Supporting Information

Broad-Scope Rh-Catalyzed Inverse-Sonogashira Reaction Directed by Weakly Coordinating Groups

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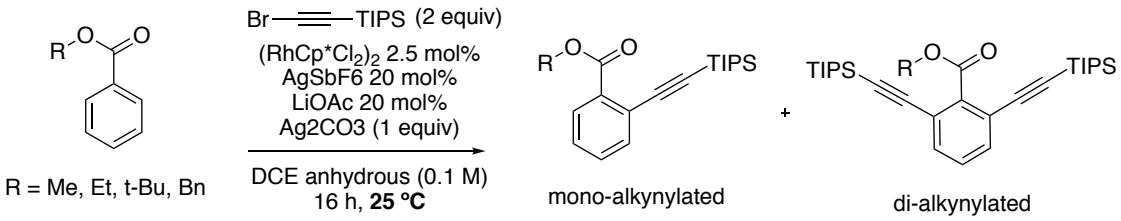
1) General Information

Catalytic reactions were carried out in 10 mL tubes under an argon atmosphere using pre-dried glassware. (Bromoethynyl)triisopropylsilane was synthesized according to previously described procedures.[1] Other chemicals were obtained from commercial sources and were used without further purification. Yields refer to isolated compounds, estimated to be > 95% pure as determined by ^{1}H-NMR. Chromatography: silica gel 60 (40-63 μm) from PanReac AppliChem. Analytical thin layer chromatography was carried out using TLC-aluminum sheets with 0.2 mm of silica gel (Merck GF_{234}) using UV light. NMR: Spectra were recorded at 298 K on a Bruker Avance 300, Bruker Avance 400 Ultrashield and Bruker Avance 500 Ultrashield apparatuses in the solvent indicated; chemical shifts (δ) are given in ppm (multiplicity, coupling constant (Hertz), number of protons). Mass spectra were recorded on a Waters Micromass LCT Premier (ESI), Waters Micromass GCT (EI, CI) and Bruker Daltonics Autoflex (MALDI) spectrometers. Melting points were determined using a Büchi melting point apparatus.

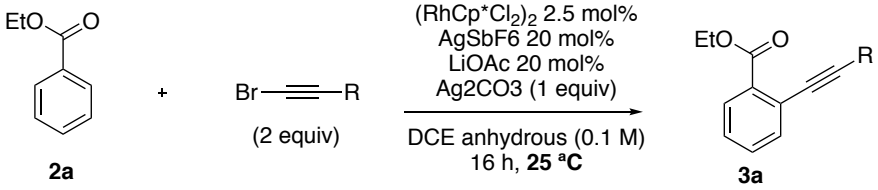
2) Optimization studies



Entry	R	Ratio mono/di[a]	Yield (mono)
1	**Et**	**30:1**	**35%[b]**
2	Me	n.d.	11%[d]
3	Bn	n.d.	6%[d]
4	*t*-Bu	26:1	42%[c]

[a] Ratio mono/di determined on the crude NMR [b] Isolated Yield of monoalkynylated compound [c]NMR Yield determined using mesitylene as internal standard
[d] NMR Yield determined using bromomesitylene as internal standard

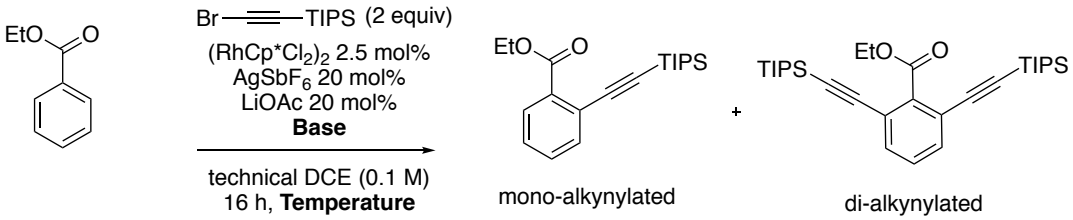
Table S2.1 - Variation of the ester chain



Entry	R	Ratio mono/di[a]	Yield (mono)
1	**TIPS**	**30:1**	**35%[b]**
2	Ph	no conversion (degradation of the alkyne)	
3	C_6H_{11}	no conversion (either at 45 °C for 3 days, 55 °C, 65 °C or 90 °C)	

[a] Ratio mono/di determined on the crude NMR [b] Isolated Yield

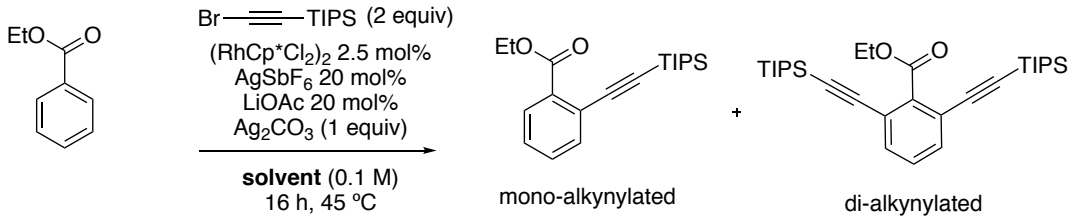
Table S2.2 - Variation of the alkyne



Entry	Temperature	Base	Ratio mono/di[a]	Yield (mono)
1	**45 ºC**	**Ag_2CO_3 1 equiv**	**3.2 : 1**	**58%[b]**
2	55 ºC	Ag_2CO_3 1 equiv	1.2 : 1	44%[b]
3	65 ºC	Ag_2CO_3 1 equiv	1 : 3	16%[b]
4	75 ºC	Ag_2CO_3 1 equiv	1 : 2.5	16%[b]
5	45 ºC	Ag_2CO_3 0.5 equiv	14 : 1	41%[b]
6	45 ºC	Ag_2CO_3 (0.5 equiv) x 2	4 : 1	54%[c]
7	45 ºC	Ag_2CO_3 1 equiv	4 : 1	69%[b]
8	45 ºC	K_2CO_3 1 equiv	-	5%[c]

[a] Ratio mono/di determined on the crude NMR [b] NMR Yield determined using mesitylene as internal standard [c] NMR Yield determined using bromomesitylene as internal standard

Table S2.3 - Temperature and base stoichiometry screening



Entry	Solvent	Ratio mono/di[a]	Yield (mono)
1	Hexafluoroisopropanol	-	no conv.
2	Trifluoroethanol	-	no conv.
3	Dichloromethane	n.d.	8-14%[b]
4	Toluene	-	no conv.
5	*tert*-amyl alcohol	-	no conv.
6	Methanol	-	no conv.
7	Ethanol	-	no conv.
8	Chlorobenzene	-	no conv.
9	Acetonitrile	-	no conv.
10	Diethylether	n.d.	4%[c]
11	Ethyl acetate	n.d.	18%[c]
12	Dioxane	-	no conv.
13	Dimethylformamide	-	no conv.
14	**Dichloroethane (technical)**	**3.6:1**	**58%[c]**
15	Dichloroethane (anhydrous)	3:1	51%[c]

[a] Ratio mono/di determined on the crude NMR [b] NMR Yield determined using mesitylene as internal standard [c] NMR Yield determined using bromomesitylene as internal standard

Table S2.4 - Solvent Screening

3) General Procedures for the Rhodium(III)-Catalyzed C–H Alkynylation

3.1 - General Procedure for Ester (3a-aa, 9a-e) and Ether (5a-w)

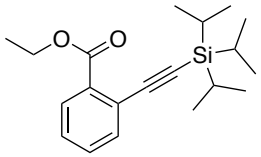
$(RhCp^*Cl_2)_2$, $AgSbF_6$, LiOAc, Ag_2CO_3, were weighted in a 10 mL tube inside a glovebox and dissolved in technical DCE (2 mL). Benzoic esters (0.20 mmol) and 1-bromo-2-(triisopropylsilyl)acetylene **1** were then added with a Hamilton syringe and the reaction mixture was stirred for corresponding time (16-72h) and temperature (45-100 ºC) according to the conversion estimated by TLC (100% Toluene). After cooling at ambient temperature, bromomesitylene (1 eq) was added as internal standard through an Hamilton syringe and the crude mixture was filtrated in a pipette through a short plug of silica and washed with DCM. After filtration, the solvents were removed under vacuum. The residue was purified by silica gel chromatography column with Toluene 100% as eluent to yield the corresponding mono alkynylated products and depending on the selectivity of the reaction some dialkynylated products which most of the time came along in the first fractions with some residual 1-bromo-2-(triisopropylsilyl)acetylene. In this case, when dialkynylated compound was present, it was then re-purified from residual 1-bromo-2-(triisopropylsilyl)acetylene with a second silica gel chromatography column using Cyclohexane 100% to Cyclohexane/EtOAc 90:10 as eluent.

3.2 - General Procedure for Ketone (7a-v, 9f-g)

$[Cp^*RhCl_2]_2$ (3.72 mg, 6.00 µmol, 3 mol %), Ag_2CO_3 (55.1 mg, 0.20 mmol, 1 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.2 equiv), $AgSbF_6$ (13.74 mg, 0.04 mmol, 0.2 equiv) were weighted in a vial inside a glovebox and dichloroethane (1 mL) is added. Corresponding ketone (0.20 mmol) and 1-Bromo-2-(triisopropylsilyl)acetylene **1** (57.5 mg, 0.22 mmol, 1.1 equiv) are then added and the vial is sealed. The reaction mixture is stirred at the appointed temperature for 16 h. After cooling to the appointed temperature, the reaction mixture is filtrated through celite and purified by column chromatography, with a gradient from cyclohexane 100% to 1/1 cyclohexane/ethyl acetate to yield corresponding product.

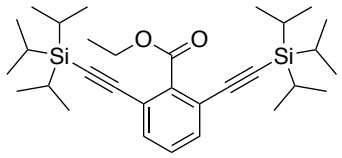
4) Characterization Data of Products

Ethyl 2-((triisopropylsilyl)ethynyl)benzoate (**3a**)



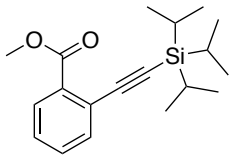
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl benzoate (**2a**) (30.0 mg, 28.7 μL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (37 mg, 0.11 mmol, 56% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.85 (dd, J = 7.7, 1.5 Hz, 1H), 7.59 (dd, J = 7.6, 1.5 Hz, 1H), 7.42 (td, J = 7.5, 1.6 Hz, 1H), 7.34 (td, J = 7.6, 1.5 Hz, 1H), 4.39 (q, J = 7.1 Hz, 2H), 1.38 (t, J = 7.1 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 166.7, 135.1, 133.2, 131.3, 130.0, 128.1, 123.5, 105.3, 96.5, 61.4, 18.8 (6C), 14.5, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{31}O_2Si^+$ $[M+H]^+$: 331.2088; found: 331.2080.

Ethyl 2,6-bis((triisopropylsilyl)ethynyl)benzoate (**3a"**)



Compound **3a"** was obtained as a white crystalline solid (14 mg, 0.03 mmol, 14% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.45 (d, *J* = 7.8 Hz, 2H), 7.27 (dd, *J* = 7.6, 7.5 Hz, 1H), 4.36 (q, *J* = 7.2 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.5, 139.8, 132.7 (2C), 128.9, 121.2 (2C), 103.3 (2C), 95.5 (2C), 62.0, 18.8 (12C), 14.2, 11.4 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{31}H_{51}O_2Si_2^+$ $[M+H]^+$: 511.3422; found: 511.3433. **Mp** 58-60 ºC.

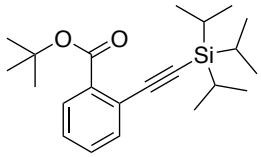
Methyl 2-((triisopropylsilyl)ethynyl)benzoate (**3b**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv),

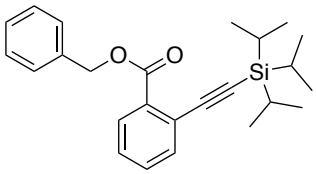
Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), methyl benzoate (**2b**) (27.2 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (29 mg, 0.09 mmol, 45% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.88 (d, J = 8.0 Hz, 1H), 7.59 (d, J = 7.7 Hz, 1H), 7.46 – 7.40 (td, J = 7.6, 1.3 Hz, 1H), 7.35 (td, J = 7.6, 1.3 Hz, 1H), 3.91 (d, J = 1.0 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 167.3, 135.1, 132.8, 131.5, 130.3, 128.1, 123.5, 105.3, 96.4, 52.3, 18.8 (6C), 11.5 (3C). Data were in agreement with existing literature.[2]

Tert-butyl 2-((triisopropylsilyl)ethynyl)benzoate (**3c**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), *tert*-butyl benzoate (**2c**) (35.6 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (29 mg, 0.11 mmol, 53% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.72 (dd, J = 7.7, 0.9 Hz, 1H), 7.56 (d, J = 7.6 Hz, 1H), 7.38 (td, J = 7.5, 0.9 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 1.60 (s, 9H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 165.9, 135.04, 135.01, 130.7, 129.5, 127.9, 123.1, 105.4, 96.1, 81.7, 28.3 (3C), 18.8 (6C), 11.6 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{22}H_{34}NaO_2Si^+$ $[M+Na]^+$: 381.2220; found: 381.2220.

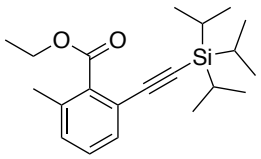
Benzyl 2-((triisopropylsilyl)ethynyl)benzoate (**3d**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), benzyl benzoate (**2d**) (42.4 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (22 mg, 0.06 mmol, 28% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.89 (dd, J = 7.9, 1.4 Hz, 1H), 7.61 (dd, J = 7.9, 1.3 Hz, 1H),

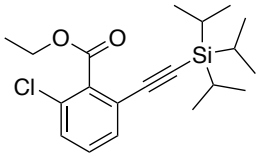
7.48 – 7.40 (m, 3H), 7.40 – 7.28 (m, 4H), 5.38 (s, 2H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 166.2, 136.3, 135.2, 132.7, 131.5, 130.2, 128.6 (2C), 128.3 (2C), 128.2, 128.0, 123.9, 105.2, 96.9, 66.9, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{25}H_{32}NaO_2Si^+$ $[M+Na]^+$: 415.2064; found: 415.2059. **HRMS** (ESI+) *m/z* calc. for $C_{25}H_{32}NaO_2Si^+$ $[M+Na]^+$: 415.2064; found: 415.2059.

Ethyl 2-methyl-6-((triisopropylsilyl)ethynyl)benzoate (**3e**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 2-methylbenzoate (**2e**) (32.8 mg, 31.8 μL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 60 ºC for 48h, and obtained as a colorless oil (62 mg, 0.18 mmol, 90% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.35 (ddd, *J* = 7.7, 1.2, 0.6 Hz, 1H), 7.22 (t, *J* = 7.7 Hz, 1H), 7.15 (ddd, *J* = 7.7, 1.3, 0.7 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.32 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H), 1.12 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 168.6, 136.8, 134.8, 130.4, 130.1, 128.9, 120.8, 104.2, 94.2, 61.3, 19.4, 18.6 (6C), 14.2, 11.3 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{33}O_2Si^+$ $[M+H]^+$: 345.2244; found: 345.2259.

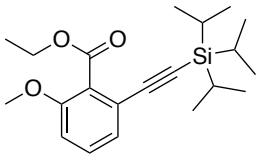
Ethyl 2-chloro-6-((triisopropylsilyl)ethynyl)benzoate (**3f**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 2-chlorobenzoate (**2f**) (36.9 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 60 ºC for 48 h, and obtained as a colorless oil (50 mg, 0.14 mmol, 69% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.41 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.34 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.26 (dd, *J* = 8.2, 7.7 Hz, 1H), 4.41 (q, *J* = 7.1 Hz, 2H), 1.39 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 166.1, 136.8, 131.2, 130.8, 130.0, 129.4, 122.8, 102.7, 96.4, 62.1, 18.7 (6C), 14.2, 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{30}ClO_2Si^+$ $[M+H]^+$:

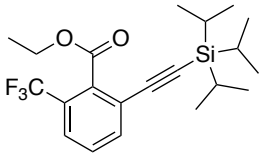
365.1698; found: 365.1701.

Ethyl 2-methoxy-6-((triisopropylsilyl)ethynyl)benzoate (**3g**)



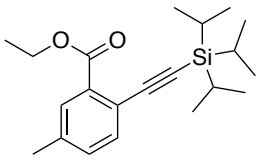
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 2-methoxybenzoate (**2g**) (36.0 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (62 mg, 0.18 mmol, 90% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.26 (t, J = 8.0 Hz, 1H), 7.10 (d, J = 7.7 Hz, 1H), 6.88 (d, J = 8.4 Hz, 1H), 4.37 (q, J = 7.1 Hz, 2H), 3.81 (s, 3H), 1.36 (t, J = 7.1 Hz, 3H), 1.11 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 167.0, 156.1, 130.2, 126.9, 125.2, 122.1, 111.6, 103.6, 94.8, 61.6, 56.2, 18.7 (6C), 14.2, 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{33}O_3Si^+$ $[M+H]^+$: 361.2193; found: 361.2183.

Ethyl 2-(trifluoromethyl)-6-((triisopropylsilyl)ethynyl)benzoate (**3h**)



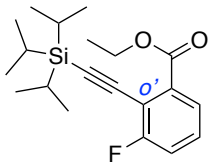
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 2-(trifluoromethyl)benzoate (**2h**) (43.6 mg, 39.3 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 60 ºC for 48 h, and obtained as a slightly yellow oil (55 mg, 0.14 mmol, 69% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.69 (ddd, *J* = 7.8, 1.2, 0.6 Hz, 1H), 7.61 (ddd, *J* = 8.0, 1.2, 0.6 Hz, 1H), 7.46 (tq, *J* = 7.9, 0.9 Hz, 1H), 4.40 (q, *J* = 7.2 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H), 1.12 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 166.4, 136.3, 135.3 (q, *J* = 2.2 Hz), 129.3, 127.7 (q, *J* = 32.5 Hz), 125.8 (q, *J* = 4.6 Hz), 124.4 (q, *J* = 273 Hz), 122.8, 102.4, 97.2, 62.4, 18.7 (6C), 14.0, 11.4 (3C). **^{19}F NMR** ($^{19}F\{^1H\}$, 376 MHz, Chloroform-*d*) δ -60.25. **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{29}F_3NaO_2Si^+$ $[M+Na]^+$: 421.1781; found: 421.1782.

Ethyl 5-methyl-2-((triisopropylsilyl)ethynyl)benzoate (**3i**)



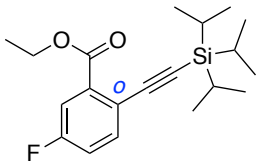
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 3-methylbenzoate (**2i**) (32.8 mg, 31.9 µL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 µL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (33 mg, 0.10 mmol, 48% yield). **^{1}H NMR** (400 MHz, Chloroform-d) δ 7.65 (dt, J = 1.9, 0.8 Hz, 1H), 7.47 (d, J = 7.9 Hz, 1H), 7.22 (ddd, J = 7.9, 1.9, 0.8 Hz, 1H), 4.38 (q, J = 7.1 Hz, 2H), 2.37 (s, 3H), 1.38 (t, J = 7.1 Hz, 3H), 1.14 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-d) δ 166.7, 138.2, 134.9, 132.9, 131.9, 130.3, 120.4, 105.3, 95.1, 61.1, 21.3, 18.7 (6C), 14.3, 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{33}O_2Si^+$ $[M+H]^+$: 345.2244; found: 345.2249.

Ethyl 3-fluoro-2-((triisopropylsilyl)ethynyl)benzoate (**3j'**)



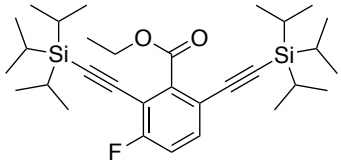
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 3-fluorobenzoate (**2j**) (33.6 mg, 29.6 µL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 µL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (37 mg, 0.11 mmol, 53% yield). **^{1}H NMR** (^{1}H{^{19}F}, 400 MHz, Chloroform-*d*) δ 7.64 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.31 (dd, *J* = 8.1, 7.9 Hz, 1H), 7.21 (dd, *J* = 8.3, 1.3 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.16 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-d) δ 165.7 (d, J = 3.3 Hz), 164.4 (d, J = 252.2 Hz), 135.1, 128.9 (d, J = 8.5 Hz), 125.6 (d, J = 3.6 Hz), 118.5 (d, J = 22.1 Hz), 112.4 (d, J = 17.8 Hz), 103.5 (d, J = 4.9 Hz), 97.2, 61.6, 18.8 (6C), 14.4, 11.4 (3C). **^{19}F NMR** (^{19}F{^{1}H}, 376 MHz, Chloroform-*d*) δ -107.23. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{30}FO_2Si^+$ $[M+H]^+$: 349.1994; found: 349.2003.

Ethyl 5-fluoro-2-((triisopropylsilyl)ethynyl)benzoate (**3j**)



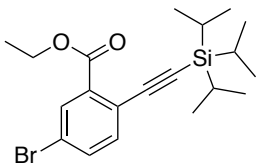
Compound **3j** was obtained as a colorless oil (8.3 mg, 0.02 mmol, 12% yield). **^{1}H NMR** (^{1}H{^{19}F}, 400 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 8.9 Hz, 1H), δ 7.55 (d, *J* = 2.7 Hz, 1H), 7.13 (dd, *J* = 8.6, 2.8 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.14 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-d) δ 165.4, 161.8 (d, J = 250.7 Hz), 137.1, 135.1, 119.8, 118.8 (d, J = 21.9 Hz), 117.1 (d, J = 24.1 Hz), 104.2, 96.3, 61.7, 18.8 (6C), 14.4, 11.5 (3C). **^{19}F NMR** (^{19}F{^{1}H}376 MHz, Chloroform-*d*) δ -110.66. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}FNaO_2Si^+$ $[M+Na]^+$: 371.1813; found: 371.1819.

Ethyl 3-fluoro-2,6-bis((triisopropylsilyl)ethynyl)benzoate (**3j"**)



Compound **3j"** was obtained as a colorless oil (7.5 mg, 0.01 mmol, 7% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.41 (dd, *J* = 8.6, 5.0 Hz, 1H), 7.04 (t, *J* = 8.6 Hz, 1H), 4.36 (q, *J* = 7.2 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H), 1.12 (s, 21H), 1.10 (s, 21H). 13C NMR (126 MHz, Chloroform-d) δ 166.36 (d, J = 3.1 Hz), 162.72 (d, J = 256.9 Hz), 141.69, 134.26 (d, J = 8.3 Hz), 117.24 (d, J = 4.2 Hz), 116.45 (d, J = 22.2 Hz), 110.56 (d, J = 19.1 Hz), 102.28, 101.96 (d, J = 3.7 Hz), 96.0, 95.1, 62.2, 18.74 (6C), 18.70 (6C), 14.1, 11.4 (3C), 11.3 (3C). **^{19}F NMR** (376 MHz, Chloroform-*d*) δ -106.42 **HRMS** (ESI+) *m/z* calc. for $C_{31}H_{49}FNaO_2Si_2^+$ $[M+Na]^+$: 551.3147; found: 551.3154. **Mp** 61-66 ºC.

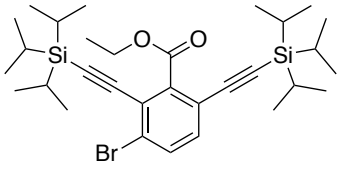
Ethyl 5-bromo-2-((triisopropylsilyl)ethynyl)benzoate (**3k**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv),

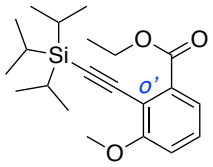
Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 3-bromobenzoate (**2k**) (45.8 mg, 32 µL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 µL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 72 h, and obtained as a colorless oil (50 mg, 0.12 mmol, 61% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.99 (d, *J* = 2.1 Hz, 1H), 7.54 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.44 (d, *J* = 8.3 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 165.1, 136.2, 134.5, 134.2, 132.8, 122.4, 121.9, 104.1, 98.0, 61.6, 18.7 (6C), 14.3, 11.3 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}BrNaO_2Si^+$ $[M+Na]^+$: 431.1012; found: 431.1012.

Ethyl 3-bromo-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3k")**



Compound **3k"** was obtained as a colorless oil (17 mg, 0.03 mmol, 14% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.4 Hz, 1H), 7.26 (d, *J* = 8.3 Hz, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.13 (s, 21H), 1.10 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 166.7, 141.5, 133.1, 133.0, 126.5, 123.1, 120.1, 102.4, 101.7, 101.3, 96.7, 62.3, 18.8 (6C), 18.7 (6C), 14.1, 11.40 (3C), 11.37 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{31}H_{50}BrO_2Si_2^+$ $[M+H]^+$: 589.2527; found: 589.2519.

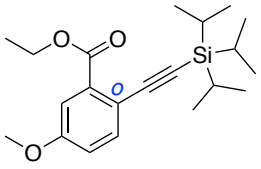
Ethyl 3-methoxy-2-((triisopropylsilyl)ethynyl)benzoate **(3l')**



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 3-methoxybenzoate (**2l**) (36 mg, 32.8 µL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 µL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 20 h, and obtained as an inseparable mixture with its monoalkynylated regioisomer (**3l**) in a ratio 1.4:1 as a colorless oil (39 mg, 0.11 mmol, 55% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.36 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.28 (dd, *J* = 8.3, 7.8 Hz, 1H), 6.99 (dd, *J* = 8.3, 1.1 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.1, 162.0, 135.5, 128.8, 121.5,

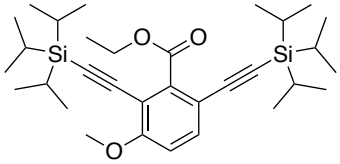
113.7, 112.8, 101.7, 100.2, 61.4, 56.3, 18.8 (6C), 14.4, 11.6 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{32}NaO_3Si^+$ $[M+Na]^+$: 383.2013; found: 383.2011.

Ethyl 5-methoxy-2-((triisopropylsilyl)ethynyl)benzoate (**3l**)



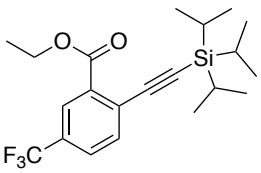
Compound **3l** was obtained in an inseparable mixture with its monoalkynylated regioisomer (**3l'**) in a ratio 1:1.4 as a colorless oil (39 mg, 0.11 mmol, 55% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 8.5 Hz, 1H), 7.35 (d, *J* = 2.7 Hz, 1H), 6.96 (dd, *J* = 8.6, 2.8 Hz, 1H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.84 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 166.6, 159.2, 136.5, 134.6, 117.9, 115.8, 114.6, 105.3, 94.2, 61.5, 55.7, 18.9 (6C), 14.5, 11.6 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{32}NaO_3Si^+$ $[M+Na]^+$: 383.2013; found: 383.2016.

Ethyl 3-methoxy-2,6-bis((triisopropylsilyl)ethynyl)benzoate (**3l"**)



Compound **3l"** was obtained as a slightly beige solid (15 mg, 0.03 mmol, 14% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.40 (d, *J* = 8.6 Hz, 1H), 6.81 (d, *J* = 8.7 Hz, 1H), 4.34 (q, *J* = 7.2 Hz, 2H), 3.86 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 21H), 1.10 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.2, 160.8, 141.6, 134.1, 113.0, 111.4, 111.0, 103.3, 100.1, 99.1, 93.0, 62.0, 56.4, 18.77 (6C), 18.75 (6C), 14.1, 11.4 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{32}H_{52}NaO_3Si_2^+$ $[M+Na]^+$: 563.3347; found: 563.3359. **Mp**: 85-90 ºC.

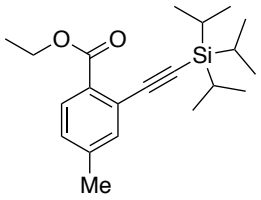
Ethyl 5-(trifluoromethyl)-2-((triisopropylsilyl)ethynyl)benzoate (**3m**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv),

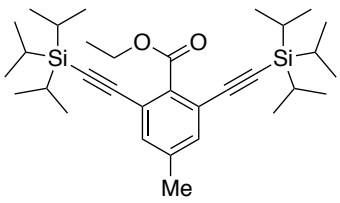
Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 3-(trifluoromethyl)benzoate (**2m**) (43.6 mg, 35.5 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 72 h, and obtained as a colorless oil (62 mg, 0.16 mmol, 78% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 8.12 (d, *J* = 1.6 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.65 (dd, *J* = 8.3, 1.6 Hz, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 165.3, 135.6, 133.7, 130.0 (q, *J* = 33.4 Hz), 127.7 (q, *J* = 3.6 Hz), 127.2, 127.1 (q, *J* = 3.6 Hz), 123.6 (q, *J* = 273 Hz), 103.91, 100.3, 61.8, 18.8 (6C), 14.4, 11.5 (3C). **^{19}F NMR** (^{19}F{^{1}H}, 376 MHz, Chloroform-d) δ -63.05. **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{29}F_3NaO_2Si^+$ $[M+Na]^+$: 421.1781; found: 421.1782.

Ethyl 4-methyl-2-((triisopropylsilyl)ethynyl)benzoate (**3n**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 4-methylbenzoate (**2n**) (32.8 mg, 32 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 24 h, and obtained as a colorless oil (37 mg, 0.11 mmol, 54% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 8.0 Hz, 1H), 7.39 (dt, *J* = 1.8, 0.7 Hz, 1H), 7.15 (ddd, *J* = 8.0, 1.8, 0.7 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 2.36 (brt, *J* = 0.7 Hz, 3H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 166.6, 141.8, 135.6, 130.28, 130.26, 129.0, 123.5, 105.6, 95.9, 61.1, 21.3, 18.8 (6C), 14.5, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{32}NaO_2Si^+$ $[M+Na]^+$: 367.2064; found: 367.2067.

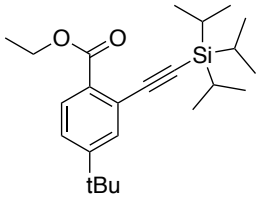
Ethyl 4-methyl-2,6-bis((triisopropylsilyl)ethynyl)benzoate (**3n"**)



Compound **3n"** was obtained as a colorless oil (14 mg, 0.03 mmol, 13% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.26 (brq, *J* = 0.7 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 2.30 (brt, *J* = 0.7 Hz, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.7, 139.1,

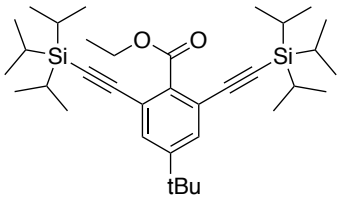
137.2, 133.3 (2C), 121.1 (2C), 103.5 (2C), 94.8 (2C), 61.8, 21.0, 18.8 (12C), 14.2, 11.4 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{32}H_{53}O_2Si_2^+$ $[M+H]^+$: 525.3579; found: 525.3579.

Ethyl 4-(tert-butyl)-2-((triisopropylsilyl)ethynyl)benzoate (**3o**)



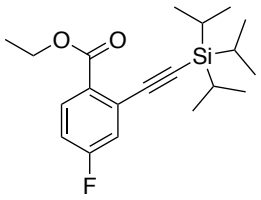
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 4-(*tert*-butyl)benzoate (**2o**) (41.3 mg, 42.5 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 16 h, and obtained as a colorless oil (44 mg, 0.11 mmol, 57% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.80 (d, J = 8.3 Hz, 1H), 7.57 (d, J = 2.0 Hz, 1H), 7.37 (dd, J = 8.3, 2.0 Hz, 1H), 4.38 (q, J = 7.1 Hz, 2H), 1.37 (t, J = 7.1 Hz, 3H), 1.32 (s, 9H), 1.16 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 166.6, 154.8, 132.0, 130.4, 130.0, 125.5, 123.2, 105.9, 95.5, 61.1, 34.9, 31.1 (3C), 18.8 (6C), 14.5, 11.6 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{24}H_{38}NaO_2Si^+$ $[M+Na]^+$: 409.2533; found: 409.2536.

Ethyl 4-(tert-butyl)-2,6-bis((triisopropylsilyl)ethynyl)benzoate (**3o"**)



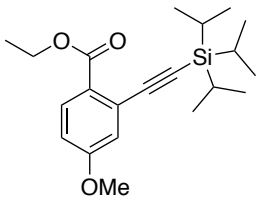
Compound 3**o"** was obtained as a colorless oil (17 mg, 0.03 mmol, 15% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.43 (s, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.30 (s, 9H), 1.12 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.7, 152.3, 137.3, 129.9 (2C), 120.9 (2C), 103.8 (2C), 94.5 (2C), 61.8, 34.8, 31.1 (3C), 18.8 (12C), 14.1, 11.5 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{35}H_{58}NaO_2Si_2^+$ $[M+Na]^+$: 589.3868; found: 589.3878.

Ethyl 4-fluoro-2-((triisopropylsilyl)ethynyl)benzoate (**3p**)



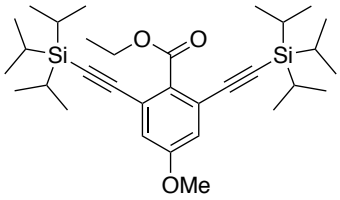
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 4-fluorobenzoate (**2p**) (33.6 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 20 h, and obtained as a colorless oil (34 mg, 0.14 mmol, 48% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.90 (dd, *J* = 8.8, 5.8 Hz, 1H), 7.26 (dd, *J* = 9.1, 2.7 Hz, 1H), 7.04 (ddd, *J* = 8.8, 7.9, 2.7 Hz, 1H), 4.38 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 165.6, 164.1 (d, J = 253.3 Hz), 132.7 (d, *J* = 9.5 Hz), 129.2 (d, *J* = 3.2 Hz), 126.2 (d, *J* = 10.2 Hz), 121.7 (d, *J* = 23.0 Hz), 115.6 (d, *J* = 21.7 Hz), 104.1 (d, *J* = 2.5 Hz), 98.4, 61.4, 18.8 (6C), 14.5, 11.5 (3C). **^{19}F NMR** ($^{19}F\{^1H\}$, 376 MHz, Chloroform-d) δ -108.41. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}FNaO_2Si^+$ $[M+Na]^+$: 371.1813; found: 371.1816.

Ethyl 4-methoxy-2-((triisopropylsilyl)ethynyl)benzoate (**3q**)



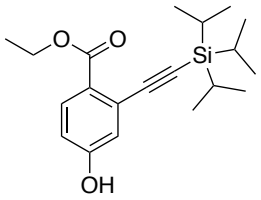
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 4-methoxybenzoate (**2q**) (36.0 mg, 32.7 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 24 h, and obtained as a colorless oil (36 mg, 0.1 mmol, 50% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 8.8 Hz, 1H), 7.06 (d, *J* = 2.7 Hz, 1H), 6.86 (dd, *J* = 8.8, 2.7 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 3.84 (s, 3H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 166.1, 161.8, 132.4, 125.5, 125.3, 120.0, 114.1, 105.4, 96.5, 60.9, 55.6, 18.8 (6C), 14.6, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{32}NaO_3Si^+$ $[M+Na]^+$: 383.2013; found: 383.2016.

Ethyl 4-methoxy-2,6-bis((triisopropylsilyl)ethynyl)benzoate (**3q"**)



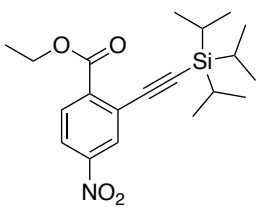
Compound **3q"** was obtained as a colorless oil (17 mg, 0.03 mmol, 16% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 6.96 (s, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 3.81 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.5, 159.4, 132.7, 122.7 (2C), 118.4 (2C), 103.4 (2C), 95.2 (2C), 61.8, 55.7, 18.7 (12C), 14.2, 11.4 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{32}H_{52}NaO_3Si_2^+$ $[M+Na]^+$: 563.3347; found: 563.3346.

Ethyl 4-hydroxy-2-((triisopropylsilyl)ethynyl)benzoate (**3r**)



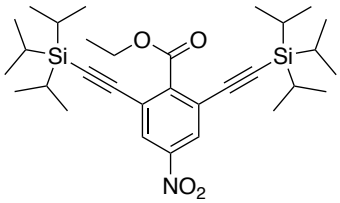
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 4-hydroxybenzoate (**2r**) (33.2 mg, 42.5 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 48 h, and obtained as a white solid (16 mg, 0.05 mmol, 23% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.83 (d, *J* = 8.7 Hz, 1H), 7.05 (d, *J* = 2.6 Hz, 1H), 6.81 (dd, *J* = 8.6, 2.6 Hz, 1H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 166.5, 158.5, 132.8, 125.8, 125.0, 121.8, 115.6, 105.2, 96.9, 61.2, 18.8 (6C), 14.5, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{30}NaO_3Si^+$ $[M+Na]^+$: 369.1856; found: 369.1859. **Mp**: 64-68 ºC.

Ethyl 4-nitro-2-((triisopropylsilyl)ethynyl)benzoate (**3s**)



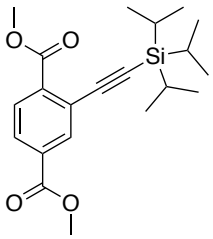
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 4-nitrobenzoate (**2s**) (39.0 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 20 h, and obtained as an orange oil (37 mg, 0.07 mmol, 36% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.36 (d, *J* = 2.3 Hz, 1H), 8.15 (dd, *J* = 8.6, 2.3 Hz, 1H), 7.97 (d, *J* = 8.6 Hz, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 165.1, 149.2, 138.6, 131.0, 129.4, 125.1, 122.5, 102.6, 100.6, 62.2, 18.8 (6C), 14.4, 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}NNaO_4Si^+$ $[M+Na]^+$: 398.1758; found: 398.1761.

Ethyl 4-nitro-2,6-bis((triisopropylsilyl)ethynyl)benzoate (**3s"**)



Compound **3s"** was obtained as an orange oil (14 mg, 0.03 mmol, 13% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.22 (s, 2H), 4.38 (q, *J* = 7.2 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H), 1.12 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 167.1, 147.7, 144.7, 126.9 (2C), 123.1 (2C), 101.0 (2C), 99.3 (2C), 62.6, 18.7 (12C), 12.8, 11.3 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{31}H_{49}NNaO_4Si_2^+$ $[M+Na]^+$: 578.3092; found: 578.3102.

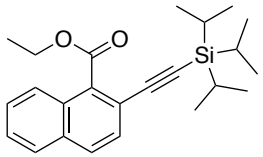
Dimethyl 2-((triisopropylsilyl)ethynyl)terephthalate (**3t**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), dimethyl terephthalate (**2t**) (38.8 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 20 h, and obtained as a colorless oil (36 mg, 0.1 mmol, 48% yield).

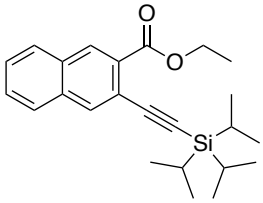
^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.20 (dd, *J* = 1.7, 0.6 Hz, 1H), 7.98 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.90 (dd, *J* = 8.2, 0.5 Hz, 1H), 3.94 (s, 3H), 3.92 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 166.6, 165.8, 136.5, 135.8, 132.8, 130.3, 128.8, 123.8, 104.1, 97.8, 52.7, 52.6, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{30}NaO_4Si^+$ $[M+Na]^+$: 397.1806; found: 397.1811.

Ethyl 2-((triisopropylsilyl)ethynyl)-1-naphthoate (**3u**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 1-naphthoate (**2u**) (40.0 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 70 ºC for 24 h, and obtained as a colorless oil (62 mg, 0.16 mmol, 81% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.86 – 7.75 (m, 3H), 7.57 – 7.45 (m, 3H), 4.53 (q, *J* = 7.2 Hz, 2H), 1.46 (t, *J* = 7.2 Hz, 3H), 1.17 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 168.5, 135.1, 132.8, 129.5, 129.4, 129.0, 128.3, 127.7, 127.1, 125.1, 119.0, 104.7, 96.1, 61.9, 18.8 (6C), 14.4, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{24}H_{33}O_2Si^+$ $[M+H]^+$: 381.2244; found: 381.2250.

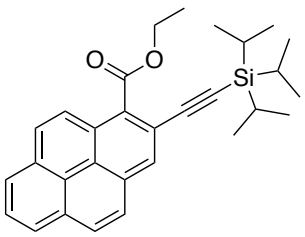
Ethyl 3-((triisopropylsilyl)ethynyl)-2-naphthoate (**3v**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 2-naphthoate (**2v**) (40.0 mg, 42.2 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 20 h, and obtained as a colorless oil (47 mg, 0.12 mmol, 62% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.39 (s, 1H), 8.10 (s, 1H), 7.87 (ddd, *J* = 8.0, 1.5, 0.7 Hz, 1H), 7.80 (ddd, *J* = 7.9, 1.4, 0.7 Hz, 1H), 7.58-7.50 (m, 2H), 4.45 (q, *J* = 7.1 Hz, 2H), 1.44 (t, *J* = 7.1 Hz, 3H), 1.19 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 166.7, 135.3, 134.2,

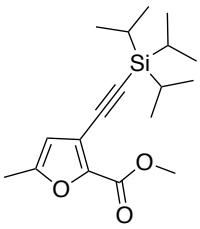
131.8, 131.1, 130.0, 128.9, 128.5, 127.5, 127.4, 119.5, 105.6, 95.2, 61.4, 18.9 (6C), 14.5, 11.6 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{24}H_{32}NaO_2Si^+$ $[M+Na]^+$: 403.2064; found: 403.2070.

Ethyl 5-((triisopropylsilyl)ethynyl)-5a1,10-dihydropyrene-4-carboxylate (**3w**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (2.25 mg, 0.004 mmol, 0.025 equiv), $AgSbF_6$, (10 mg, 0.03 mmol, 0.20 equiv), LiOAc (1.92 mg, 0.03 mmol, 0.20 equiv), Ag_2CO_3 (40.2 mg, 0.15 mmol, 1 equiv), ethyl pyrene-1-carboxylate (**2w**) (40 mg, 0.146 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (76 mg, 66 µL, 0.29 mmol, 2 equiv) according to general procedure, at 45 ºC for 48 h, and obtained as a beige solid (56 mg, 0.12 mmol, 84% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.28 (s, 1H), δ 8.17 (d, *J* = 7.6 Hz, 1H), δ 8.16 (d, *J* = 7.5 Hz, 1H), 8.11 (d, *J* = 9.2 Hz, 1H), 8.08 (d, *J* = 9.2 Hz, 1H), 8.05 (d, *J* = 8.9 Hz, 1H), 8.00 (t, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 8.9 Hz, 1H), 4.64 (q, *J* = 7.2 Hz, 2H), 1.53 (t, *J* = 7.2 Hz, 3H), 1.23 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 168.9, 131.7, 131.3, 131.1, 130.8, 129.3, 129.1, 129.0, 128.1, 126.8, 126.6, 126.2, 126.0, 124.2, 124.0, 123.9, 118.7, 105.1, 95.2, 62.0, 18.9 (6C), 14.5, 11.6 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{30}H_{35}O_2Si^+$ $[M+H]^+$: 455.2401; found: 455.2404. *m/z* calc. for $C_{30}H_{34}NaO_2Si^+$ $[M+Na]^+$: 477.2220; found: 477.2213. **Mp**: 96-100 ºC.

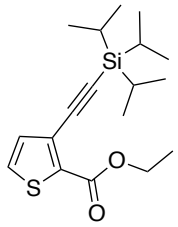
Methyl 5-methyl-3-((triisopropylsilyl)ethynyl)furan-2-carboxylate (**3x**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), methyl 5-methylfuran-2-carboxylate (**2x**) (28.0 mg, 25.6 µL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 µL, 0.40 mmol, 2 equiv) according to general procedure, at 70 ºC for 72 h, and obtained as a slightly yellow oil (42 mg, 0.13 mmol, 66% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 6.18 (q, *J* = 1.0 Hz, 1H), 3.88 (s,

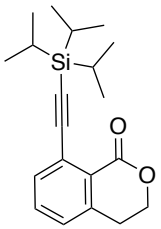
3H), 2.33 (d, *J* = 1.0 Hz, 3H), 1.12 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 158.8, 156.2, 144.3, 116.0, 112.4, 99.2, 97.4, 51.9, 18.7 (6C), 13.8, 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{18}H_{28}NaO_3Si^+$ $[M+Na]^+$: 343.1700; found: 343.1706.

Methyl 3-((triisopropylsilyl)ethynyl)thiophene-2-carboxylate (**3y**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl thiophene-2-carboxylate (**2y**) (31.2 mg, 26.9 μL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 70 ºC for 48 h, and obtained as a yellow oil (57 mg, 0.17 mmol, 85% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.41 (d, *J* = 5.1 Hz, 1H), 7.15 (d, *J* = 5.1 Hz, 1H), 4.40 (q, *J* = 7.1 Hz, 2H), 1.39 (t, *J* = 7.1 Hz, 3H), 1.17 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 161.5, 135.1, 133.4, 130.1, 126.9, 100.6, 97.8, 61.4, 18.8 (6C), 14.5, 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{18}H_{28}NaO_2SSi^+$ $[M+Na]^+$: 359.1471; found: 359.1475.

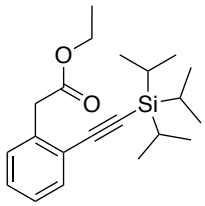
8-((Triisopropylsilyl)ethynyl)isochroman-1-one (**3z**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), isochroman-1-one (**2z**) (29.6 mg, 24.96 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 72 h, and obtained as a colorless oil (22 mg, 0.05 mmol, 25% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.56 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.17 (dd, *J* = 7.6, 1.1 Hz, 1H), 4.44 (t, *J* = 5.9 Hz, 2H), 3.00 (t, *J* = 5.9 Hz, 2H), 1.16 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 162.4, 140.7, 134.9, 132.2, 127.0, 126.4, 125.9,

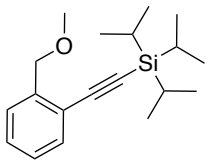
104.7, 99.0, 66.6, 29.0, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}O_2Si^+$ $[M+H]^+$: 329.1931; found: 329.1948.

Ethyl 2-(2-((triisopropylsilyl)ethynyl)phenyl)acetate (**3aa**)



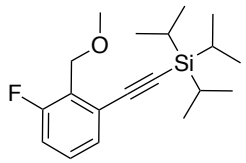
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 2-phenylacetate (**2aa**) (32.8 mg, 31.9 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 90ºC for 72 h, and obtained as a colorless oil (12 mg, 0.04 mmol, 18% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.50 (dt, *J* = 7.6, 1.0 Hz, 1H), 7.29-7.28 (m, 2H), 7.24-7.19 (m, 1H), 4.14 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 2H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.13 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 171.2, 136.5, 132.9, 129.8, 128.6, 127.1, 124.0, 105.1, 95.2, 61.0, 39.9, 18.8 (6C), 14.3, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{33}O_2Si^+$ $[M+H]^+$: 345.2244; found: 345.2234.

Triisopropyl((2-(methoxymethyl)phenyl)ethynyl)silane (**5a**)



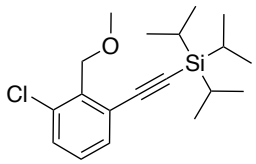
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), (methoxymethyl)benzene (**4a**) (24.4 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (39 mg, 0.13 mmol, 64% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.48 (dd, J = 7.7, 1.3 Hz, 1H), 7.46 (dd, J = 7.7, 0.9 Hz, 1H), 7.33 (td, J = 7.6, 1.4 Hz, 1H), 7.22 (td, J = 7.5, 1.3 Hz, 1H), 4.67 (s, 2H), 3.44 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 140.5, 132.7, 128.7, 127.3, 127.2, 122.2, 104.6, 95.6, 72.9, 58.7, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{30}NaOSi^+$ $[M+Na]^+$: 325.1958; found: 325.1963.

((3-Fluoro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5h**)



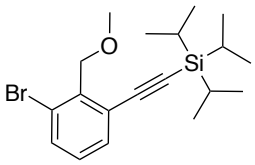
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-fluoro-2-(methoxymethyl)benzene (**4h**) (28 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (43,1 mg, 0.13 mmol, 67% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.31 (dd, J = 7.7, 1.1 Hz, 1H), 7.23 (td, J = 8.0, 5.5 Hz, 1H), 7.04 (ddd, J = 9.4, 8.2, 1.2 Hz, 1H), 4.70 (d, J = 1.7 Hz, 2H), 3.41 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 161.9 (d, J = 248.7 Hz), 129.7 (d, J = 9.5 Hz), 128.9 (d, J = 3.4 Hz), 126.7 (d, J = 16.5 Hz), 126.6 (d, J = 5.5 Hz), 116.1 (d, J = 22.9 Hz), 103.8 (d, J = 4.0 Hz), 96.0, 66.4 (d, J = 3.1 Hz), 58.4, 18.8 (6C), 11.5 (3C). **^{19}F NMR** (^{19}F{^{1}H}, 376 MHz, Chloroform-d) δ -116.64. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}FNaOSi^+$ $[M+Na]^+$: 343.1864; found: 343.1861.

((3-Chloro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5i**)



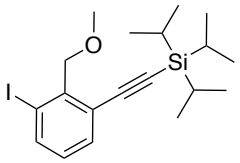
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-chloro-2-(methoxymethyl)benzene (**4i**) (31.3 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (45mg, 0.13 mmol, 67% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.42 (dd, J = 7.7, 1.3 Hz, 1H), 7.36 (dd, J = 8.1, 1.3 Hz, 1H), 7.19 (t, J = 7.9 Hz, 1H), 4.79 (s, 2H), 3.42 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 136.9, 136.1, 131.7, 130.1, 129.2, 126.7, 104.3, 96.0, 70.1, 58.5, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}ClNaOSi^+$ $[M+Na]^+$: 359.1568; found: 359.1563.

((3-Bromo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5j**)



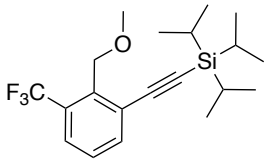
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-bromo-2-(methoxymethyl)benzene (**4j**) (40.2 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (54 mg, 0.14 mmol, 71% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.54 (dd, J = 8.0, 1.2 Hz, 1H), 7.46 (dd, J = 7.7, 1.2 Hz, 1H), 7.10 (t, J = 7.9 Hz, 1H), 4.79 (s, 2H), 3.43 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 138.5, 133.4, 132.3, 129.4, 126.7, 126.2, 104.4, 96.1, 72.4, 58.5, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}BrNaOSi^+$ $[M+Na]^+$: 403.1063; found: 403.1063.

((3-Iodo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5k**)



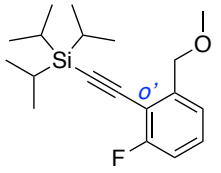
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-iodo-2-(methoxymethyl)benzene (**4k**) (49.6 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (47 mg, 0.11 mmol, 55% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.82 (dd, J = 7.9, 1.2 Hz, 1H), 7.48 (dd, J = 7.7, 1.2 Hz, 1H), 6.92 (t, J = 7.8 Hz, 1H), 4.77 (s, 2H), 3.43 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 141.4, 140.2, 133.2, 129.5, 125.8, 104.7, 101.4, 95.9, 76.3, 58.5, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}INaOSi^+$ $[M+Na]^+$: 451.0925; found: 451.0922.

