502 | -1.749296 | 0.989591 |
| 23 | 1 | 0 | -1.154316 | 0.738111 | -2.357315 |
| 24 | 1 | 0 | -3.183467 | -0.001382 | -3.558579 |
| 25 | 1 | 0 | -4.250278 | -2.507296 | -0.226531 |
| 26 | 1 | 0 | -4.737898 | -1.629546 | -2.502917 |
| 27 | 6 | 0 | 1.198650 | -1.290981 | -0.128755 |
| 28 | 6 | 0 | 3.135093 | -3.190898 | -0.850468 |
| 29 | 6 | 0 | 2.300371 | -1.533285 | 0.703840 |
| 30 | 6 | 0 | 1.073084 | -2.016359 | -1.325736 |
| 31 | 6 | 0 | 2.036584 | -2.962145 | -1.680812 |
| 32 | 6 | 0 | 3.265174 | -2.473170 | 0.340278 |
| 33 | 1 | 0 | 2.377031 | -1.004800 | 1.648777 |
| 34 | 1 | 0 | 0.224196 | -1.849969 | -1.980615 |
| 35 | 1 | 0 | 1.923412 | -3.522435 | -2.605066 |
| 36 | 1 | 0 | 4.112187 | -2.652903 | 0.996740 |
| 37 | 1 | 0 | 3.881730 | -3.930897 | -1.126264 |

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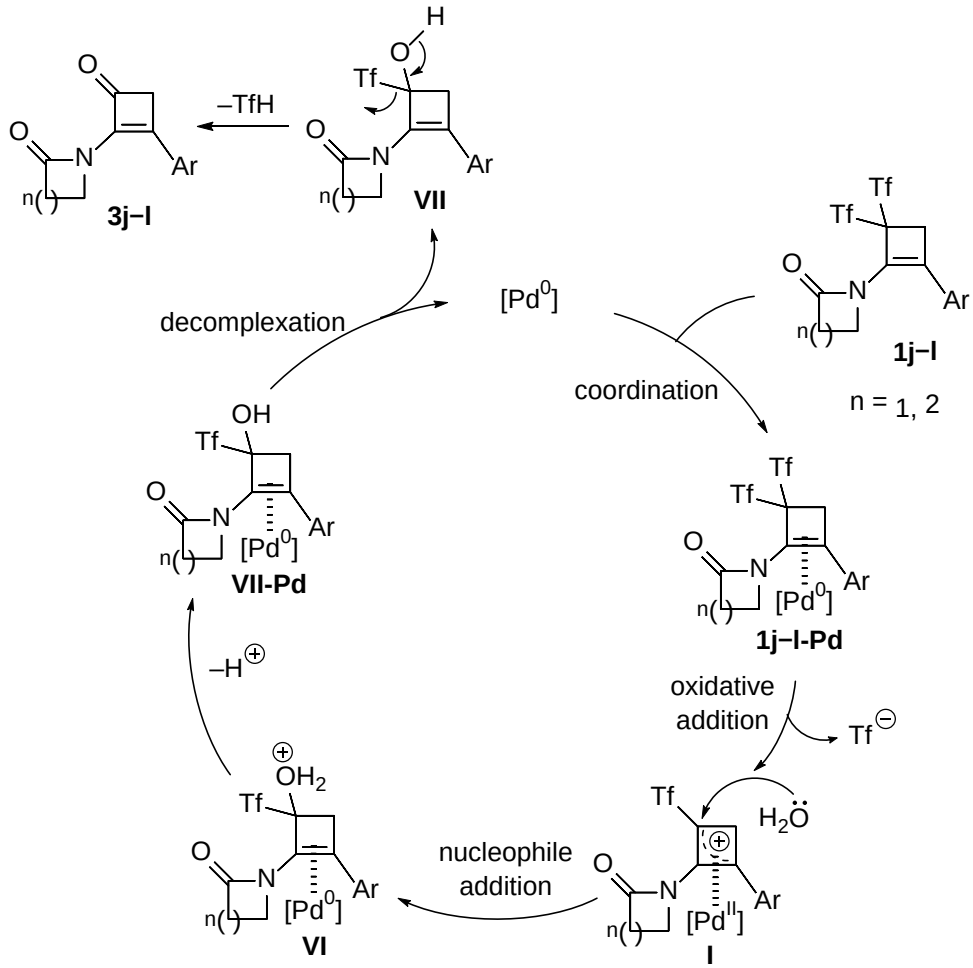
| | | |
|---|---|---|
| Zero-point correction= | 0.289351 | (Hartree/Particle) |
| Thermal correction to Energy= | 0.308195 | |
| Thermal correction to Enthalpy= | 0.309139 | |
| Thermal correction to Gibbs Free Energy= | 0.238669 | |
| Sum of electronic and zero-point Energies= | -1163.907637 | |
| Sum of electronic and thermal Energies= | -1163.888794 | |
| Sum of electronic and thermal Enthalpies= | -1163.887850 | |
| Sum of electronic and thermal Free Energies= | -1163.958320 | |

The rationale enabling the formation of cyclobutenones **3j–l** from bis(triflyl)cyclobutenes **1j–l** is outlined in Supplementary Scheme 8. After coordination to give **1-Pd**, the Pd(0) species should promote oxidative addition with the allyl sulphones **1j–l** which bear a leaving group (Tf) by generation of π-allyl palladium species **I**. These formed Pd(II) species are very reactive and suffer a selective nucleophilic attack by water at the 1-position to form intermediates **VI**, which after proton loss and decomplexation should liberate Tf-cyclobutenols **VII** with concomitant regeneration of the Pd(0) complex to close the palladium catalytic cycle. Ultimately, TfH release generates the observed 2,3-disubstituted-cyclobut-2-en-1-ones **3**.




**Supplementary Scheme 8**. Proposed reaction pathway for the Pd-catalyzed formation of cyclobutenones **3j–l**.