Triisopropyl((2-(methoxymethyl)-3-(trifluoromethyl)phenyl)ethynyl)silane (**5l**)



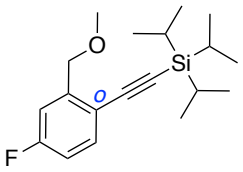
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-iodo-2-(methoxymethyl)benzene (**4l**) (49.6 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 µL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (47 mg, 0.11 mmol, 55% yield). **^{1}H NMR** (5 00 MHz, Chloroform-d) δ 7.70 (dd, J = 7.8, 1.3 Hz, 1H), 7.63 (dd, J = 7.9, 0.6 Hz, 1H), 7.37 (td, J = 7.8, 0.9 Hz, 1H), 4.77 (d, J = 1.2 Hz, 2H), 3.45 (s, 3H), 1.16 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 137.7 (d, J = 1.5 Hz), 136.8, 130.4 (q, J = 30.8 Hz), 128.21, 127.4, 126.2 (q, J = 5.7 Hz), 124.0 (q, J = 270 Hz), 104.0, 96.8, 69.1 (q, J = 1.9 Hz), 59.0, 18.8 (6C), 11.5 (3C). **^{19}F NMR** (^{19}F{^{1}H}, 376 MHz, Chloroform-d) δ -59.15. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}F_3NaOSi^+$ $[M+Na]^+$: 393.1832; found: 393.1820.

((2-Fluoro-6-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5m'**)



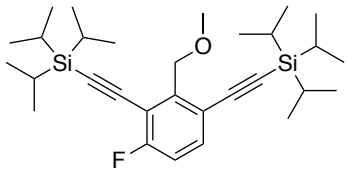
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-(methoxymethyl)-4-(trifluoromethyl)benzene (**4m**) (38 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 µL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (15.4 mg, 0.05 mmol, 24% yield). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}FNaOSi^+$ $[M+Na]^+$: 343.1864; found: 343.1856. **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.34 – 7.22 (m, 2H), 6.99 (td, J = 8.4, 7.9, 1.4 Hz, 1H), 4.65 (s, 2H), 3.45 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 163.5 (d, J = 251.6 Hz), 143.0, 129.6 (d, J = 8.6 Hz), 122.6 (d, J = 3.4 Hz), 114.2 (d, J = 21.2 Hz), 110.9 (d, J = 16.3 Hz), 102.0 (d, J = 3.6 Hz), 97.3, 72.4 (d, J = 3.2 Hz), 58.8, 18.8 (6C), 11.4 (3C). **^{19}F NMR** (^{19}F{^{1}H}, 376 MHz, Chloroform-d) δ -109.84. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}FNaOSi^+$ $[M+Na]^+$: 343.1864; found: 343.1856.

((4-Fluoro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5m**)



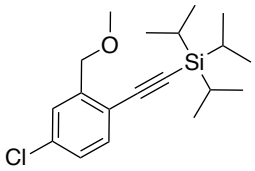
Compound **5m** was obtained as a colorless oil (10.2 mg, 0.03mmol, 16% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.44 (dd, J = 8.5, 5.6 Hz, 1H), 7.19 (dd, J = 9.7, 2.7 Hz, 1H), 6.91 (td, J = 8.4, 2.7 Hz, 1H), 4.64 (s, 2H), 3.45 (s, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 163.0 (d, J = 249.6 Hz), 143.7, 134.4 (d, J = 8.6 Hz), 117.63, 114.183, 114.177 (d, J = 45.1 Hz), 103.4, 95.4 (d, J = 1.5 Hz), 72.4, 58.8, 18.8 (6C), 11.4 (3C).**^{19}F NMR** (^{19}F{^{1}H}, 376 MHz, Chloroform-d) δ -110.32. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}FNaOSi^{+}$ $[M+Na]^{+}$: 343.1864; found: 343.1867.

((4-Fluoro-2-(methoxymethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) (**5m"**)



Compound **5m"** was obtained as a colorless oil (10.2 mg, 0.03mmol, 16% yield). **^{1}H NMR** (400 MHz, Chloroform-d) δ 7.42 (dd, J = 8.6, 5.5 Hz, 1H), 6.98 (t, J = 8.5 Hz, 1H), 4.78 (s, 2H), 3.41 (s, 3H), 1.15 (s, 21H), 1.14 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-d) δ 163.2 (d, J = 255.4 Hz), 143.5, 134.0 (d, J = 8.4 Hz), 121.0 (d, J = 3.7 Hz), 115.4 (d, J = 22.3 Hz), 114.0 (d, J = 16.5 Hz), 103.8, 101.7 (d, J = 4.1 Hz), 97.3, 94.6, 70.9 (d, J = 2.4 Hz), 58.7, 18.81 (6C), 18.77 (6C), 11.5 (3C), 11.4 (3C). **^{19}F NMR** (376 MHz, Chloroform-d) δ -106.12. **HRMS** (ESI+) *m/z* calc. for $C_{30}H_{49}FNaOSi2^{+}$ $[M+Na]^{+}$: 523.3198; found: 523.3214.

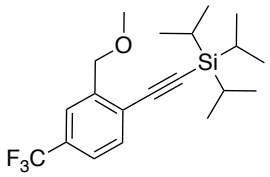
((4-Chloro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5n**)



The title compound was prepared by reaction between $(RhCp^{*}Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-chloro-3-(methoxymethyl)benzene (**4n**) (31.3 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv)

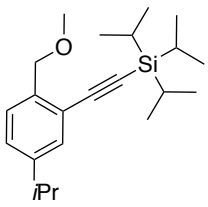
according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (37 mg, 0.11 mmol, 55% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.47 (d, J = 2.2 Hz, 1H), 7.39 (d, J = 8.2 Hz, 1H), 7.19 (dd, J = 8.2, 2.2 Hz, 1H), 4.62 (s, 2H), 3.45 (s, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 142.6, 134.8, 133.7, 127.4, 127.2, 120.2, 103.3, 96.9, 72.3, 58.8, 18.8 (6C), 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}ClNaOSi^+$ $[M+Na]^+$: 359.1568; found: 359.1573.

Triisopropyl((2-(methoxymethyl)-4-(trifluoromethyl)phenyl)ethynyl)silane (**5o**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-(methoxymethyl)-4-(trifluoromethyl)benzene (**4o**) (38 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (52 mg, 0.14 mmol, 70% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.75 (brs, 1H), 7.56 (d, J = 8.0 Hz, 1H), 7.47 (brd, J = 8.1, 1H), 4.69 (s, 2H), 3.48 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 141.7, 132.8 (2C), 130.5 (q, J = 32.5 Hz), 125.30, 124.0 (q, J = 271 Hz), 123.9 (q, J = 3.6 Hz), 103.0, 99.0, 72.4, 58.9, 18.8 (6C), 11.4 (3C). **^{19}F NMR** (^{19}F{^{1}H}, 376 MHz, Chloroform-d) δ -62.90. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}F_3NaOSi^+$ $[M+Na]^+$: 393.1832; found: 393.1832.

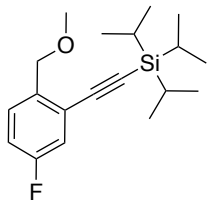
Triisopropyl((5-isopropyl-2-(methoxymethyl)phenyl)ethynyl)silane (**5p**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-(tert-butyl)-4-(methoxymethyl)benzene (**4p**) (35,7 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (29 mg,

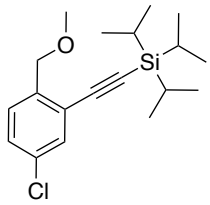
0.08 mmol, 40% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.47 (dd, J = 1.7, 0.9 Hz, 1H), 7.35 – 7.39 (m, 2H) , 4.64 (s, 2H), 3.43 (s, 3H), 1.31 (s, 9H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 150.3, 137.6, 129.5, 127.4, 126.1, 121.9, 105.2, 94.6, 72.7, 58.6, 34.6, 31.4 (9C), 18.9 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{23}H_{38}NaOSi^{+}$ $[M+Na]^{+}$: 381.2584; found: 381.2597.

((5-Fluoro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5q**)



The title compound was prepared by reaction between $(RhCp^{*}Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-fluoro-4-(methoxymethyl)benzene (**4p**) (28 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (37 mg, 0.12 mmol, 58% yield). **^{1}H NMR** ($^{1}H\{^{19}F\}$ 400 MHz, Chloroform-d) δ 7.31 (dd, J = 7.7, 1.3 Hz, 1H), 7.23 (t, J = 8.0 Hz, 1H), 7.04 (dd, J = 8.3, 1.3 Hz, 1H), 4.70 (s, 2H), 3.41 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 161.9 (d, J = 248.6 Hz), 129.7 (d, J = 9.5 Hz), 128.9 (d, J = 3.3 Hz), 126.7 (d, J = 16.6 Hz), 126.6 (d, J = 5.5 Hz), 116.1 (d, J = 22.7 Hz), 103.8 (d, J = 4.1 Hz), 96.0, 66.4 (d, J = 3.1 Hz), 58.4, 18.8 (6C), 11.5 (3C). **^{19}F NMR** ($^{19}F\{^{1}H\}$ 376 MHz, Chloroform-d) δ -116.64. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}FNaOSi^{+}$ $[M+Na]^{+}$: 343.1864; found: 343.1859.

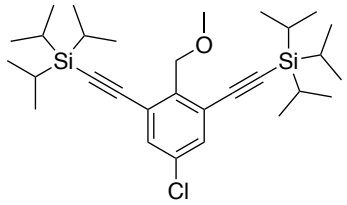
((5-Chloro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5r**)



The title compound was prepared by reaction between $(RhCp^{*}Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-chloro-4-(methoxymethyl)benzene (**4r**) (31.3 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv)

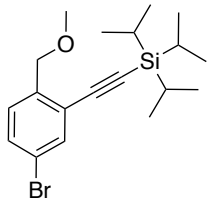
according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (32 mg, 0.09 mmol, 48% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.45 (d, J = 2.2 Hz, 1H), 7.39 (d, J = 8.3 Hz, 1H), 7.30 (dd, J = 8.3, 2.2 Hz, 1H), 4.61 (s, 2H), 3.43 (s, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 139.1, 132.9, 132.2, 128.9, 128.6, 123.6, 103.0, 97.3, 72.3, 58.7, 18.8 (6C), 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}ClNaOSi^+$ $[M+Na]^+$: 359.1568; found: 359.1569.

***((5-Chloro-2-(methoxymethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane)*(5r")**



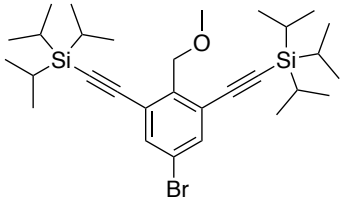
Compound **5r"** was obtained as a colorless oil (35 mg, 0.06 mmol, 34% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.43 (s, 2H), 4.75 (s, 2H), 3.39 (s, 3H), 1.14 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 139.6, 133.5, 132.7 (2C), 126.7 (2C), 103.4 (2C), 96.7 (2C), 70.5, 58.6, 18.8 (12 C), 11.5 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{30}H_{49}ClNaOSi_2^+$ $[M+Na]^+$: 539.2903; found: 539.2904.

***((5-Bromo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane* (5s)**



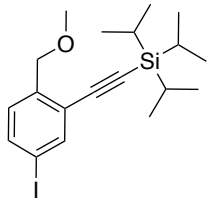
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-bromo-4-(methoxymethyl)benzene (**4s**) (40.2 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 µL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (42 mg, 0.11 mmol, 55% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.60 (d, J = 2.1 Hz, 1H), 7.45 (dd, J = 8.3, 2.1 Hz, 1H), 7.33 (d, J = 8.3 Hz, 1H), 4.60 (s, 2H), 3.43 (s, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 139.6, 135.0, 131.8, 128.8, 123.9, 120.7, 102.9, 97.4, 72.3, 58.7, 18.8 (6C), 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}BrNaOSi^+$ $[M+Na]^+$: 403.1063; found: 403.1058.

((5-Bromo-2-(methoxymethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) (**5s"**)



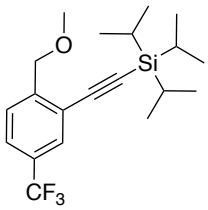
Compound **5s"** was obtained as a colorless oil (30 mg, 0.055 mmol, 28% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.58 (s, 2H), 4.74 (s, 2H), 3.39 (s, 3H), 1.14 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 140.1, 135.5 (2C), 126.9 (2C), 121.3, 103.2 (2C), 96.8 (2C), 70.6, 58.6, 18.8 (12 C), 11.4 (6C). **HRMS** (ESI+) *m/z* calc. for $C_{30}H_{49}BrNaOSi_2^+$ $[M+Na]^+$: 583.2398; found: 583.2420.

((5-Iodo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5t**)



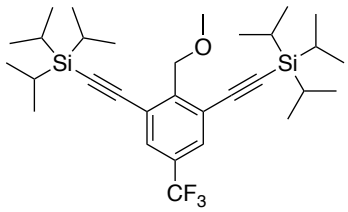
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-iodo-4-(methoxymethyl)benzene (**4t**) (49.6 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (27 mg, 0.06 mmol, 32% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.79 (d, J = 1.8 Hz, 1H), 7.65 (dd, J = 8.2, 1.8 Hz, 1H), 7.19 (d, J = 8.2 Hz, 1H), 4.59 (s, 2H), 3.43 (s, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 140.8, 140.3, 137.7, 128.9, 124.1, 102.7, 97.5, 91.9, 72.4, 58.7, 18.8, 11.4. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{29}INaOSi^+$ $[M+Na]^+$: 451.0925; found: 451.0929.

Triisopropyl((2-(methoxymethyl)-5-(trifluoromethyl)phenyl)ethynyl)silane (**5u**)



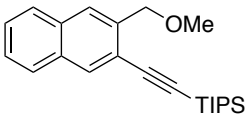
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 1-(methoxymethyl)-4-(trifluoromethyl)benzene (**4u**) (38 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 μL, 0.420 mmol, 2.1 equiv) according to general procedure, at 100 ºC for 20 h, and obtained as a yellow oil (33 mg, 0.09 mmol, 45% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.70 (dt, J = 1.7, 0.8 Hz, 1H), 7.61 (dt, J = 8.2, 0.7 Hz, 1H), 7.57 (dd, J = 8.2, 1.8 Hz, 1H), 4.69 (s, 2H), 3.47 (s, 3H), 1.15 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 144.6, 129.7 (q, J = 33 Hz), 129.3 (q, J = 3.7 Hz), 127.2, 125.2 (q, J = 3.8 Hz), 123.9 (q, J = 272 Hz), 122.4, 102.7, 98.0, 72.4, 58.9, 18.8 (6C), 11.4 (3C). **^{19}F NMR** ($^{19}F\{^1H\}$, 376 MHz, Chloroform-d) δ -62.80. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{29}F_3NaOSi^+$ $[M+Na]^+$: 393.1832; found: 393.1850.

((2-(Methoxymethyl)-5-(trifluoromethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsi-lane) (**5u"**)



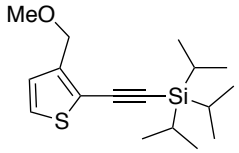
Compound **5u"** was obtained as a colorless oil (17.6 mg, 0.032 mmol, 16% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.66 (s, 2H), 4.82 (s, 2H), 3.41 (s, 3H), 1.15 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 144.4, 130.7 (q, J = 33.2 Hz), 129.3 (q, J = 3.6 Hz, 2C), 126.1 (2C), 123.4 (q, J = 272.6 Hz), 103.2 (2C), 97.3 (2C), 70.7, 58.8, 18.8 (12C), 11.4 (6C). **^{19}F NMR** ($^{19}F\{^1H\}$, 376 MHz, Chloroform-d) δ -63.22. **HRMS** (ESI+) *m/z* calc. for $C_{31}H_{49}F_3NaOSi_2^+$ $[M+Na]^+$: 573.3166; found: 573.3187.

Triisopropyl((3-(methoxymethyl)naphthalen-2-yl)ethynyl)silane (**5v**)



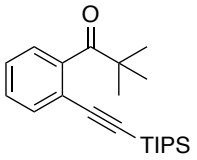
General procedure starting from 2-(methoxymethyl)naphthalene (**4v**) (34.4 mg, 0.2 mmol) at 100 ºC. Yellow liquid (75 mg, 70 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 7.90 (s, 1H), 7.85 – 7.75 (m, 2H), 7.52 – 7.43 (m, 2H), 4.82 (s, 2H), 3.55 (s, 3H), 1.20 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 136.47, 132.97, 132.68, 132.12, 127.80, 127.34, 126.81, 126.24, 125.66, 119.74, 104.57, 95.17, 72.98, 58.72, 18.71, 11.36. **HRMS** (ESI+) *m/z* calc. for $C_{23}H_{32}NaOSi$ $[M+Na]^+$: 375.2115. Found: 375.2116.

Triisopropyl((3-(methoxymethyl)thiophen-2-yl)ethynyl)silane (**5w**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.71 mg, 0.006 mmol, 0.03 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 3-(methoxymethyl)thiophene (**4w**) (25,6 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 95 µL, 0.420 mmol, 2.1 equiv) according to general procedure, at 45 ºC for 20 h, and obtained as a yellow oil (19 mg, 0.06 mmol, 31% yield). **^{1}H NMR** (300 MHz, Chloroform-d) δ 7.18 (d, J = 5.2 Hz, 1H), 7.03 (d, J = 5.2 Hz, 1H), 4.53 (s, 2H), 3.36 (s, 3H), 1.13 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 143.8, 127.8, 126.4, 121.7, 98.7, 98.1, 68.4, 58.2, 18.8 (6C), 11.4 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{17}H_{28}NaOSSi$ $[M+Na]^+$: 331.1522. Found: 331.1524.

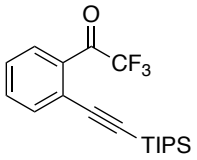
2,2-Dimethyl-1-(2-((triisopropylsilyl)ethynyl)phenyl)propan-1-one (**7a**)



General procedure starting from 2,2-dimethyl-1-phenylpropan-1-one (**6a**) (32.4 mg, 0.2 mmol) at 45 ºC. Colorless liquid (65 mg, 95 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.55 – 7.48 (m, 1H), 7.33 – 7.25 (m, 2H), 7.13 (m, 1H), 1.27 (s, 9H), 1.10 (m, 21H). **^{13}C NMR** (75 MHz,

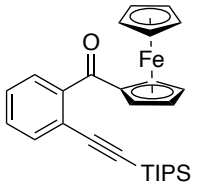
$CDCl_3$) δ 212.30, 144.13, 133.50, 128.10, 127.51, 124.43, 120.04, 104.76, 94.92, 45.08, 26.89, 18.59, 11.28. **HRMS** (ESI+) *m/z* calc. for $C_{22}H_{34}NaO_2Si$ $[M+Na]^+$: 365.2271. Found: 365.2272.

2,2,2-Trifluoro-1-(2-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7b**)



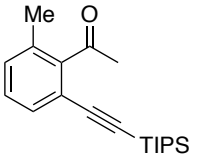
General procedure at 90 ºC starting from 2,2,2-trifluoro-1-phenylethan-1-one (**6b**) (34.8 mg, 0.2 mmol) at 90 ºC. Yellow liquid (35.0 mg, 0.10 mmol, 50 % yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.78 (dt, *J* = 8.0, 1.3 Hz, 1H), 7.71 – 7.66 (m, 1H), 7.56 (td, *J* = 7.7, 1.3 Hz, 1H), 7.43 (td, *J* = 7.7, 1.3 Hz, 1H), 1.15 (m, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.86 (q, *J* = 33 Hz), 135.51, 133.02, 132.59, 129.11 (q, *J* = 3 Hz), 127.86, 124.42, 116.19 (q, *J* = 289 Hz), 103.50, 98.86, 18.57, 11.28. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -71.90. **HRMS** (ESI+) *m/z* calc. for $C_{22}H_{29}F_3NaO_2Si$ $[M+Na+OMe]^+$: 409.1781. Found: 409.1790.

2-((Triisopropylsilyl)ethynyl)benzoyl ferrocene (**7c**)



General procedure starting from (**6c**) (67.0 mg, 0.237 mmol) at 45 ºC. Brown liquid (90 mg, 83 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.54 (m, 2H), 7.39 (m, 2H), 4.77 (t, *J* = 1.9 Hz, 2H), 4.51 (t, *J* = 1.9 Hz, 2H), 4.21 (s, 5H), 1.00 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 200.00, 143.20, 133.53, 129.29, 127.84, 126.98, 120.90, 104.53, 96.66, 78.52, 72.56, 71.34, 69.93, 18.56, 11.12. **HRMS** (ESI+) *m/z* calc. for $C_{28}H_{34}NaOSiFe$ $[M+Na]^+$: 491.1667. Found: 491.1670.

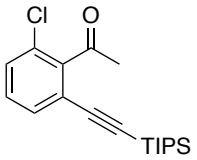
1-(2-Methyl-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7d**)



General procedure starting from 1-(*o*-tolyl)ethan-1-one (**6d**) (26.8 mg, 0.2 mmol) at 45 ºC. Yellow liquid (55 mg, 87 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.36 – 7.30 (m, 1H), 7.23 – 7.11 (m, 2H), 2.59 (s, 3H), 2.24 (s, 3H), 1.11 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 205.69,

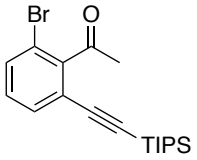
144.77, 133.10, 130.55, 130.37, 128.41, 119.08, 104.22, 95.85, 31.72, 19.04, 18.54, 11.23. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{30}NaOSi$ $[M+Na]^+$: 337.1958. Found: 337.1954.

1-(2-Chloro-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7e**)



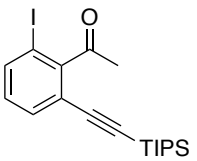
General procedure starting from 1-(2-chlorophenyl)ethan-1-one (**6e**) (35.0 mg, 0.226 mmol) at 45 ºC. Light yellow liquid (70 mg, 92 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.39 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.32 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.23 (dd, *J* = 8.1, 7.6 Hz, 1H), 2.58 (s, 3H), 1.10 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 201.36, 143.78, 131.09, 129.49, 129.44, 128.74, 121.02, 102.37, 97.32, 31.06, 18.49, 11.17. **HRMS** (ESI+) *m/z* calc. for $C_{17}H_{27}NaClOSi$ $[M+Na]^+$: 357.1412. Found: 357.1414.

1-(2-Bromo-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7f**)



General procedure starting from 1-(2-bromophenyl)ethan-1-one (**6f**) (40.0 mg, 0.2 mmol) at 45 ºC. Colorless liquid (75 mg, 95 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.49 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.43 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.16 (t, *J* = 7.9 Hz, 1H), 2.58 (s, 3H), 1.09 (m, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 202.08, 145.77, 132.56, 131.61, 129.58, 121.02, 116.64, 102.41, 97.49, 30.76, 18.52, 11.19. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{28}BrOSi$ $[M+H]^+$: 379.1087. Found: 379.1087.

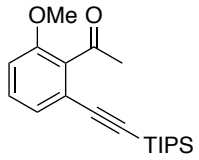
1-(2-Iodo-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7g**)



General procedure starting from 1-(2-iodophenyl)ethan-1-one (**6g**) (53.0 mg, 0.215 mmol) at 45 ºC. Yellow liquid (88 mg, 95 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.75 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.46 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.00 (t, *J* = 7.9 Hz, 1H), 2.59 (s, 3H), 1.09 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 203.72, 149.55, 138.89, 132.30, 129.63, 120.29, 102.65, 97.51,

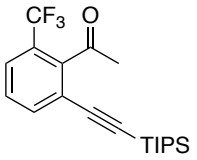
88.61, 30.20, 18.50, 11.17. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{27}NaIOSi$ $[M+Na]^+$: 449.0768. Found: 449.0773.

1-(2-Methoxy-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7h**)



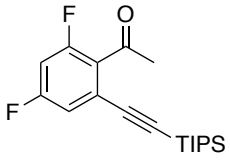
General procedure starting from 1-(2-methoxyphenyl)ethan-1-one (**6h**) (35.0 mg, 0.233 mmol) at 45 ºC. Light yelow liquid (70 mg, 91 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.23 (dd, *J* = 8.4, 7.7 Hz, 1H), 7.08 (dd, *J* = 7.7, 0.9 Hz, 1H), 6.87 (dd, *J* = 8.4, 0.9 Hz, 1H), 3.79 (s, 3H), 2.52 (s, 3H), 1.10 (s, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 202.64, 155.23, 134.46, 129.61, 125.03, 120.42, 111.29, 103.41, 95.35, 55.72, 31.54, 18.50, 11.18. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{30}NaO_2Si$ $[M+Na]^+$: 353.1907. Found: 353.1902.

1-(2-(Trifluoromethyl)-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7i**)



General procedure starting from 1-(2-(trifluoromethyl)phenyl)ethan-1-one (**6i**) (37.6 mg, 0.2 mmol) at 45 ºC. Light yellow liquid (60 mg, 81 % yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.44 (tq, *J* = 7.9, 0.9 Hz, 1H), 2.62 (s 3H), 1.13 – 1.08 (m, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 201.94, 143.54 (q, *J* = 2 Hz), 136.20, 128.69, 126.42 (q, *J* = 32 Hz), 125.87 (q, J = 5 Hz) 123.22 (q, J = 275 Hz), 120.81, 102.13, 98.62, 31.41, 18.52, 11.21. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -58.84. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{27}NaF_3OSi$ $[M+Na]^+$: 391.1675. Found: 391.1690.

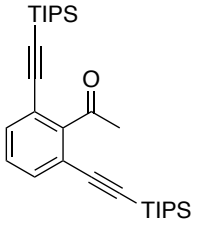
1-(2,4-Difluoro-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7j**)



General procedure starting from 1-(2,4-difluorophenyl)ethan-1-one (**6j**) (31.2 mg, 0.2 mmol) at 45 ºC. Yellow liquid (64 mg, 95 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.03 (ddd, *J* =

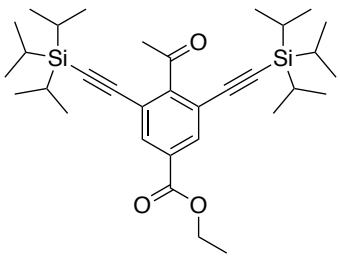
8.6, 2.4, 1.3 Hz, 1H), 6.82 (ddd, *J* = 9.7, 8.6, 2.4 Hz, 1H), 2.59 (d, *J* = 1.6 Hz, 3H), 1.11 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 197.41, 162.69 (dd, *J* = 245 Hz, *J* = 15 Hz), 159.36 (dd, *J* = 245 Hz, *J* = 15 Hz), 128.45 (dd, *J* = 18 Hz, *J* = 4 Hz), 123.68 (dd, *J* = 18 Hz, *J* = 4 Hz), 116.40 (dd, *J* = 23 Hz, *J* = 4 Hz), 104.87 (t, 25 Hz), 101.79 (dd, *J* =3 Hz, *J* = 1Hz), 99.04, 31.73, 18.52, 11.18. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -107.20, -111.35. **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{26}NaF_2OSi$ $[M+Na]^+$: 359.1613. Found: 359.1604.

1-***(2,6-bis((Triisopropylsilyl)ethynyl)phenyl)ethan-1-one*** (**7k**)



General procedure at room temperature starting from acetophenone (**6k**) (24.0 mg, 0.2 mmol), using 1-Bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 0.42 mmol). Colorless oil (90 mg, 0.2 mmol, 94 % yield). **^{1}H NMR** (300 MHz, Chloroform-d) δ 7.43 (d, J = 7.7 Hz, 2H), 7.24 (t, J = 7.7, 1H), 2.60 (s, 3H), 1.10 (m, 42H). **^{13}C NMR** (75 MHz, CDCl3) δ 203.11, 148.08, 132.48, 128.32, 119.30, 102.98, 96.28, 31.11, 18.55, 11.22. **HRMS** (ESI+) m/z calc. for $C_{30}H_{48}NaO_2S_{i2}$ [M+Na]+: 503.3136. Found: 503.3137.

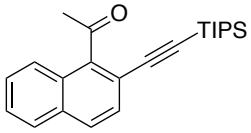
Ethyl 4-acetyl-3,5-bis((triisopropylsilyl)ethynyl)benzoate (**7l**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl 4-acetylbenzoate (**6l**) (38.4 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 45 ºC for 20 h, and obtained as a white cristalline solid (88 mg, 0.16 mmol, 80% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 8.04 (s, 2H), 4.40 (q, *J* = 7.1 Hz, 2H), 2.59 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H), 1.10 (s, 42H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 202.5, 164.9, 151.5, 133.3 (2C), 131.0, 120.0 (2C), 102.2 (2C), 97.7 (2C), 61.8, 31.0, 18.7 (12C), 14.4, 11.4

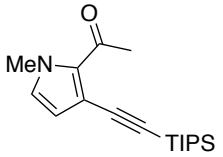
(6C). **HRMS** (ESI+) *m/z* calc. for $C_{33}H_{53}O_3Si_2^+$ $[M+H]^+$: 553.3528; found: 553.3525. **Mp**: 43-48 ºC.

1-(2-((Triisopropylsilyl)ethynyl)naphthalen-1-yl)ethan-1-one (**7m**)



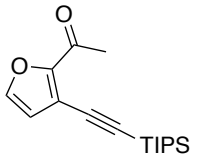
General procedure starting from 1-(naphthalen-1-yl)ethan-1-one (**6m**) (34.2 mg, 0.2 mmol) at 45 ºC. Brown liquid (65 mg, 93 % yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.84 – 7.80 (m, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.73 – 7.69 (m, 1H), 7.54 – 7.49 (m, 3H), 2.78 (s, 3H), 1.16 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 205.44, 143.28, 132.84, 128.84, 128.70, 128.35, 128.24, 127.48, 126.97, 124.58, 116.65, 104.50, 97.62, 32.31, 18.60, 11.28. **HRMS** (ESI+) *m/z* calc. for $C_{23}H_{30}NaOSi$ $[M+Na]^+$: 373.1958. Found: 373.1960.

1-(1-Methyl-3-((triisopropylsilyl)ethynyl)-1H-pyrrol-2-yl)ethan-1-one (**7n**)



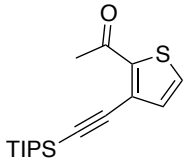
General procedure starting from 1-(1-methyl-1*H*-pyrrol-2-yl)ethan-1-one (**6n**) (24.63 mg, 0.2 mmol) at 45 ºC. Light yellow liquid (45 mg, 74 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 6.65 (d, *J* = 2.6 Hz, 1H), 6.30 (d, *J* = 2.6 Hz, 1H), 3.88 (s, 3H), 2.71 (s, 3H), 1.11 (s, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 189.40, 132.37, 129.25, 113.98, 113.63, 102.32, 96.56, 38.66, 29.93, 18.63, 11.34. **HRMS** (ESI+) *m/z* calc. for $C_{18}H_{29}NNaOSi$ $[M+Na]^+$: 326.1911. Found: 326.1908.

1-(3-((Triisopropylsilyl)ethynyl)furan-2-yl)ethan-1-one (**7o**)



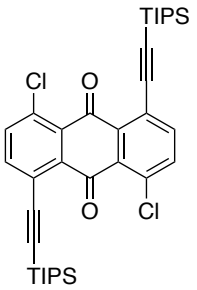
General procedure starting from 1-(furan-2-yl)ethan-1-one (**6o**) (22.22 mg, 0.2 mmol) at 45 ºC. Light yellow liquid (50 mg, 86 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.50 (d, *J* = 1.8 Hz, 1H), 6.56 (d, *J* = 1.8 Hz, 1H), 2.62 (s, 3H), 1.12 (m, 21H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 185.63, 152.94, 145.35, 116.15, 114.71, 101.64, 97.52, 27.64, 18.54, 11.18. **HRMS** (ESI+) *m/z* calc. for $C_{17}H_{26}NaO_2Si$ $[M+Na]^+$: 313.1594. Found: 313.1596.

1-(3-((Triisopropylsilyl)ethynyl)thiophen-2-yl)ethan-1-one (**7p**)



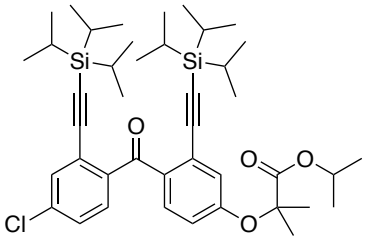
General procedure starting from 1-(thiophen-2-yl)ethan-1-one (**6p**) (25.2 mg, 0.2 mmol) at 45 ºC. Light yellow liquid (58 mg, 95 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.49 (d, *J* = 5.1 Hz, 1H), 7.16 (d, *J* = 5.1 Hz, 1H), 2.78 (s, 3H), 1.13 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 191.05, 146.12, 133.71, 131.61, 125.60, 101.17, 100.17, 28.88, 18.58, 11.23. **HRMS** (ESI+) *m/z* calc. for $C_{17}H_{27}OSSi$ $[M+H]^+$: 307.1546. Found: 307.1545.

1,5-Dichloro-4,8-bis((triisopropylsilyl)ethynyl)anthracene-9,10-dione (**7q**)



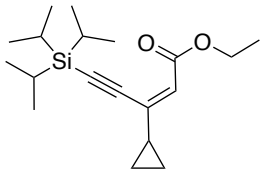
General procedure starting from 1,5-dichloroanthracene-9,10-dione (**6q**) (54.4 mg, 0.20 mmol) using $[Cp^*RhCl_2]_2$ (4.96 mg, 8.00 µmol, 4 mol %), and 1-Bromo-2-(triisopropylsilyl)acetylene (120 mg, 0.46 mmol) at 100 ºC. Yellow liquid (105 mg, 82 % yield).**^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 1.19 (m, 42H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 180.85, 138.95, 137.80, 135.07, 132.70, 131.83, 121.32, 102.93, 99.71, 18.64, 11.35. **HRMS** (ESI+) *m/z* calc. for $C_{36}H_{46}NaCl_2O_2Si_2$ $[M+Na]^+$: 659.2306. Found: 659.2334.

Isopropyl 2-(4-(4-chloro-2-((triisopropylsilyl)ethynyl)benzoyl)-3-((triisopropylsilyl)ethynyl) phenoxy) -2-methylpropanoate (**7r**)



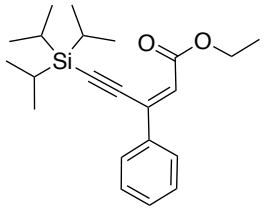
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), Fenofibrate (**6r**) (72.2 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 50ºC for 20 h, and obtained as a colorless oil (52 mg, 0.07 mmol, 36% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.52 (d, J = 8.7 Hz, 1H), 7.47 (d, J = 2.1 Hz, 1H), 7.38 (d, J = 8.3 Hz, 1H), 7.29 (dd, J = 8.3, 2.1 Hz, 1H), 6.96 (d, J = 2.6 Hz, 1H), 6.74 (dd, J = 8.8, 2.6 Hz, 1H), 5.07 (h, J = 6.3 Hz, 1H), 1.63 (s, 6H), 1.21 (d, J = 6.3 Hz, 6H), 1.09 – 0.90 (m, 42H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 193.8, 173.0, 158.5, 140.4, 136.5, 133.8, 132.75, 132.72, 131.0, 128.5, 125.2, 124.2, 124.1, 117.5, 104.8, 103.4, 98.5, 98.5, 79.6, 69.5, 25.5 (2C), 21.7 (3C), 18.7 (6C), 18.7 (6C), 11.5 (2C), 11.3 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{42}H_{61}ClNaO4Si2^+$ $[M+Na]^+$: 743.3689; found: 743.3711.

Ethyl (Z)-3-cyclopropyl-5-(triisopropylsilyl)pent-2-en-4-ynoate (**9a**)



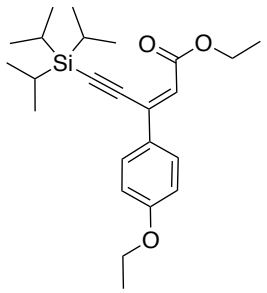
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl (*E*)-3-cyclopropylacrylate (**8a**) (28.0 mg, 31.2 μL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 85 ºC for 48 h, and obtained as a colorless oil (33 mg, 0.10 mmol, 52% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 6.12 (s, 1H), 4.19 (q, *J* = 7.1 Hz, 2H), 1.65 (tt, *J* = 8.0, 4.7 Hz, 1H), 1.26 (t, *J* = 7.1 Hz, 3H), 1.11 (s, 21H), 1.01 – 0.92 (m, 2H), 0.85 – 0.73 (m, 2H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 164.7, 141.9, 122.9, 103.9, 99.9, 60.0, 18.7 (6C), 18.3, 14.5, 11.4 (3C), 7.7 (2C). **HRMS** (ESI+) *m/z* calc. for $C_{19}H_{33}O_2Si^+$ $[M+H]^+$: 321.2244; found: 321.2246.

Ethyl (Z)-3-phenyl-5-(triisopropylsilyl)pent-2-en-4-ynoate (**9b**)



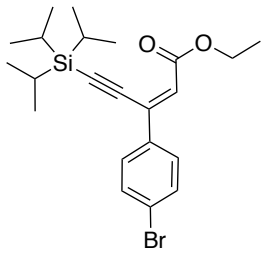
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl cinnamate (**8b**) (35.2 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 85 ºC for 48 h, and obtained as a yellow oil (43 mg, 0.12 mmol, 60% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.79 – 7.70 (m, 2H), 7.43 – 7.34 (m, 3H), 6.55 (s, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.33 (t, *J* = 7.1 Hz, 3H), 1.17 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 165.2, 137.5, 135.7, 129.8, 128.6 (2C), 127.3 (2C), 124.0, 106.0, 103.1, 60.5, 18.8 (6C), 14.5, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{22}H_{32}NaO_2Si^+$ $[M+Na]^+$: 379.2064; found: 379.2073.

Ethyl (Z)-3-(4-ethoxyphenyl)-5-(triisopropylsilyl)pent-2-en-4-ynoate (**9c**)



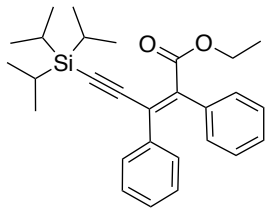
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl (*E*)-3-(4-ethoxyphenyl)acrylate (**8c**) (44.1 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 85 ºC for 48 h, and obtained as a colorless oil (35 mg, 0.09 mmol, 44% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.74 – 7.65 (m, 2H), 6.92 – 6.84 (m, 2H), 6.47 (s, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 4.06 (q, *J* = 7.0 Hz, 2H), 1.42 (t, *J* = 7.0 Hz, 3H), 1.31 (t, *J* = 7.1 Hz, 3H), 1.17 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 165.4, 160.5, 135.2, 129.6, 128.8 (2C), 121.7, 114.5 (2C), 105.5, 103.2, 63.7, 60.3, 18.8 (6C), 14.9, 14.5, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{24}H_{36}NaO_3Si^+$ $[M+Na]^+$: 423.2326; found: 423.2331.

Ethyl (Z)-3-(4-bromophenyl)-5-(triisopropylsilyl)pent-2-en-4-ynoate (**9d**)



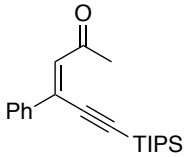
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl (*E*)-3-(4-bromophenyl)acrylate (**8d**) (51.0 mg, 37.5 μL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 85 ºC for 48 h, and obtained as a yellow oil (58 mg, 0.13 mmol, 66% yield). **^{1}H NMR** (400 MHz, Chloroform-*d*) δ 7.64 – 7.56 (m, 2H), 7.55 – 7.45 (m, 2H), 6.52 (s, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 1.32 (t, *J* = 7.1 Hz, 3H), 1.16 (s, 21H). **^{13}C NMR** (101 MHz, Chloroform-*d*) δ 164.9, 136.4, 134.5, 131.8 (2C), 128.8 (2C), 124.3, 124.2, 106.5, 102.6, 60.6, 18.8 (6C), 14.5, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{22}H_{32}BrO_2Si^+$ $[M+H]^+$: 435.1349; found: 435.1368.

***Ethyl (Z)-2,3-diphenyl-5-(triisopropylsilyl)pent-2-en-4-ynoate (*9e**)



The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), ethyl (*E*)-2,3-diphenylacrylate (**8e**) (50.5 mg, 54.3 μL 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 85 ºC for 48 h, and obtained as a colorless oil (72 mg, 0.17 mmol, 84% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.33 – 7.23 (m, 2H), 7.24 – 7.10 (m, 8H), 4.33 (q, *J* = 7.1 Hz, 2H), 1.34 (t, *J* = 7.1 Hz, 3H), 1.14 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 168.8, 140.7, 137.0, 135.2, 129.9 (2C), 129.5 (2C), 128.3 (2C), 128.1, 128.04, 127.96 (2C), 125.5, 105.9, 99.3, 61.6, 18.8 (6C), 14.2, 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{28}H_{36}NaO_2Si^+$ $[M+Na]^+$: 455.2377; found: 455.2377.

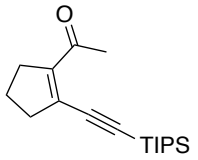
(Z)-4-Phenyl-6-(triisopropylsilyl)hex-3-en-5-yn-2-one **(9f)**



General procedure starting from (*E*)-4-phenylbut-3-en-2-one (**8f**) (29.2 mg, 0.2 mmol) at 45 ºC. Brown liquid (40 mg, 61 % yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.76 – 7.71 (m, 2H), 7.41 – 7.37 (m, 3H), 6.74 (s, 1H), 2.63 (s, 3H), 1.21 – 1.13 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$)

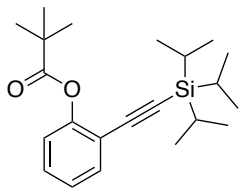
δ 198.06, 137.49, 133.89, 133.23, 129.84, 128.53, 127.24, 107.66, 103.72, 30.51, 18.60, 11.30. **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{30}NaOSi$ $[M+Na]^+$: 349.1958. Found: 349.1960.

1-(2-((Triisopropylsilyl)ethynyl)cyclopent-1-en-1-yl)ethan-1-one (**9g**)



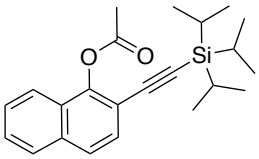
General procedure starting from 1-(cyclopent-1-en-1-yl)ethan-1-one (**8g**) (67.0 mg, 0.4 mmol) and 1-Bromo-2-(triisopropylsilyl)acetylene (**1**) (52 mg, 0.2 mmol, 1 equiv) at 45 ºC. Yellow liquid (35 mg, 60 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 2.70 (m, 4H), 2.59 (s, 3H), 1.92 – 1.78 (m, 2H), 1.09 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 196.55, 147.49, 134.11, 105.86, 103.15, 40.94, 32.86, 29.52, 21.62, 18.55, 11.19. **HRMS** (ESI+) *m/z* calc. for $C_{18}H_{30}NaOSi$ $[M+Na]^+$: 313.1958. Found: 313.1967.

2-((Triisopropylsilyl)ethynyl)phenyl pivalate (**11a**)



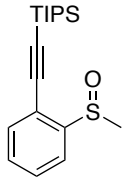
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), phenyl pivalate (**10a**) (35.6 mg, 42.4 μL, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 90ºC for 72 h, and obtained as a colorless oil (25 mg, 0.07 mmol, 35% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.53 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.31 (ddd, *J* = 8.2, 7.4, 1.7 Hz, 1H), 7.16 (td, *J* = 7.6, 1.2 Hz, 1H), 7.05 (dd, *J* = 8.2, 1.1 Hz, 1H), 1.39 (s, 9H), 1.12 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 176.5, 151.6, 134.7, 129.4, 125.6, 122.4, 117.7, 102.1, 95.8, 39.3, 27.4 (3C), 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{22}H_{35}O_2Si^+$ $[M+H]^+$: 359.2401; found: 359.2417.

2-((Triisopropylsilyl)ethynyl)naphthalen-1-yl acetate (**11b**)



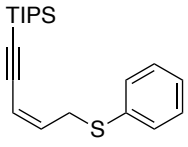
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), naphthalen-1-yl acetate (**10b**) (37.2 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 70 ºC for 24 h, and obtained as a dark yellow solid (29 mg, 0.08 mmol, 40% yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.86 – 7.78 (m, 2H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.57 – 7.43 (m, 3H), 2.48 (s, 3H), 1.17 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-*d*) δ 168.5, 148.9, 134.3, 129.2, 128.1, 127.3, 127.2, 127.1, 125.9, 121.5, 114.1, 102.4, 97.0, 21.0, 18.8 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{23}H_{30}NaO_2Si^+$ $[M+Na]^+$: 389.1907; found: 389.1918. **Mp**: 47-51 ºC.

Triisopropyl((2-(methylsulfinyl)phenyl)ethynyl)silane (**11c**)



General procedure starting from (methylsulfinyl)benzene (**10c**) (28 mg, 0.2 mmol) at 100 ºC. Yellow liquid (55 mg, 55 % yield). **^{1}H NMR** (500 MHz, Chloroform-*d*) δ 7.94 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.56 (td, *J* = 7.8, 1.3 Hz, 1H), 7.51 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.42 (td, *J* = 7.8, 1.3 Hz, 1H), 2.83 (s, 3H), 1.15 – 1.10 (m, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 147.47, 133.12, 130.18, 129.57, 123.04, 119.39, 101.17, 100.97, 42.08, 18.57, 11.19. **HRMS** (ESI+) *m/z* calc. for $C_{18}H_{28}NaOSSi$ $[M+Na]^+$: 343.1522. Found: 343.1518.

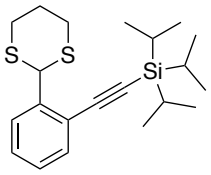
(Z)-Triisopropyl(5-(phenylthio)pent-3-en-1-yn-1-yl)silane (**11d**)



General procedure starting from allyl(phenyl)sulfane (**10d**) (30.0 mg, 0.2 mmol) at 50 ºC. Yellow liquid (55 mg, 83 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.42 – 7.37 (m, 2H), 7.32 – 7.25 (m, 2H), 7.22 – 7.16 (m, 1H), 6.00 (dt, *J* = 10.7, 7.5 Hz, 1H), 5.63 (dt, *J* = 10.7, 1.0 Hz, 1H),

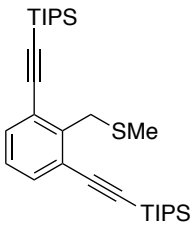
3.87 (dd, *J* = 7.5, 1.0 Hz, 2H), 1.13 (s, 21H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.26, 135.42, 129.32, 128.75, 126.05, 112.03, 102.45, 97.47, 32.96, 18.63, 11.24. **HRMS** (ESI+) *m/z* calc. for $C_{20}H_{31}SSi$ $[M+H]^+$: 331.1910. Found: 331.1909.

((2-(1,3-Dithian-2-yl)phenyl)ethynyl)triisopropylsilane (**11e**)



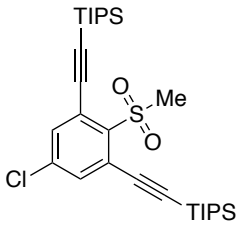
The title compound was prepared by reaction between $(RhCp^*Cl_2)_2$ (3.09 mg, 0.005 mmol, 0.025 equiv), $AgSbF_6$, (13.74 mg, 0.04 mmol, 0.20 equiv), LiOAc (2.64 mg, 0.04 mmol, 0.20 equiv), Ag_2CO_3 (55 mg, 0.2 mmol, 1 equiv), 2-phenyl-1,3-dithiane (**10e**) (39 mg, 0.20 mmol), and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 μL, 0.40 mmol, 2 equiv) according to general procedure, at 90 ºC for 16 h, and obtained as a colorless solid (40 mg, 0.11 mmol, 53% yield). **^{1}H NMR** (500 MHz, Chloroform-d) δ 7.63 (dd, J = 7.9, 1.3 Hz, 1H), 7.47 (dd, J = 7.9, 1.3 Hz, 1H), 7.32 (td, J = 7.6, 1.4 Hz, 1H), 7.23 (td, J = 7.6, 1.3 Hz, 1H), 5.87 (s, 1H), 3.04 (ddd, J = 14.9, 12.5, 2.4 Hz, 2H), 2.91 (ddd, J = 14.4, 4.2, 3.0 Hz, 2H), 2.17 (dtt, J = 13.8, 4.5, 2.4 Hz, 1H), 1.94 (dtt, J = 14.1, 12.5, 3.1 Hz, 1H), 1.18 (s, 21H). **^{13}C NMR** (126 MHz, Chloroform-d) δ 140.9, 132.8, 129.2, 128.1, 128.0, 122.2, 104.2, 96.0, 49.4, 32.5 (2C), 25.4, 18.9 (6C), 11.5 (3C). **HRMS** (ESI+) *m/z* calc. for $C_{21}H_{33}S_2Si$ $[M+H]^+$: 377.1784. Found: 377.1787. **Mp**: 56-60 ºC.

((2-((Methylthio)methyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) (**11f**)



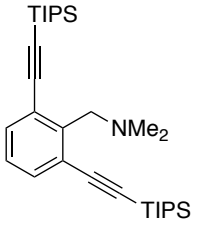
General procedure starting from benzyl(methyl)sulfane (**10f**) (27.6 mg, 0.2 mmol) using 1-Bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 0.42 mmol) at 100 ºC. Light yellow liquid (75 mg, 75 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 7.7 Hz, 2H), 7.18 – 7.10 (t, *J* = 7.7 Hz 1H), 4.14 (s, 3H), 2.13 (s, 3H), 1.16 (s, 42H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 143.31, 133.09, 126.40, 123.66, 104.70, 96.11, 34.64, 18.68, 15.35, 11.36. **HRMS** (ESI+) *m/z* calc. for $C_{30}H_{31}SSi_2$ $[M+H]^+$: 499.3245. Found: 499.3254.

((5-Chloro-2-(methylsulfonyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) (**11g**)



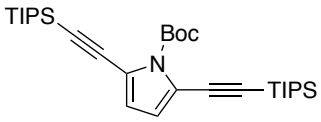
General procedure starting from 1-chloro-4-(methylsulfonyl)benzene (**10g**) (38.1 mg, 0.2 mmol) using 1-Bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 0.42 mmol)at 100 ºC. Yellow liquid (45 mg, 41 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.54 (s, 2H), 3.28 (s, 3H), 1.14 (m, 42H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 139.93, 137.84, 135.46, 125.68, 103.76, 101.47, 42.95, 18.58, 11.28. **HRMS** (ESI+) *m/z* calc. for $C_{29}H_{48}ClSO_2Si_2$ $[M+H]^+$: 551.2597. Found: 551.2613.

1-(2,6-Bis((triisopropylsilyl)ethynyl)phenyl)-N,N-dimethylmethanamine (**11h**)



General procedure at 90 ºC starting from *N*,*N*-dimethyl-1-phenylmethanamine **xx** (27.0 mg, 0.2 mmol) and 1-Bromo-2-(triisopropylsilyl)acetylene (**10h**) (110 mg, 0.42 mmol, 2.1 equiv). Yellow liquid (50 mg, 0.10 mmol, 50 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 7.7 Hz, 2H), 7.15 (t, *J* = 7.7 Hz, 1H), 3.83 (s, 2H), 2.33 (s, 6H), 1.14 (s, 42H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 142.57, 133.33, 126.74, 125.12, 105.46, 94.84, 59.44, 45.85, 18.72, 11.39. **HRMS** (ESI+) *m/z* calc. for $C_{31}H_{54}NSi_2$ $[M+H]^+$: 496.3789. Found: 496.3809.

Tert-butyl 2,5-bis((triisopropylsilyl)ethynyl)-1H-pyrrole-1-carboxylate (**11i**)



General procedure starting from *tert*-butyl 1*H*-pyrrole-1-carboxylate (**10i**) (33.4 mg, 0.2 mmol) using 1-Bromo-2-(triisopropylsilyl)acetylene (**1**) (110 mg, 0.42 mmol) at 45 ºC. Yellow liquid (70 mg, 66 % yield). **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 6.45 (s, 2H), 1.62 (s, 9H), 1.12 (m, 42H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 147.58, 119.83, 116.67, 97.91, 96.20, 84.85, 27.84, 18.63, 11.36. **HRMS** (ESI+) *m/z* calc. for $C_{31}H_{53}NaNO_2Si_2$ $[M+Na]^+$: 550.3507. Found: 550.3513.

5) Mechanistic Studies

5.1 - Intermolecular Kinetic Isotope Effects

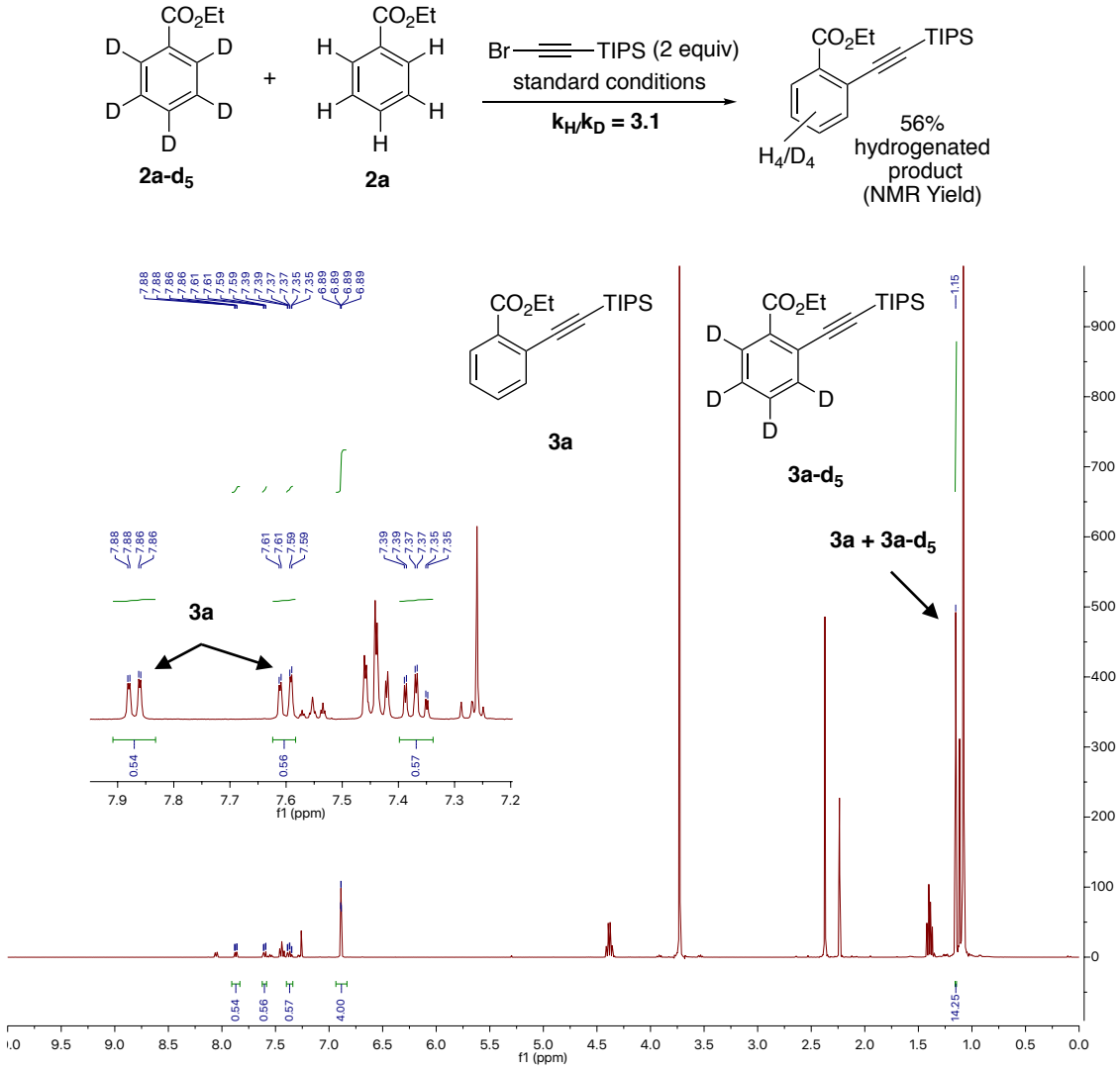


Figure S5.1.1 - ^{1}H NMR of crude reaction

$(RhCp^*Cl_2)_2$, $AgSbF_6$, LiOAc, Ag_2CO_3, were dissolved in DCE (2 mL) in a 10 mL tube. Benzoic esters **2a** (0.2 mmol) and **2a-d$_5$** (0.2 mmol) and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (0.4 mmol) were then added with a Hamilton syringe and the reaction mixture was stirred 45 ºC for 16 h. After cooling at ambient temperature, bromomesitylene (2 equiv) was added as internal standard through an Hamilton syringe and the crude mixture was filtrated in a pipette through a short plug of silica and washed with DCM. After filtration, the solvents were removed under vacuum. The yield of the mono-alkynylated product was determined by ^{1}H NMR analysis of the crude using bromomesitylene as internal standard. The residue was purified by silica gel chromatography column with Toluene 100% as eluent to yield the corresponding mono alkynylated products (**3a**+**3a-d$_5$**) KIE value (3.1) was determined by the ratio of desired products.

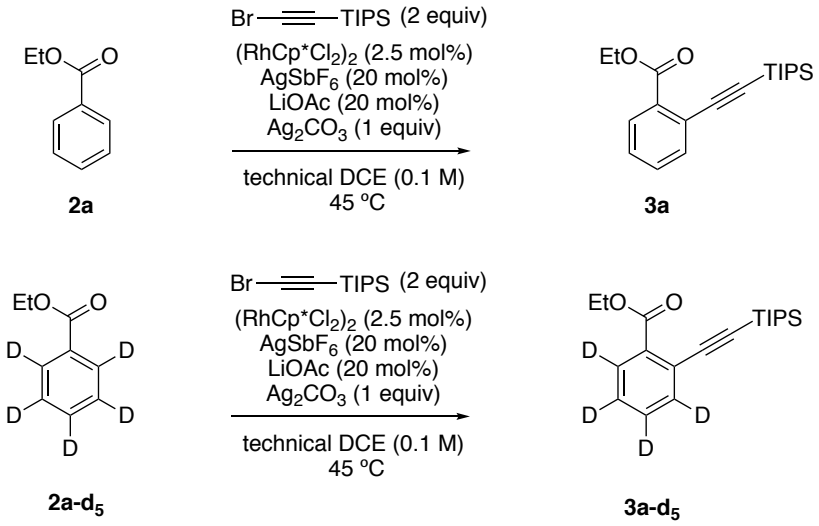


Figure S5.2 - Parallel Kinetic Isotope Effects

$(RhCp^*Cl_2)_2$, $AgSbF_6$, LiOAc, Ag_2CO_3, were dissolved in DCE (2 mL) in a 10 mL tube. Benzoic esters (**2a** or **2a-d$_5$**) (0.15 mmol) and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (0.3 mmol) were then added with a Hamilton syringe and the reaction mixture was stirred 45 ºC for the indicated time : 30 min, 1 h, 2 h, 3 h or 5 h (five parallel runs). After cooling at ambient temperature, bromomesitylene (1 equiv) was added as internal standard through an Hamilton syringe and the crude mixture was filtrated in a pipette through a short plug of silica and washed with DCM. After filtration, the solvents were removed under vacuum. The yield of the mono-alkynylated product was determined by ^{1}H NMR analysis of the crude using bromomesitylene as internal standard. For **2a**, y = 5.8281x+10.195, R^2=0.94271, for **2a-d$_5$**, y=1.9x+2.55, R^2=0.93109. KIE value (3.1) was determined by comparing the relative initial rates.

Time (h)	NMR Yield **3a** (%)	NMR Yield **3a-d$_5$** (%)
0.5	12	2.4
1	14	5
2	24	6.5
3	31	9.4
5	37	11.3

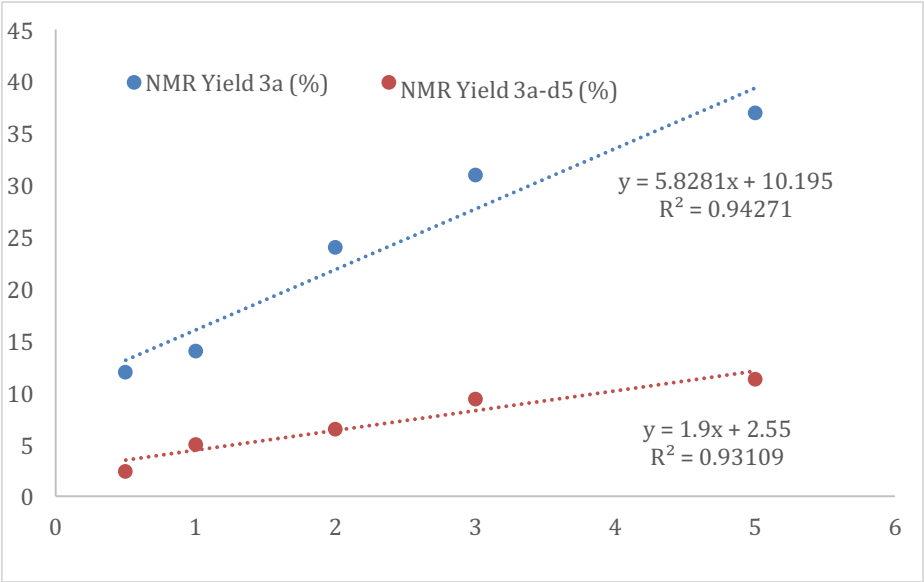
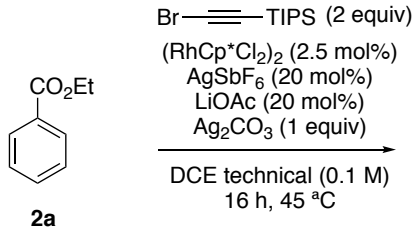
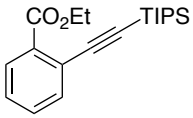


Figure S5.2.1- Initial rate data for the formation of 3a and 3a-d_5

5.3 - Reaction in the presence of a radical scavenger



Br—≡—TIPS (2 equiv)
$(RhCp^*Cl_2)_2$ (2.5 mol%)
$AgSbF_6$ (20 mol%)
LiOAc (20 mol%)
Ag_2CO_3 (1 equiv)
DCE technical (0.1 M)
16 h, 45 °C



radical scavenger	yield
none	56-58%[a]
TEMPO (1 equiv.)	3%[b]
BHT (1 equiv.)	1%[b]

[a] Isolated Yield [b] NMR Yield determined using bromomesitylene as internal standard

The inhibition of the reaction in presence of a radical scavenger as TEMPO or BHT doesn't allow us to conclude about the possible intervention of a radical intermediate. Indeed, TEMPO and BHT could inhibit the activity of the catalyst through for example coordination. In order to check this last hypothesis, a mixture of Rhodium catalyst in presence of BHT under standard conditions was analyzed by ^{1}H NMR after 16 h at 45 ºC. The ^{1}H NMR clearly showed major changes in both catalyst and BHT ^{1}H NMR. Concerning the chemical shifts of the BHT substrate: the singlet of H_a protons is shifted to 6.98 ppm to 6.08 ppm in presence of the catalyst and OH peak disappears. For the Rhodium catalyst, we can also notice a shift of the cyclopentadienyl proton peak from 1.61 ppm to 2.02 ppm. These significant NMR shifts could suggest that the catalyst interact directly with the BHT in order to form a new complex, through the hydroxyle function, which could also inhibit the reaction.

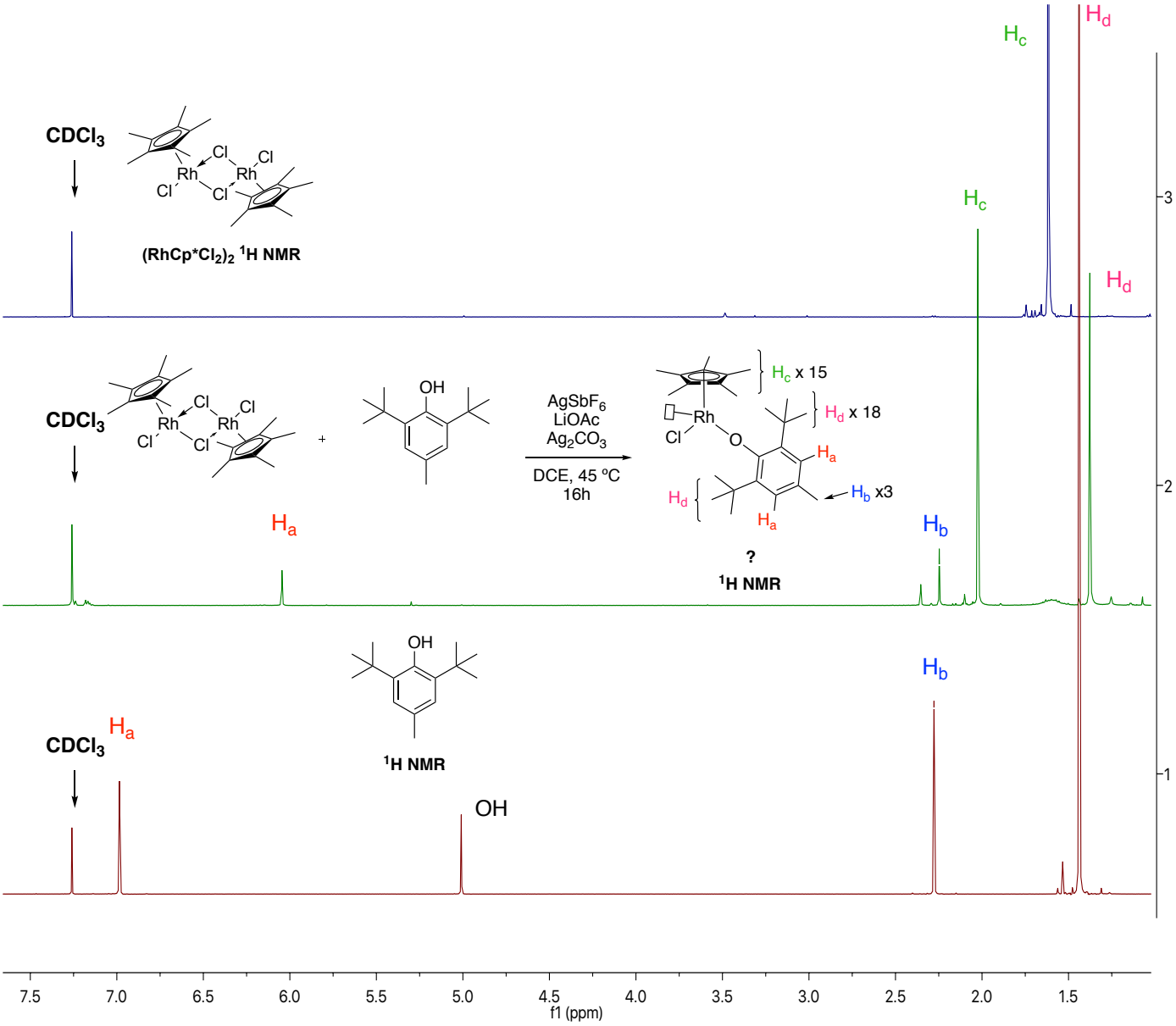
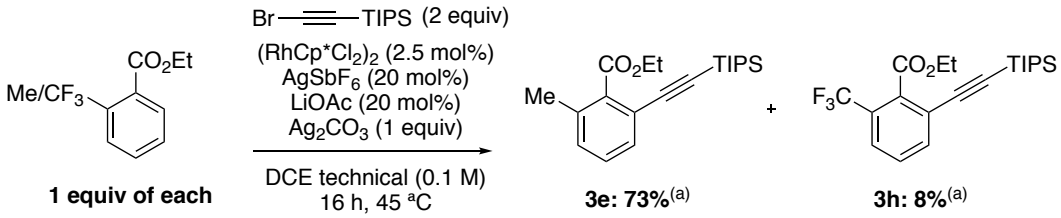


Figure S5.3.1 - Comparison of the ^{1}H NMR of $(RhCpCl_2)_2$, BHT and the mixture of both

5.4 - Competition experiments



(a) NMR Yield determined using bromomesitylene as internal standard

$(RhCp^*Cl_2)_2$, $AgSbF_6$, LiOAc, Ag_2CO_3, were dissolved in DCE (2 mL) in a 10 mL tube. ethyl 2-methylbenzoate (**2e**) (32.8 mg, 31.8 µL, 0.2 mmol, 1 equiv), ethyl 2-(trifluoromethyl)benzoate (**2h**) (43.6 mg, 39.3 µL, 0.2 mmol, 1 equiv) and 1-bromo-2-(triisopropylsilyl)acetylene (**1**) (105 mg, 90 µL, 0.40 mmol, 2 equiv) were then added with a Hamilton syringe and the reaction mixture was stirred 45 ºC for 16 h. After cooling at ambient temperature, bromomesitylene (1 equiv) was added as internal standard through an Hamilton syringe and the crude mixture was filtrated in a pipette through a short plug of silica and washed with DCM. After filtration, the solvents were removed under vacuum. The yield of each mono-alkynylated product (**3e** and **3 h**) was determined by ^{1}H NMR analysis of the crude using bromomesitylene as internal standard (Figure S5.4.1).

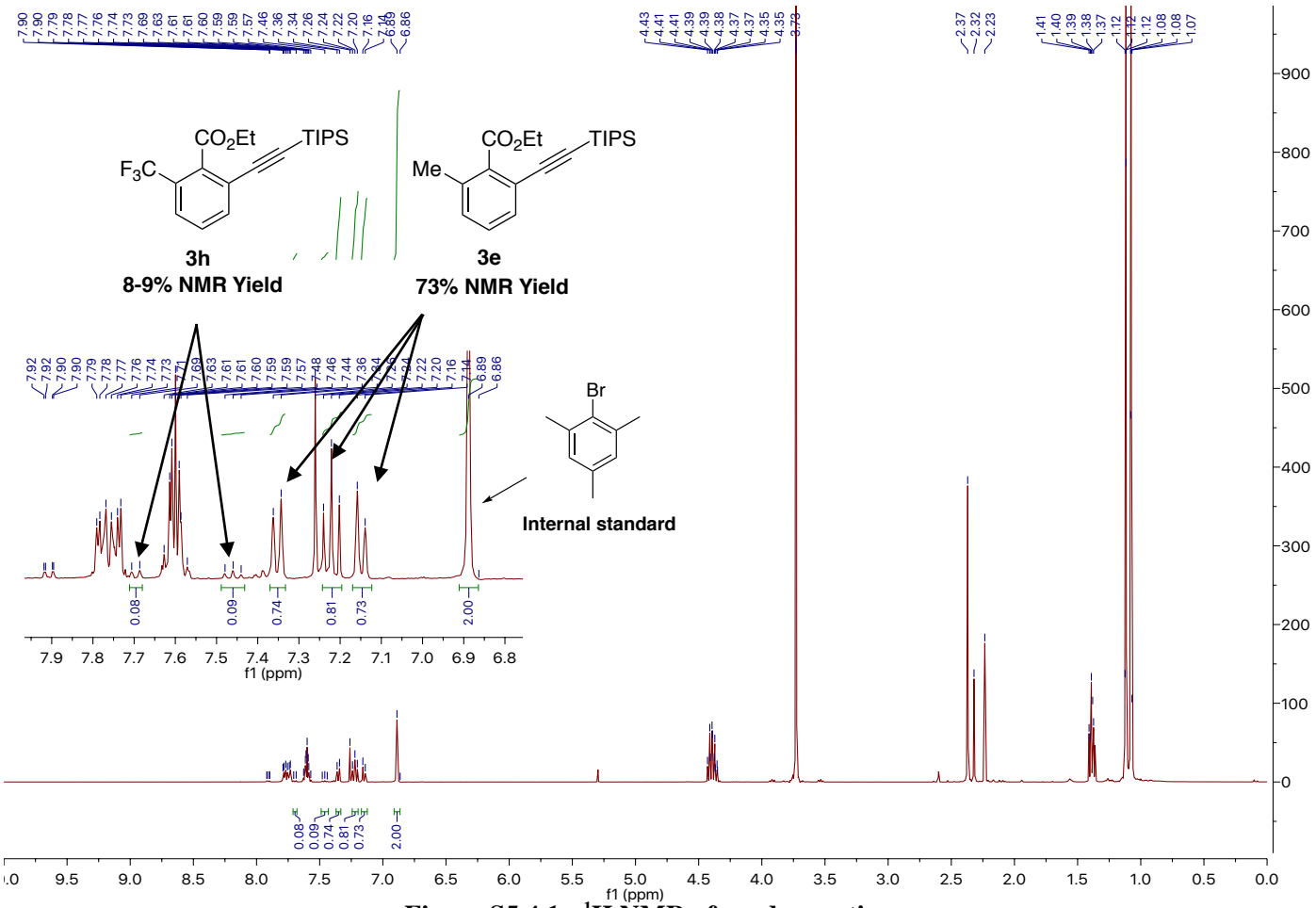
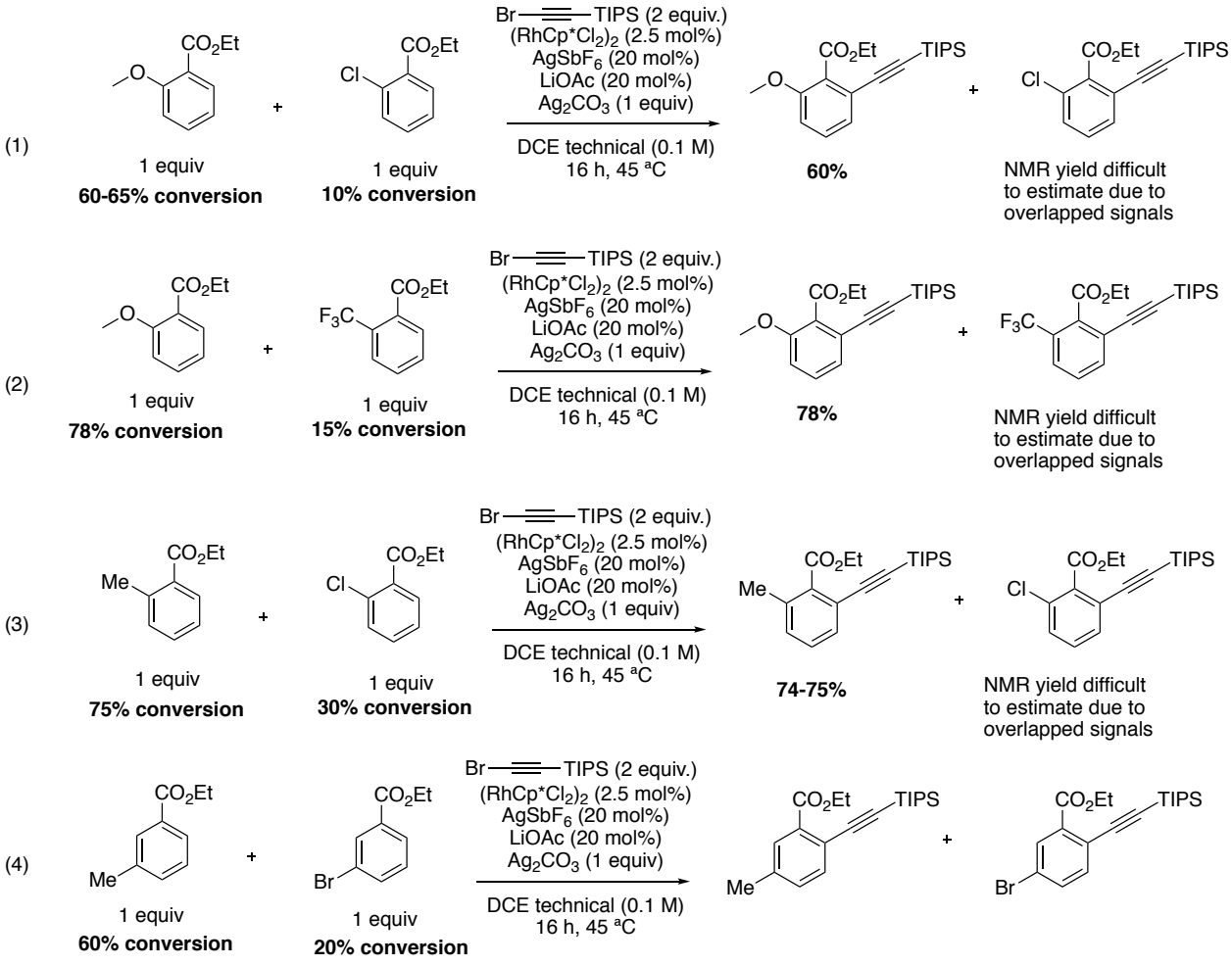


Figure S5.4.1 - ^{1}H NMR of crude reaction

Other competition experiments:



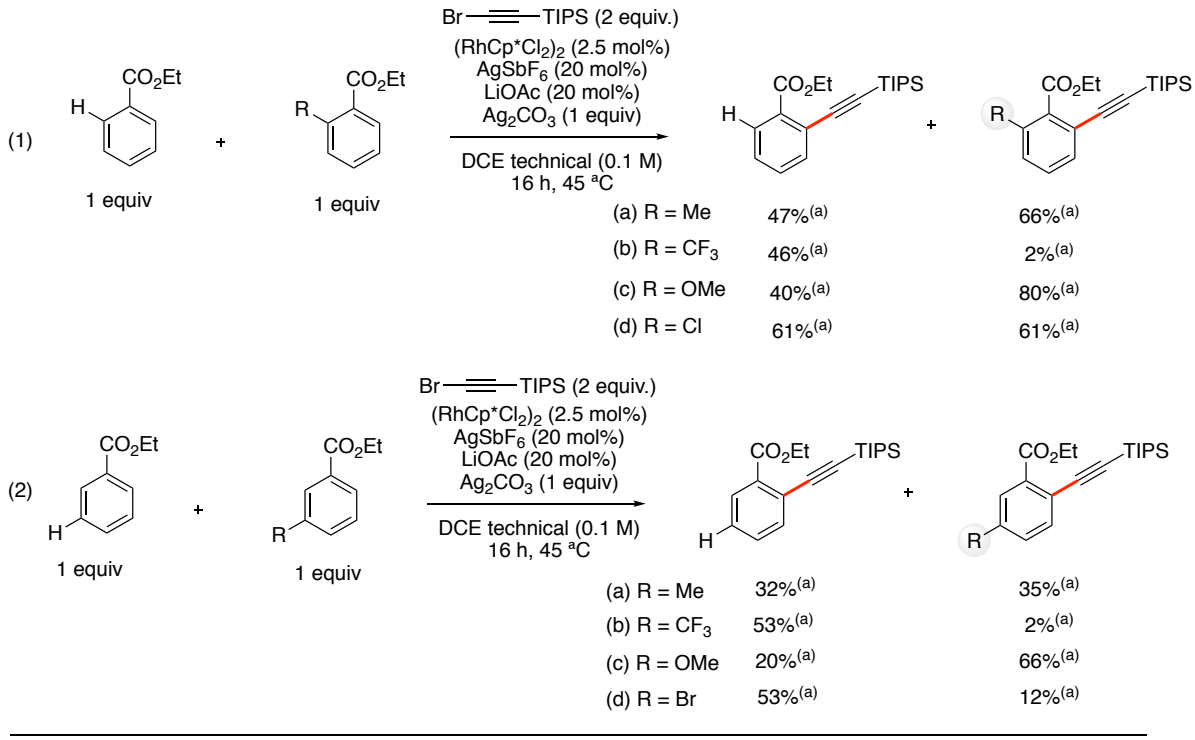
Conversion and NMR Yield were determined using bromomesitylene as internal standard in the crude mixture

Scheme S5.4.1 - Competition experiments

The intermolecular competition between electron rich and electron poor substrates suggests that substrates bearing electrodonating group in *meta* position of the CH functionalization site are more reactive. This result could indicate that the CH-activation step might occur through an electrophilic type mechanism.

In order to check that there is no steric bias when using *ortho* substituted ester, meta substituted were also used (Scheme S5.4.1, eq. 4) with weak activating or deactivating functional group still show the same tendency as previous experiments.

5.5 - Hammett Plot



(a)NMR Yield were determined using bromomesitylene as internal standard in the crude mixture

Scheme S5.5.1 - Hammett plot experiments: determination of k/k_0

The product ratios (k/k_0) were correlated with σ-values (σ_m^+, σ_p^+ or σ_p) to ascertain the existence of any linear free energy relationships.

$R_{(meta)}$	k/k_0	$\log(k/k_0)$	σ_m^+
Me	1.40	0.146	-0.07
CF_3	0.04	-1.39	0.43
OMe	2	0.3	0.12
Cl	1	0	0.37

$R_{(para)}$	k/k_0	$\log(k/k_0)$	σ_p^+	σ_p
Me	1.10	0.041	-0.31	-0.27
CF_3	0.04	-1.39	0.61	0.54
OMe	3.3	0.52	-0.78	-0.27
Br	0.23	-0.64	0.15	0.23

A Hammett correlation ($R^2 = 0.99$ using σ_p^+ or $R^2 = 0.98$ using σ_p) (Figures S5.5.1 and S5.5.2 respectively) was validated for substrates bearing substituants in *para* position to the reaction center. A negative ρ value also suggests that electron density is leaving the aromatic system in the product-determining step which is in accordance with an electrophilic mechanism occurring for the C-H activation step.[3]

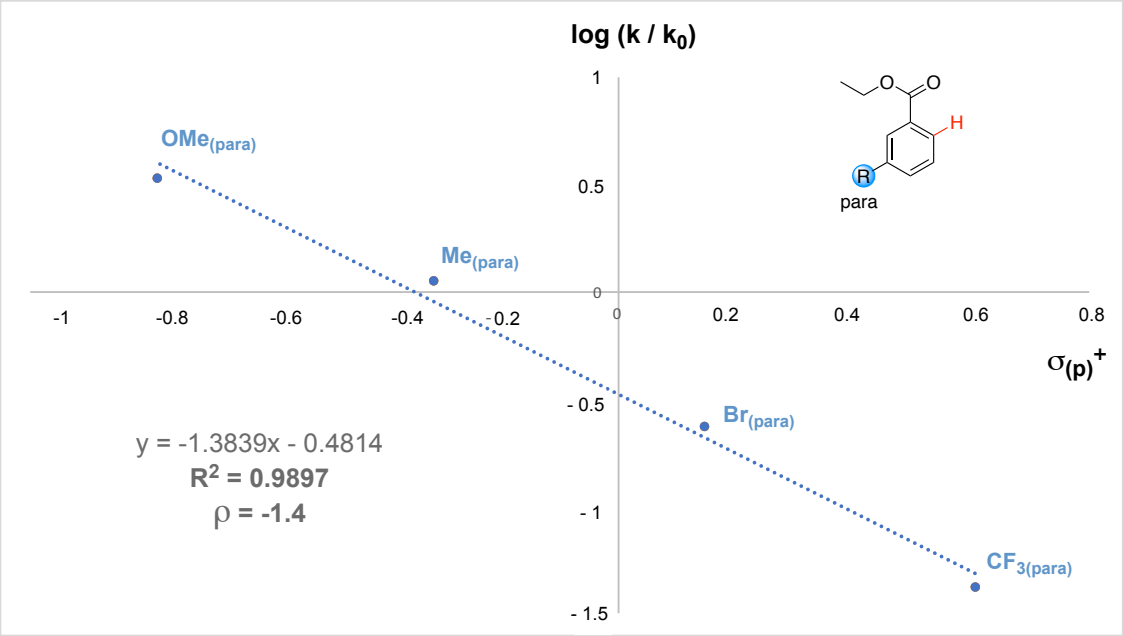


Figure S5.5.1 - Hammett plot using $\sigma_{(p)}^{+}$

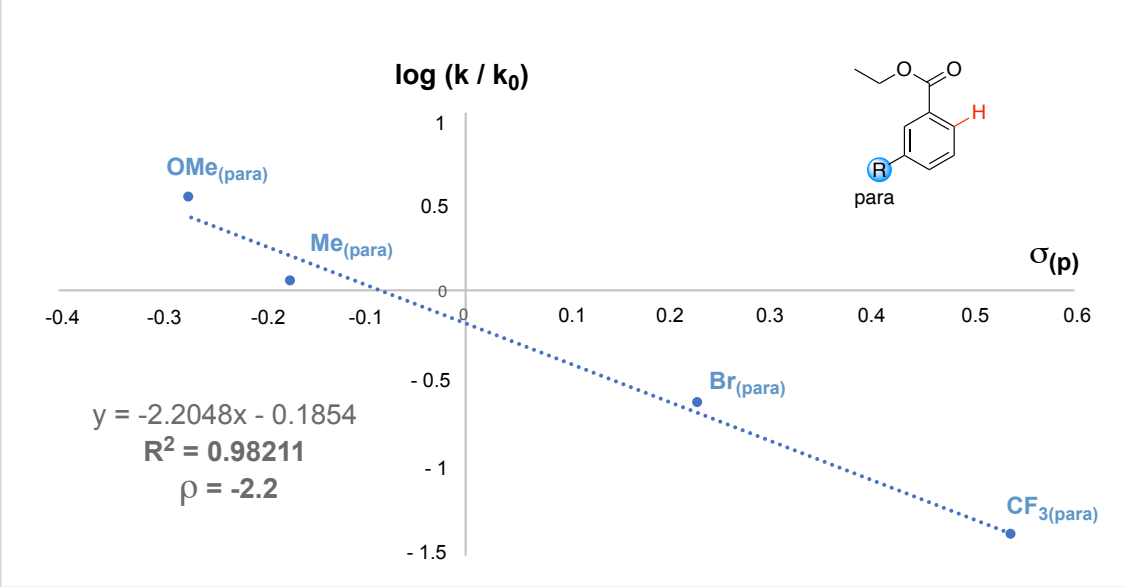


Figure S5.5.2 - Hammett plot using $\sigma_{(p)}$

However, this correlation could not be validated for substrates bearing functional groups in *meta* position to the C-H activation site (Figure S5.5.3).

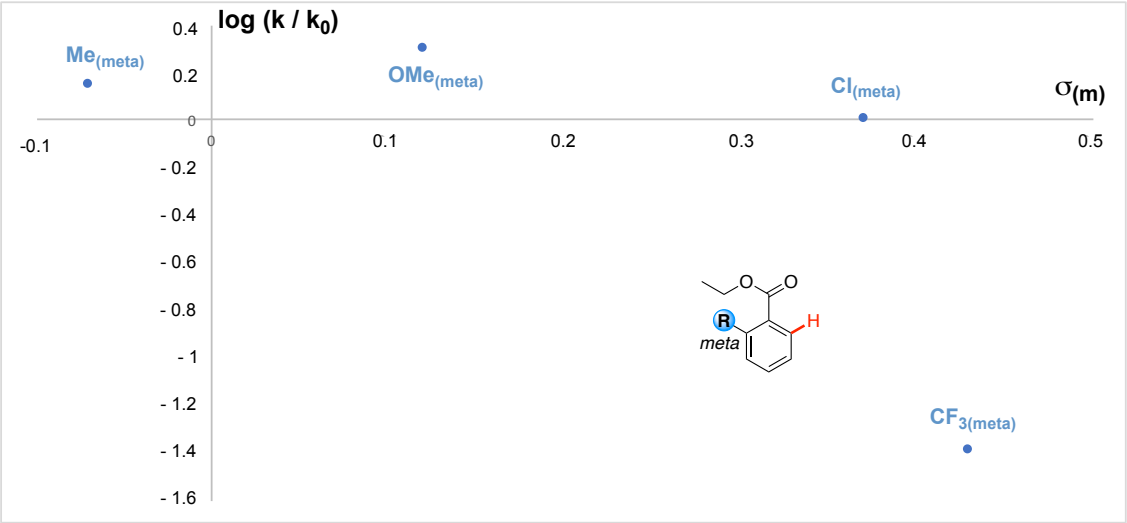


Figure S5.5.3 - Hammett plot using $\sigma_{(m)}$

A plausible explanation could be that, in this case, steric factors could also be involved. To validate this hypothesis a correlation was tested between $\log(k/k_0)$ and different steric parameters (Taft parameters and Charton size values) (Figure S5.5.4).

$R_{(meta)}$	$\log(k/k_0)$	E_s (Taft)	σv (Charton)
Me	0.146	-1.24	0.52
CF_3	-1.39	-2.4	0.91
OMe	0.3	-0.55	0.36
Cl	0	-0.97	0.55

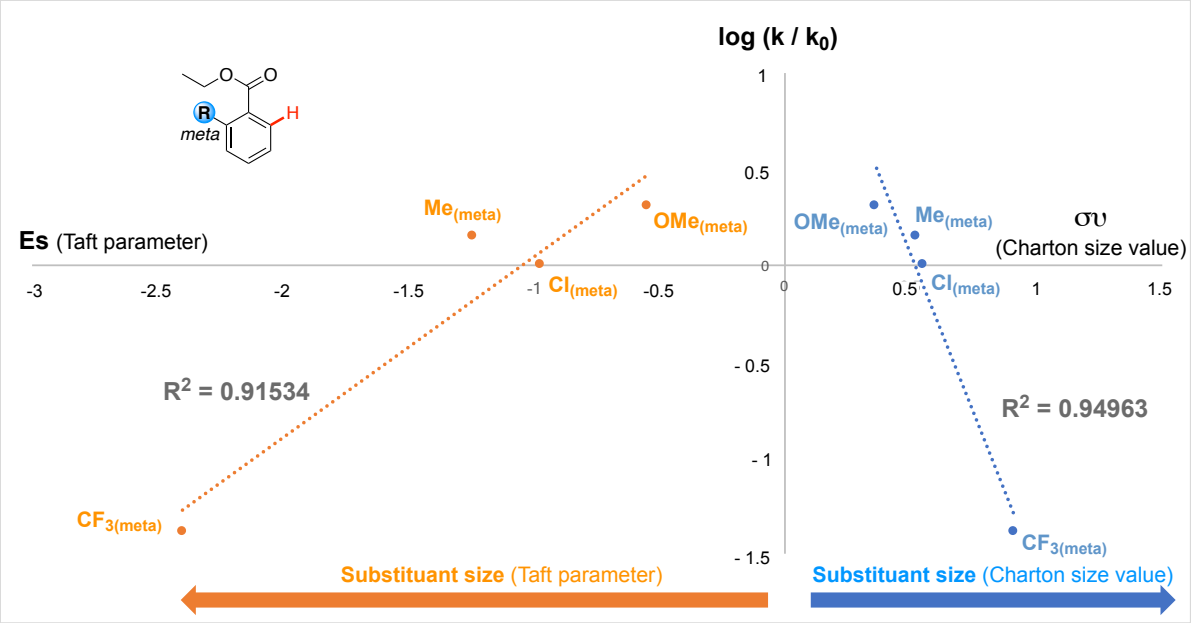
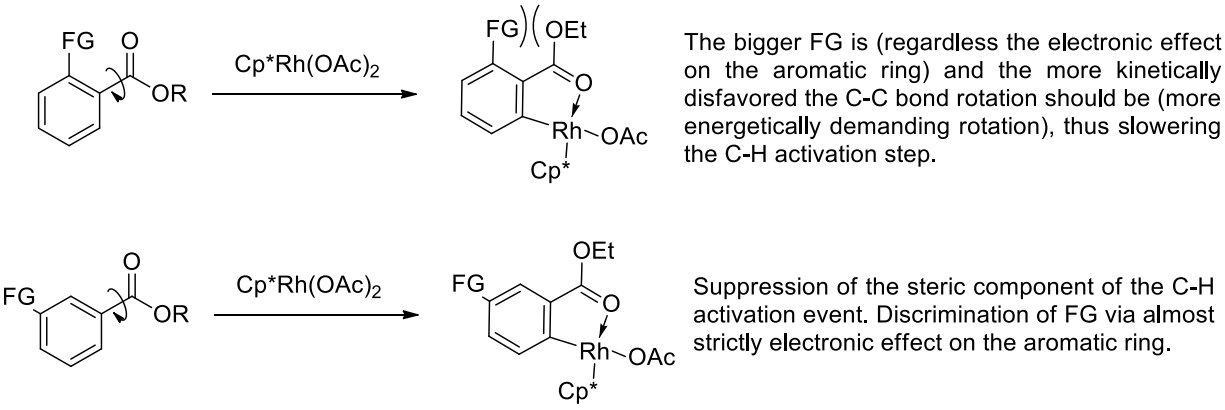


Figure S5.5.4 - Correlation between k/k_0 and substituant size parameter

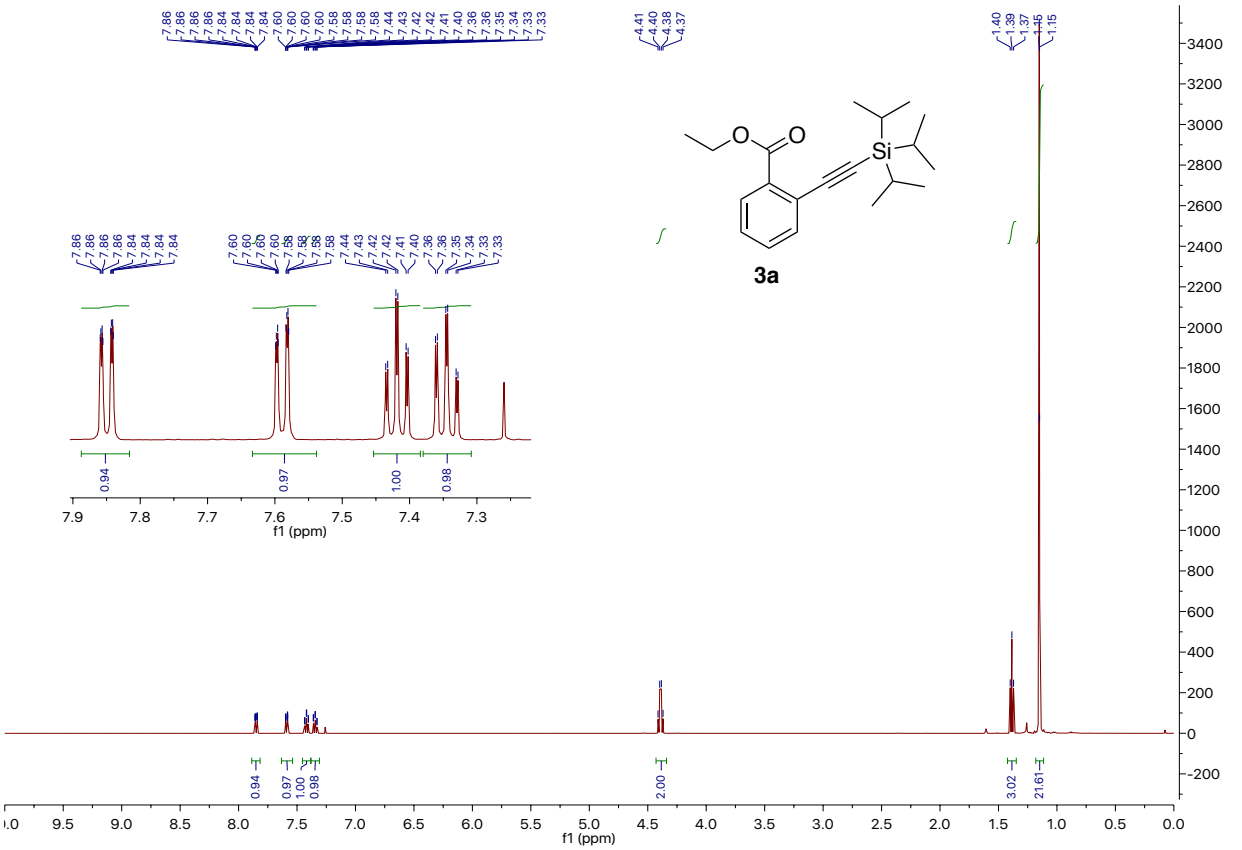
For both steric parameters, a correlation could be found ($R^2 = 0.92$ and $R^2 = 0.95$), which could validate the involvement of a steric bias in the case of substrates bearing functional group in meta position to the C-H activation site (Scheme S5.5.2).

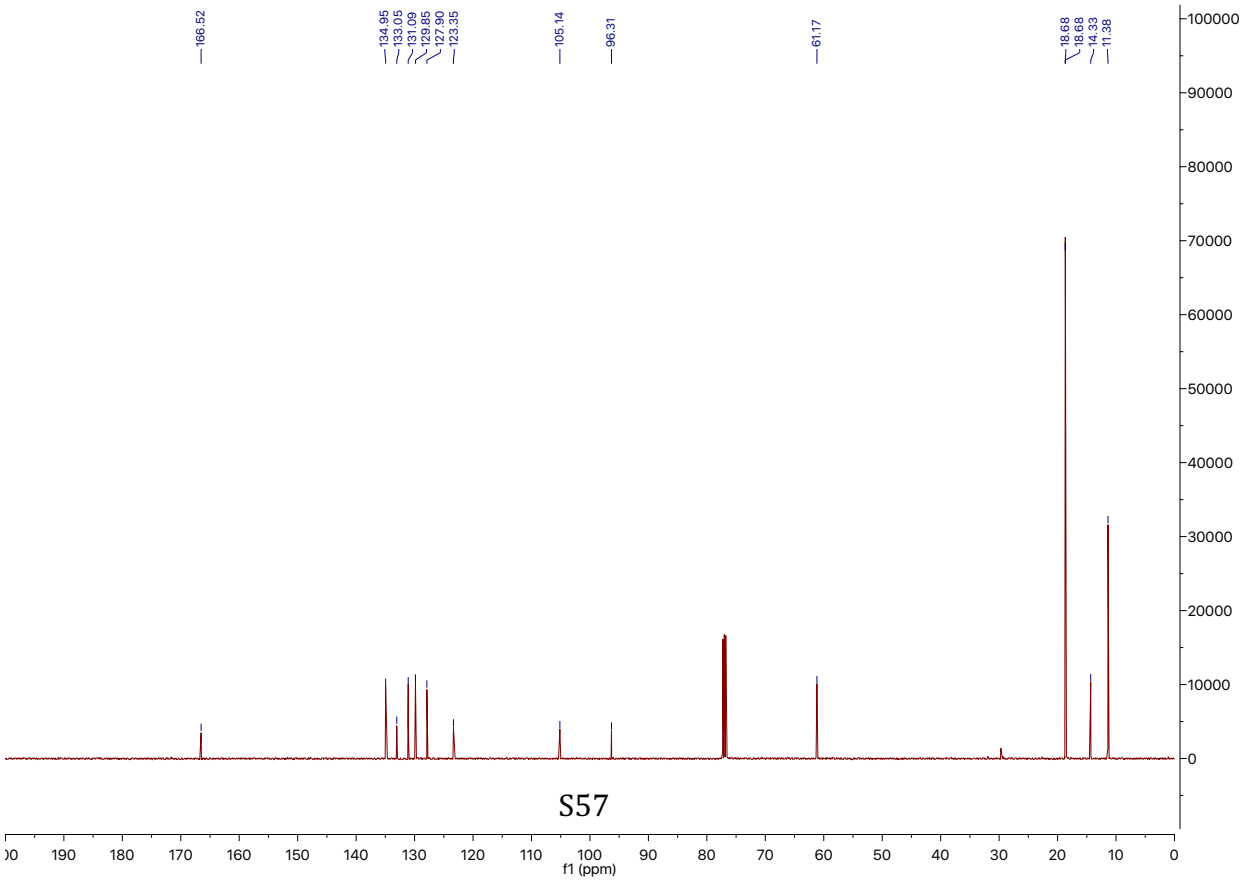


Scheme S5.5.2 - Steric Bias Hypothesis

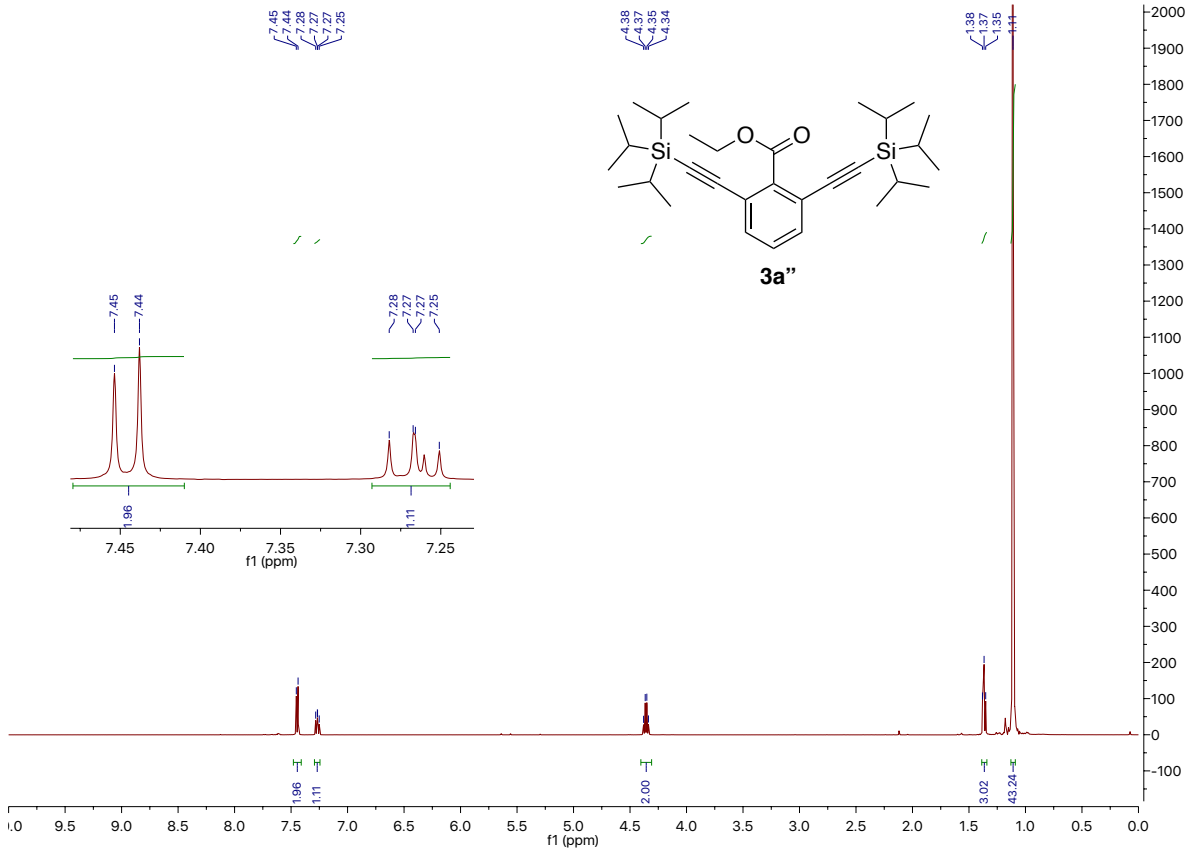
6) ^{1}H and ^{13}C NMR Spectra

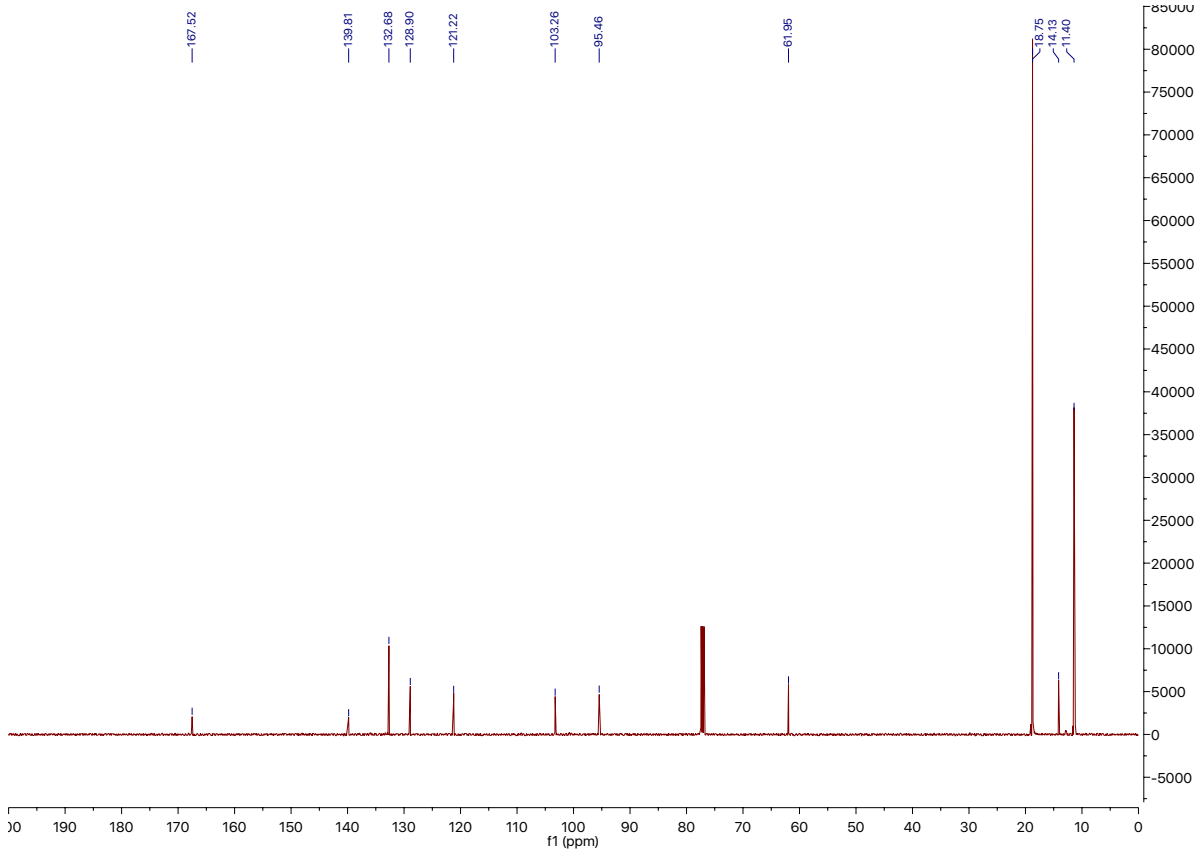
Ethyl 2-((triisopropylsilyl)ethynyl)benzoate **(3a)**



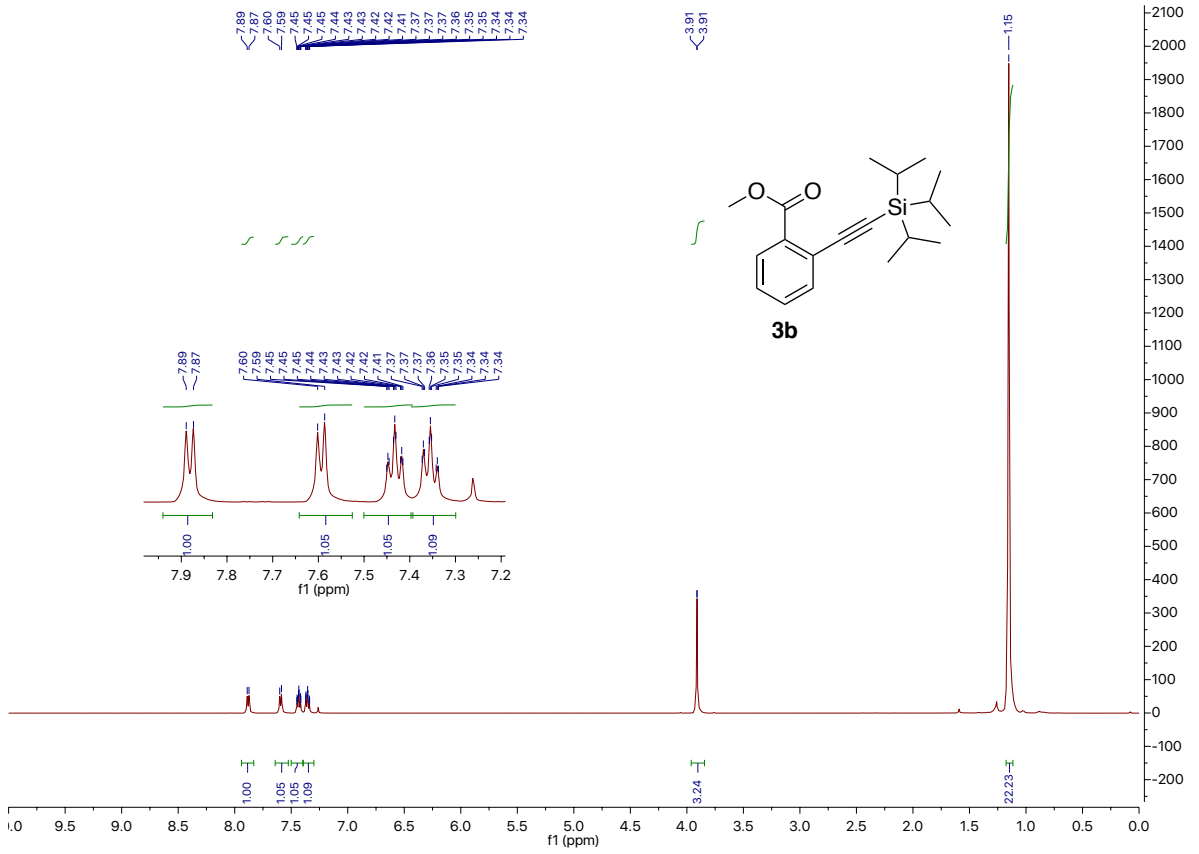


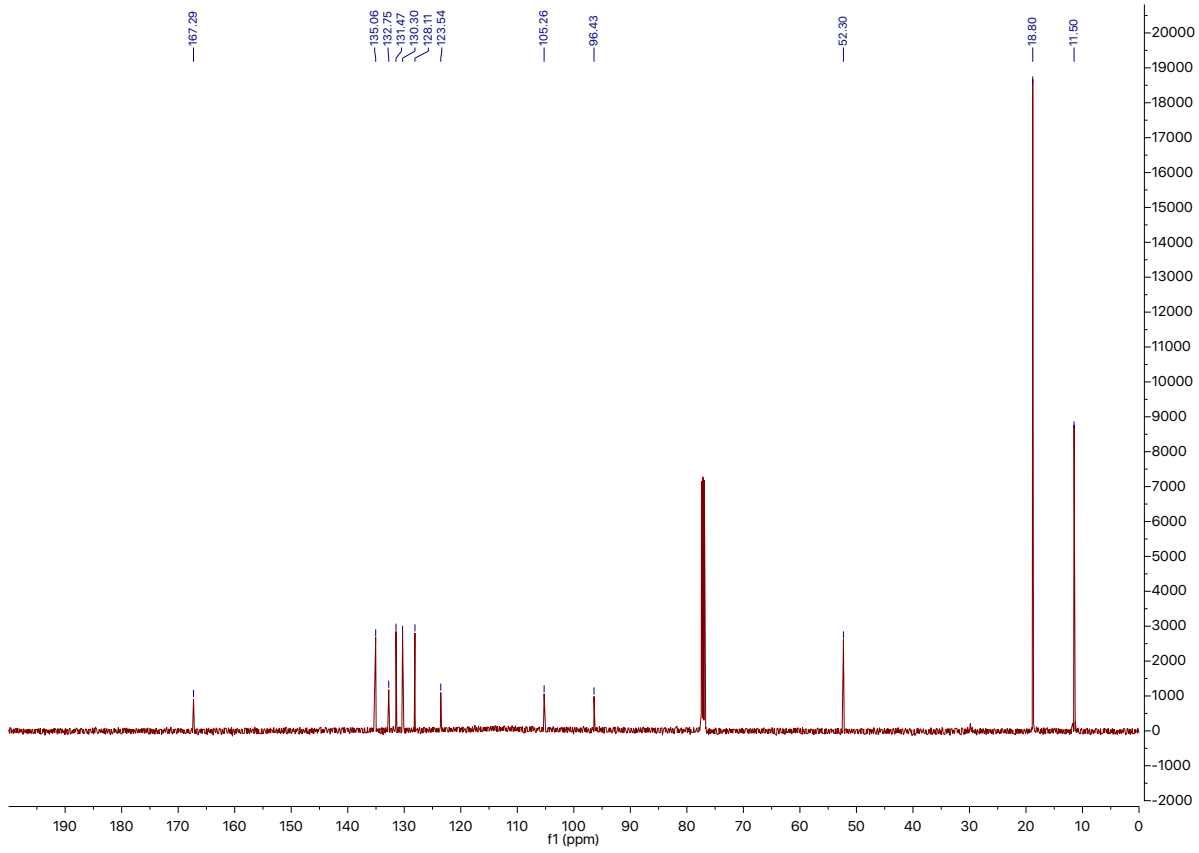
***Ethyl 2,6-bis((triisopropylsilyl)ethynyl)benzoate* (3a")**



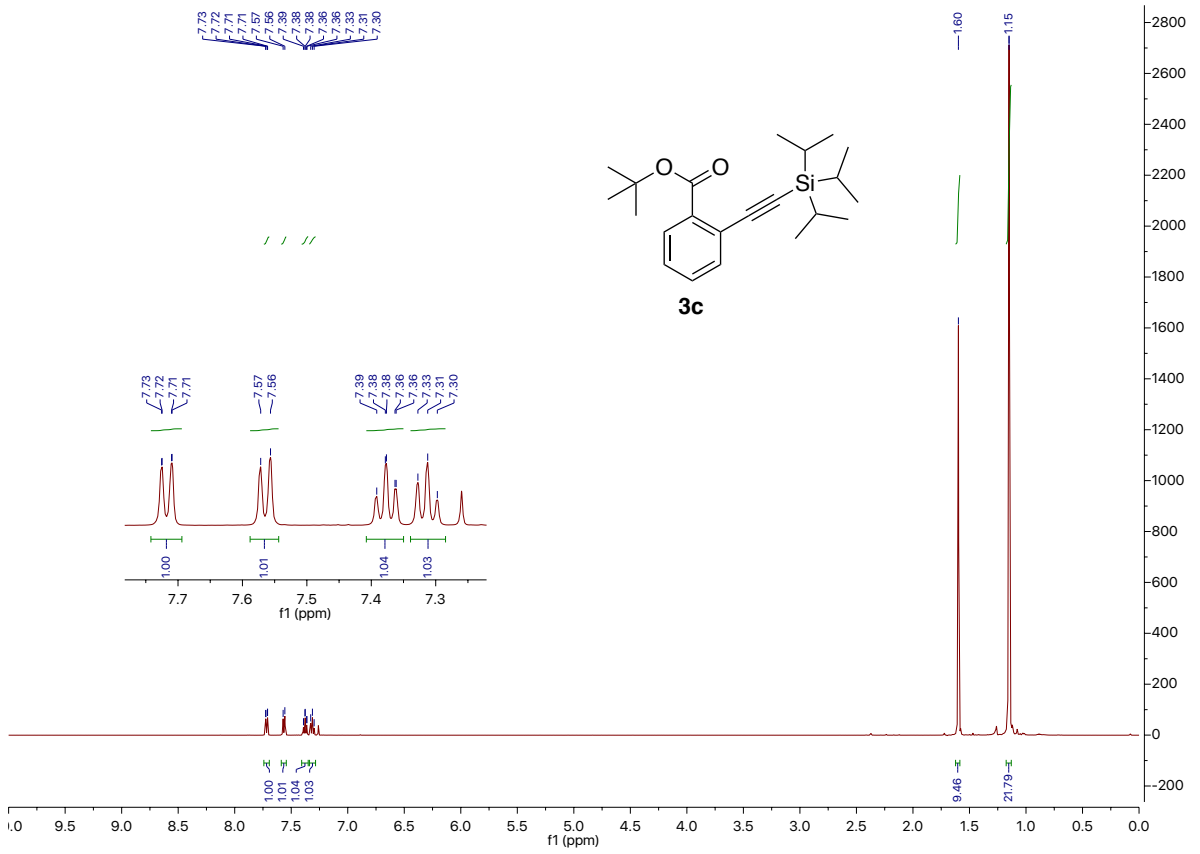


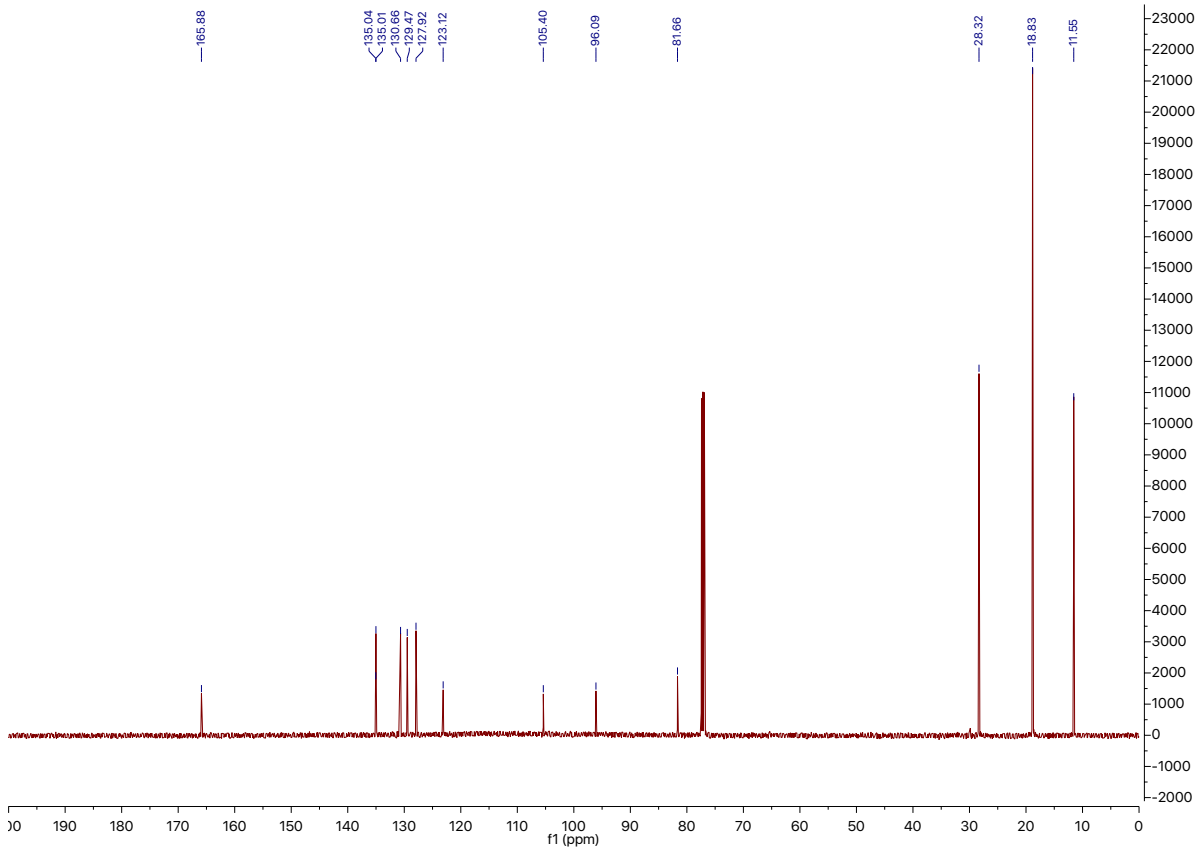
***Methyl 2-((triisopropylsilyl)ethynyl)benzoate* (3b)**



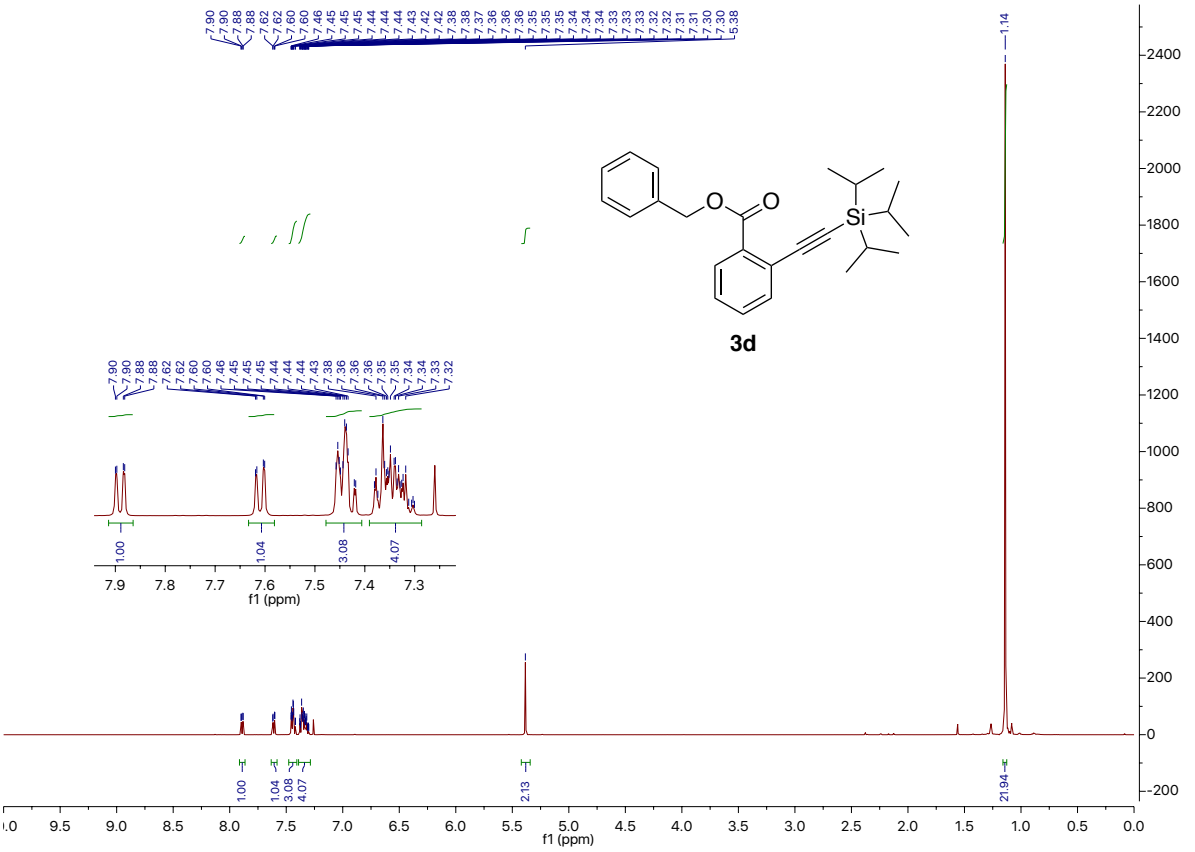


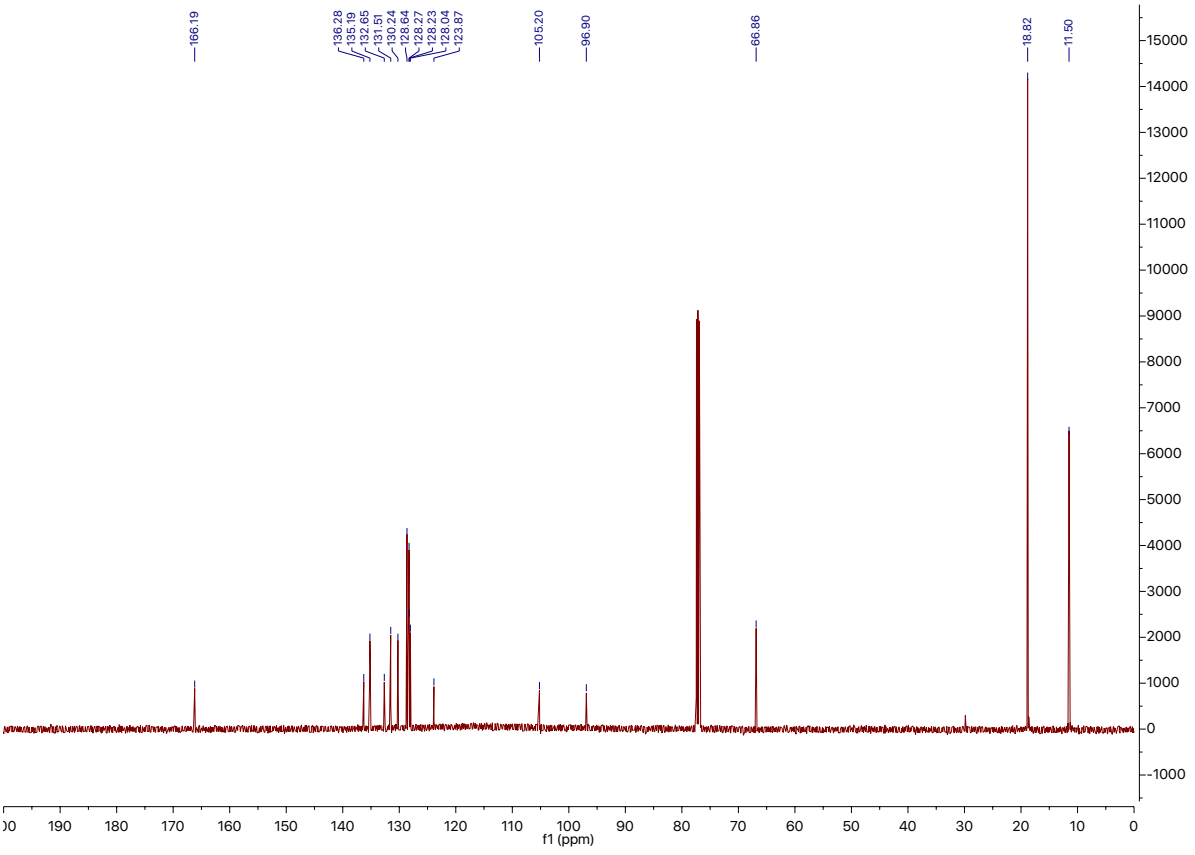
***Tert-butyl 2-((triisopropylsilyl)ethynyl)benzoate* (3c)**



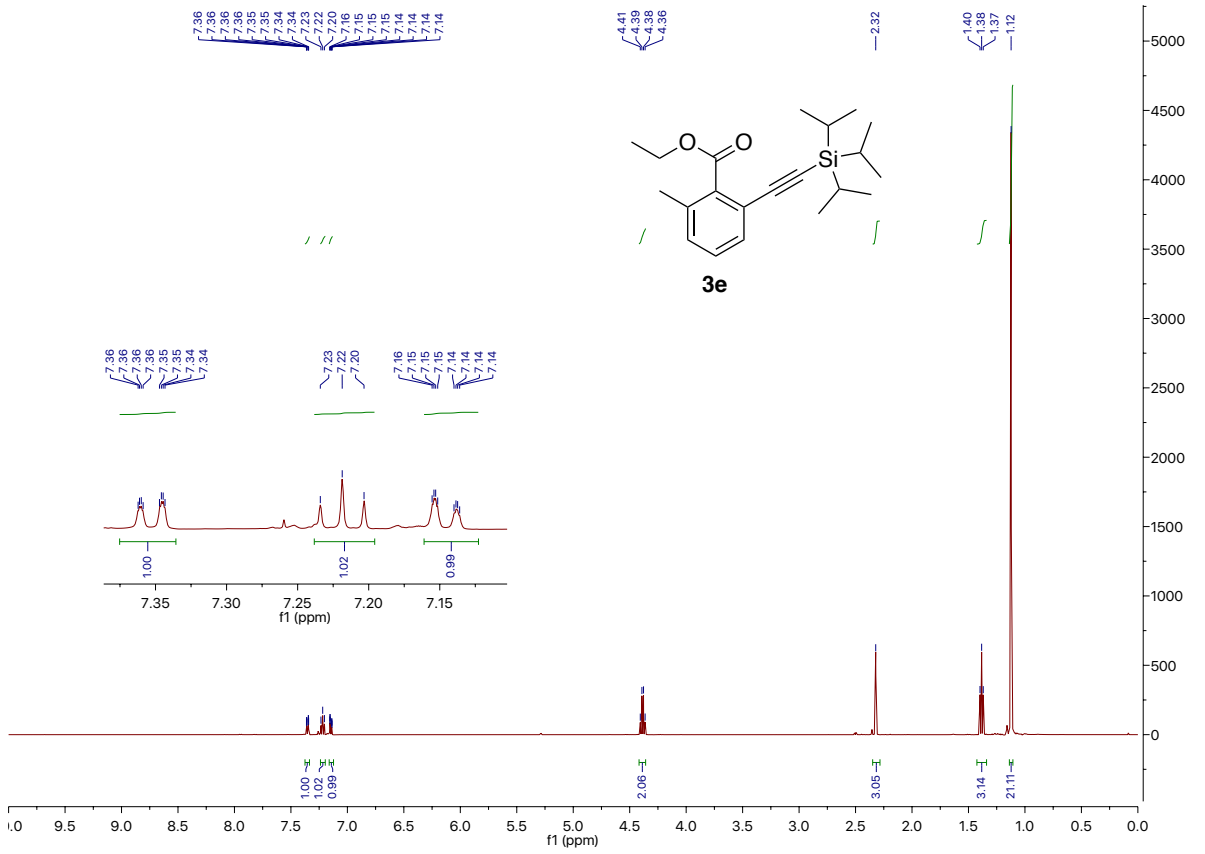


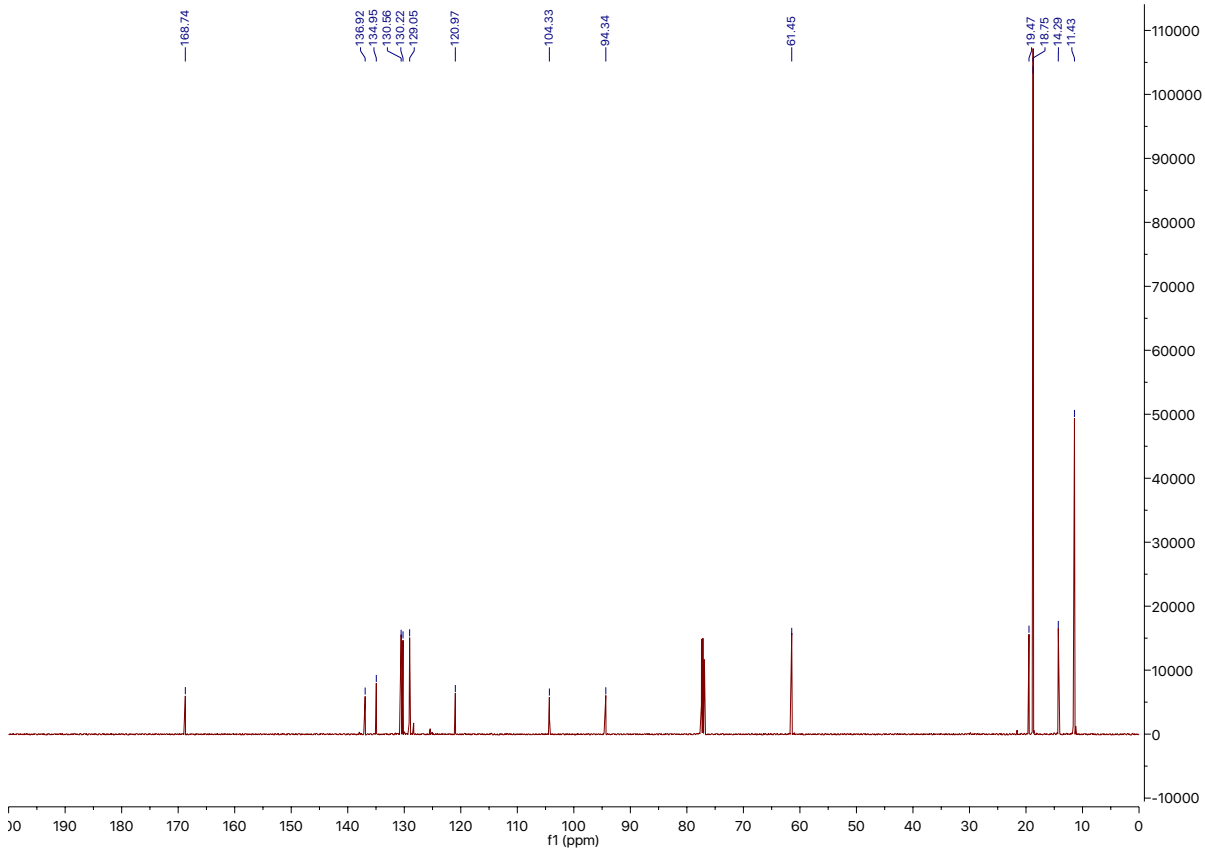
***Benzyl 2-((triisopropylsilyl)ethynyl)benzoate* (3d)**



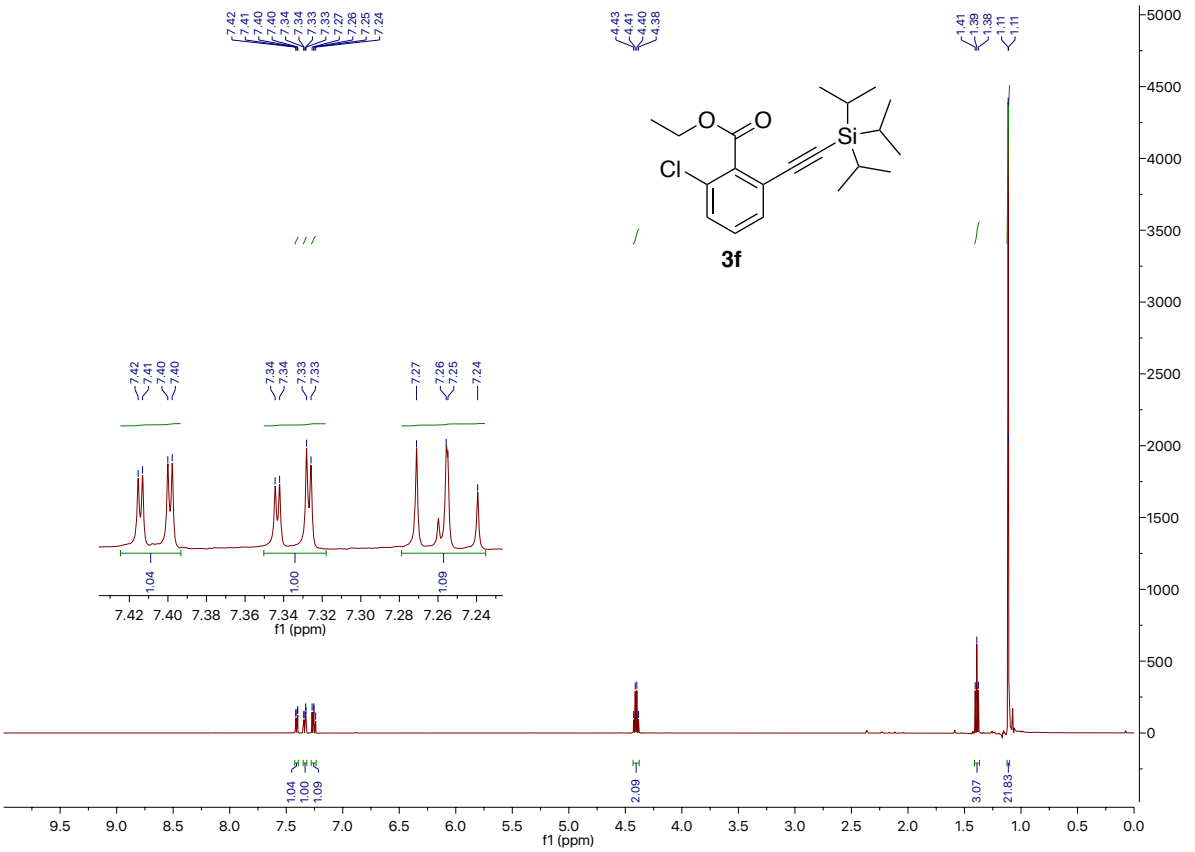


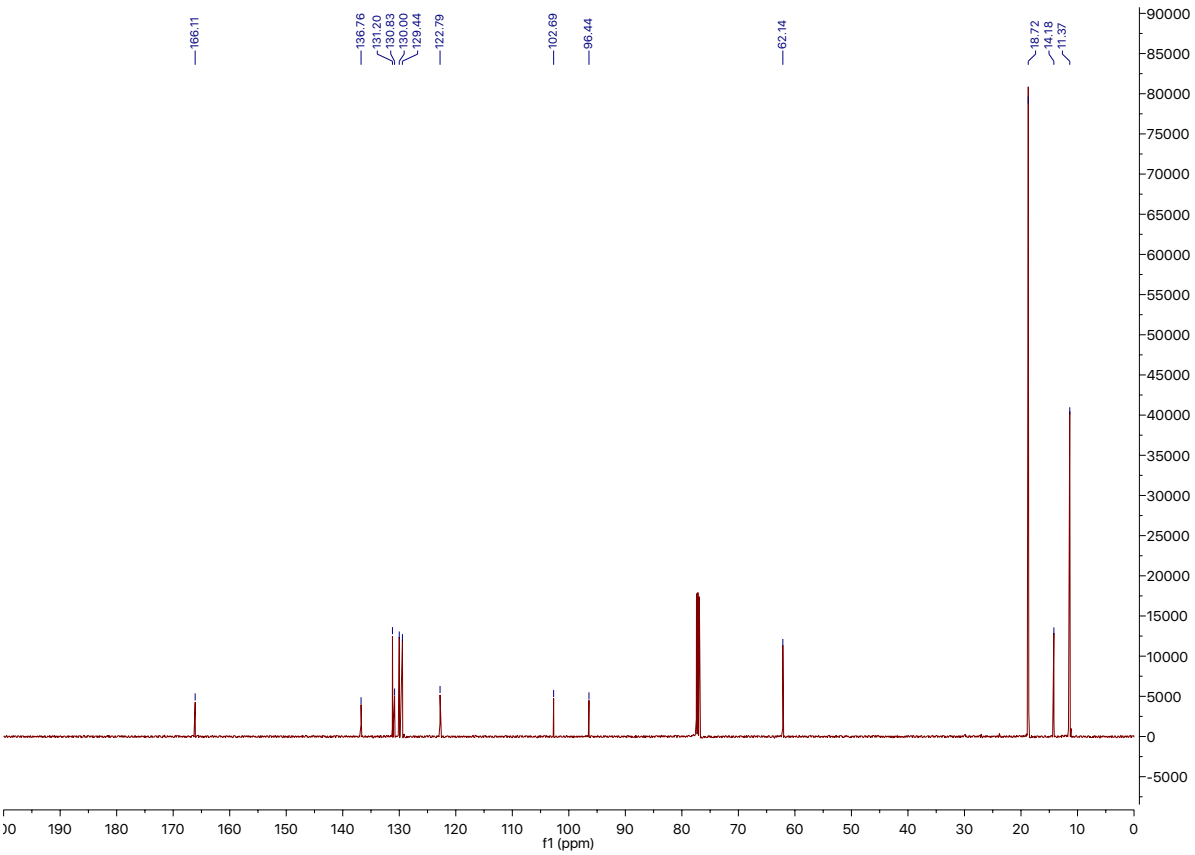
***Ethyl 2-methyl-6-((triisopropylsilyl)ethynyl)benzoate* (3e)**



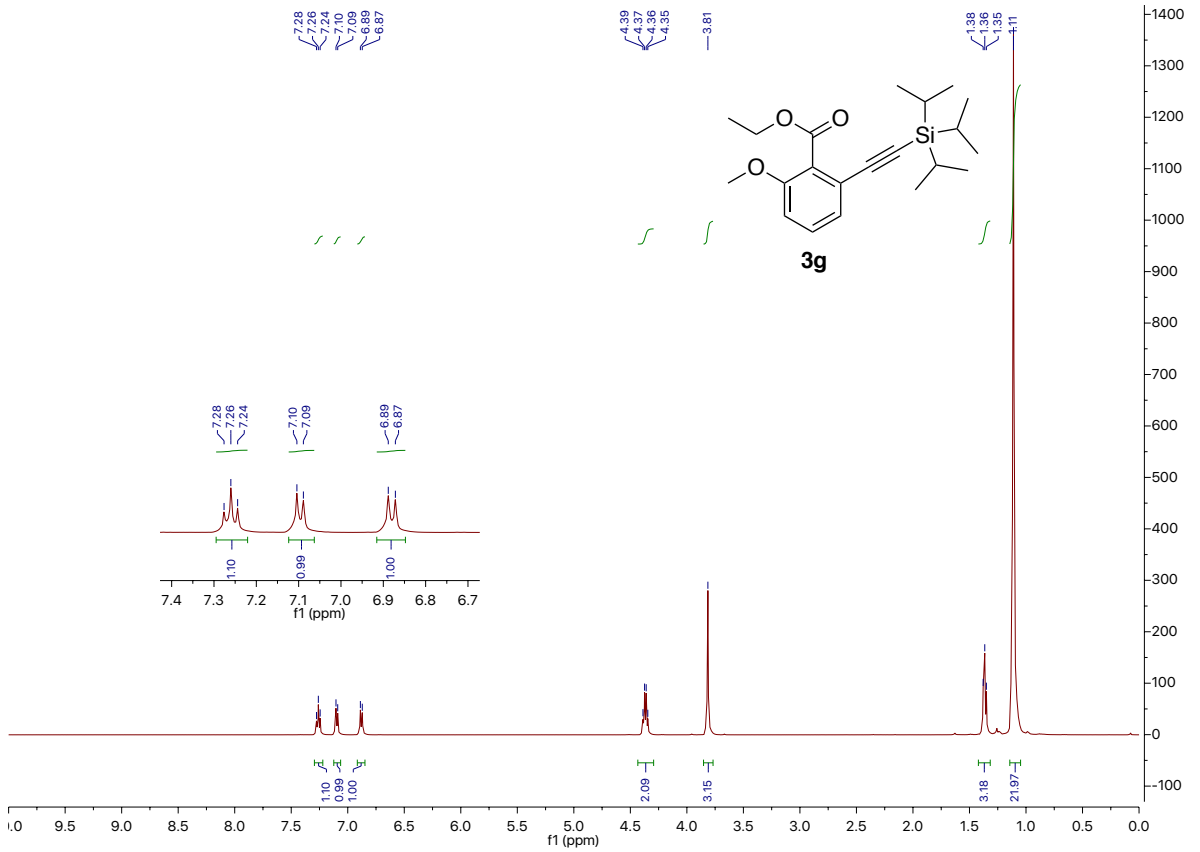


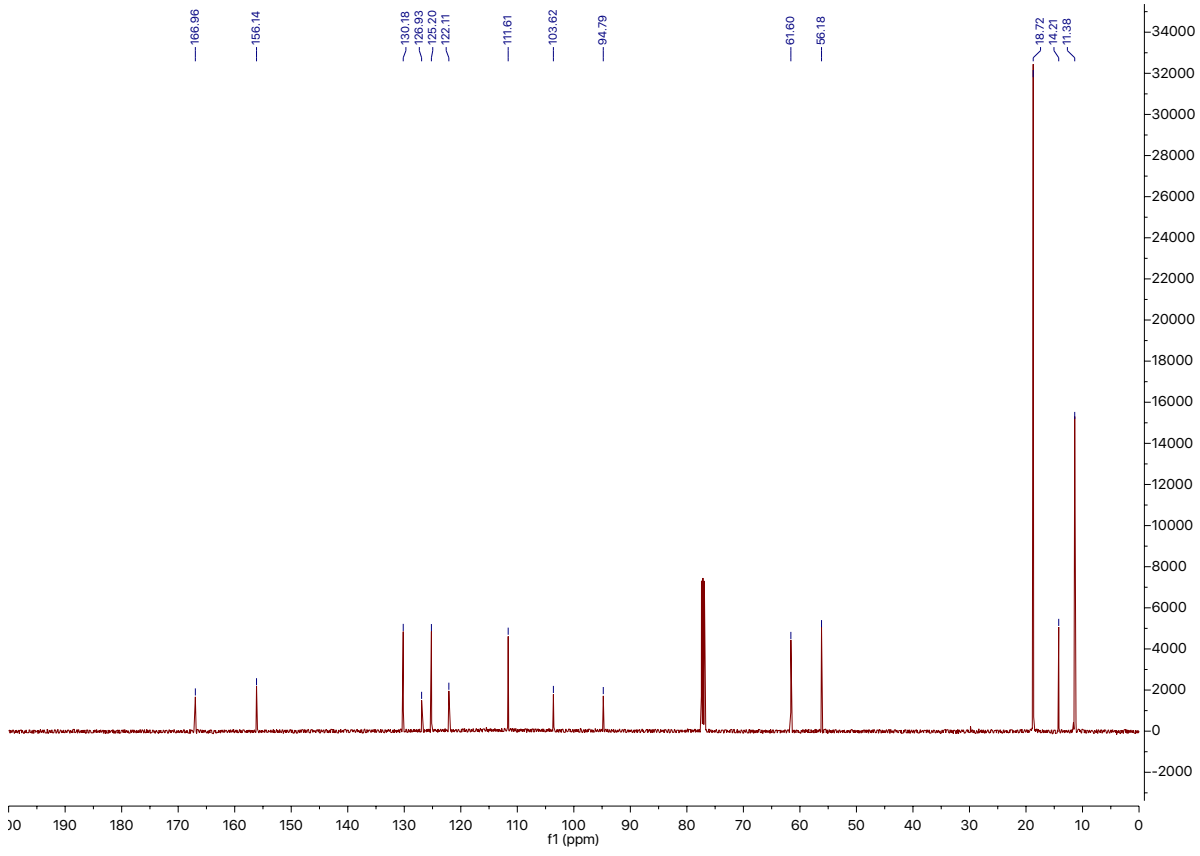
***Ethyl 2-chloro-6-((triisopropylsilyl)ethynyl)benzoate* (3f)**



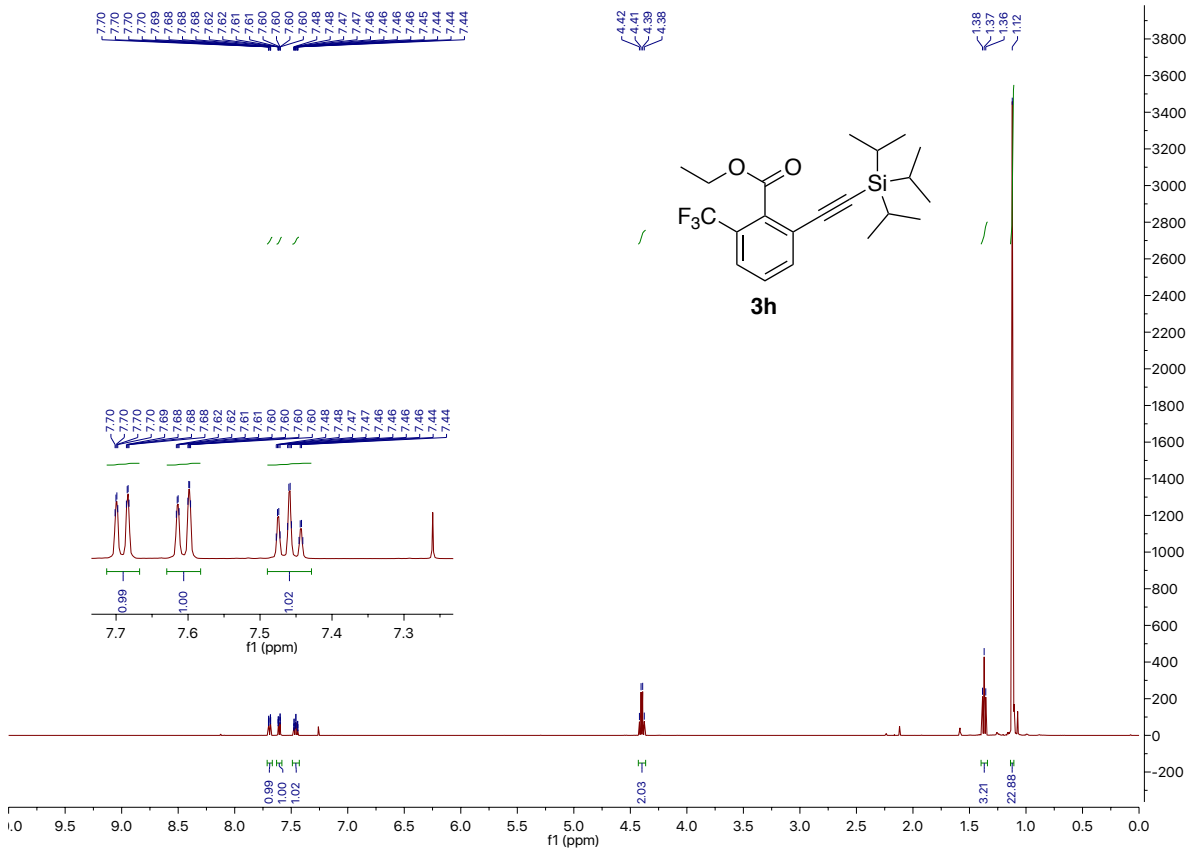


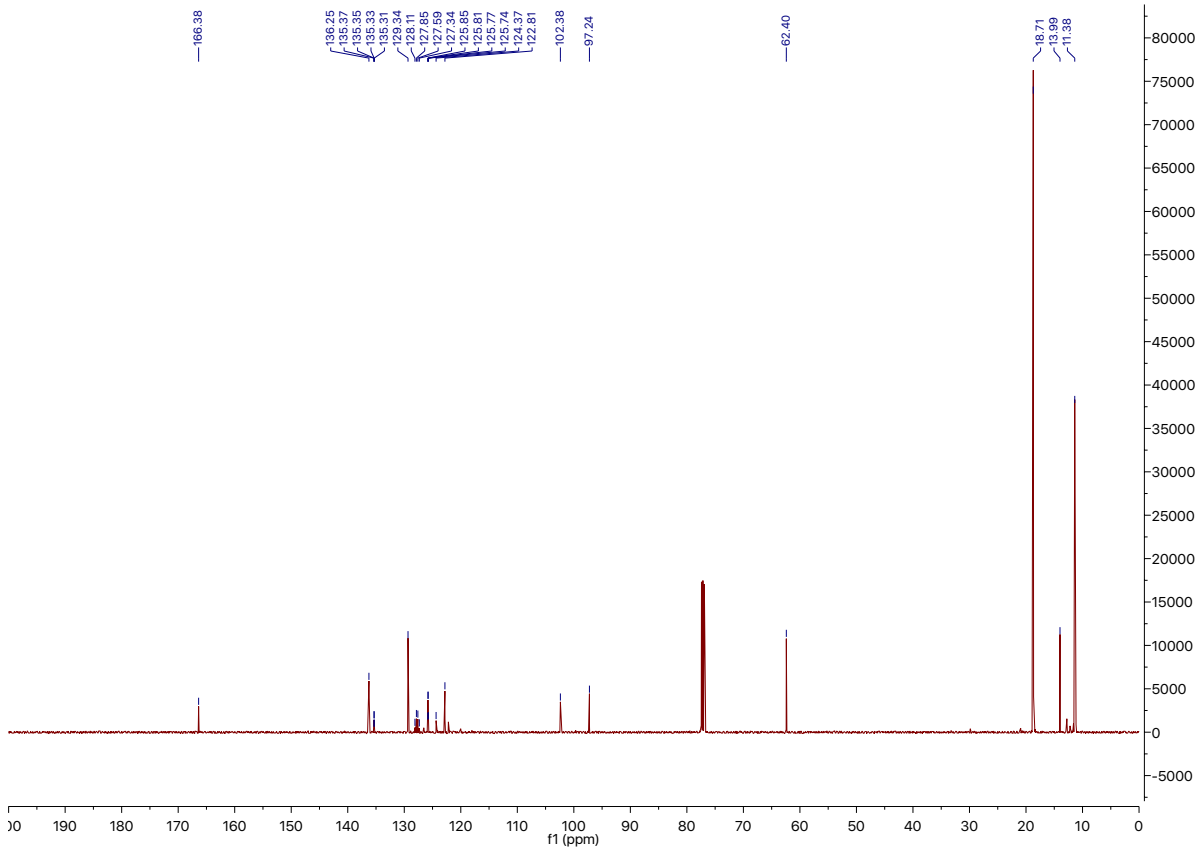
***Ethyl 2-methoxy-6-((triisopropylsilyl)ethynyl)benzoate* (3g)**



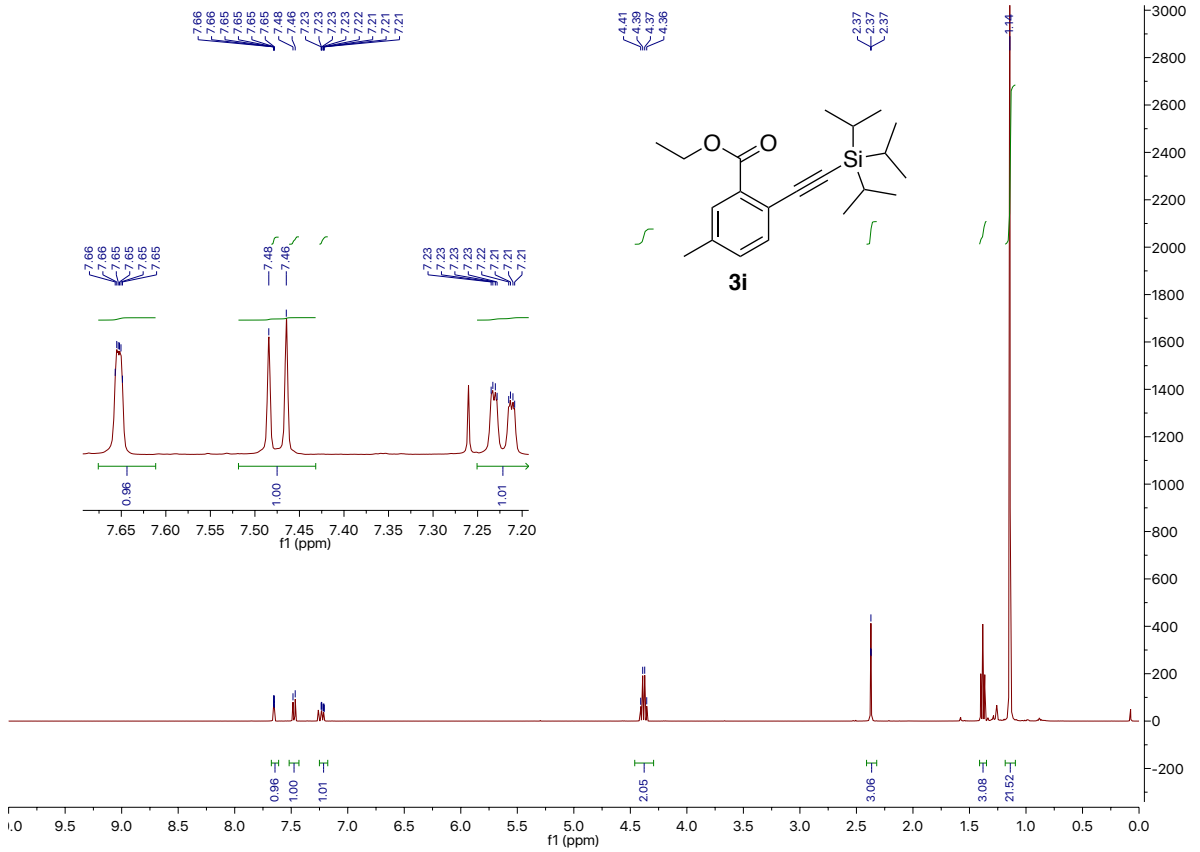


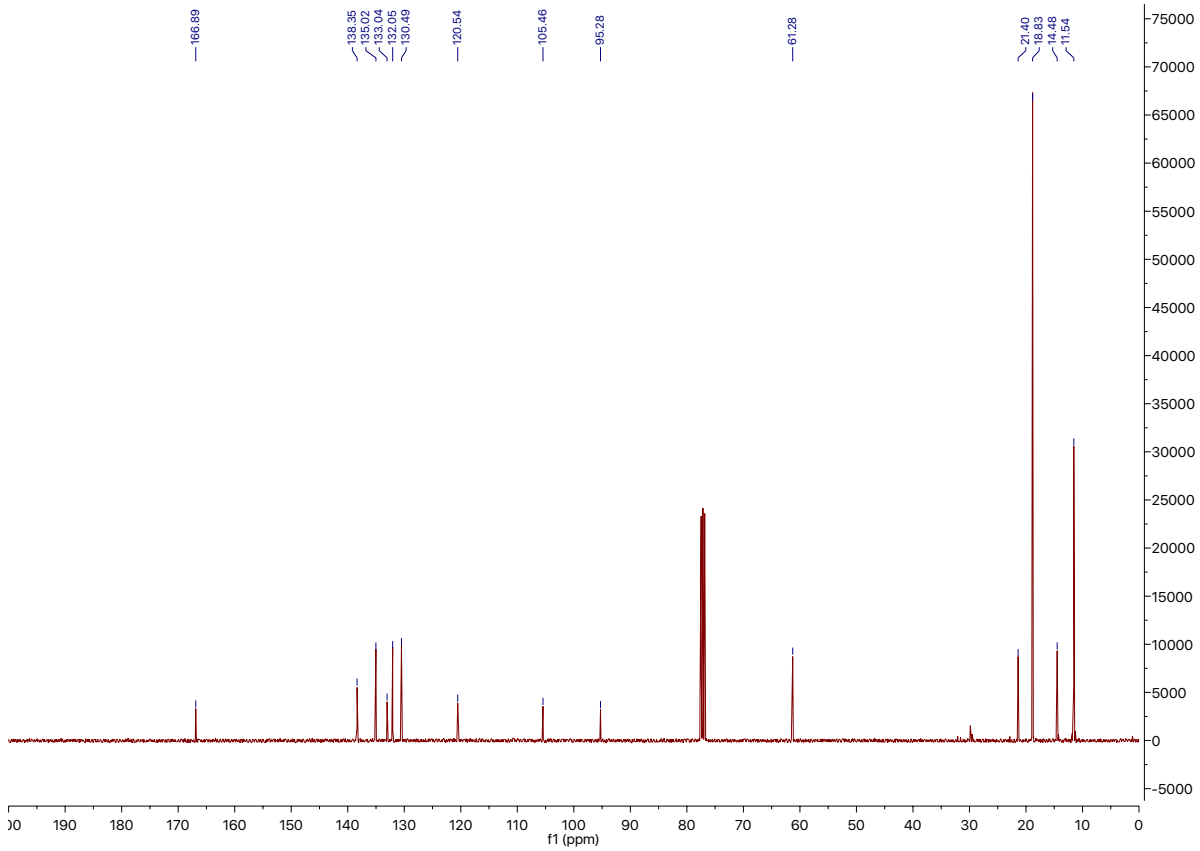
***Ethyl 2-(trifluoromethyl)-6-((triisopropylsilyl)ethynyl)benzoate* (3h)**



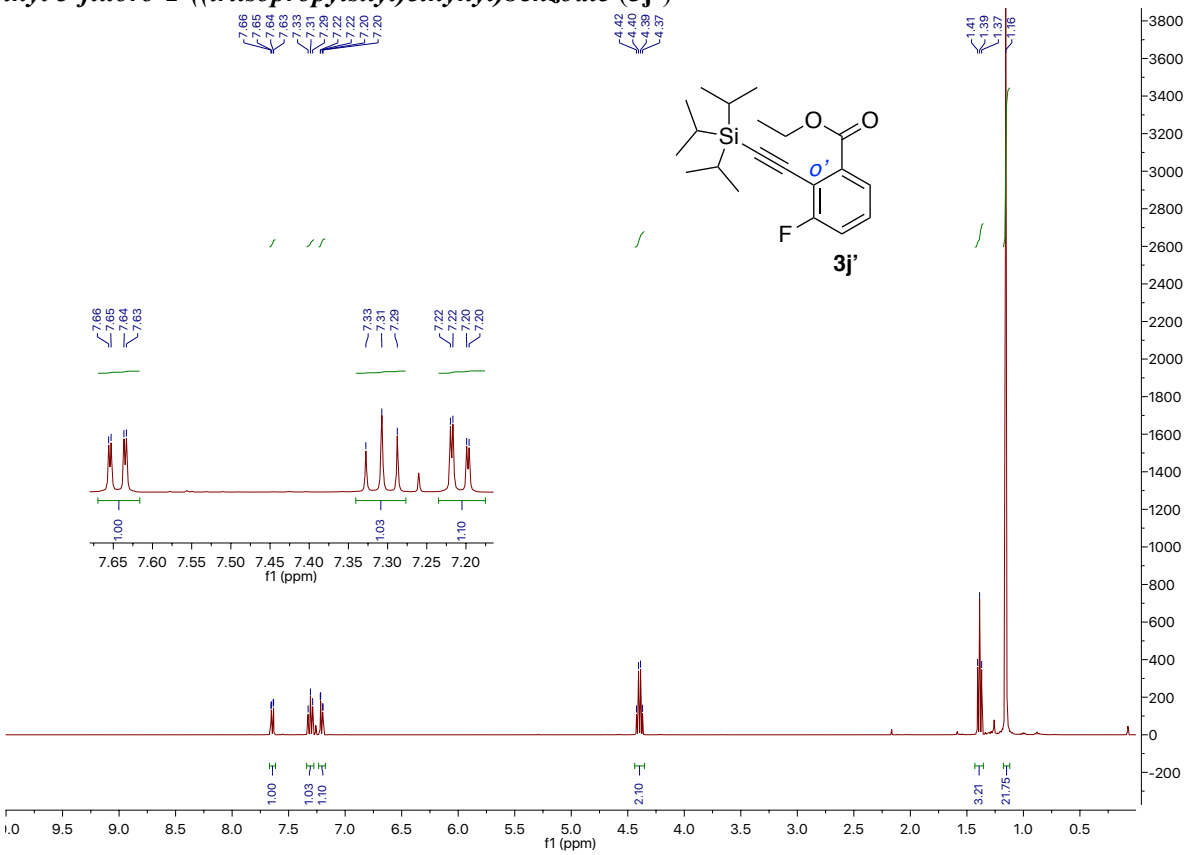


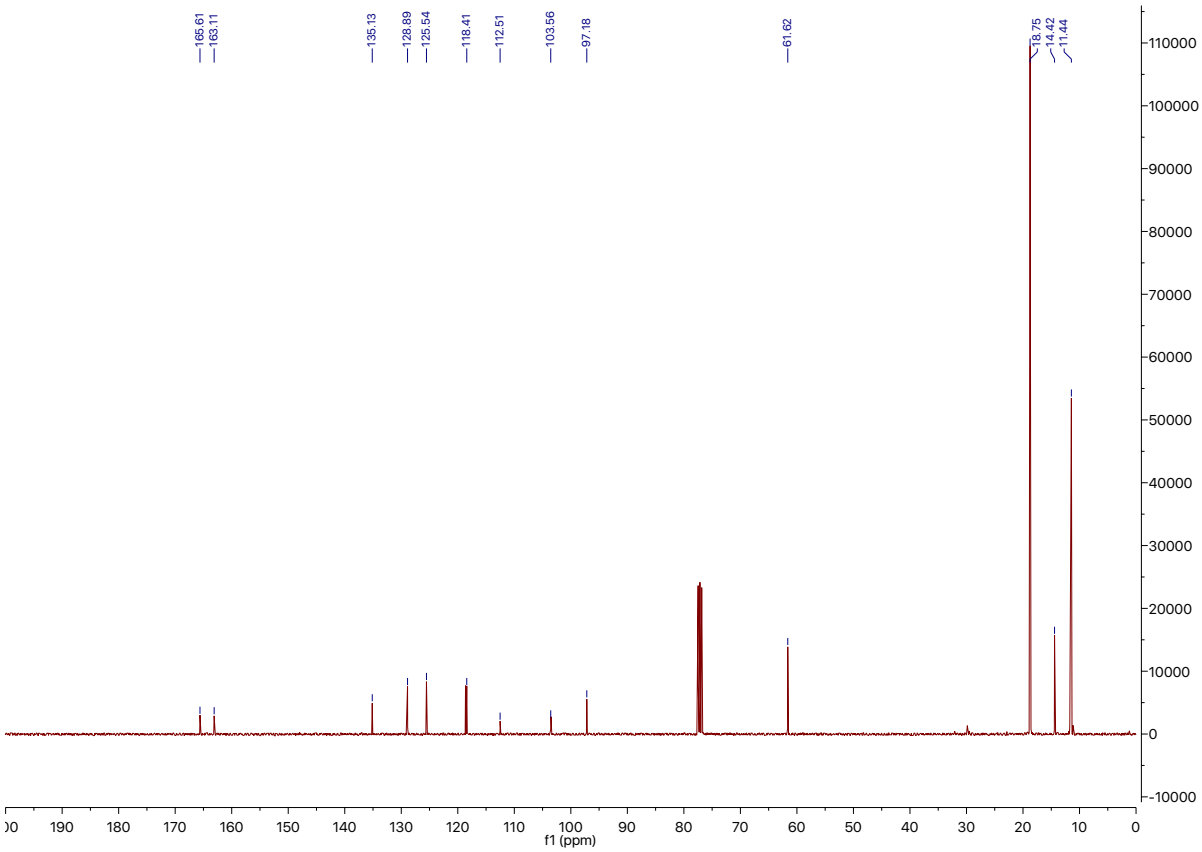
***Ethyl 5-methyl-2-((triisopropylsilyl)ethynyl)benzoate* (3i)**



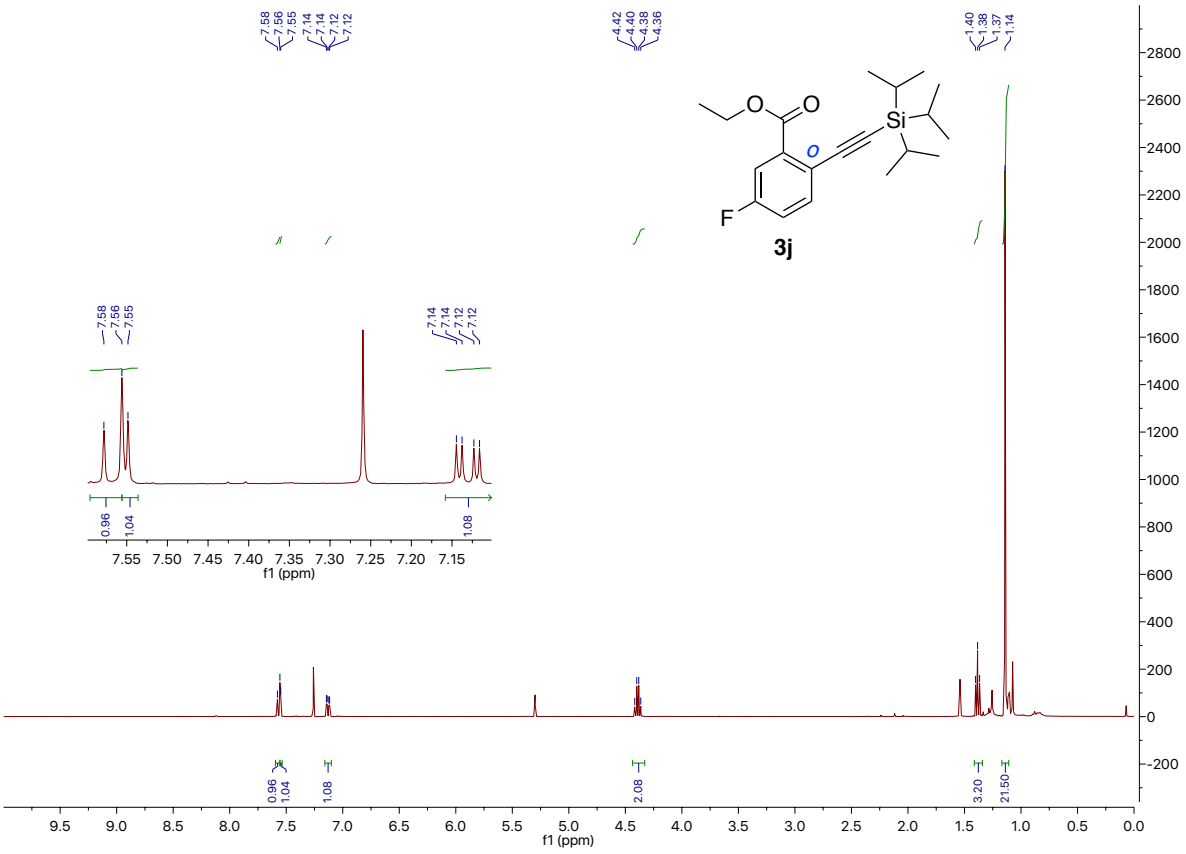


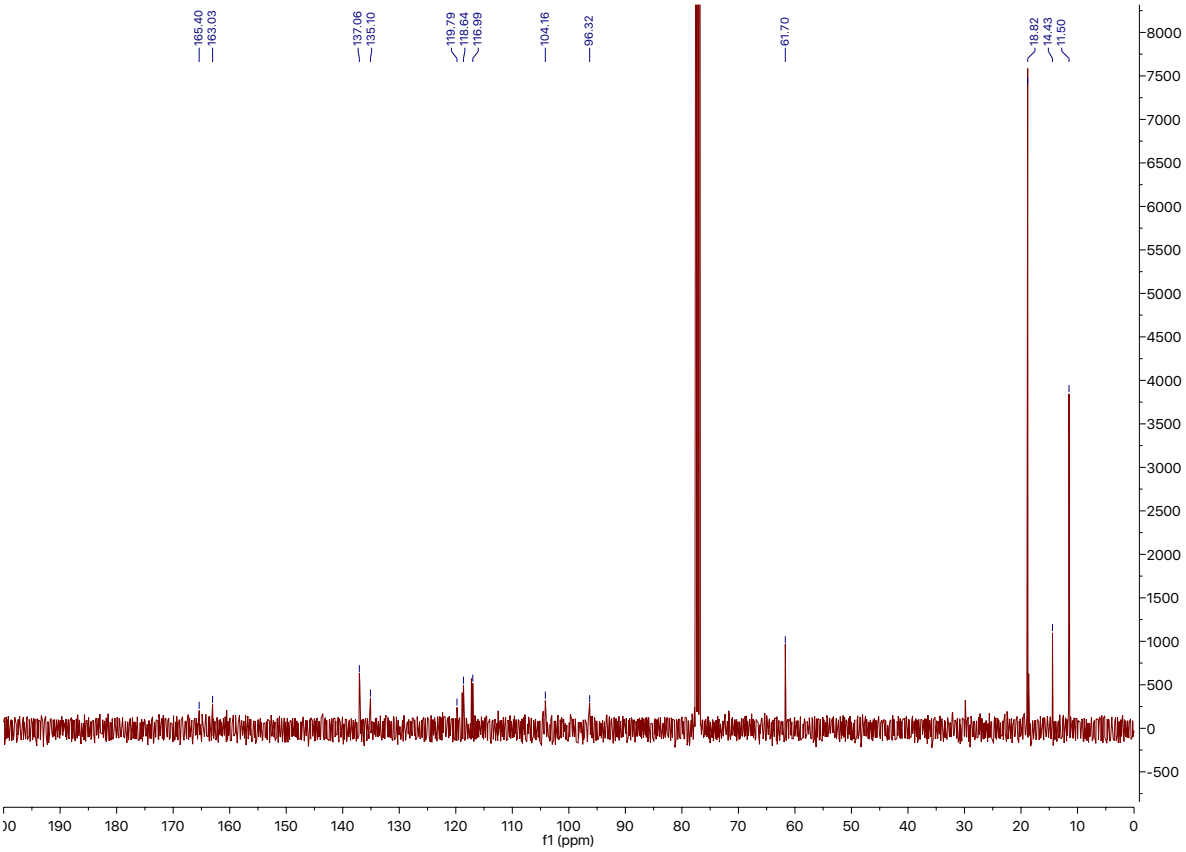
***Ethyl 3-fluoro-2-((triisopropylsilyl)ethynyl)benzoate* (3j')**



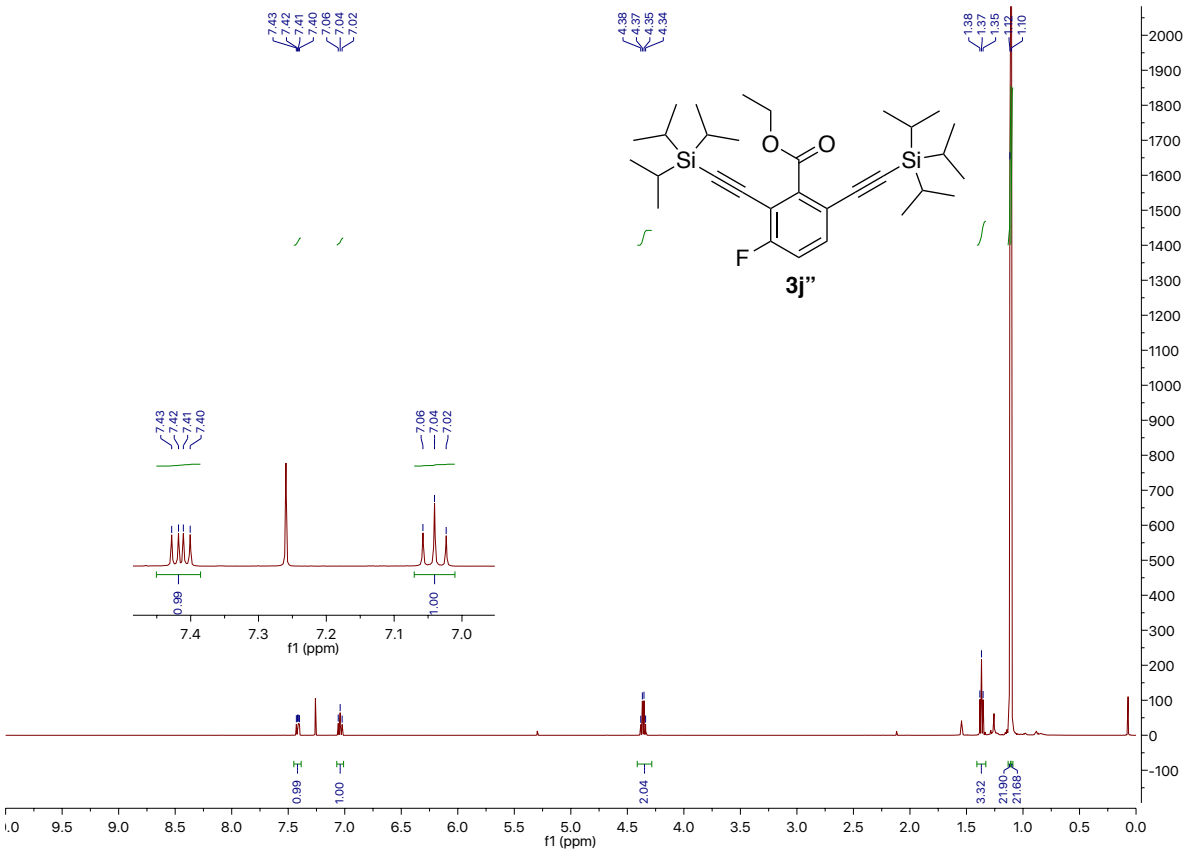


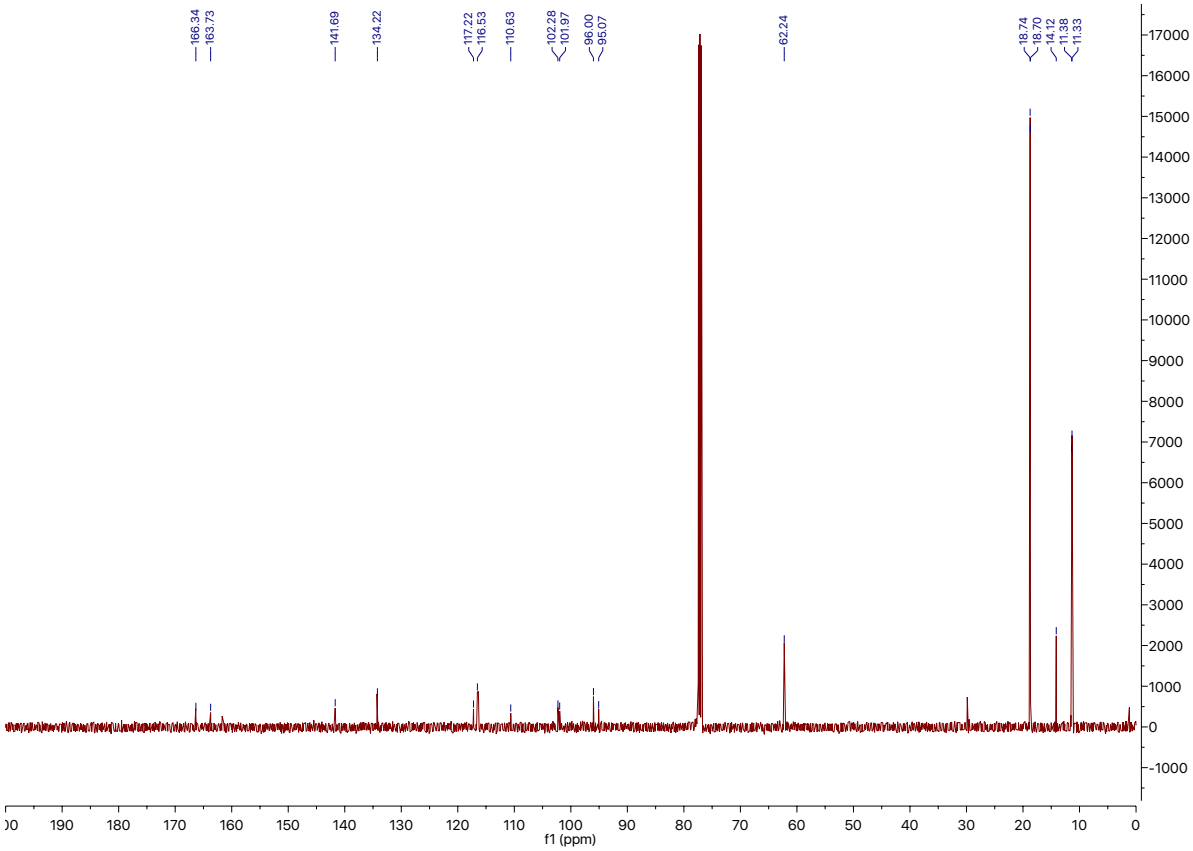
***Ethyl 5-fluoro-2-((triisopropylsilyl)ethynyl)benzoate* (3j)**



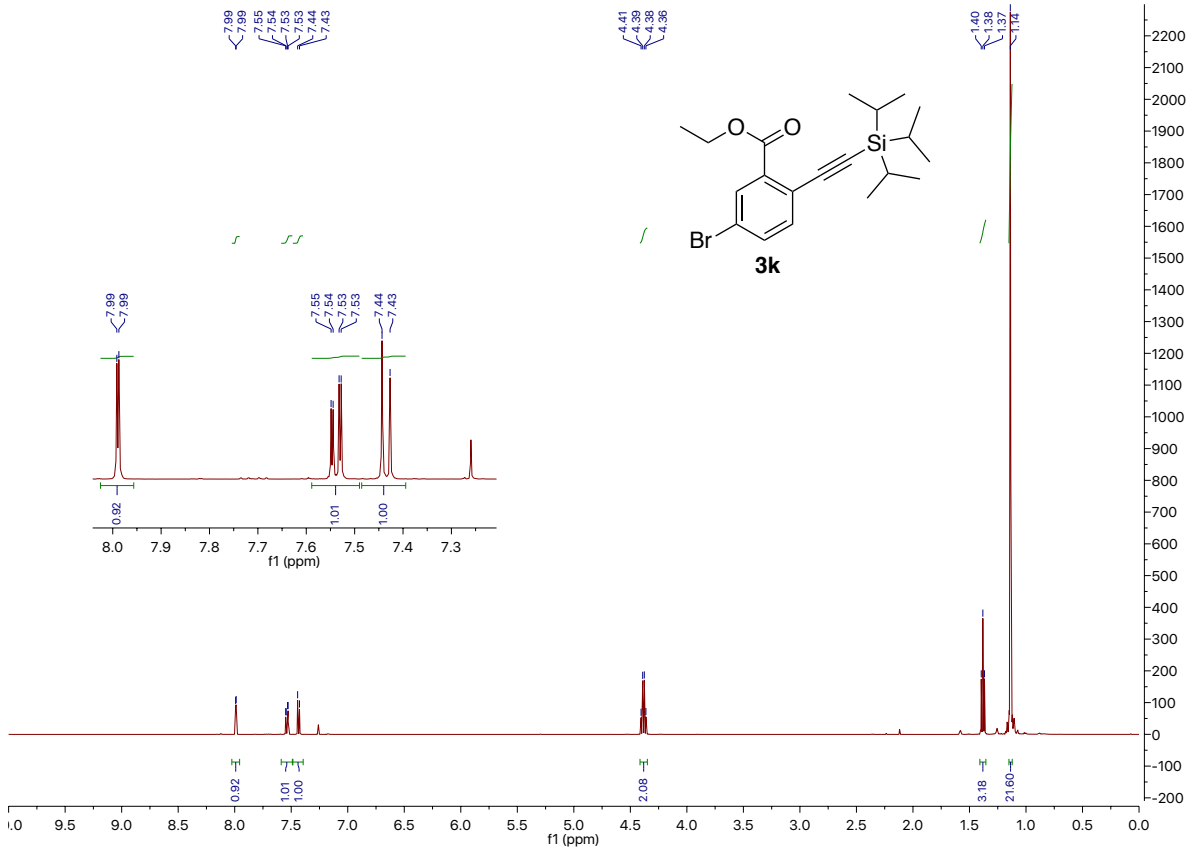


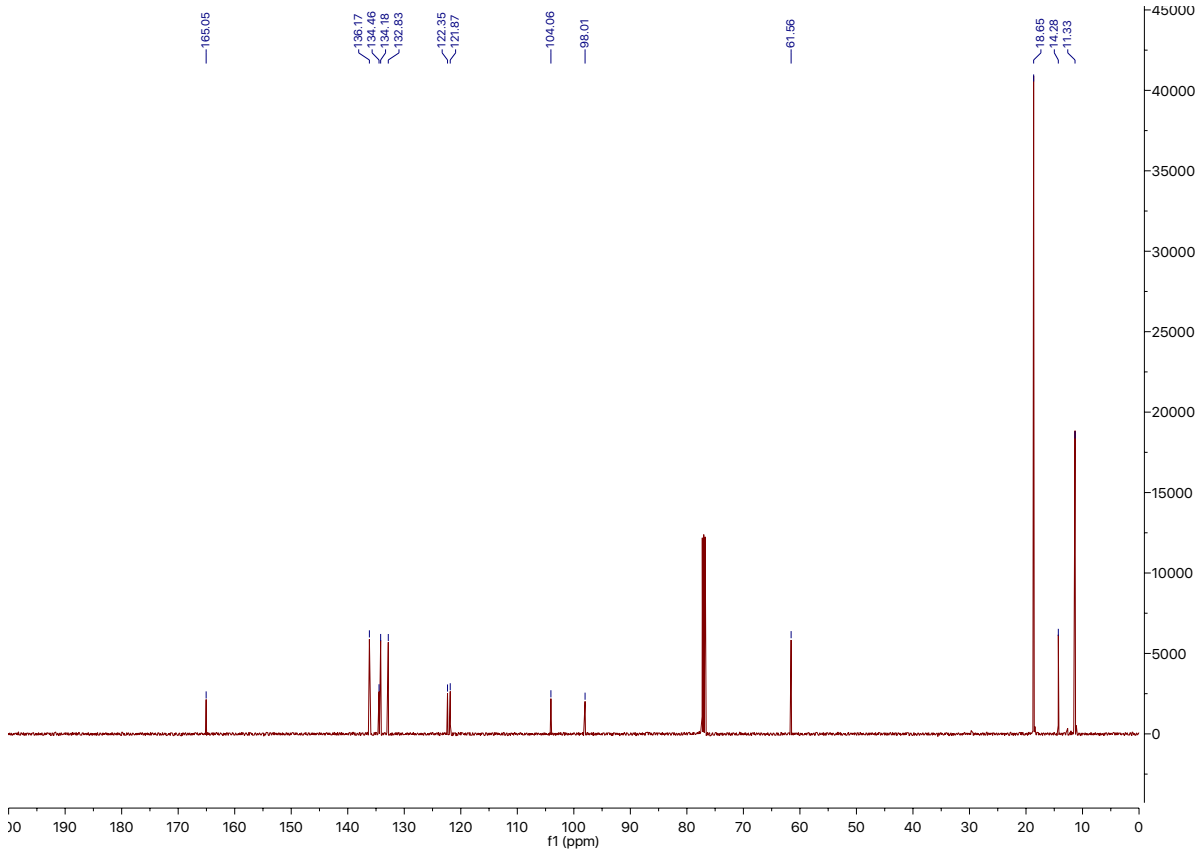
Ethyl 3-fluoro-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3j")**



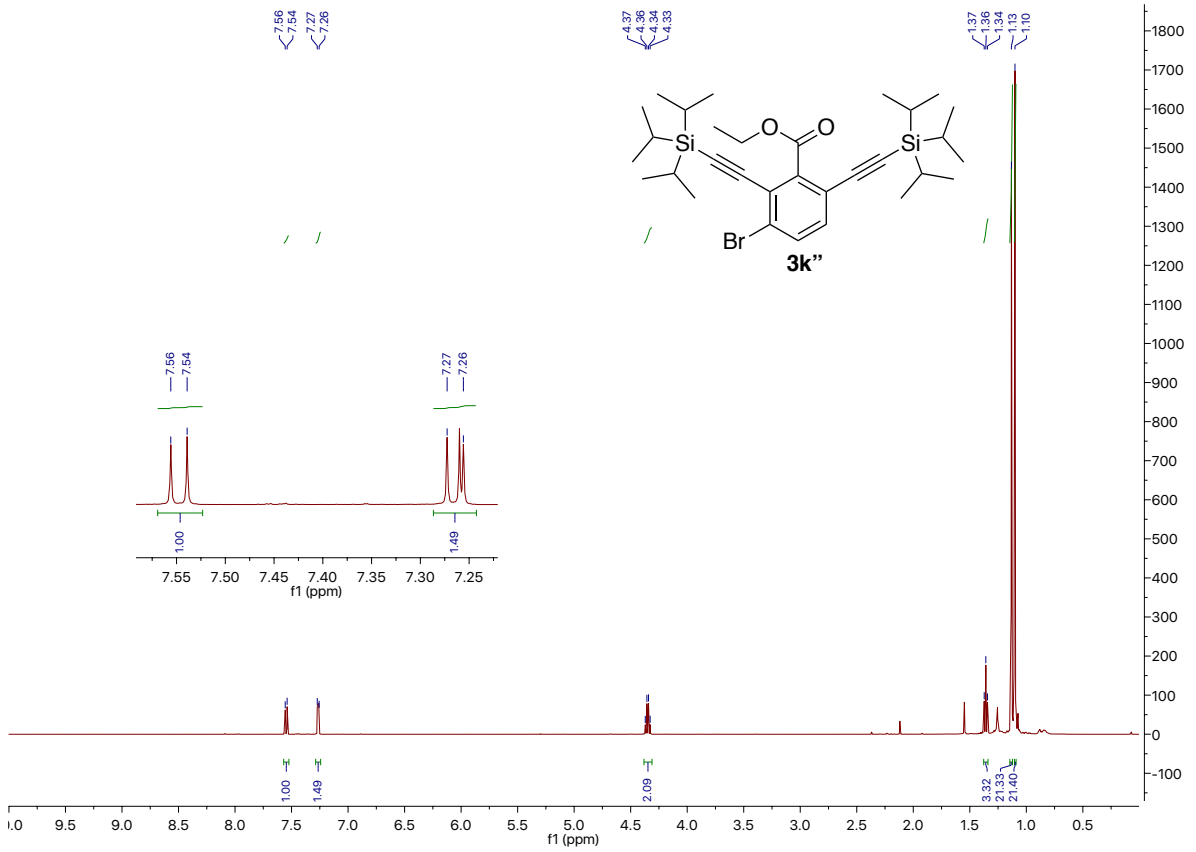


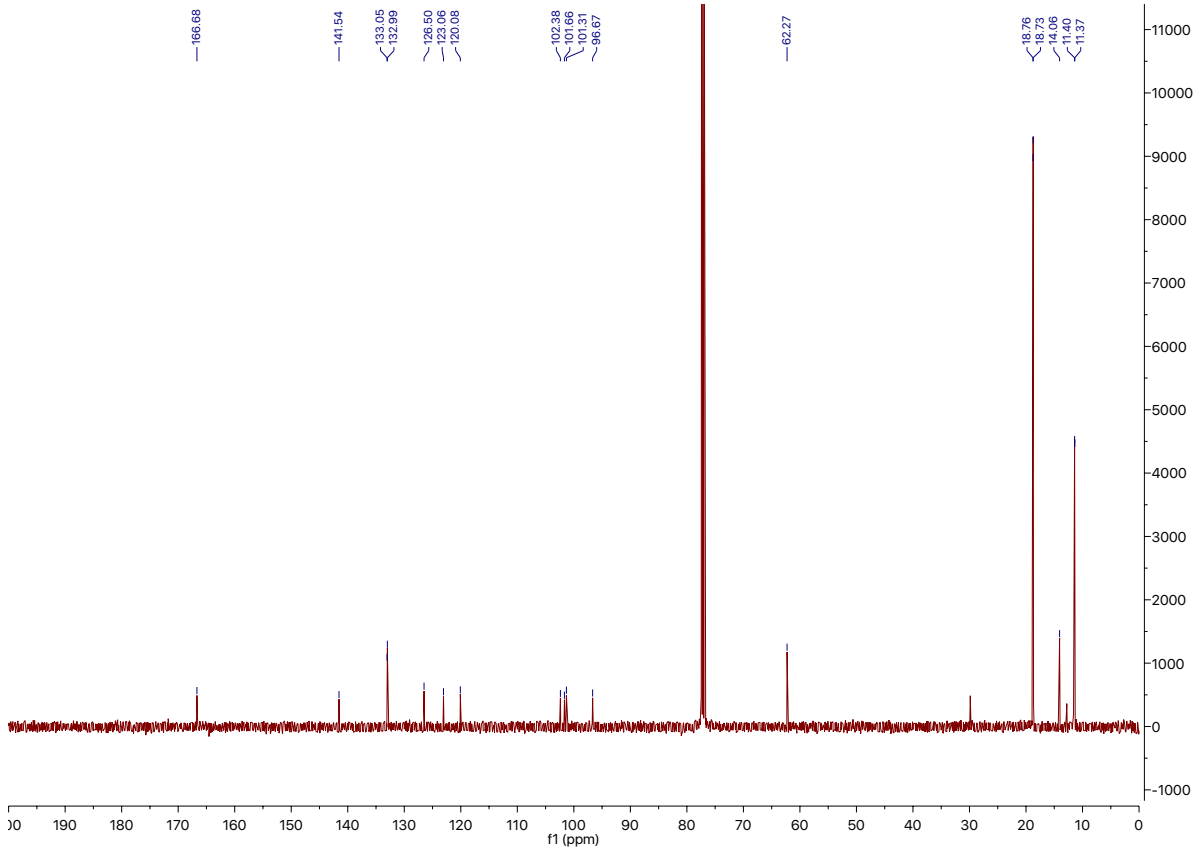
Ethyl 5-bromo-2-((triisopropylsilyl)ethynyl)benzoate **(3k)**



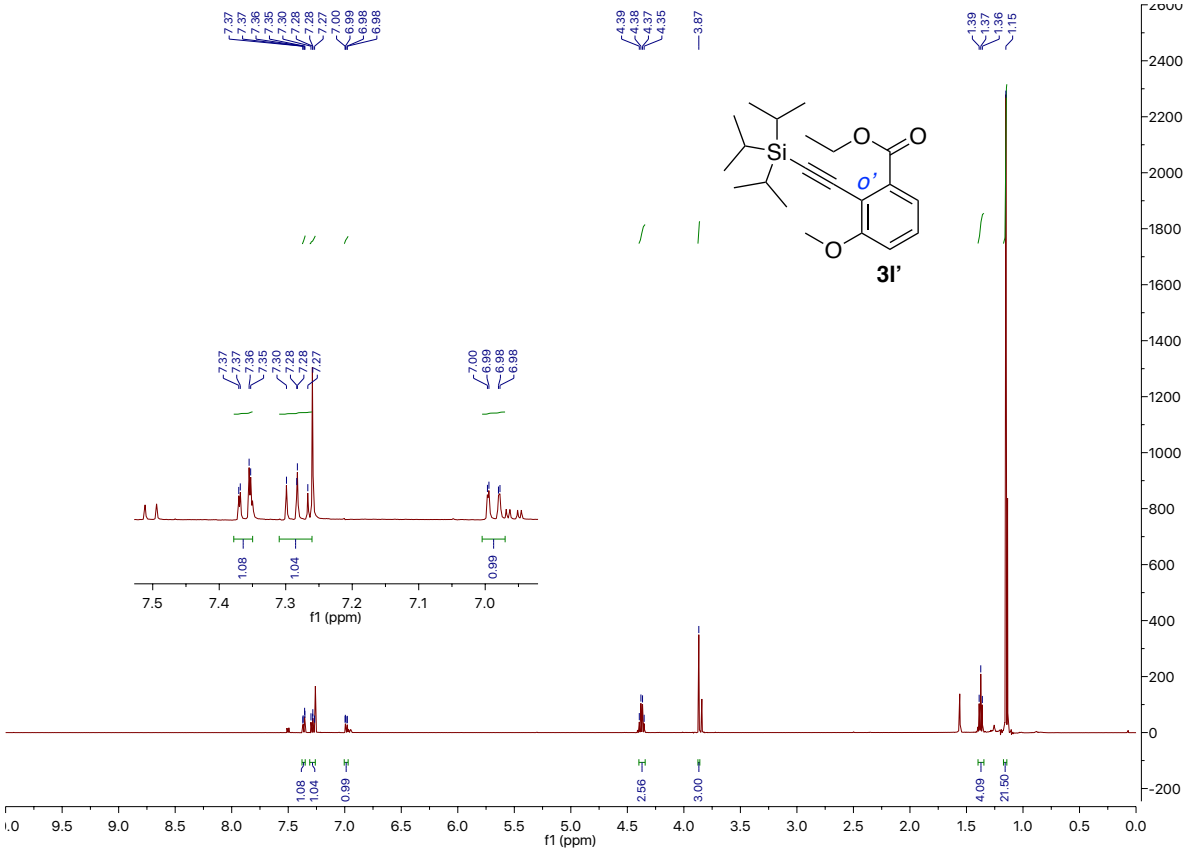


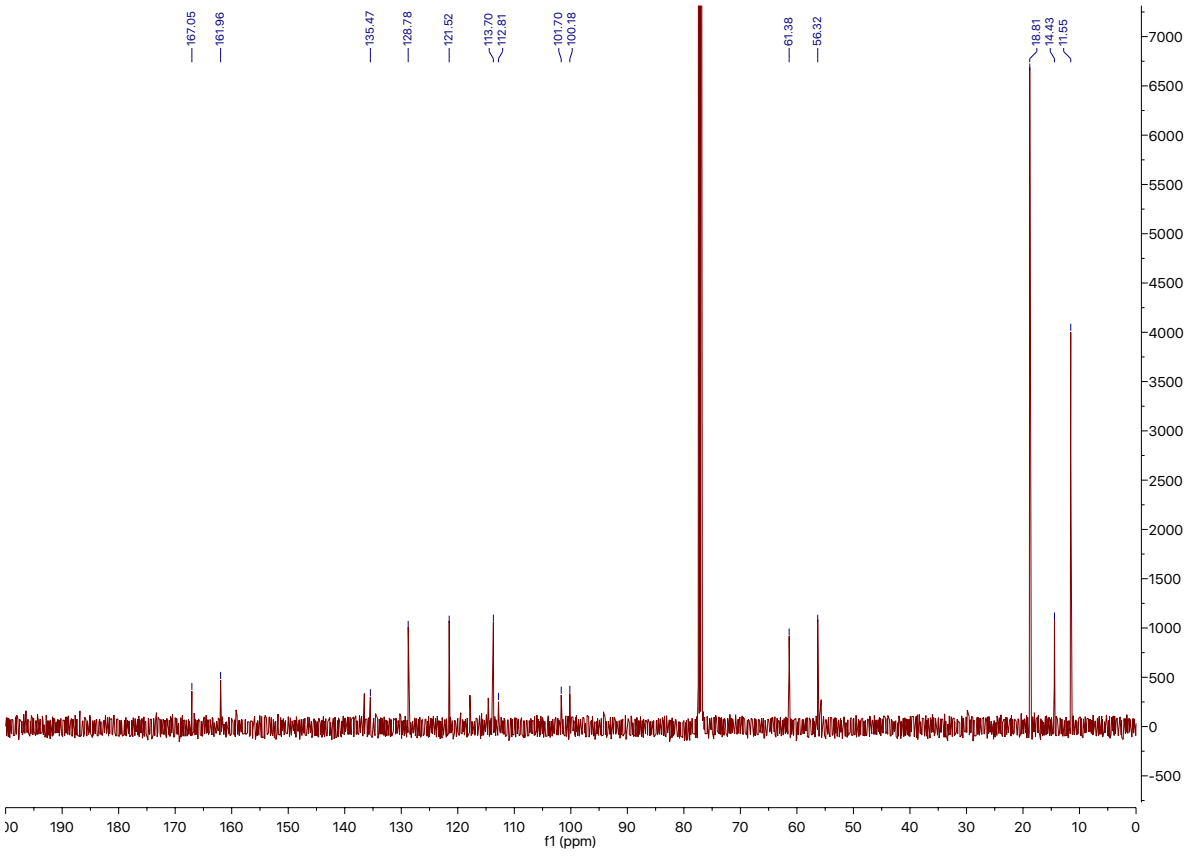
Ethyl 3-bromo-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3k")**



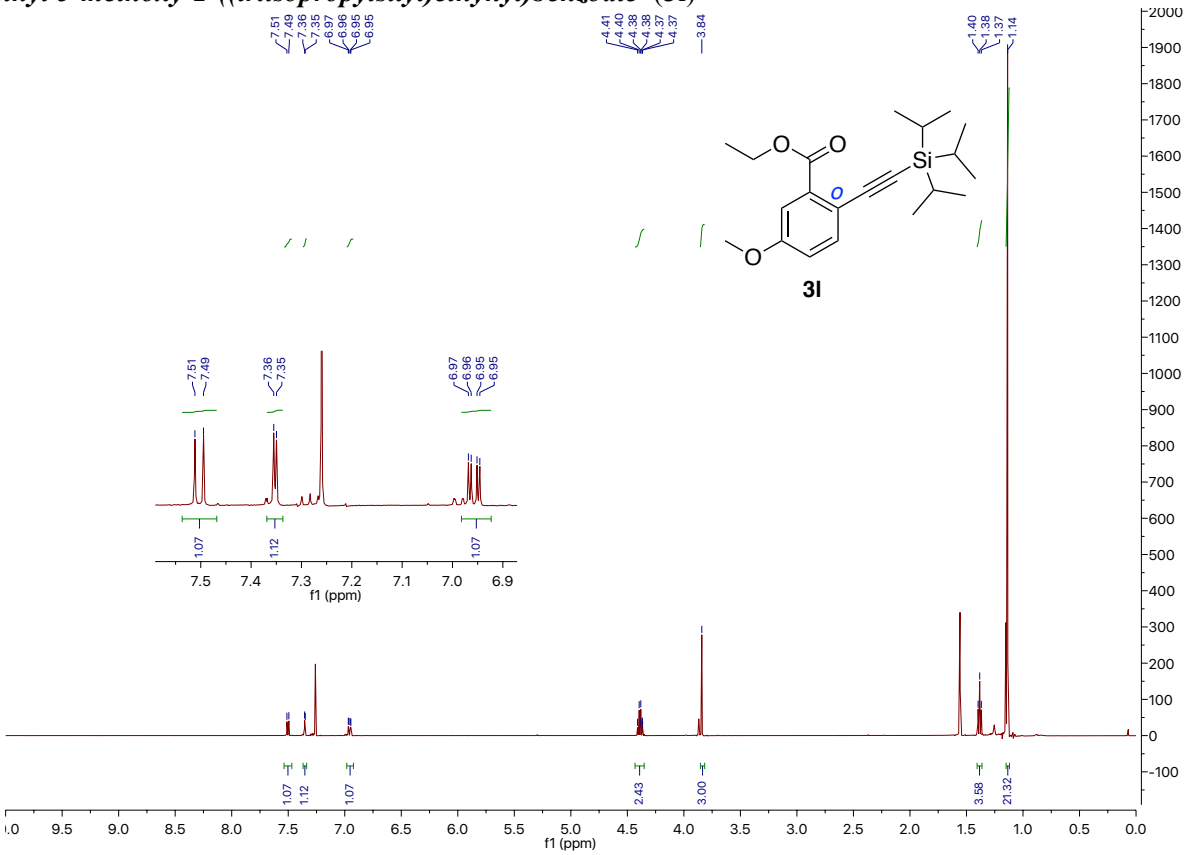


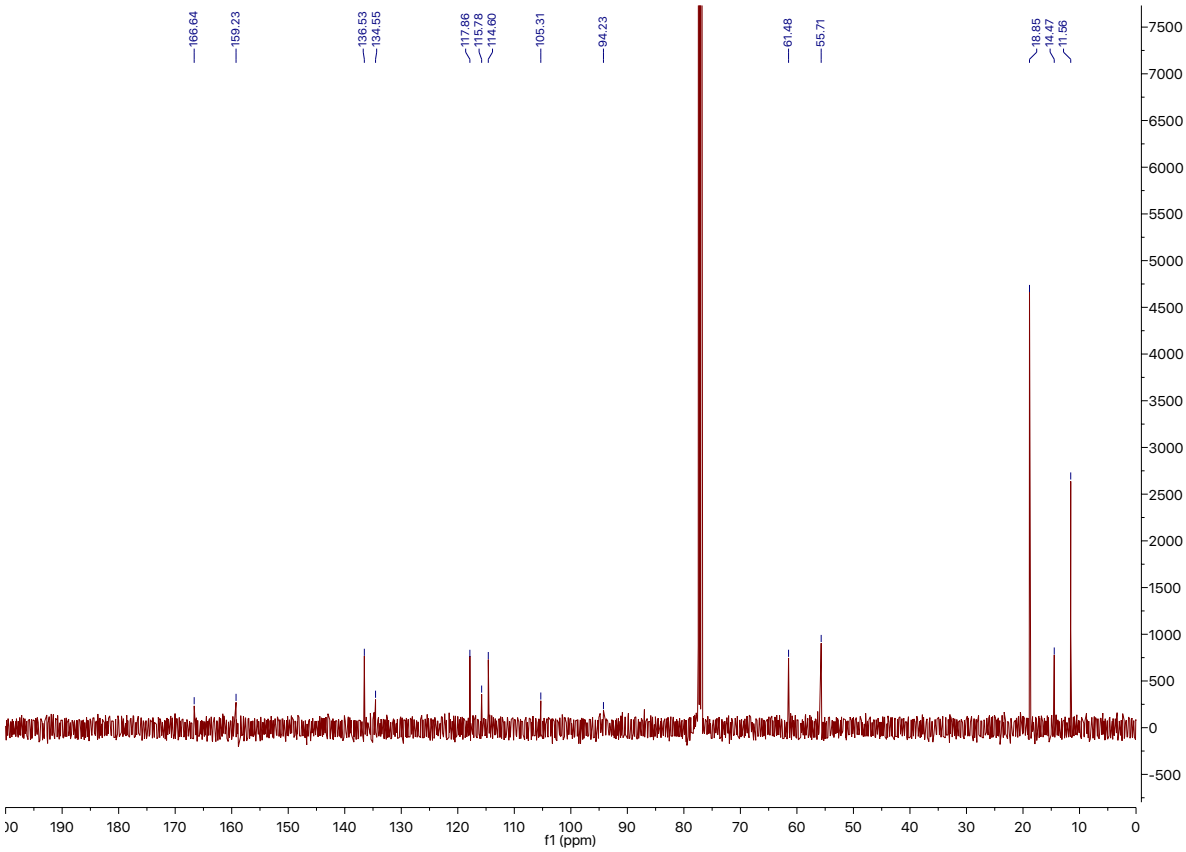
Ethyl 3-methoxy-2-((triisopropylsilyl)ethynyl)benzoate **(3l')**



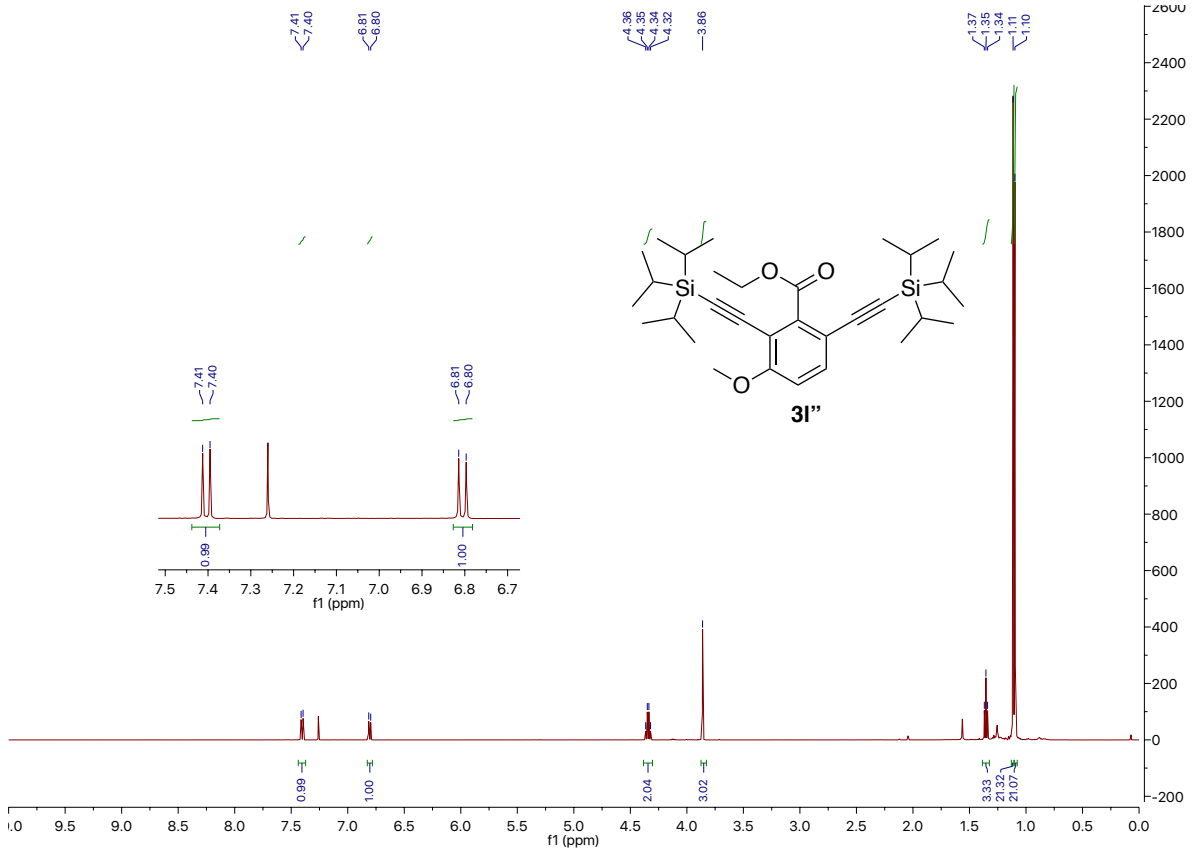


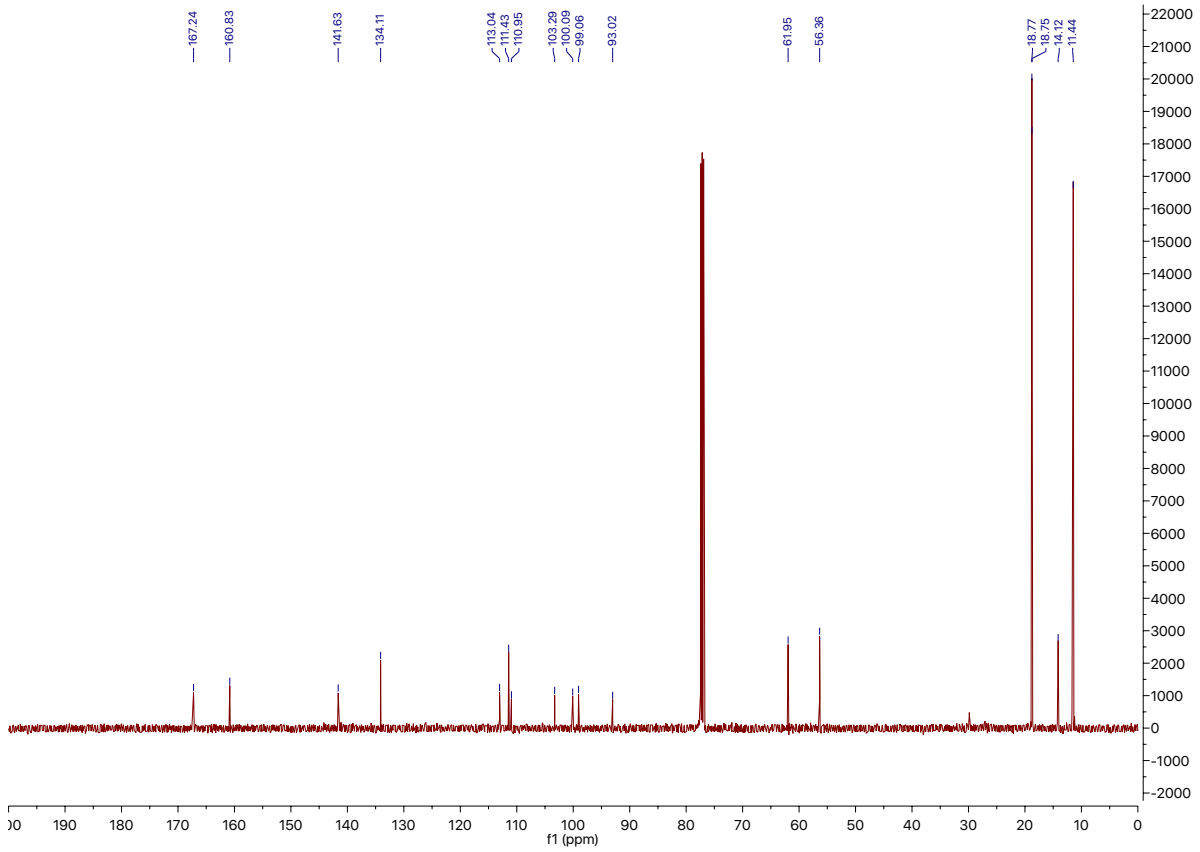
Ethyl 5-methoxy-2-((triisopropylsilyl)ethynyl)benzoate **(3l)**



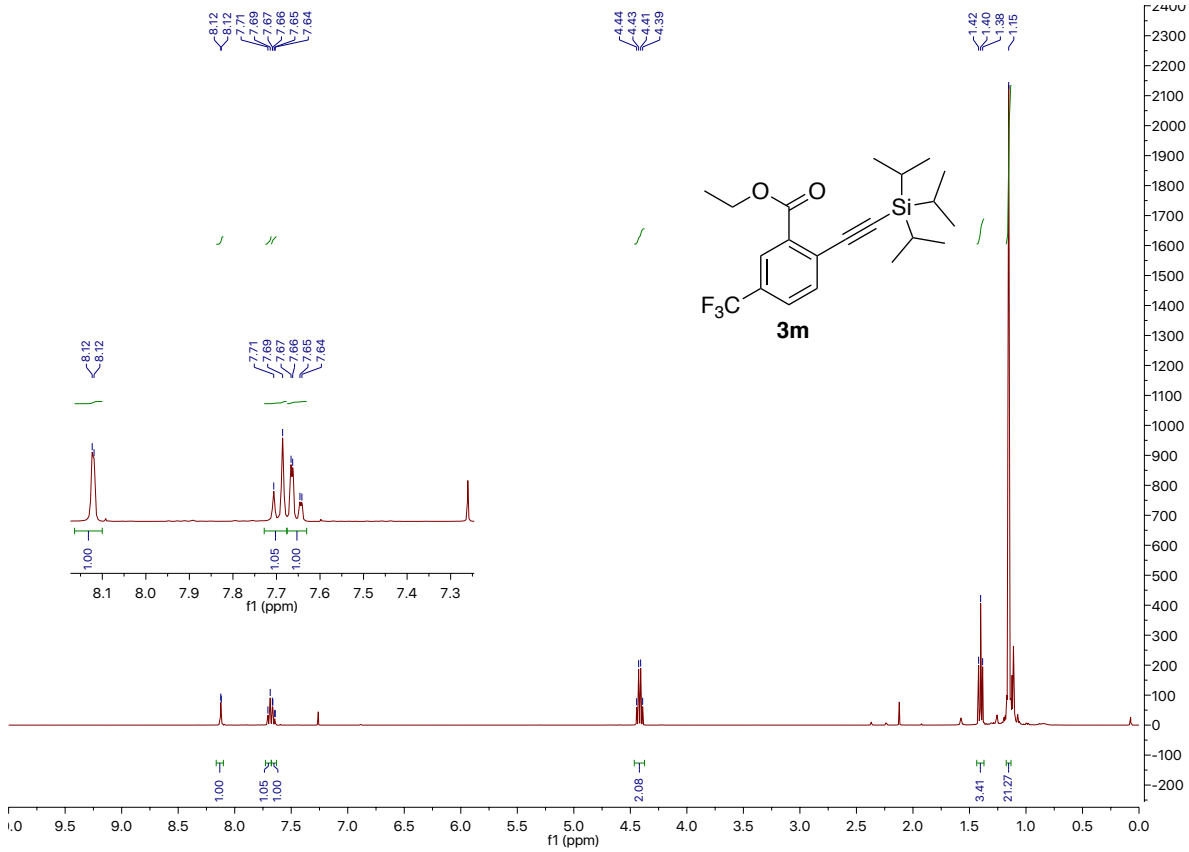


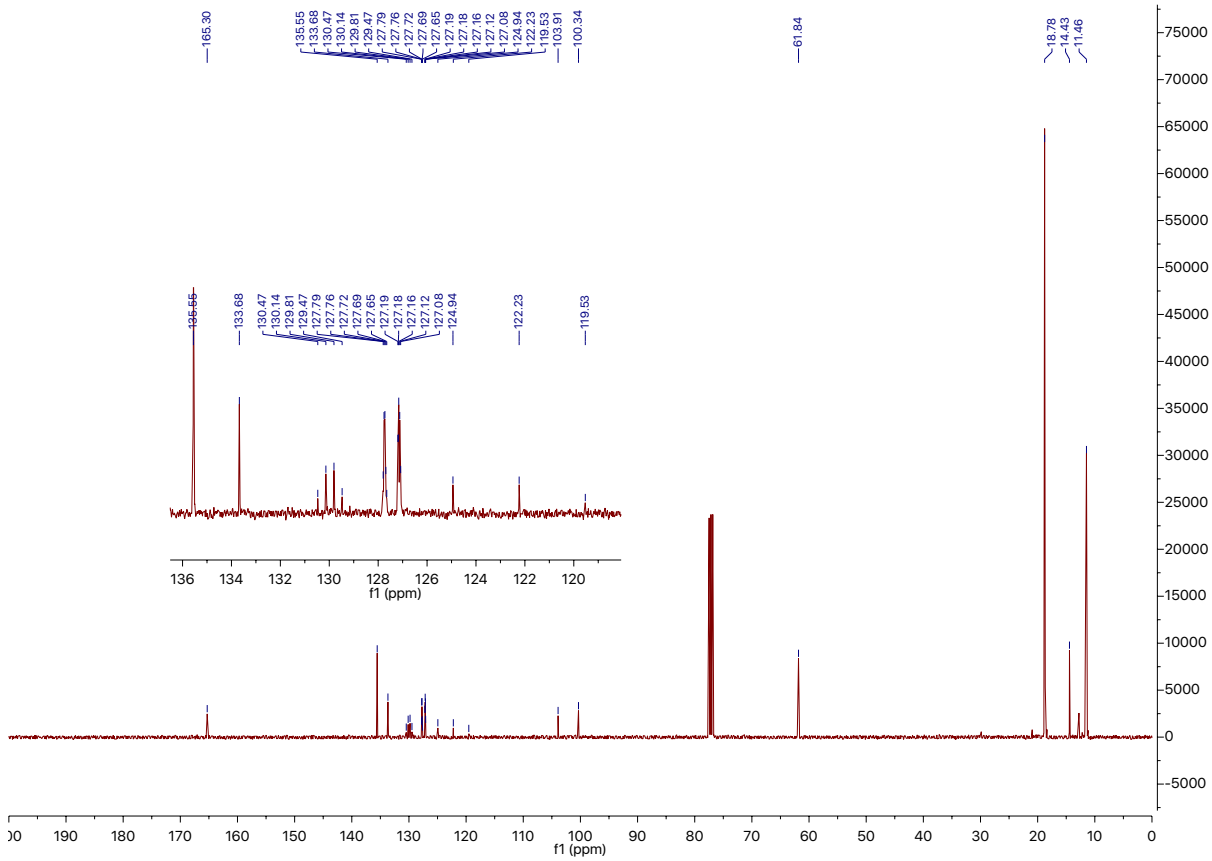
Ethyl 3-methoxy-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3l")**



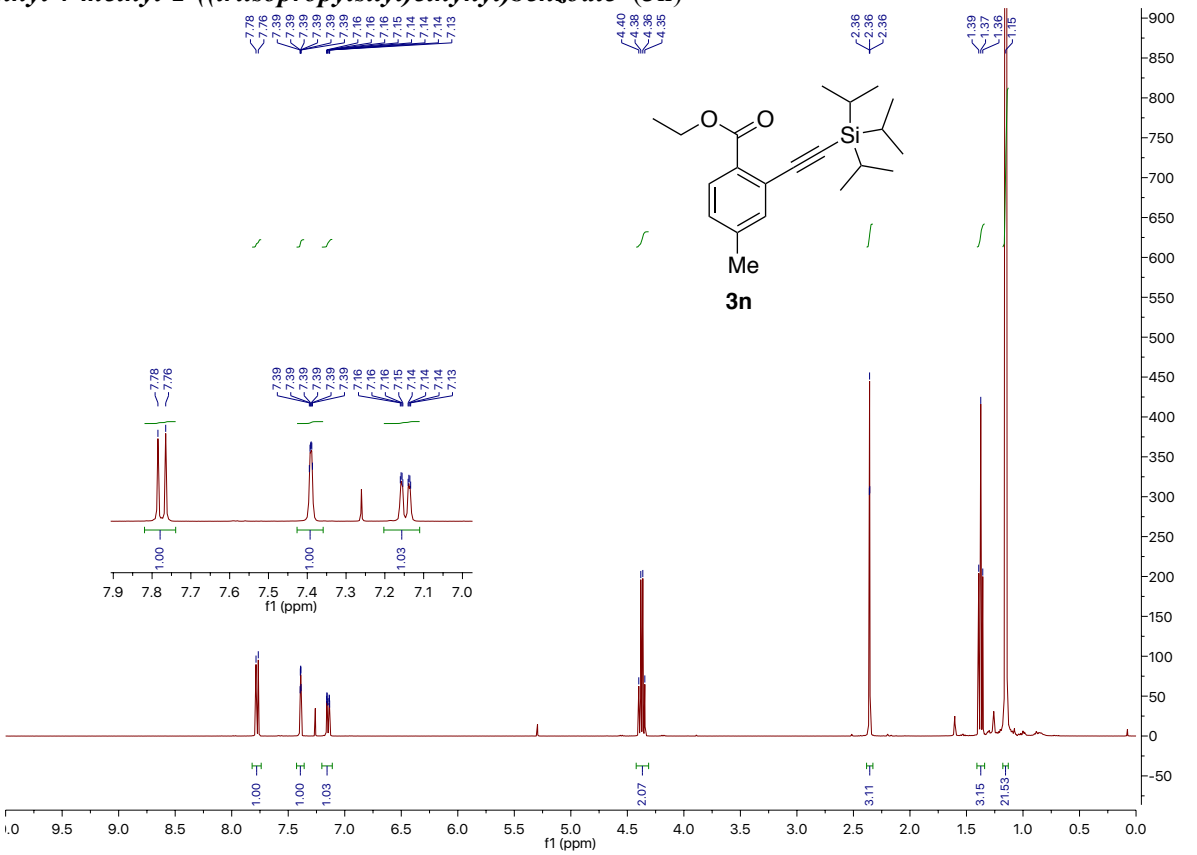


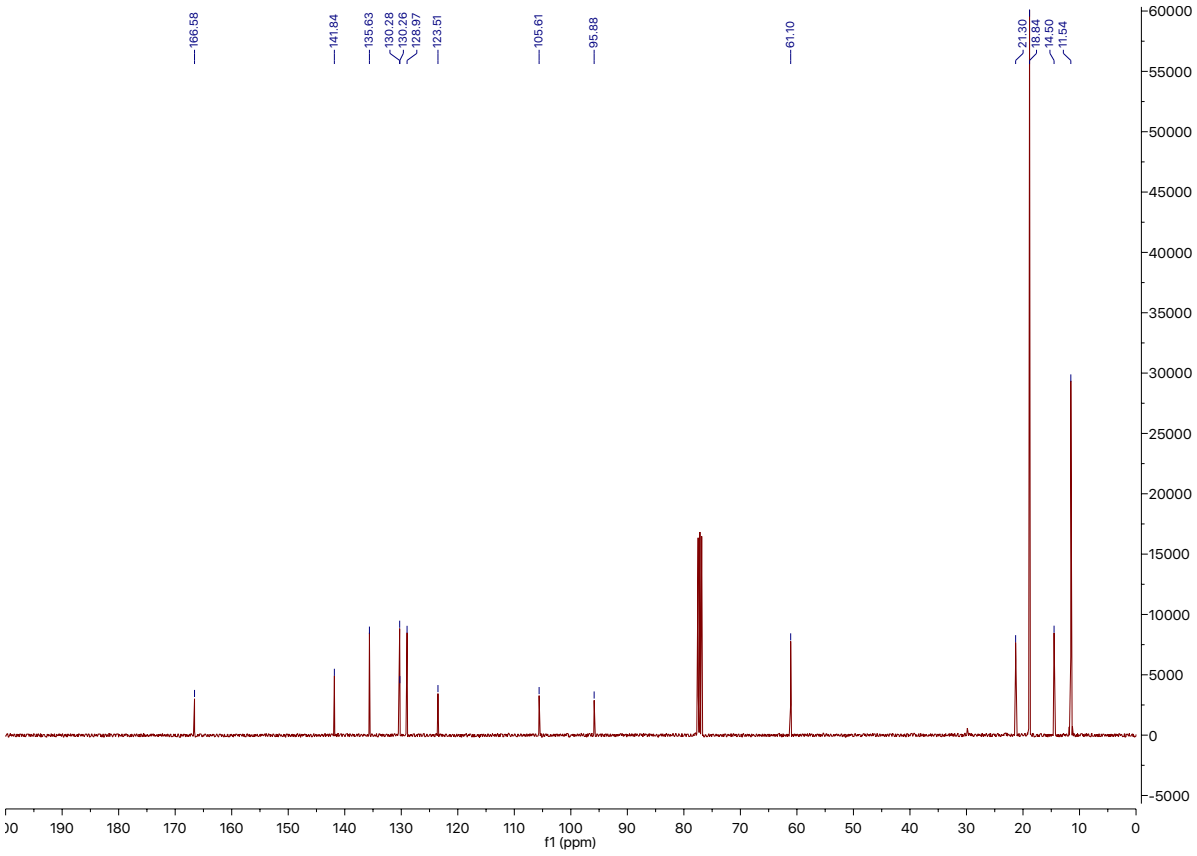
Ethyl 5-(trifluoromethyl)-2-((triisopropylsilyl)ethynyl)benzoate **(3m)**



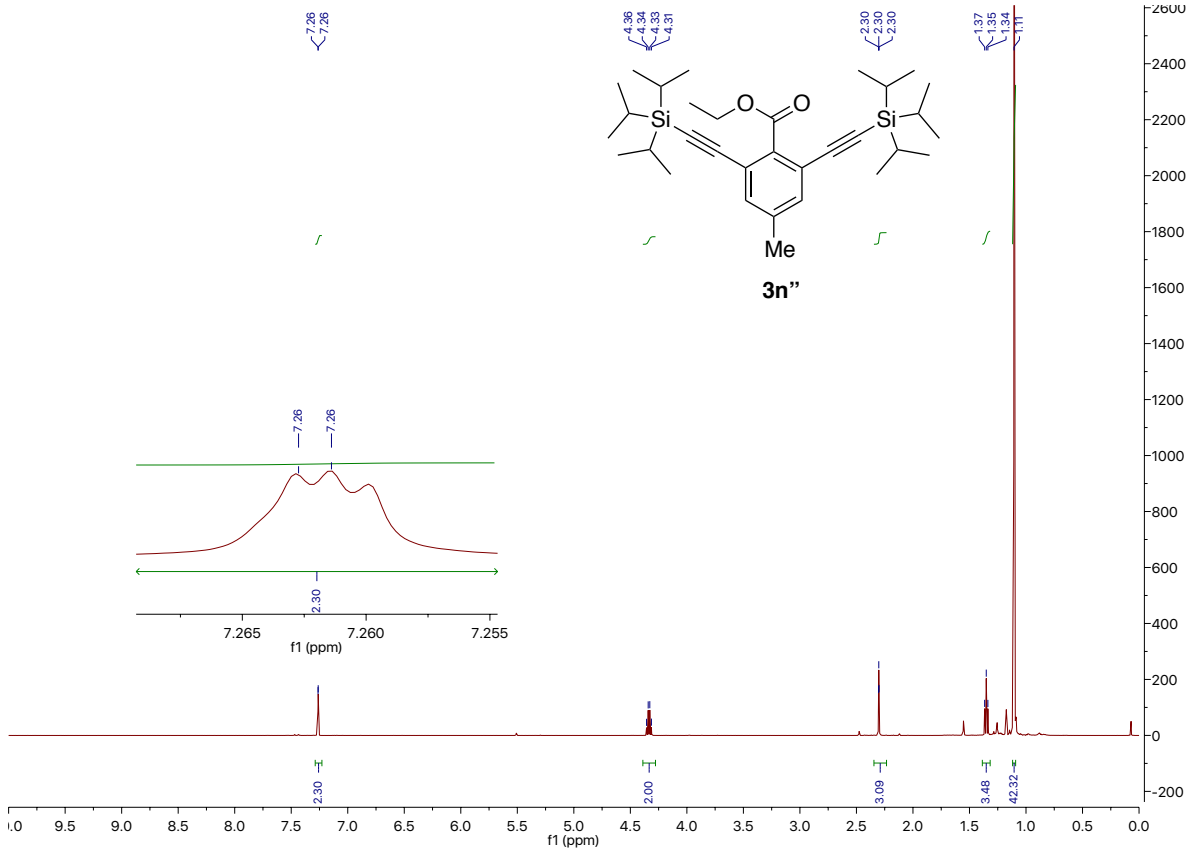


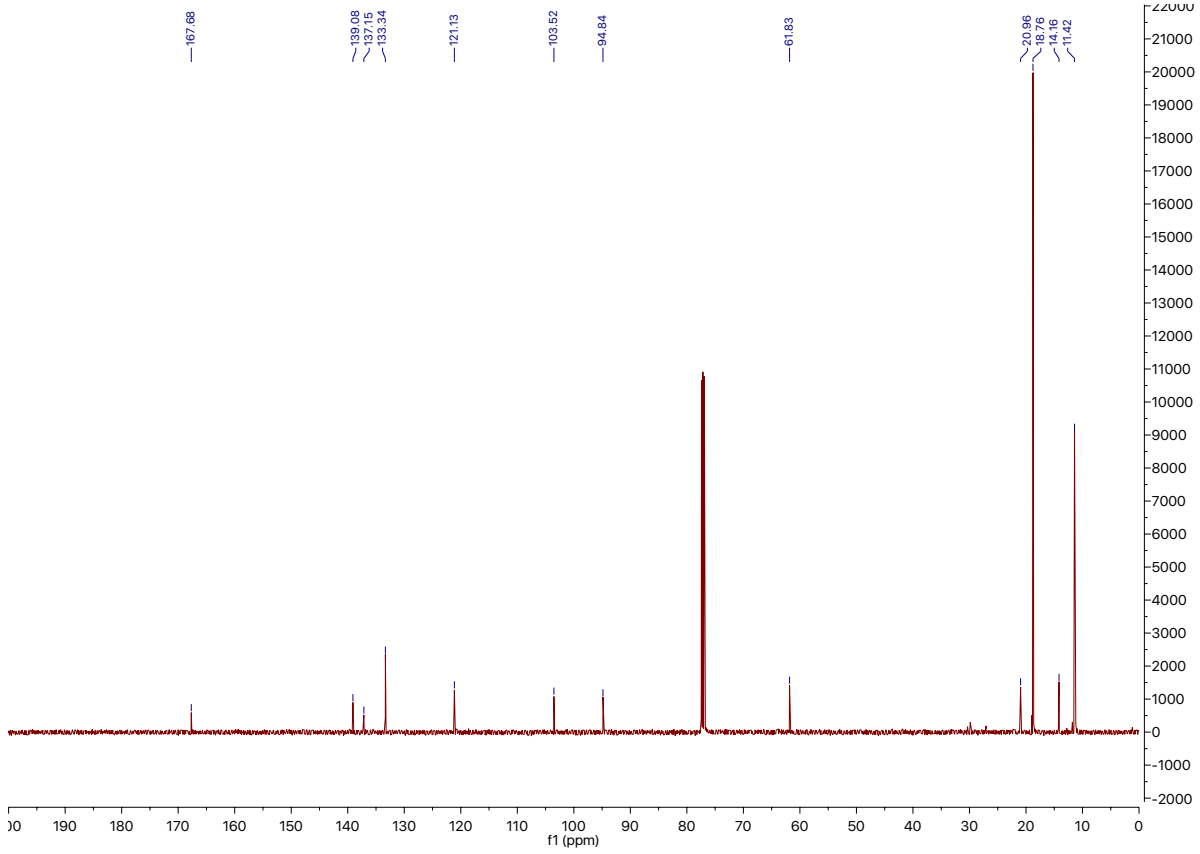
Ethyl 4-methyl-2-((triisopropylsilyl)ethynyl)benzoate **(3n)**



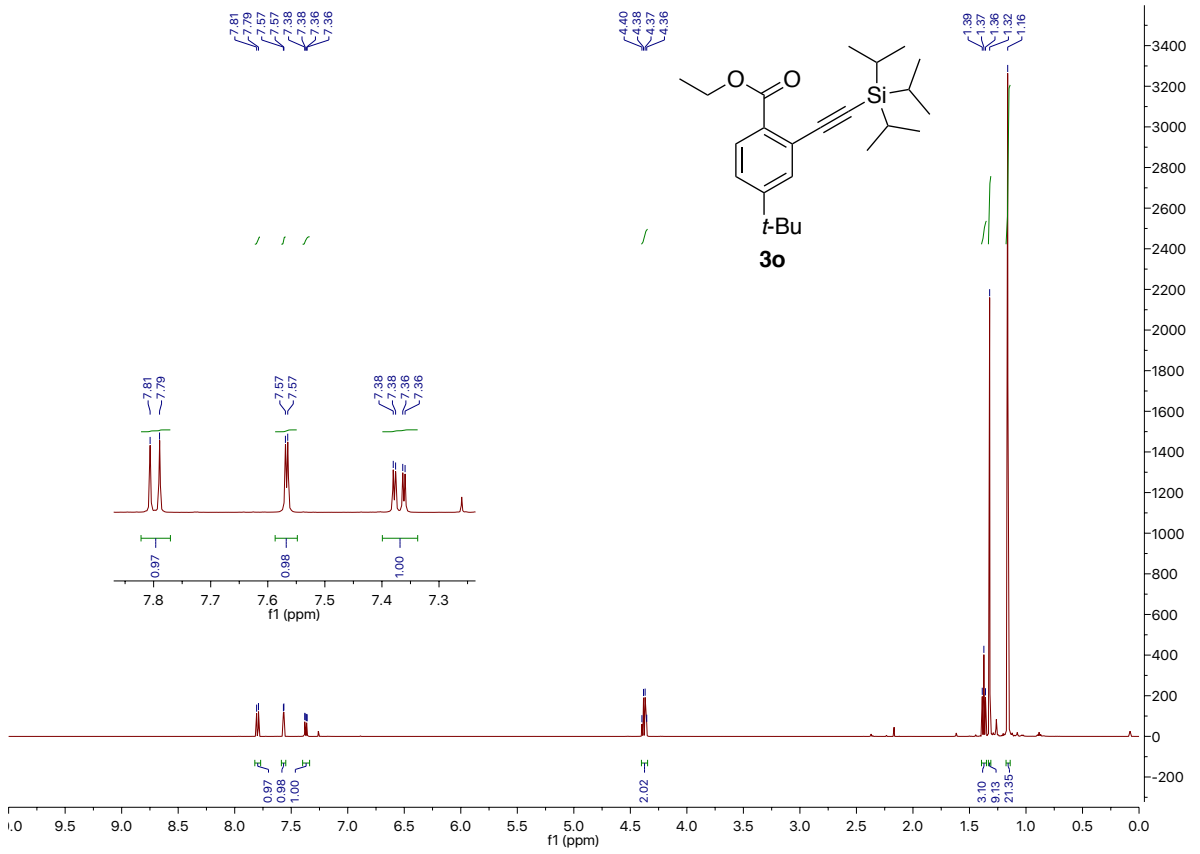


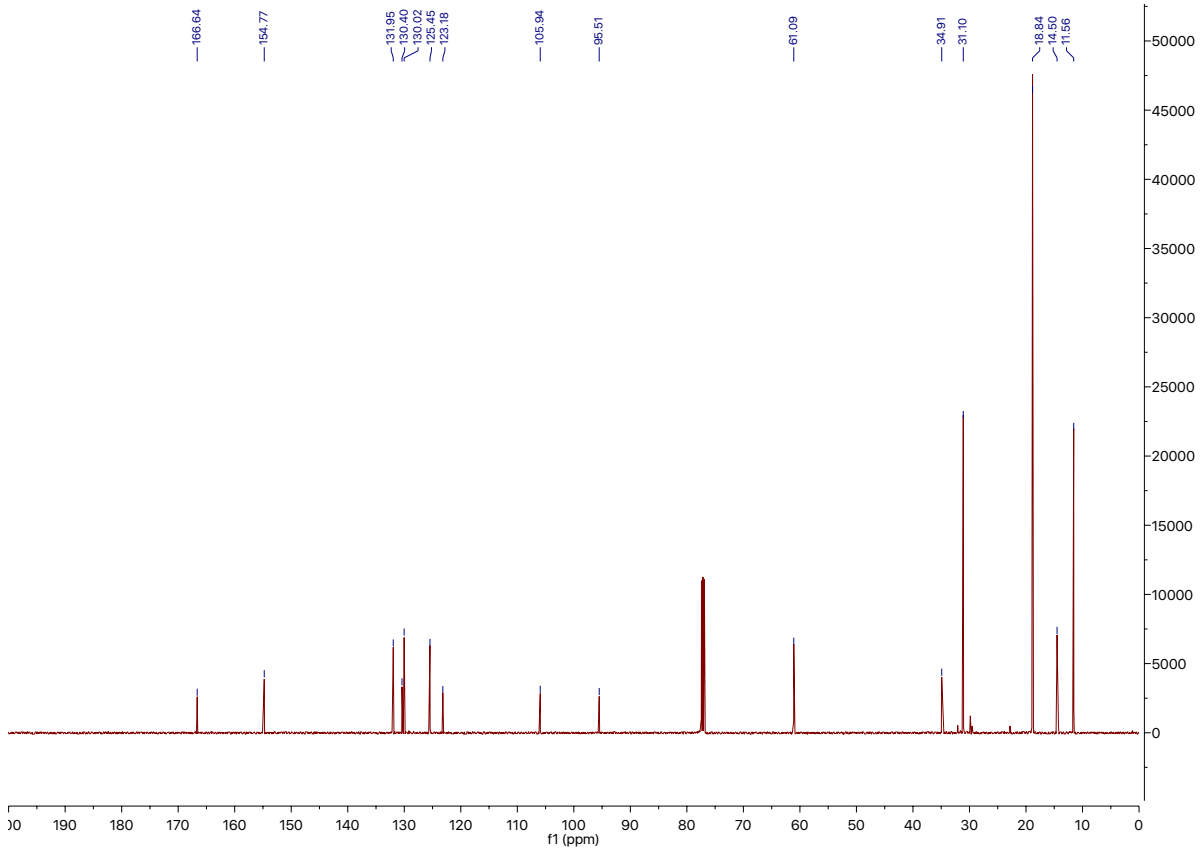
Ethyl 4-methyl-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3n")**



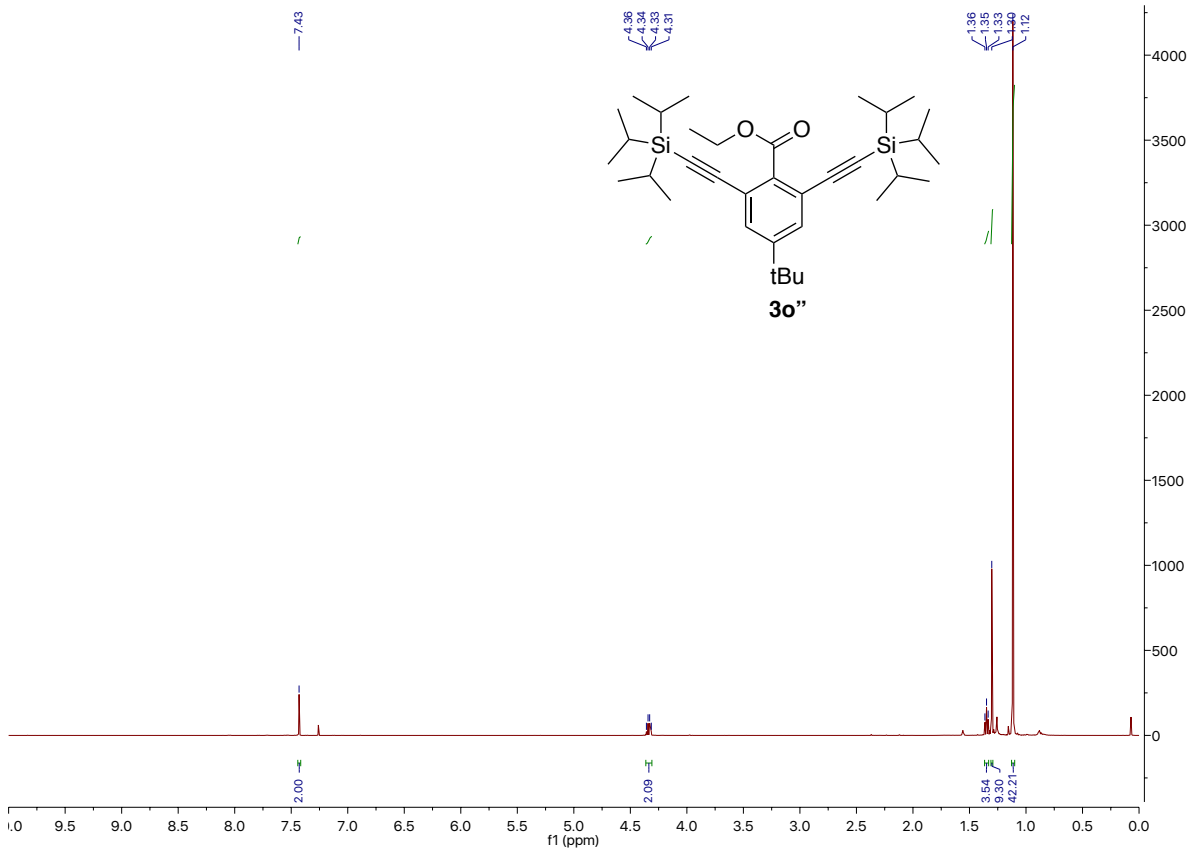


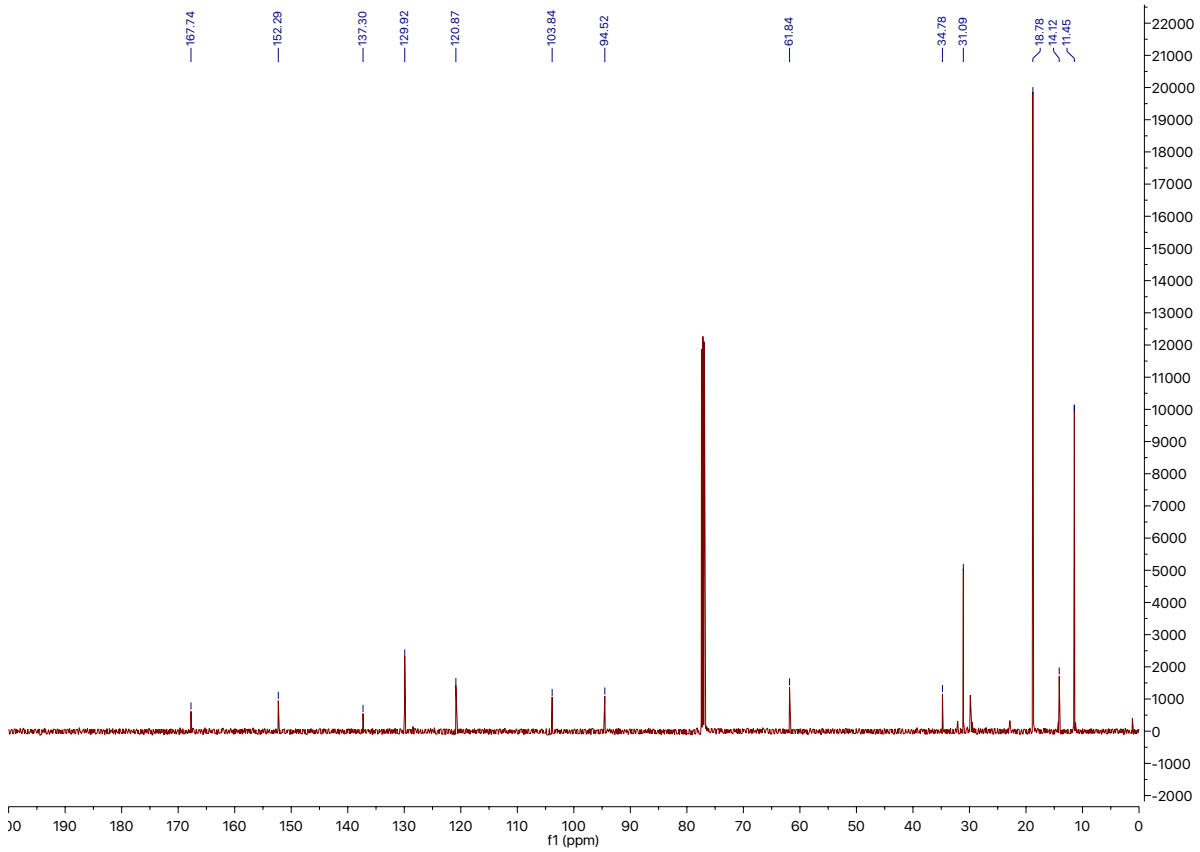
Ethyl 4-(tert-butyl)-2-((triisopropylsilyl)ethynyl)benzoate **(3o)**



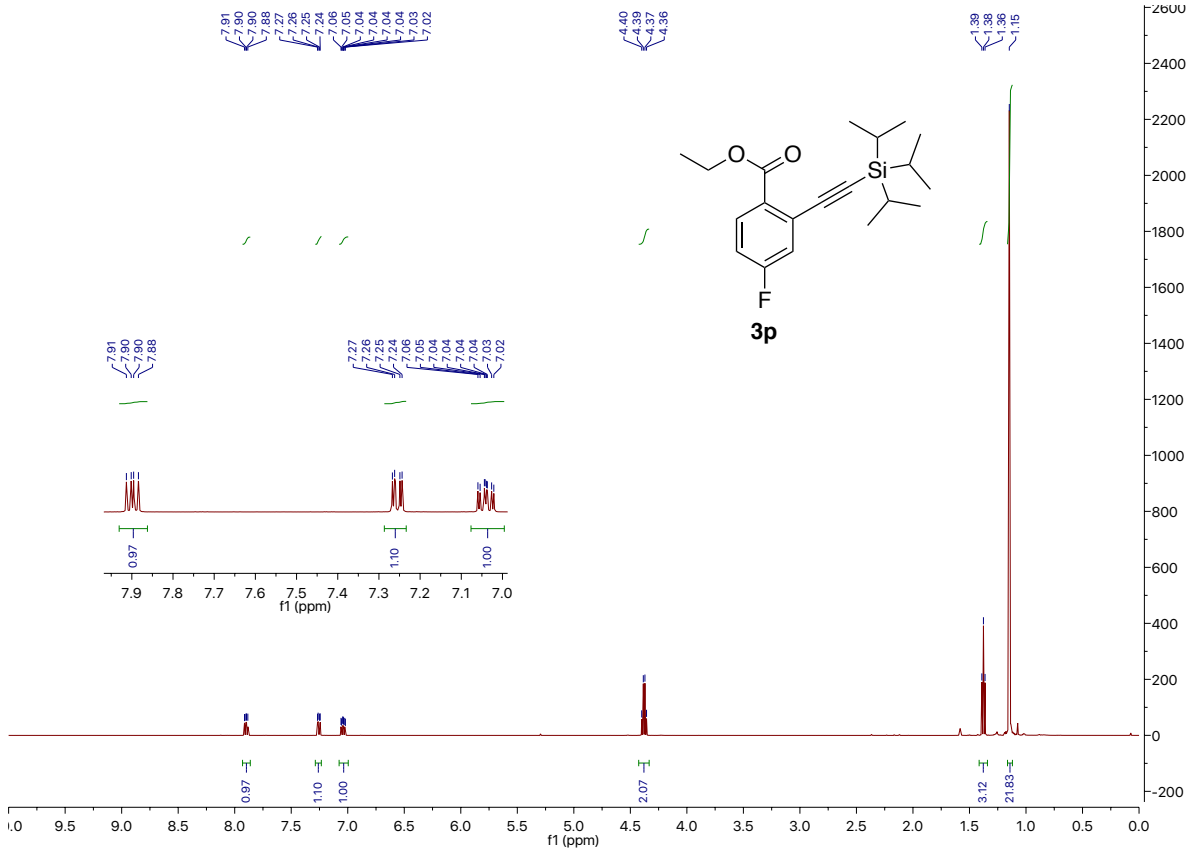


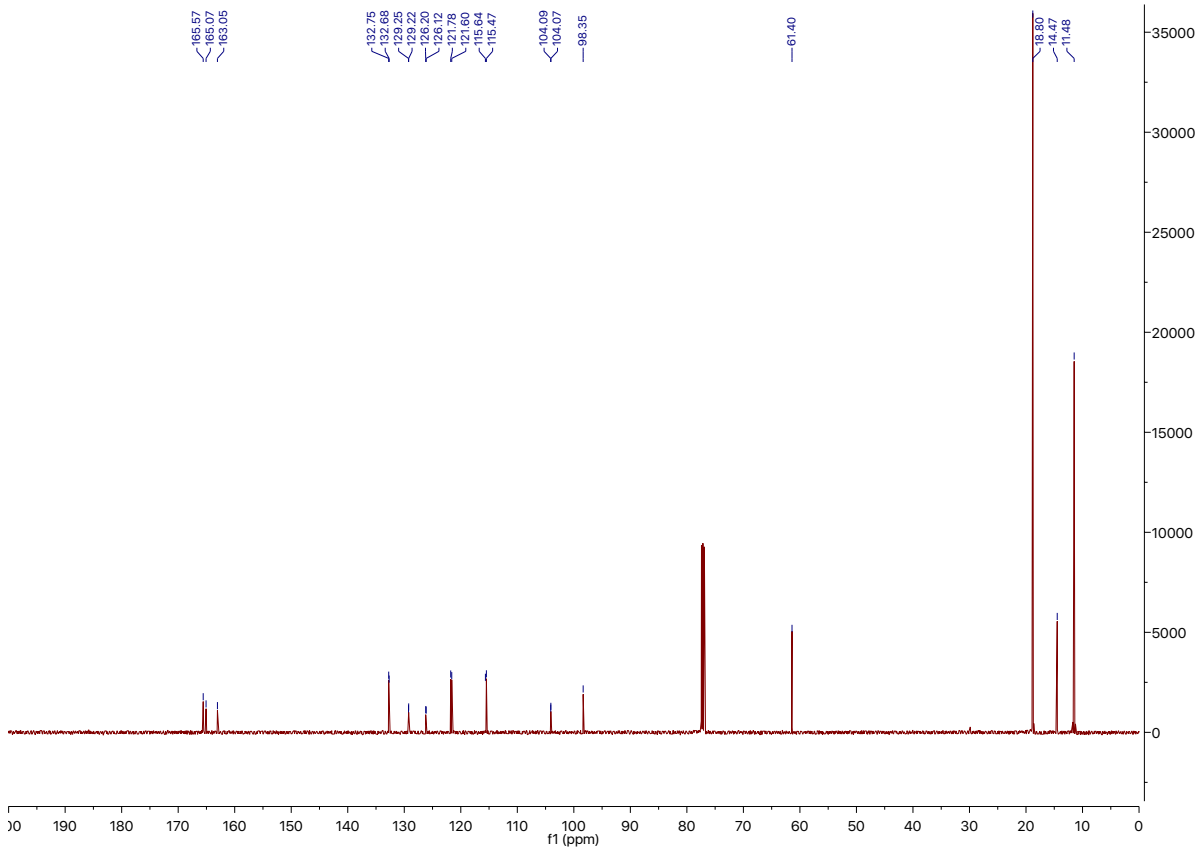
Ethyl 4-(tert-butyl)-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3o")**



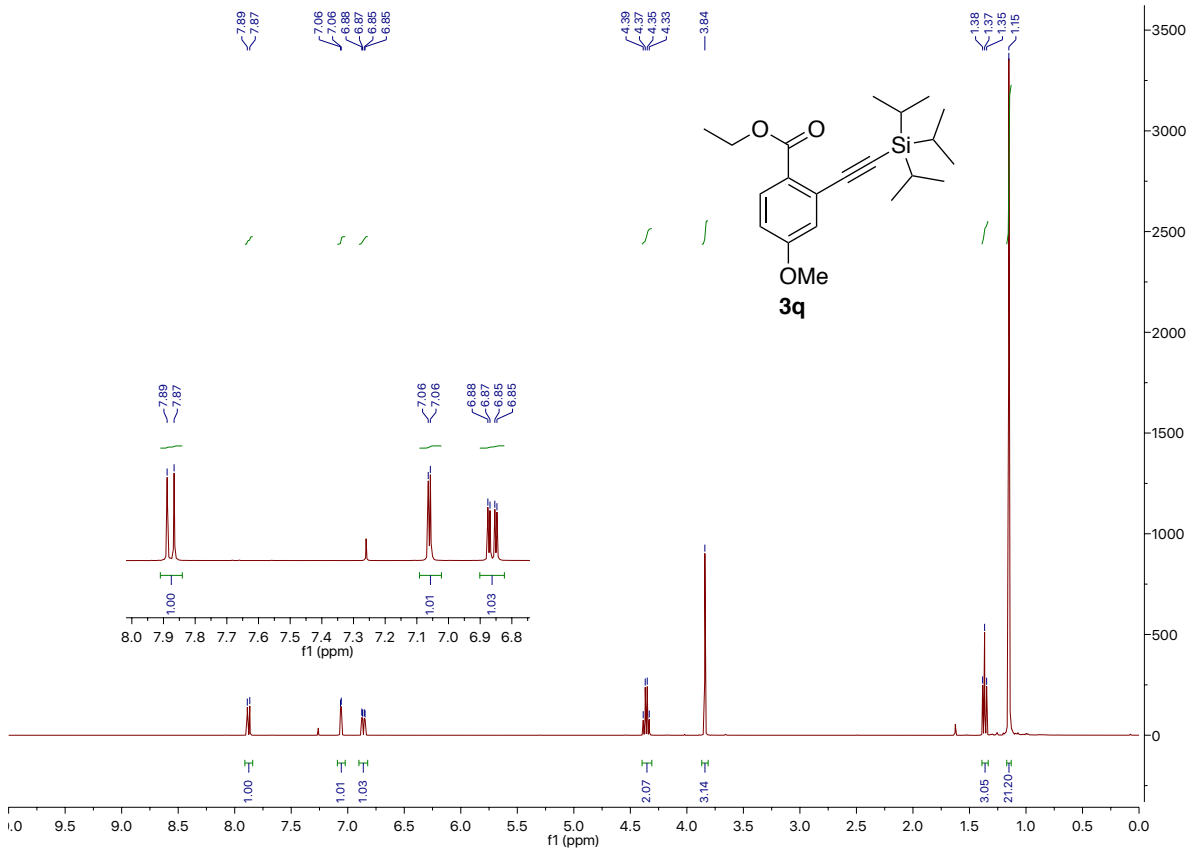


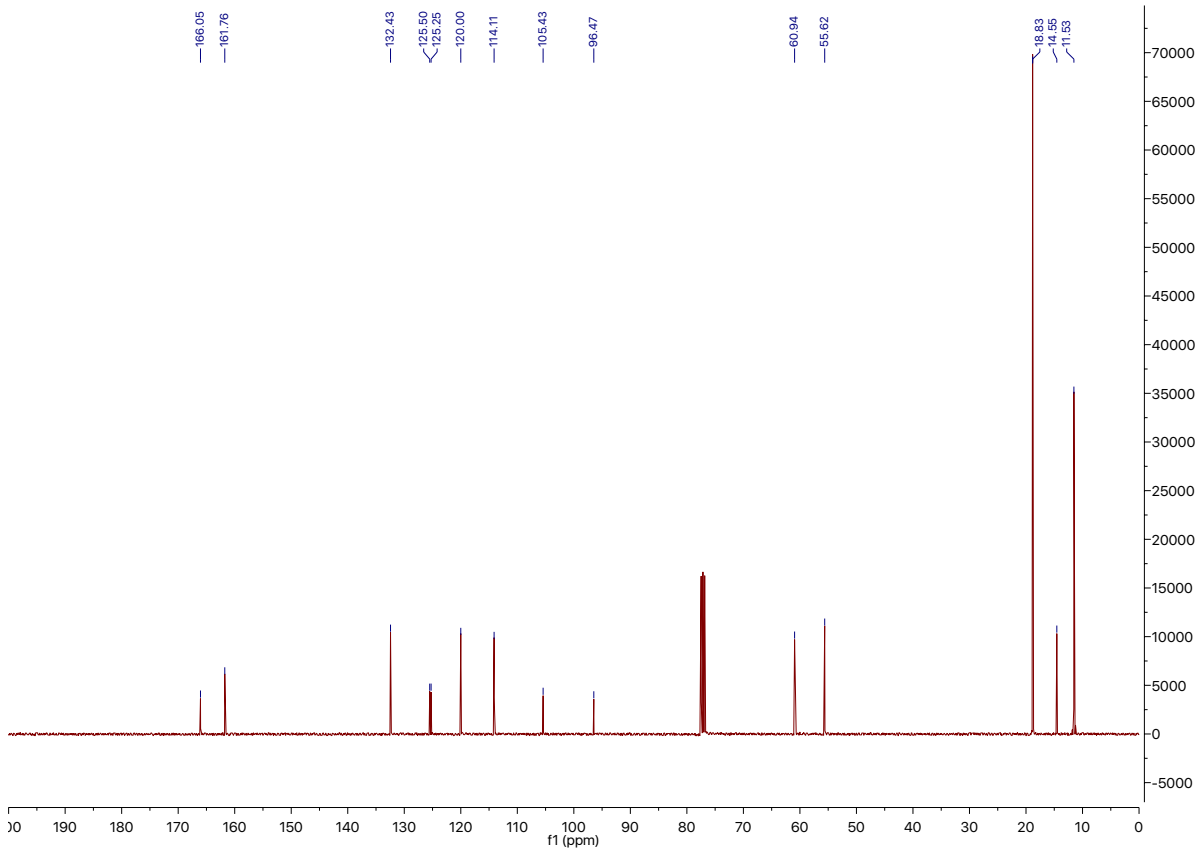
Ethyl 4-fluoro-2-((triisopropylsilyl)ethynyl)benzoate **(3p)**



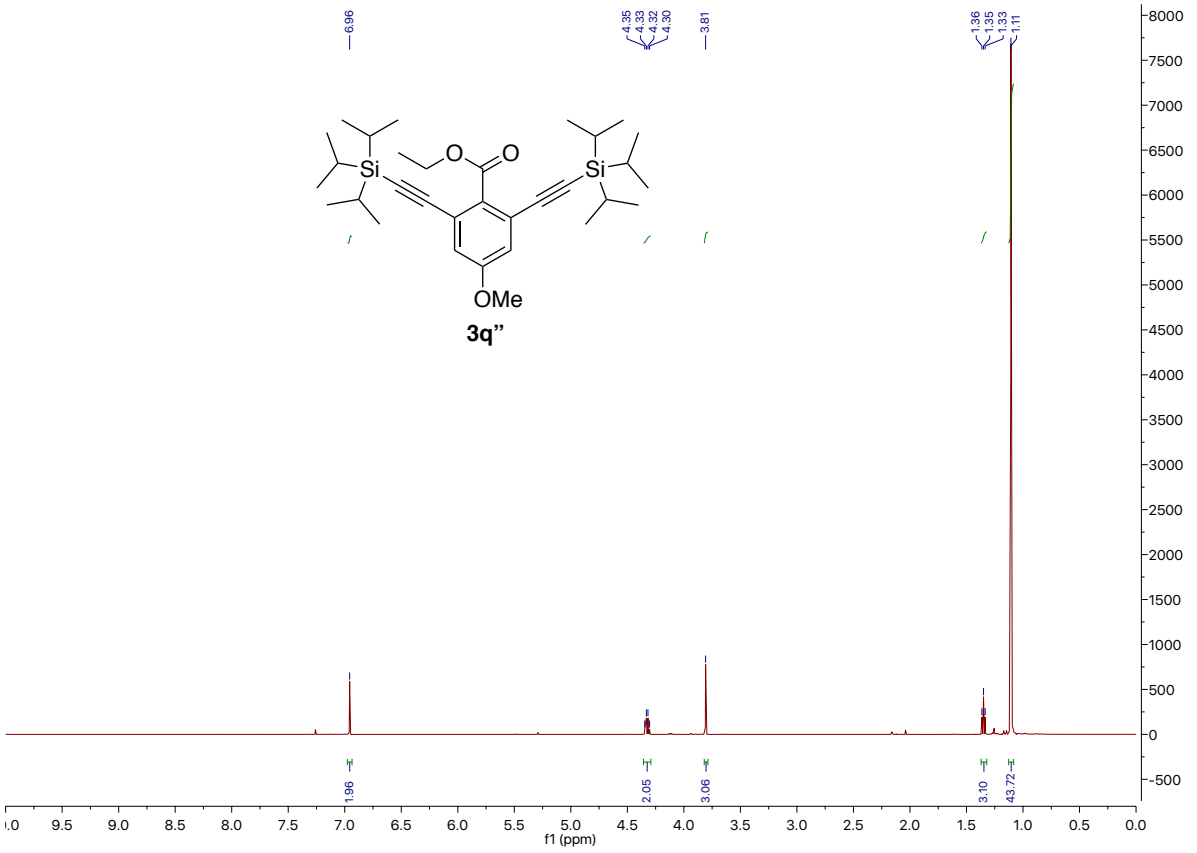


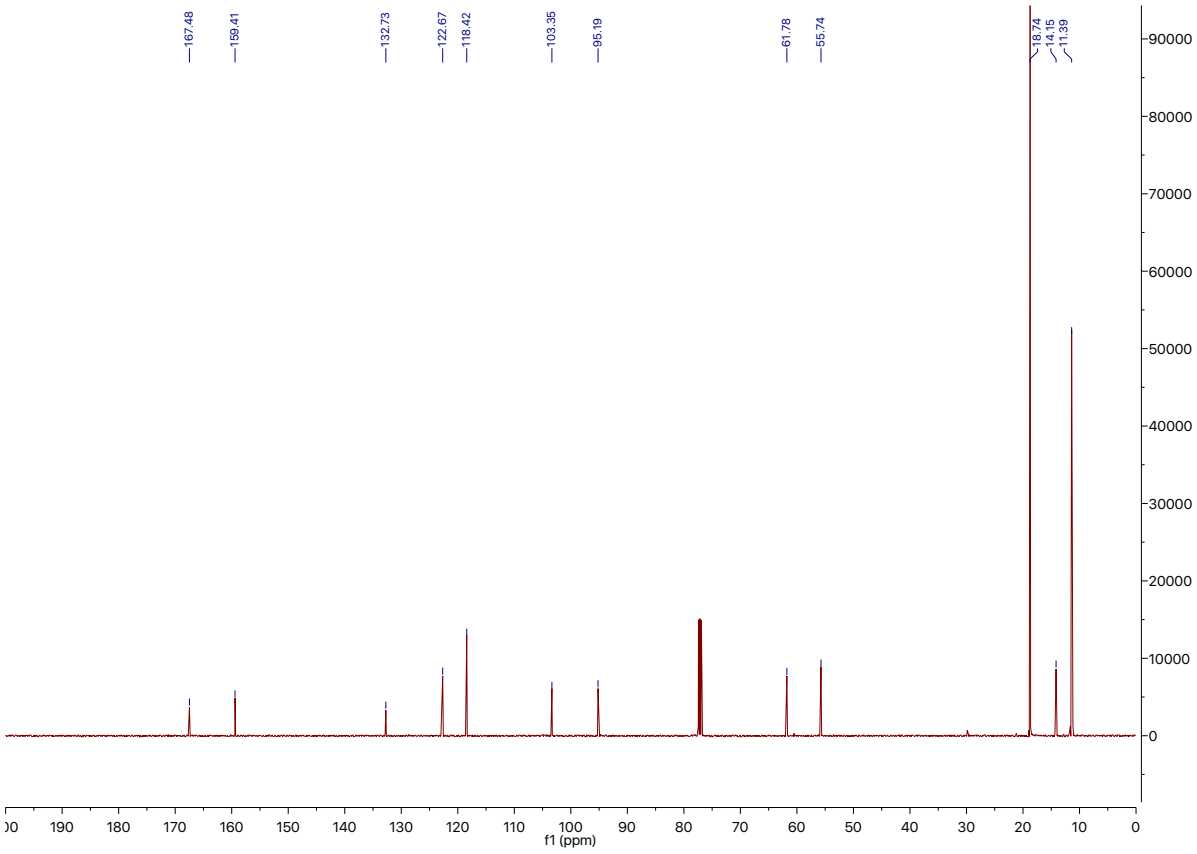
Ethyl 4-methoxy-2-((triisopropylsilyl)ethynyl)benzoate **(3q)**



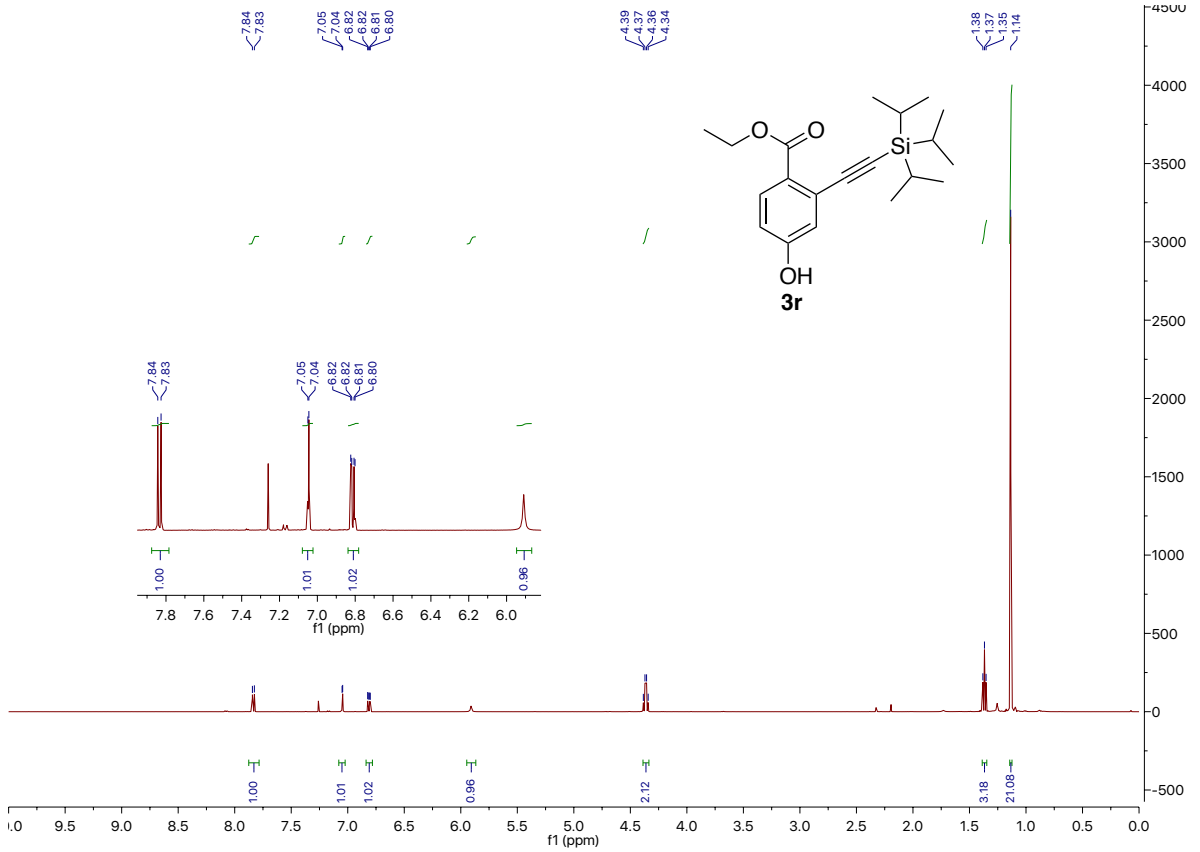


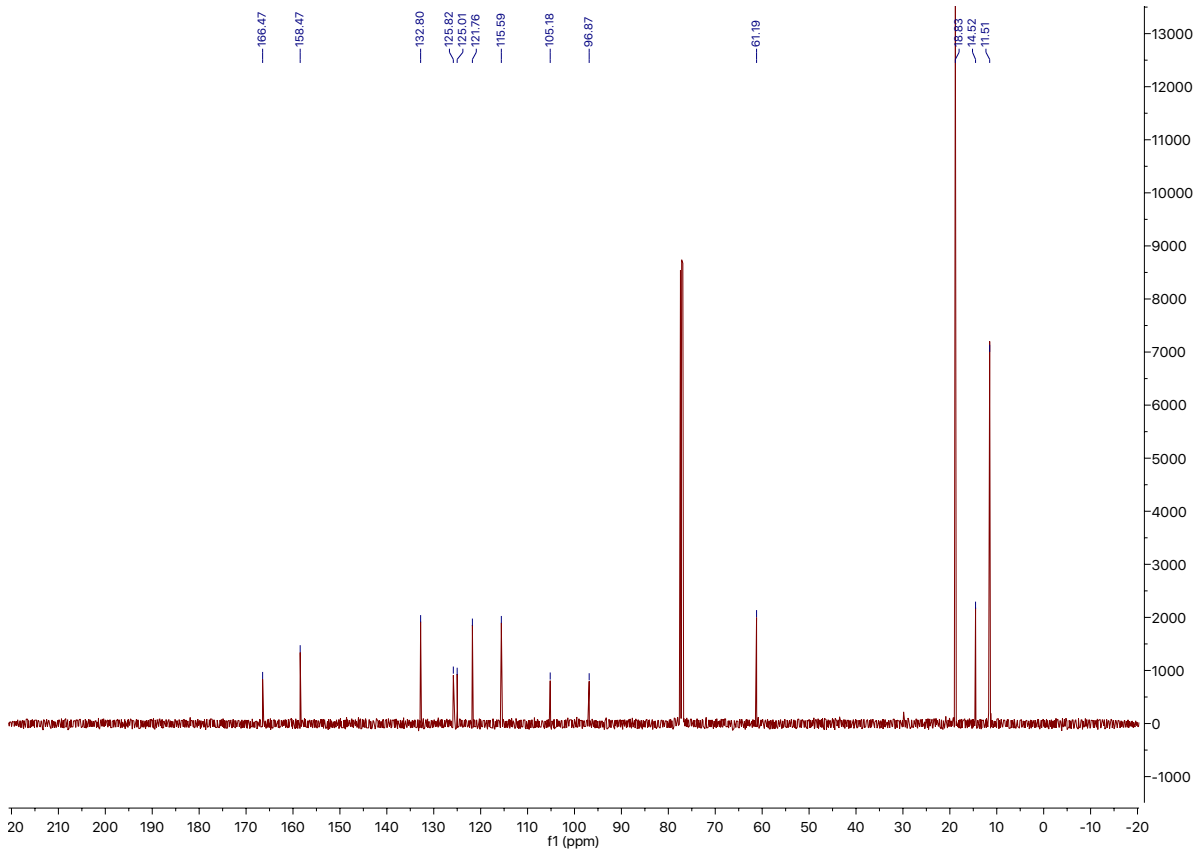
Ethyl 4-methoxy-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3q")**



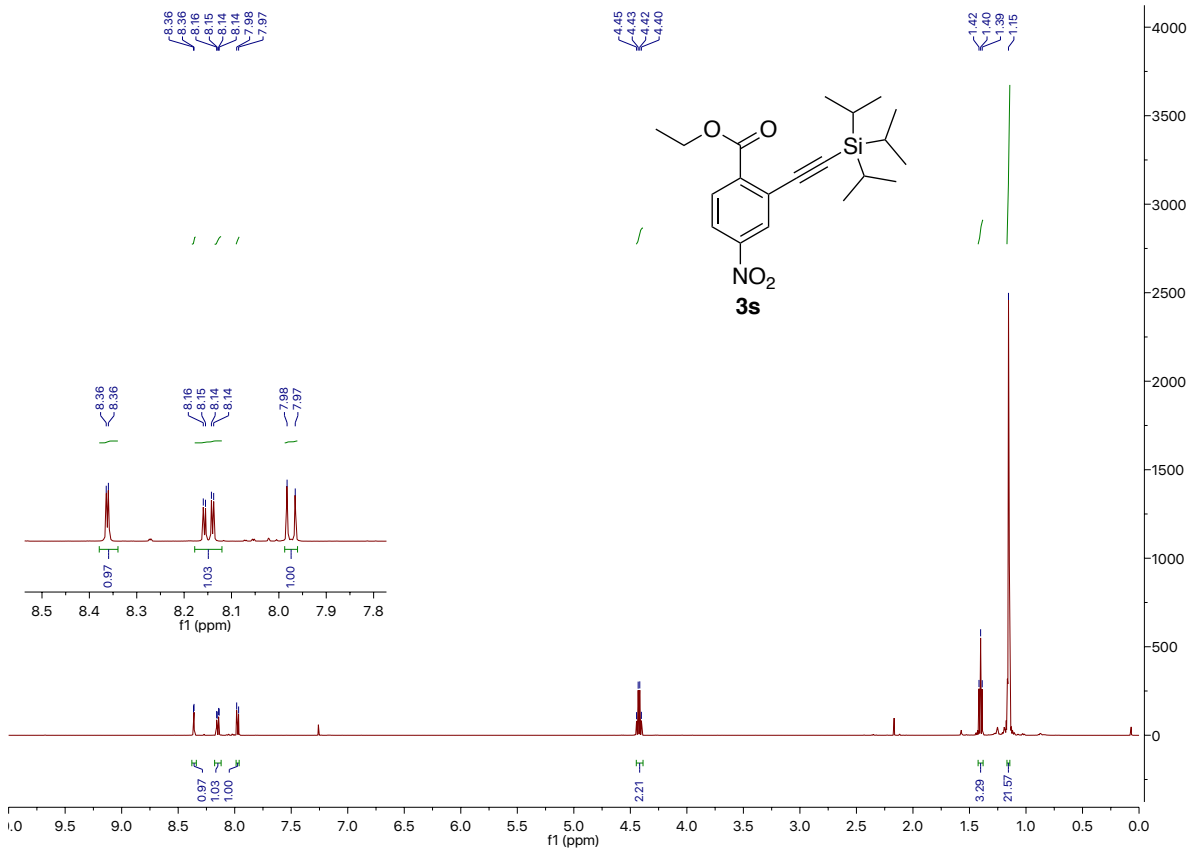


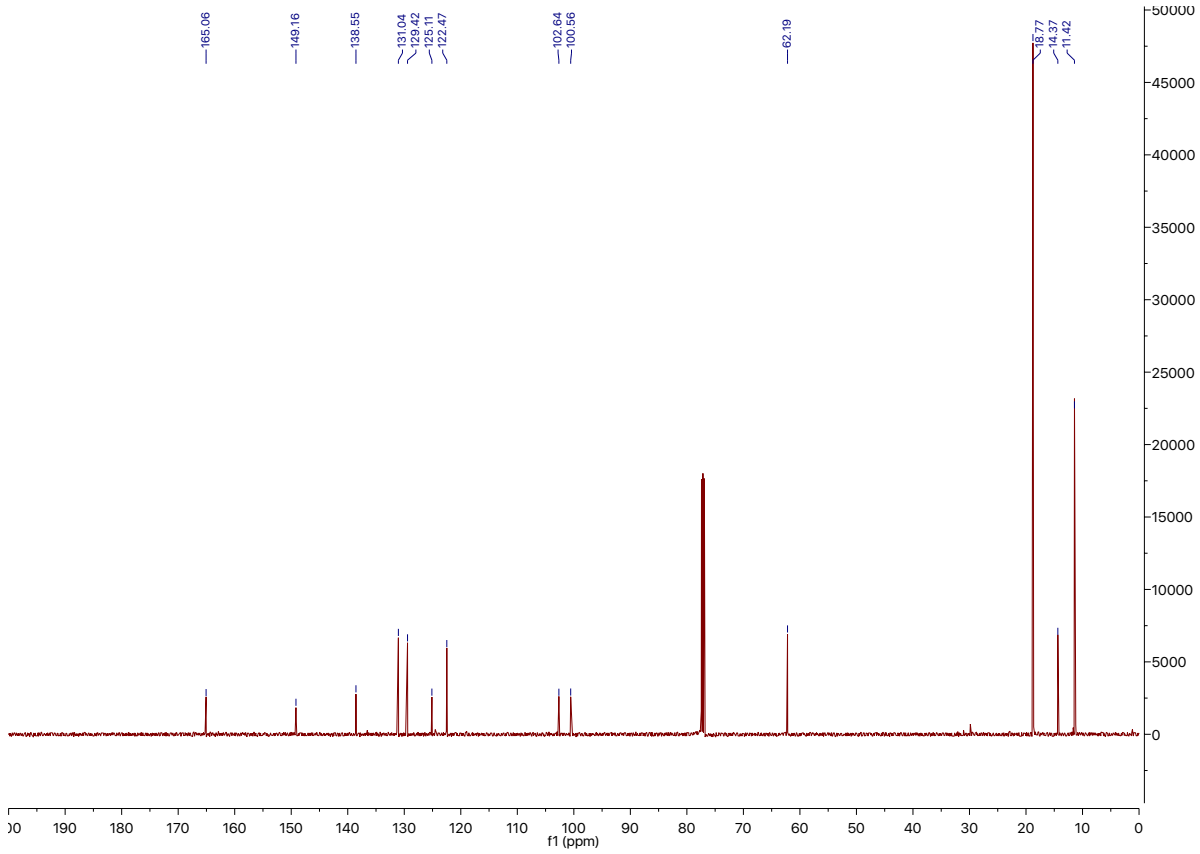
Ethyl 4-hydroxy-2-((triisopropylsilyl)ethynyl)benzoate **(3r)**



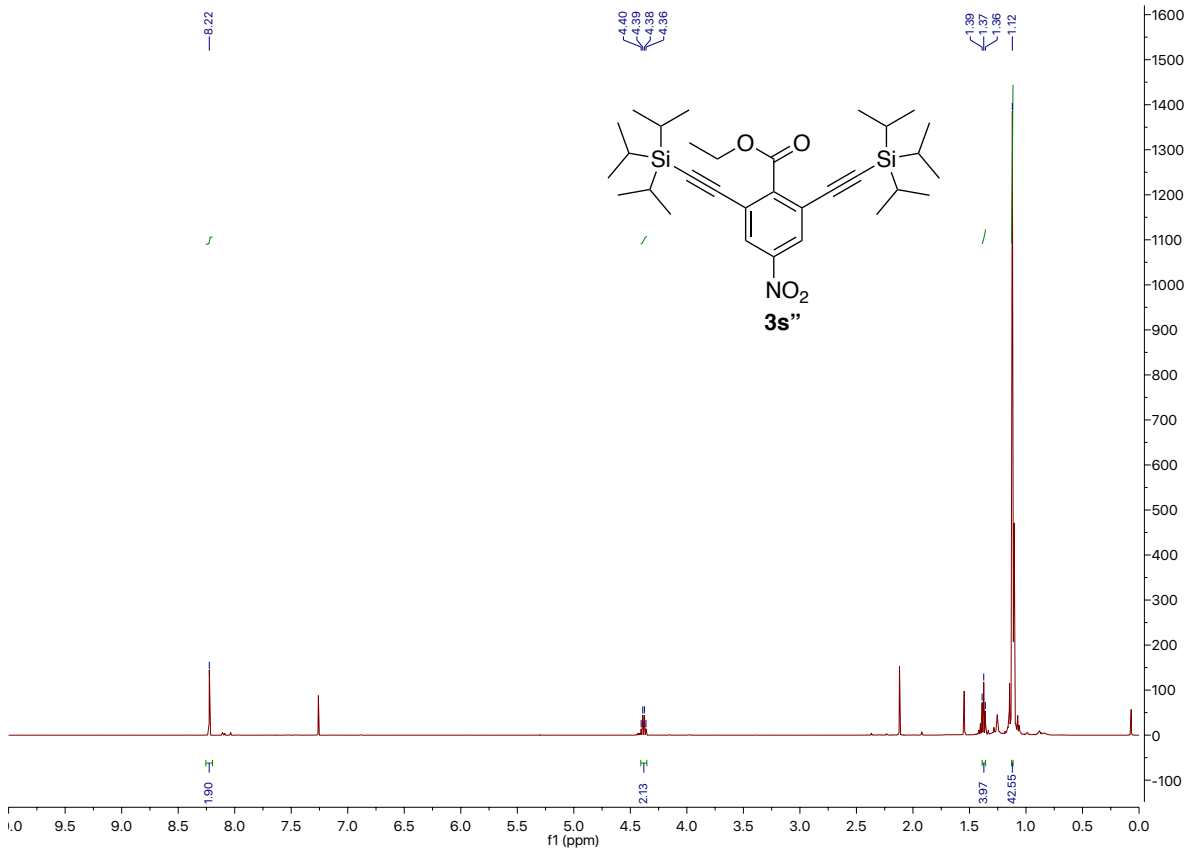


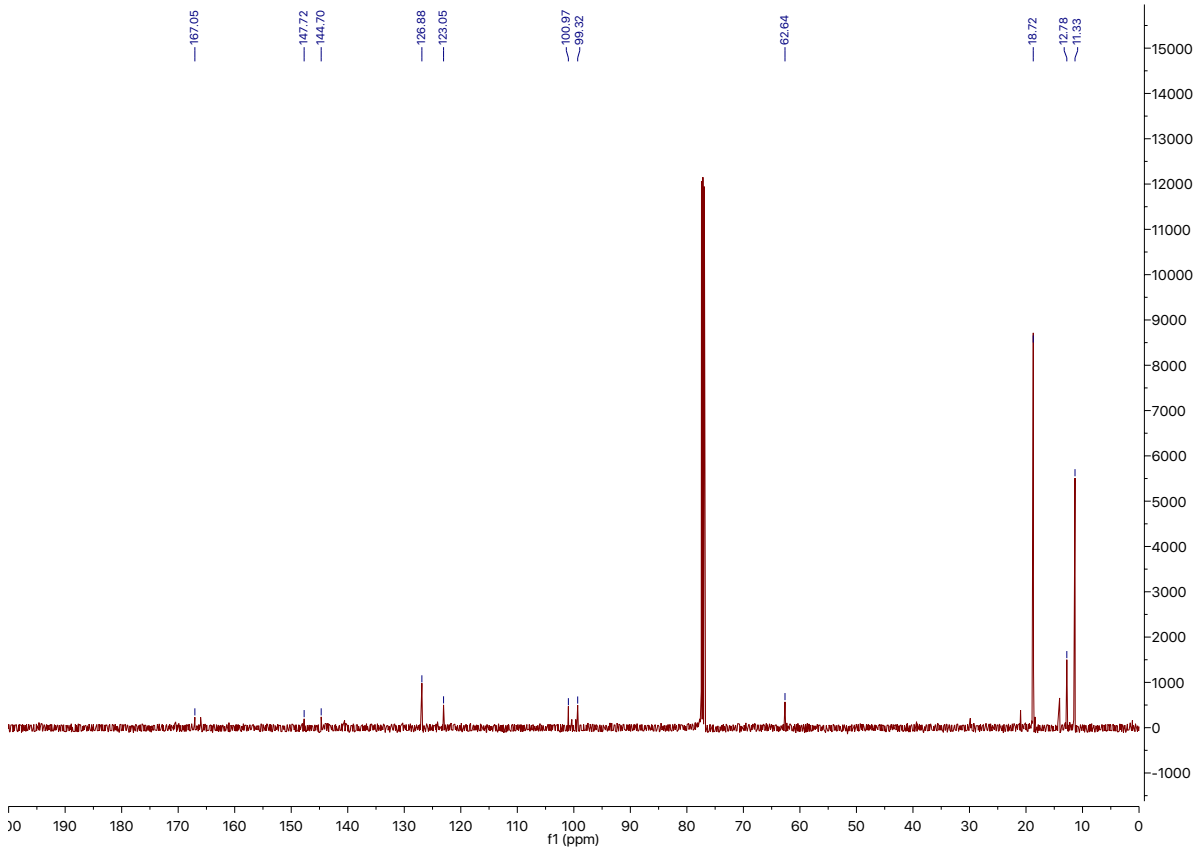
Ethyl 4-nitro-2-((triisopropylsilyl)ethynyl)benzoate **(3s)**



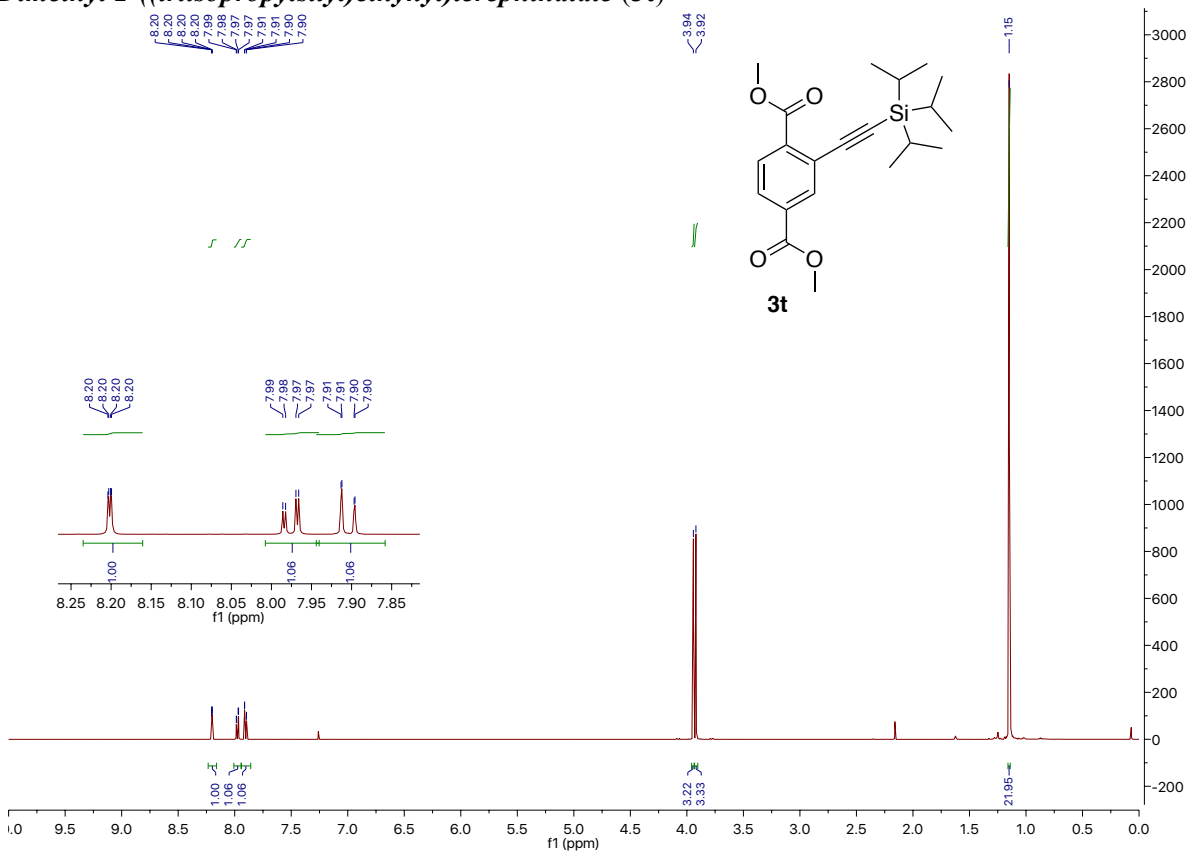


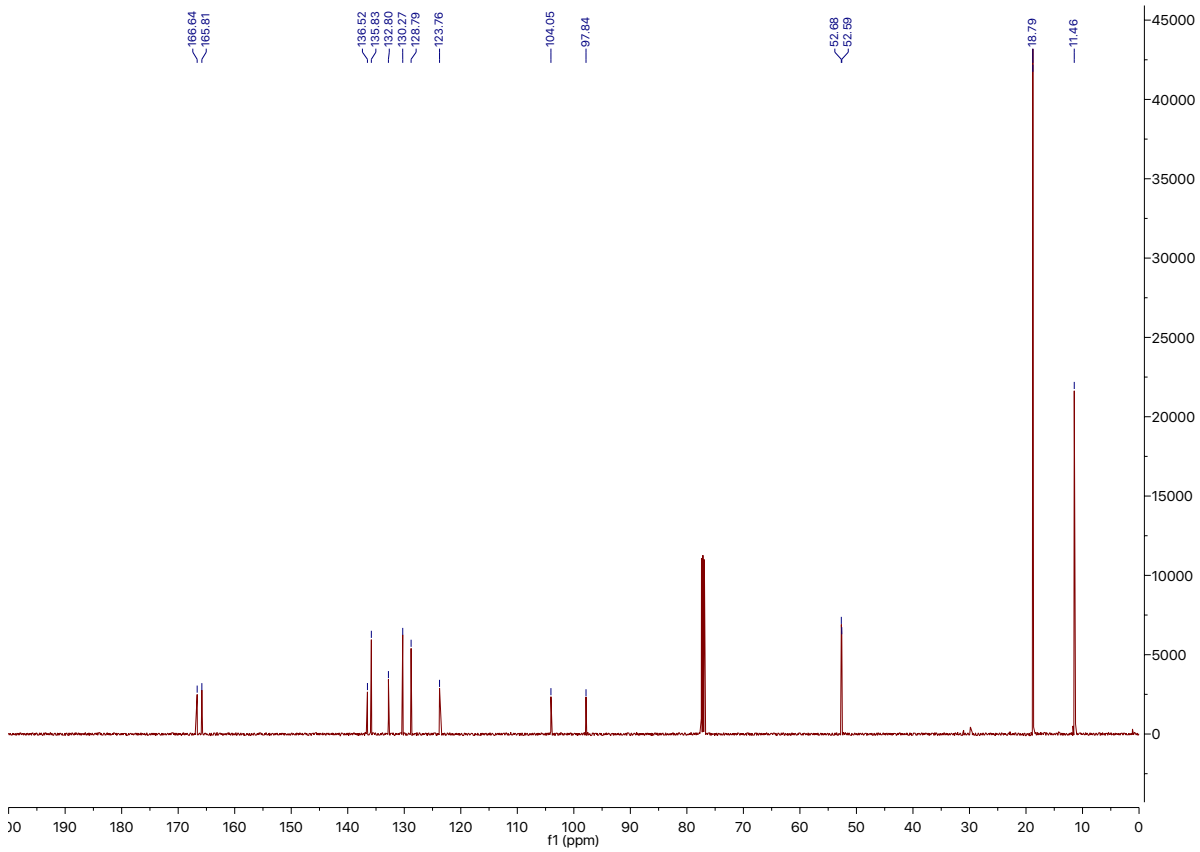
Ethyl 4-nitro-2,6-bis((triisopropylsilyl)ethynyl)benzoate **(3s")**



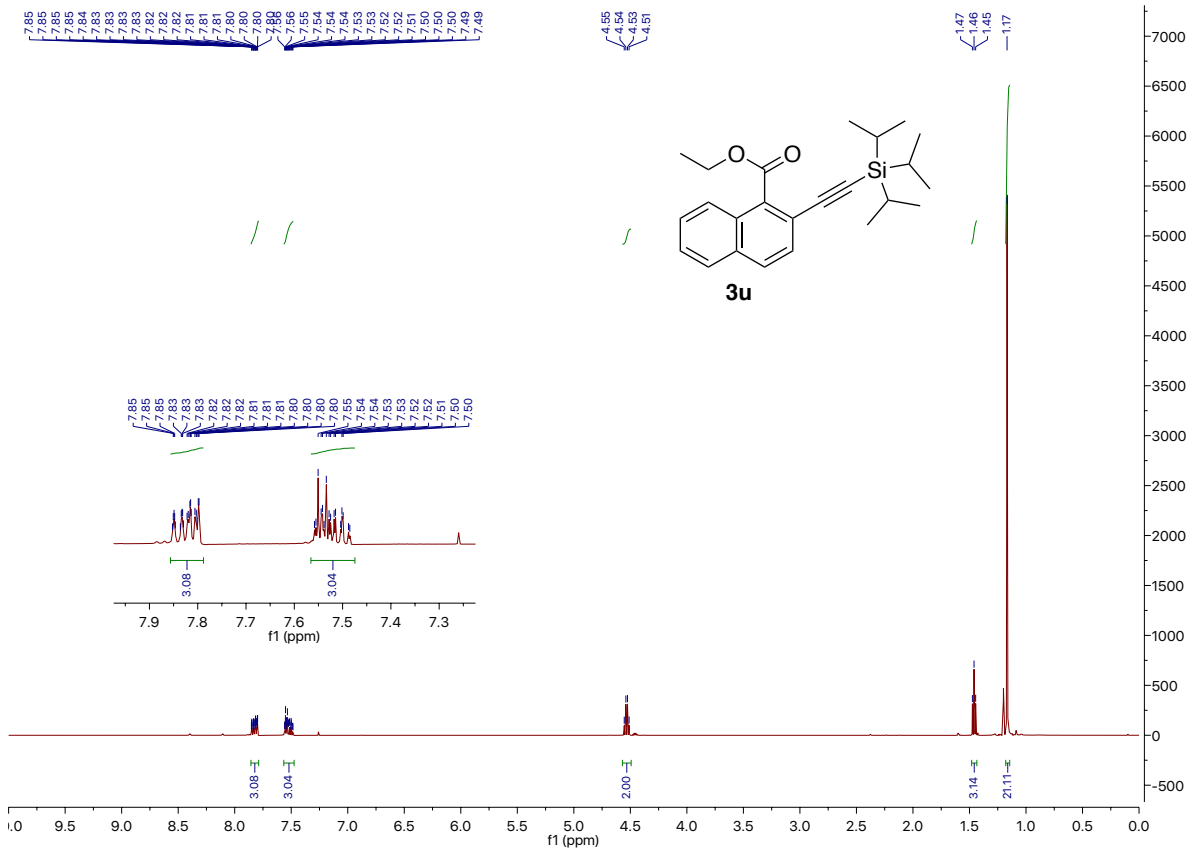


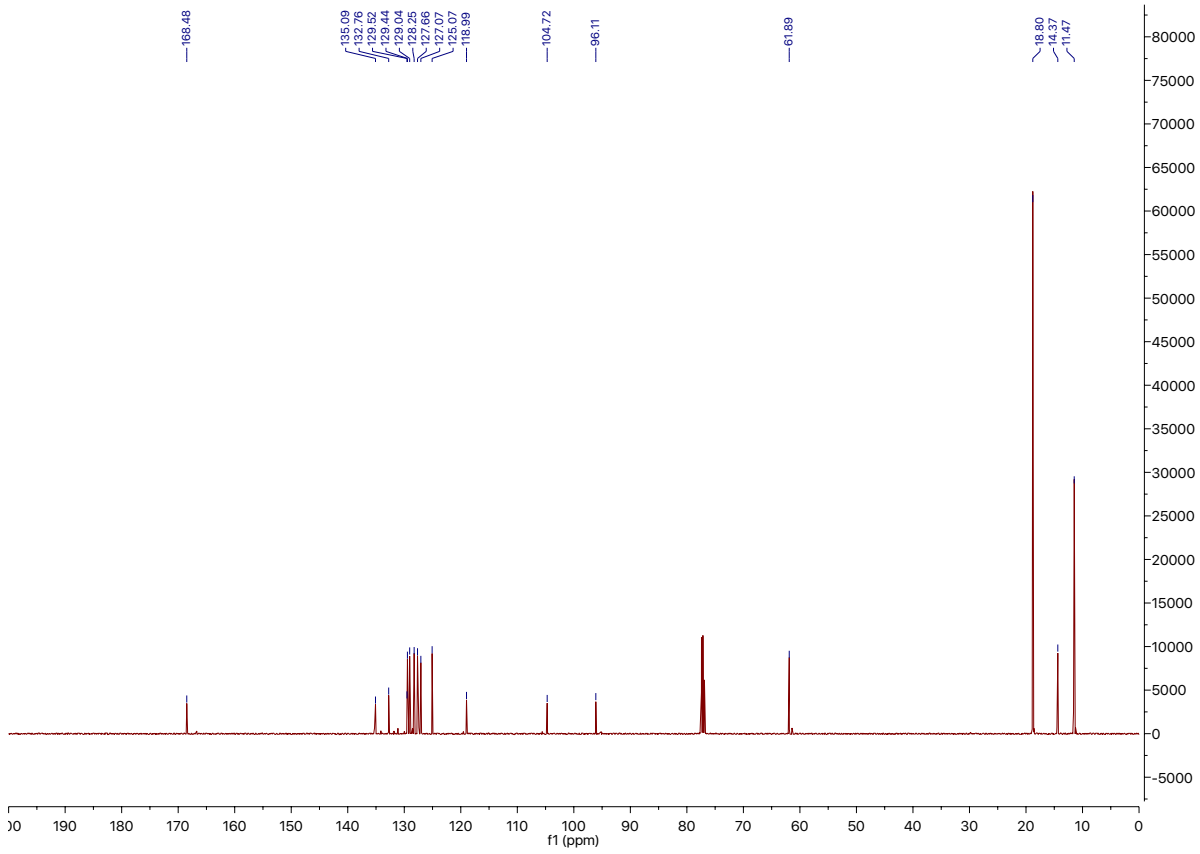
***Dimethyl 2-((triisopropylsilyl)ethynyl)terephthalate* (3t)**



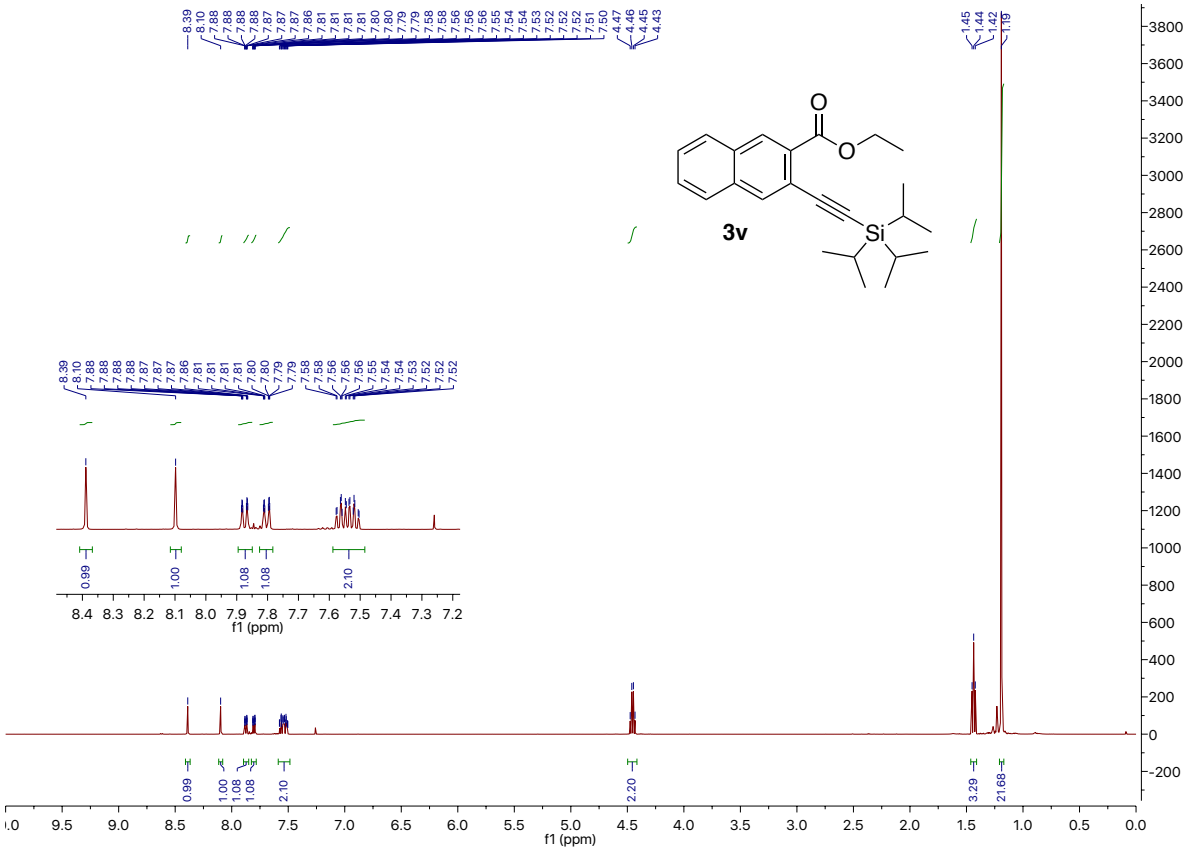


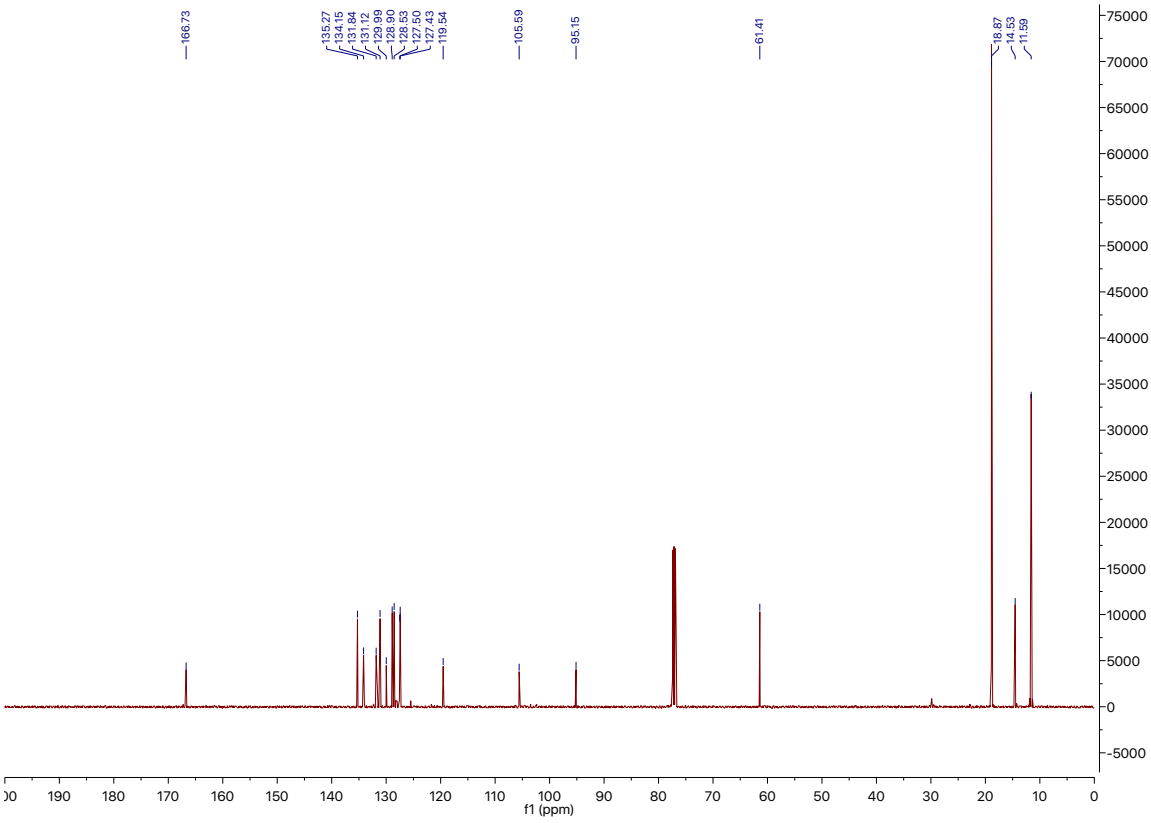
***Ethyl 2-((triisopropylsilyl)ethynyl)-1-naphthoate* (3u)**



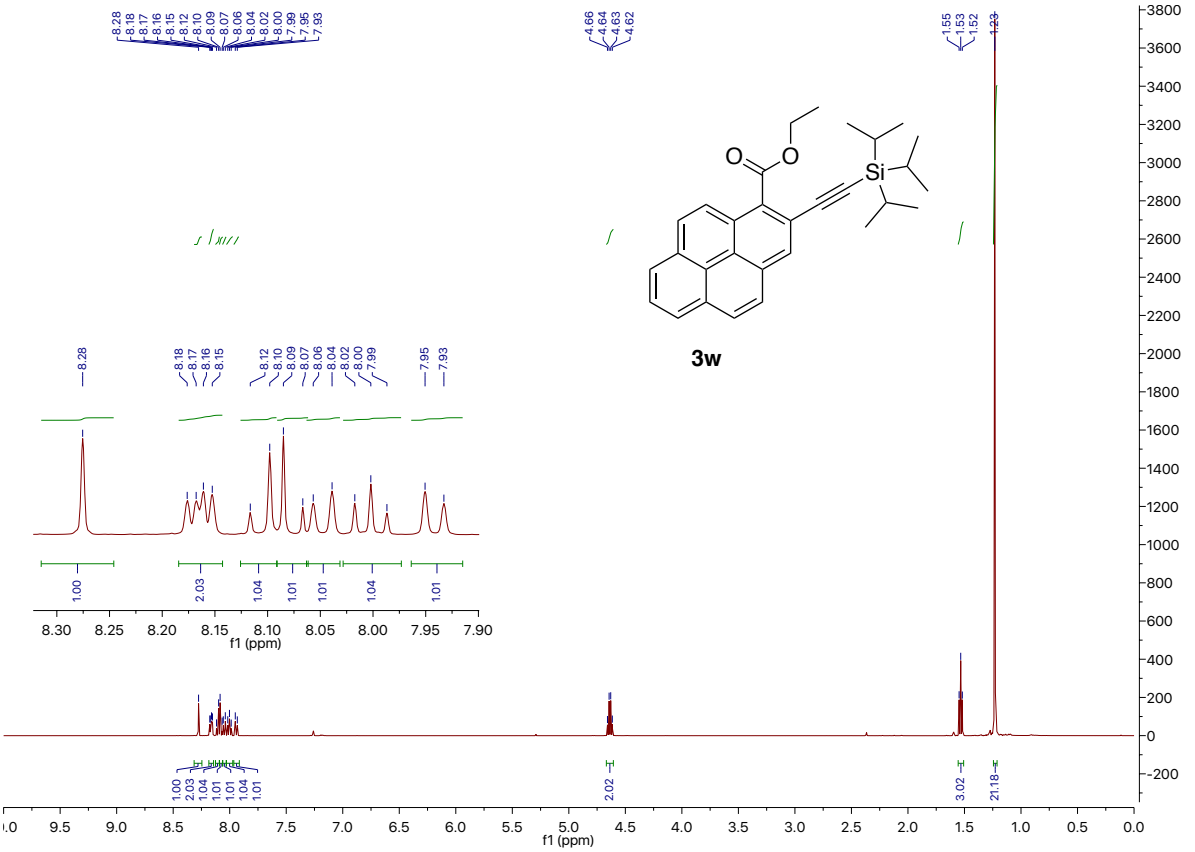


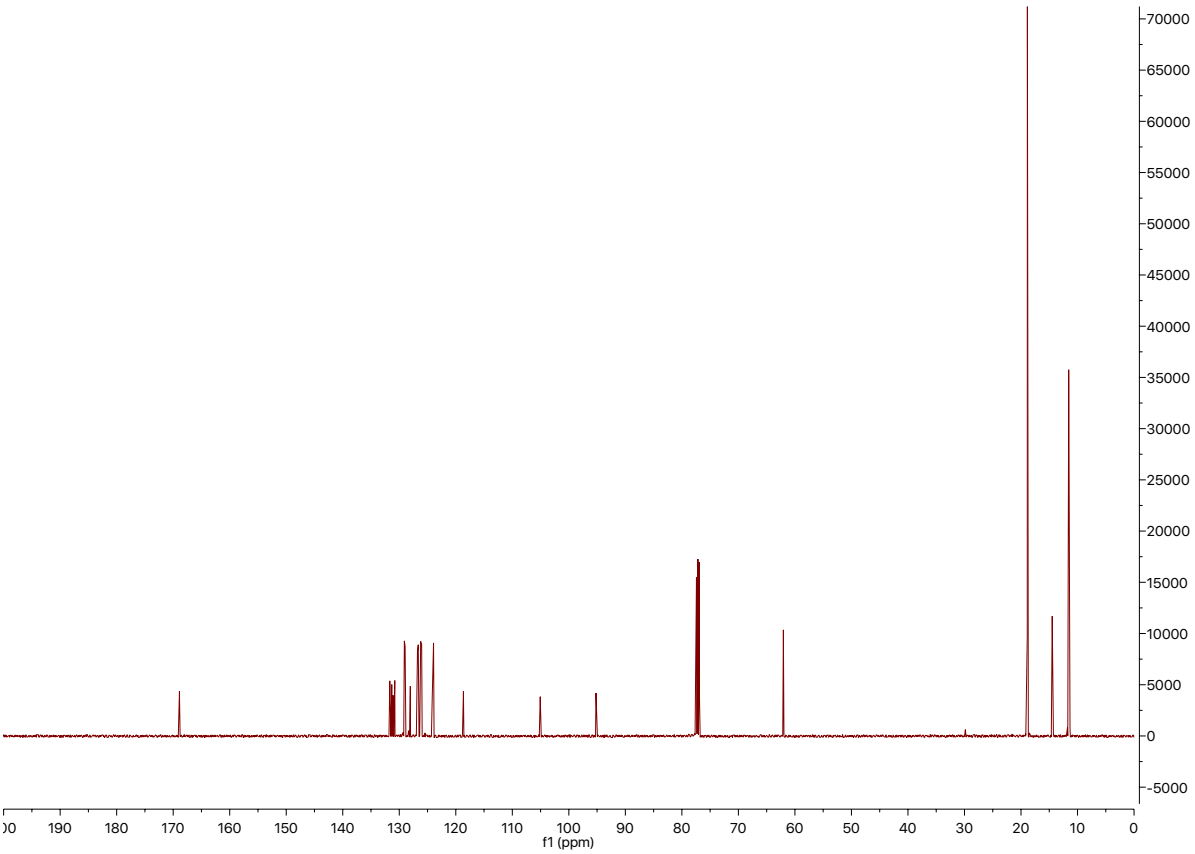
***Ethyl 3-((triisopropylsilyl)ethynyl)-2-naphthoate* (3v)**



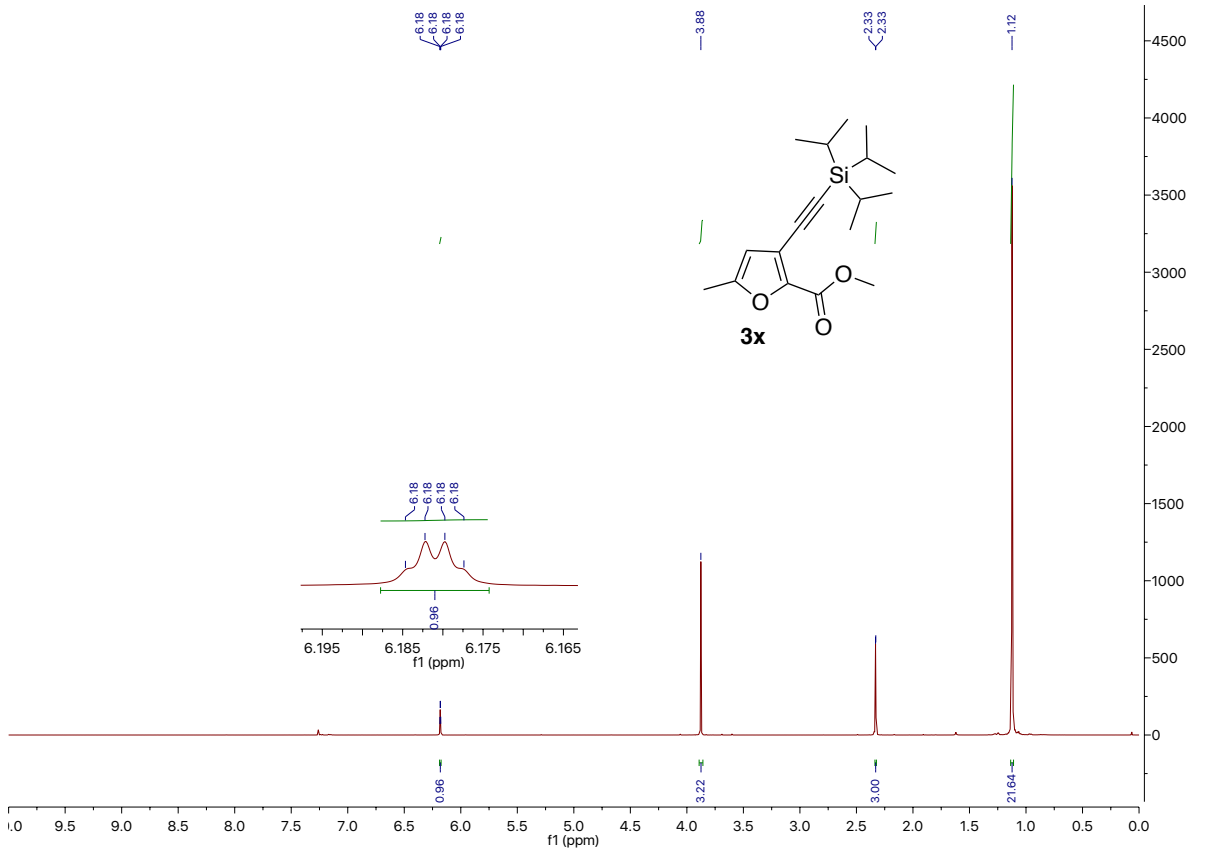


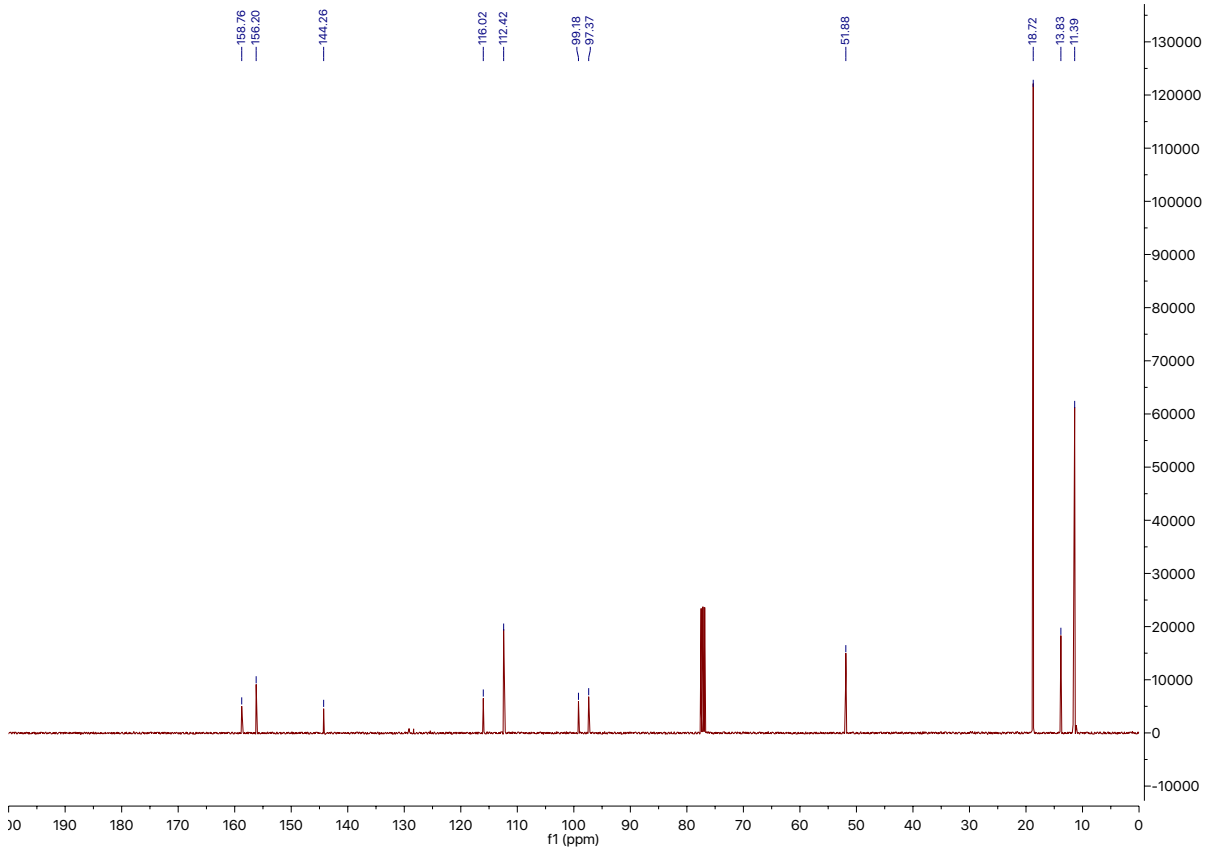
***Ethyl 5-((triisopropylsilyl)ethynyl)-5a1,10-dihydropyrene-4-carboxylate* (3w)**



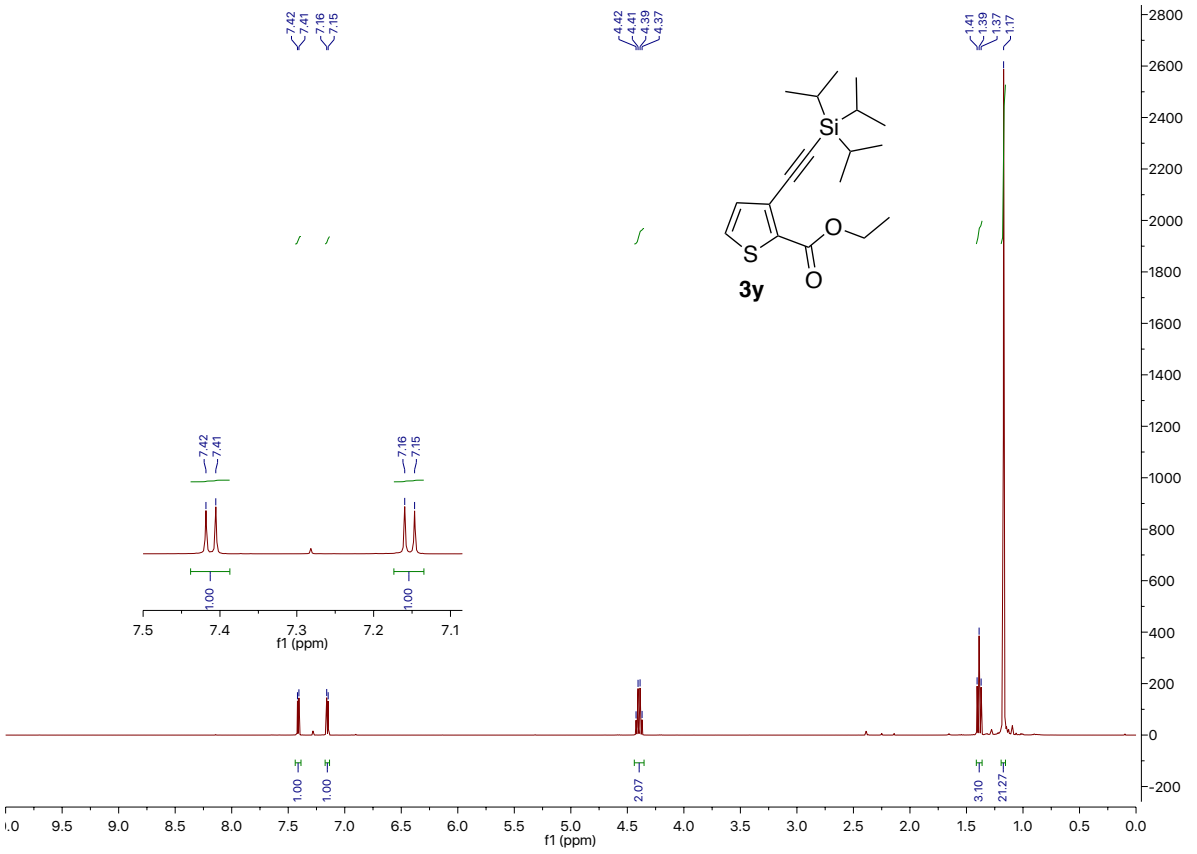


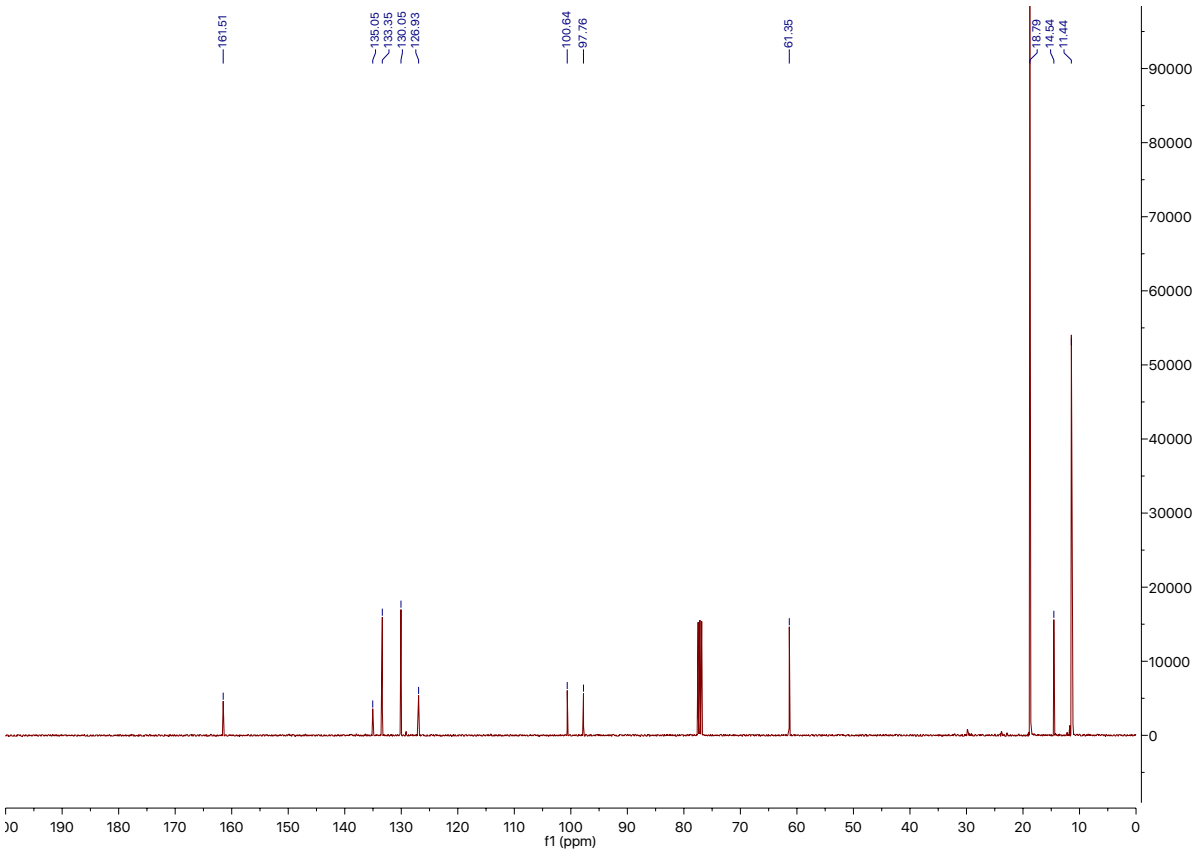
***Methyl 5-methyl-3-((triisopropylsilyl)ethynyl)furan-2-carboxylate* (3x)**



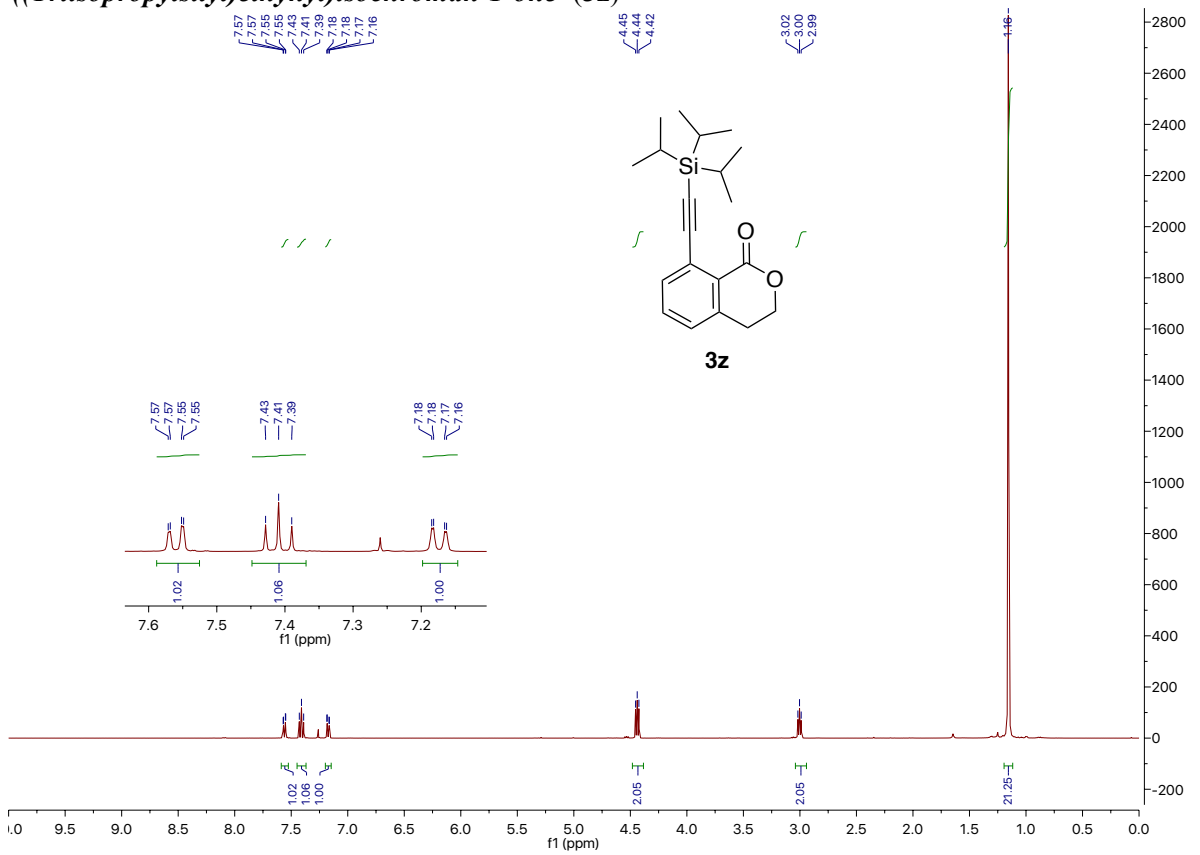


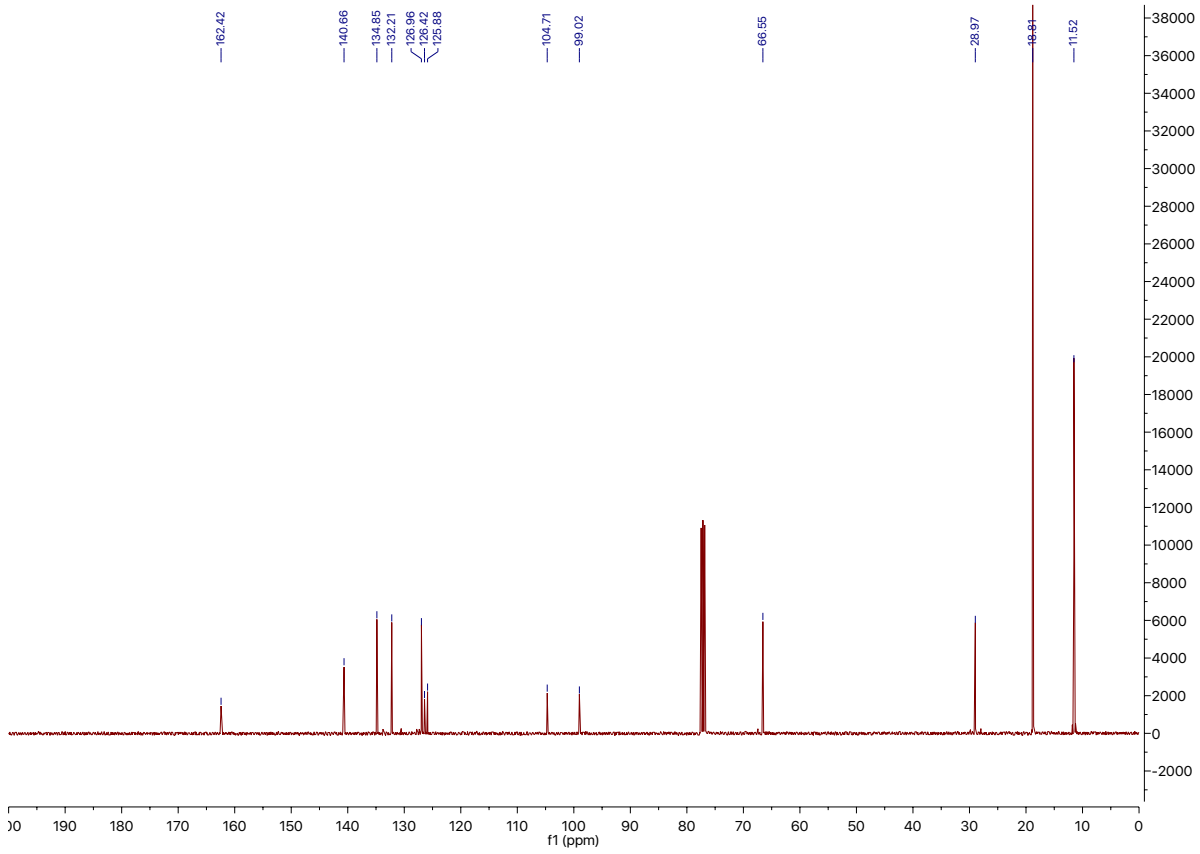
***Methyl 3-((triisopropylsilyl)ethynyl)thiophene-2-carboxylate* (3y)**



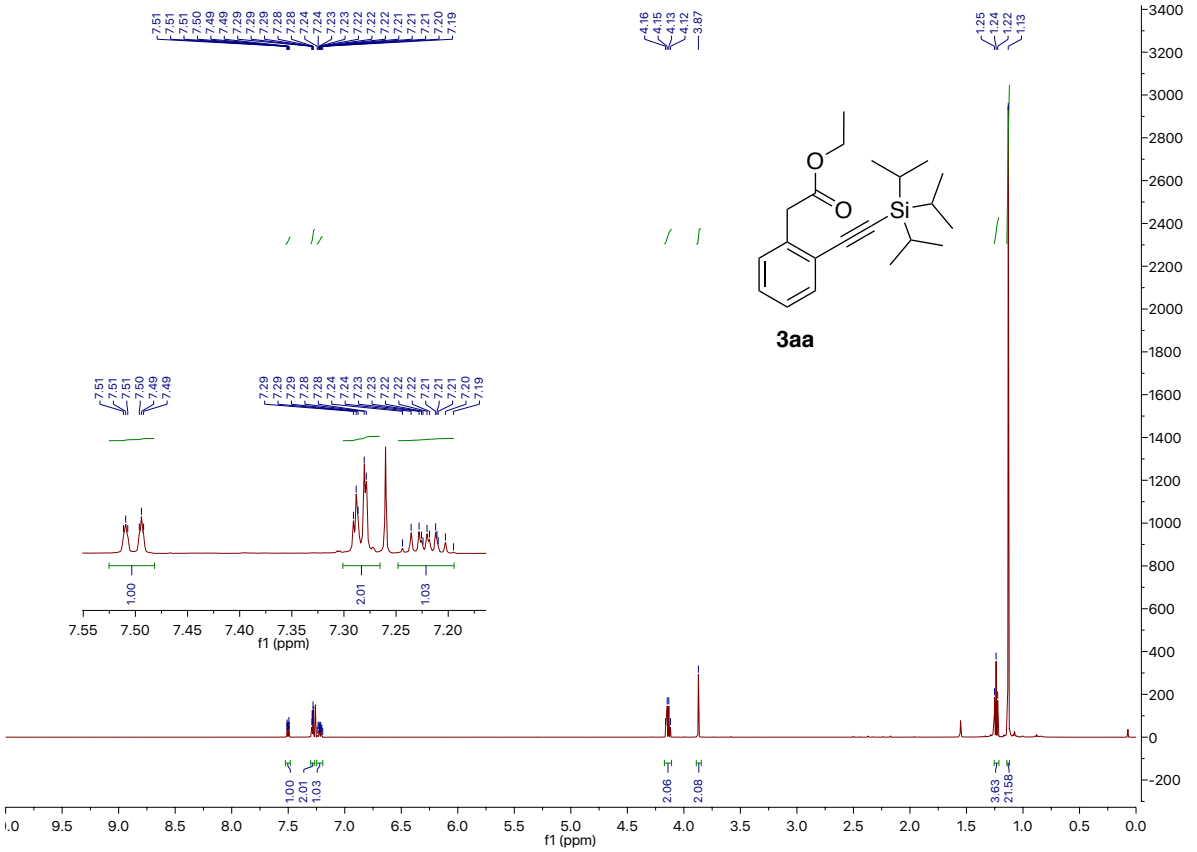


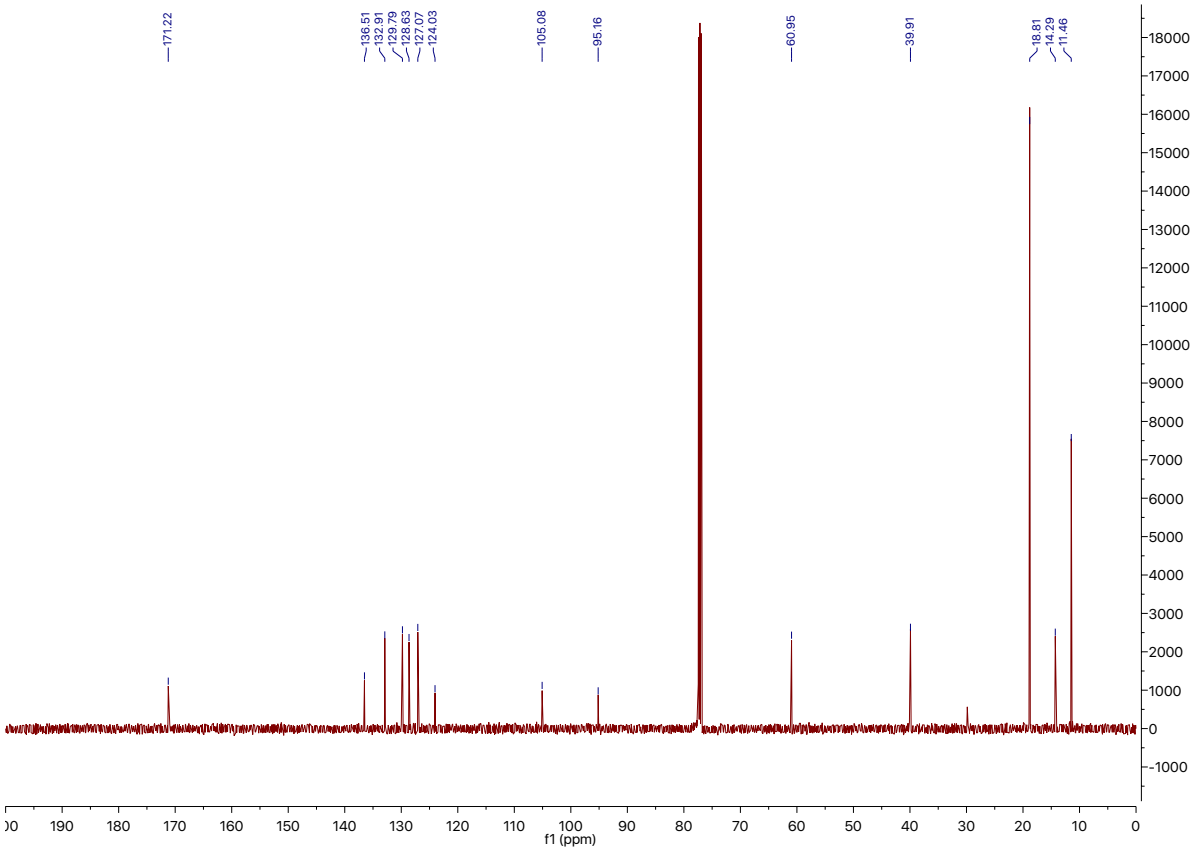
***8-((Triisopropylsilyl)ethynyl)isochroman-1-one* (3z)**



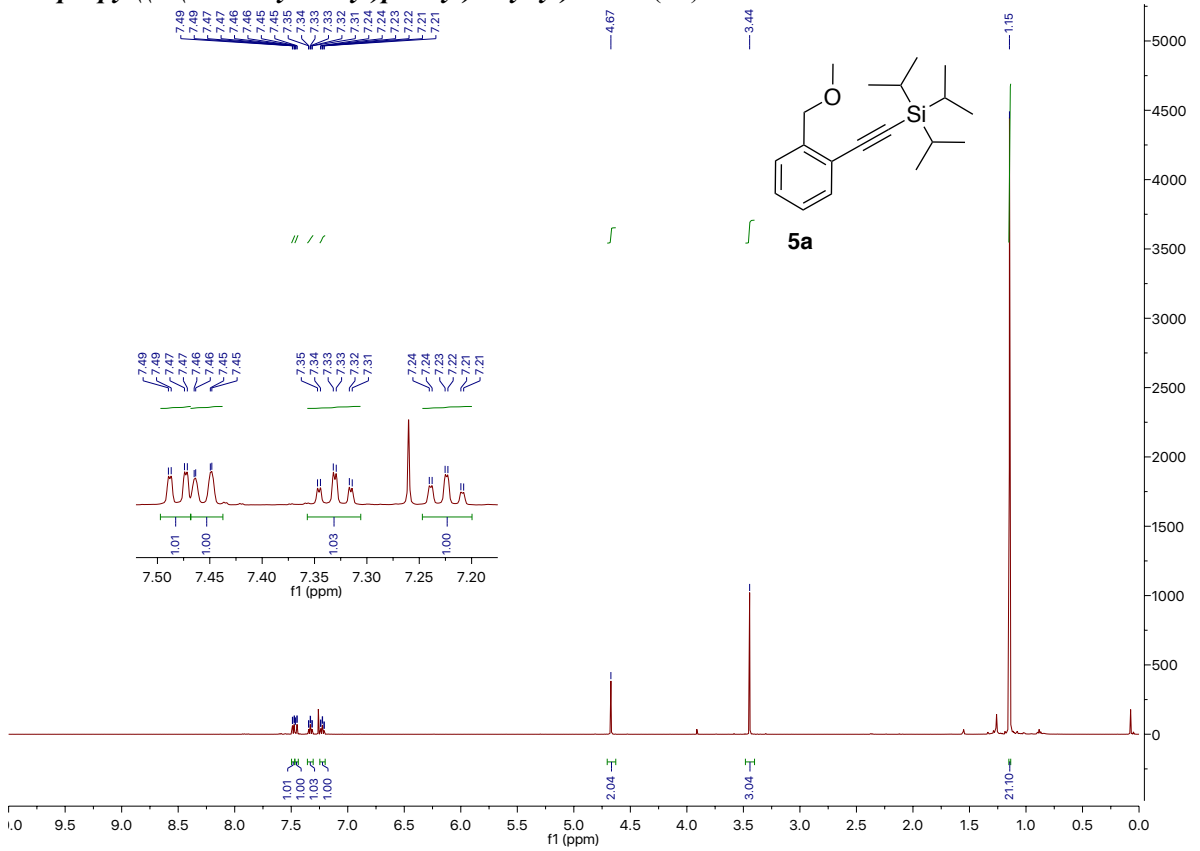


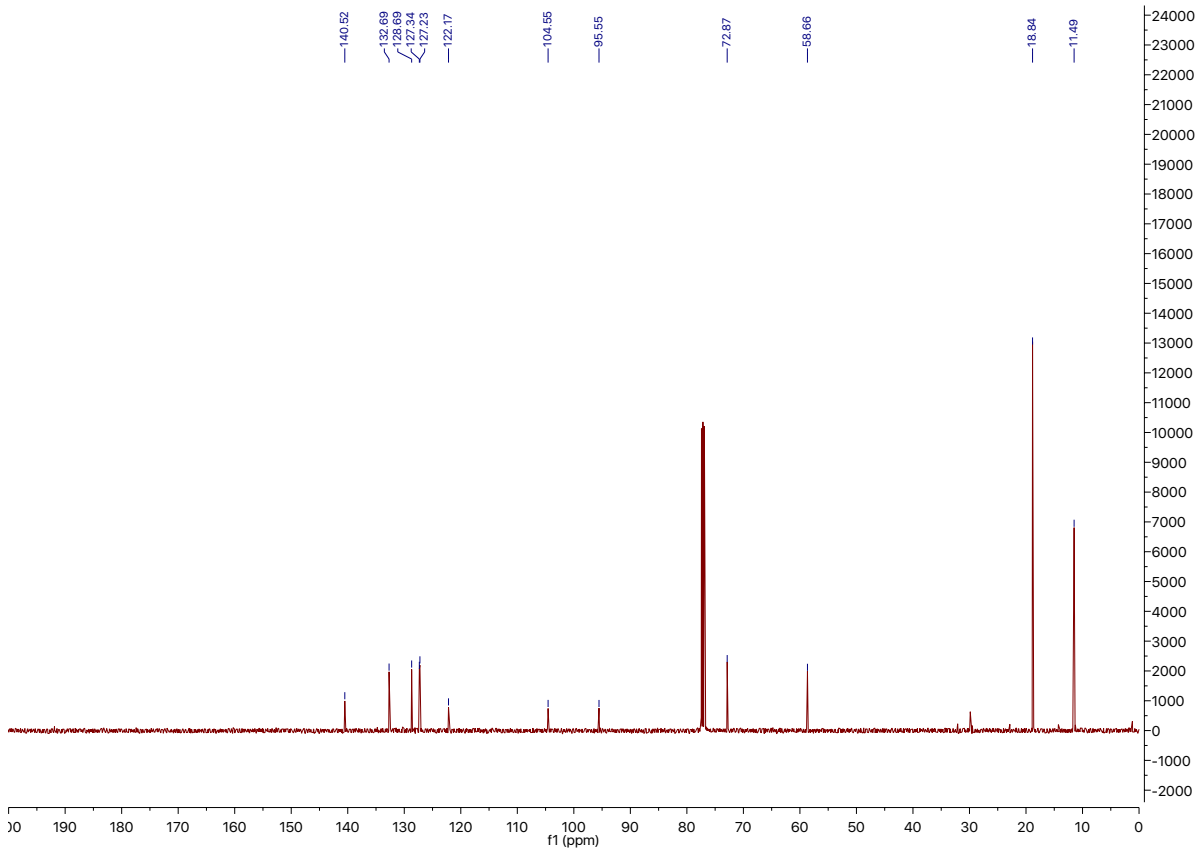
Ethyl 2-(2-((triisopropylsilyl)ethynyl)phenyl)acetate **(3aa)**



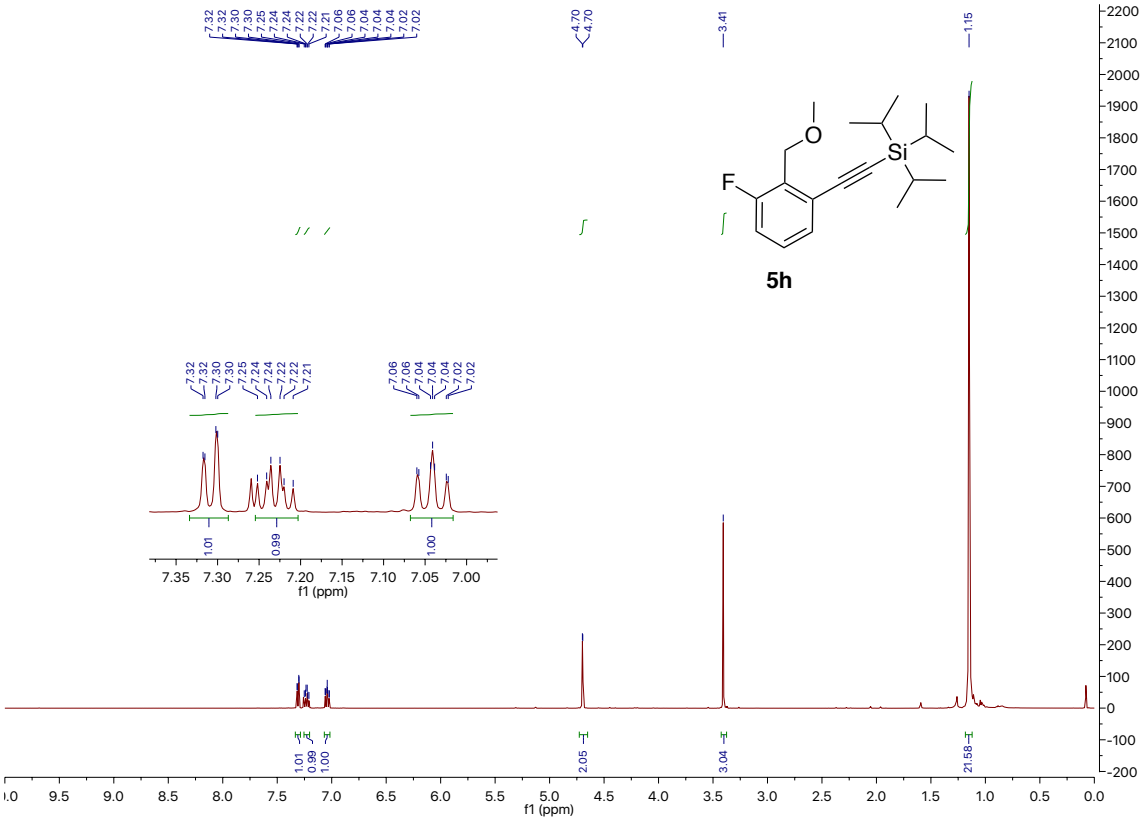


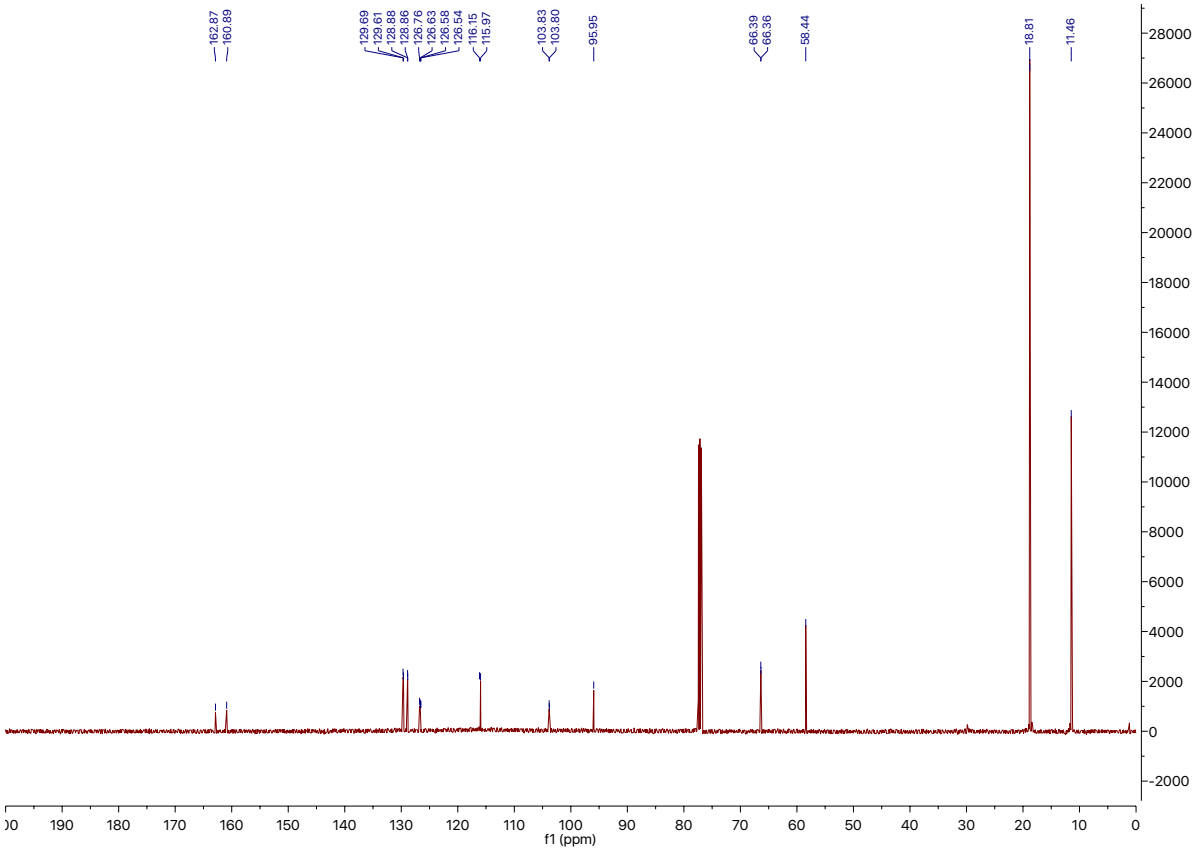
***Triisopropyl((2-(methoxymethyl)phenyl)ethynyl)silane* (5a)**



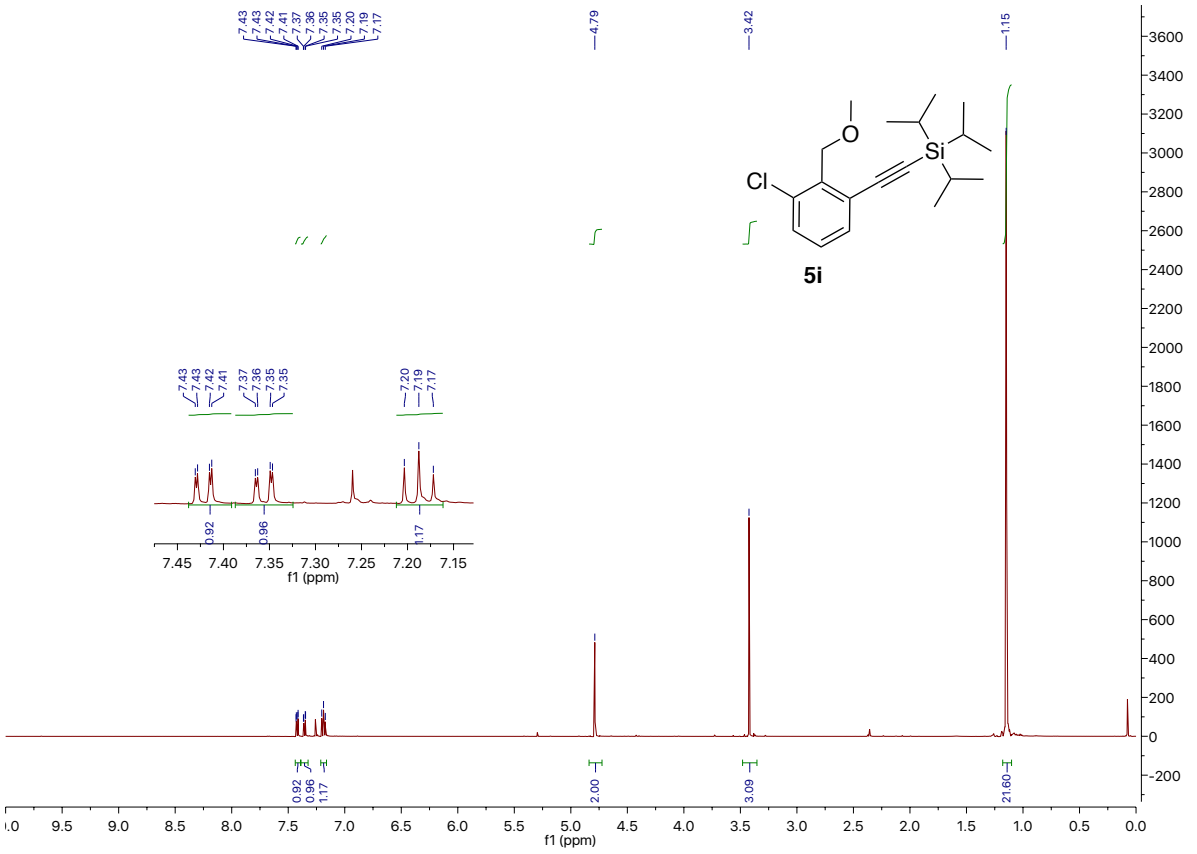


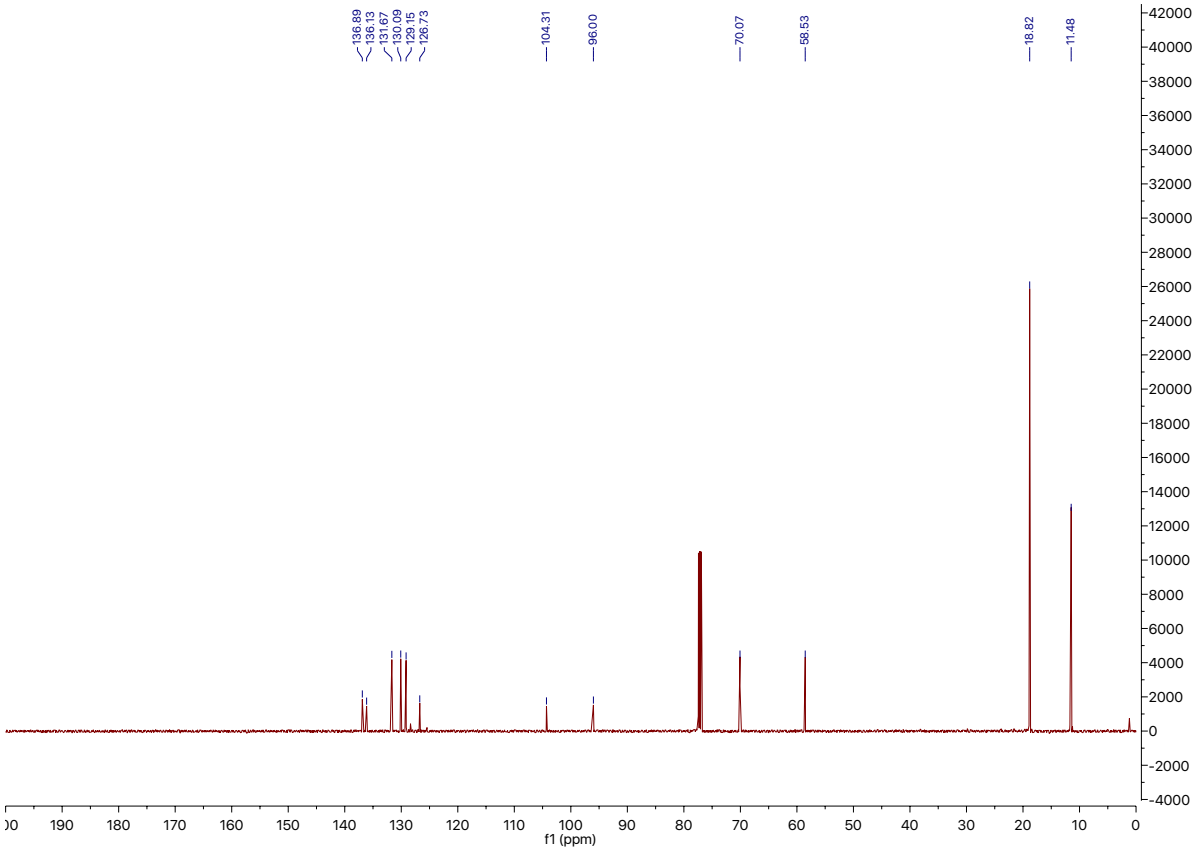
((3-Fluoro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5h**)



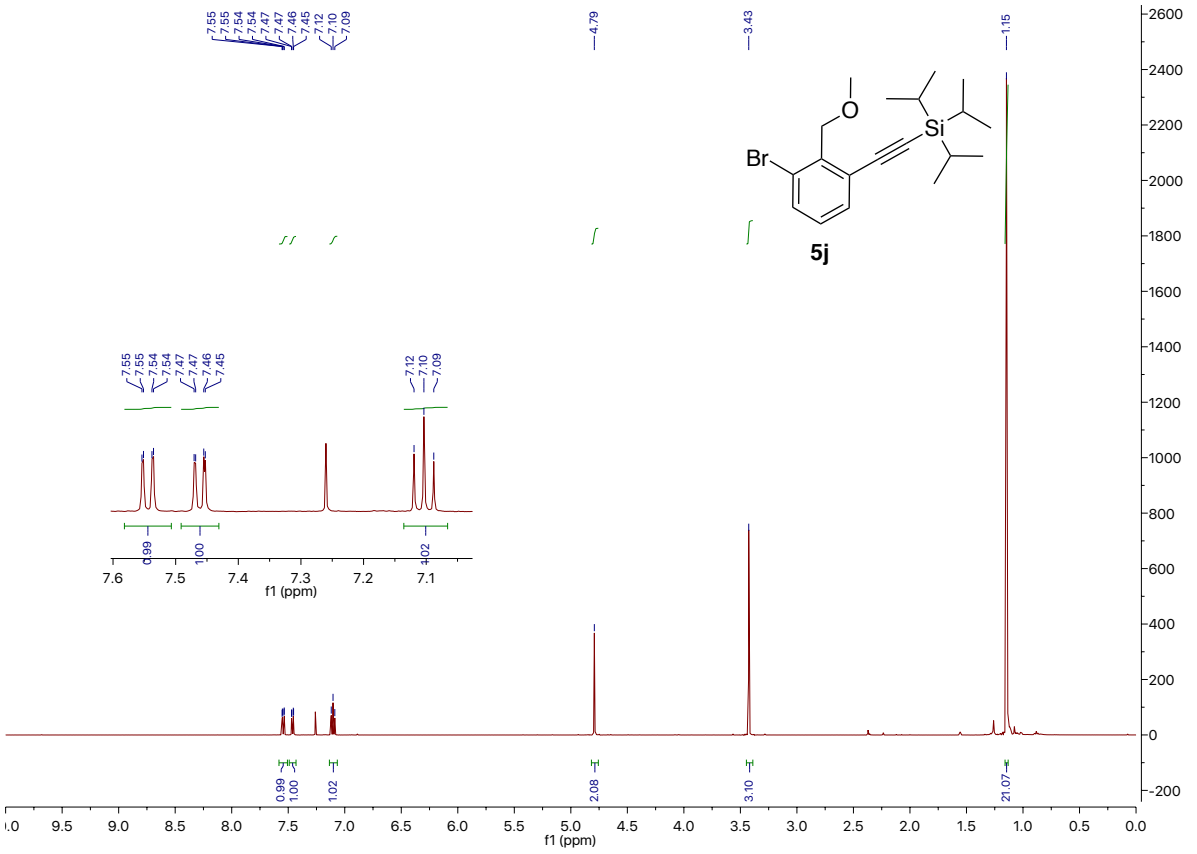


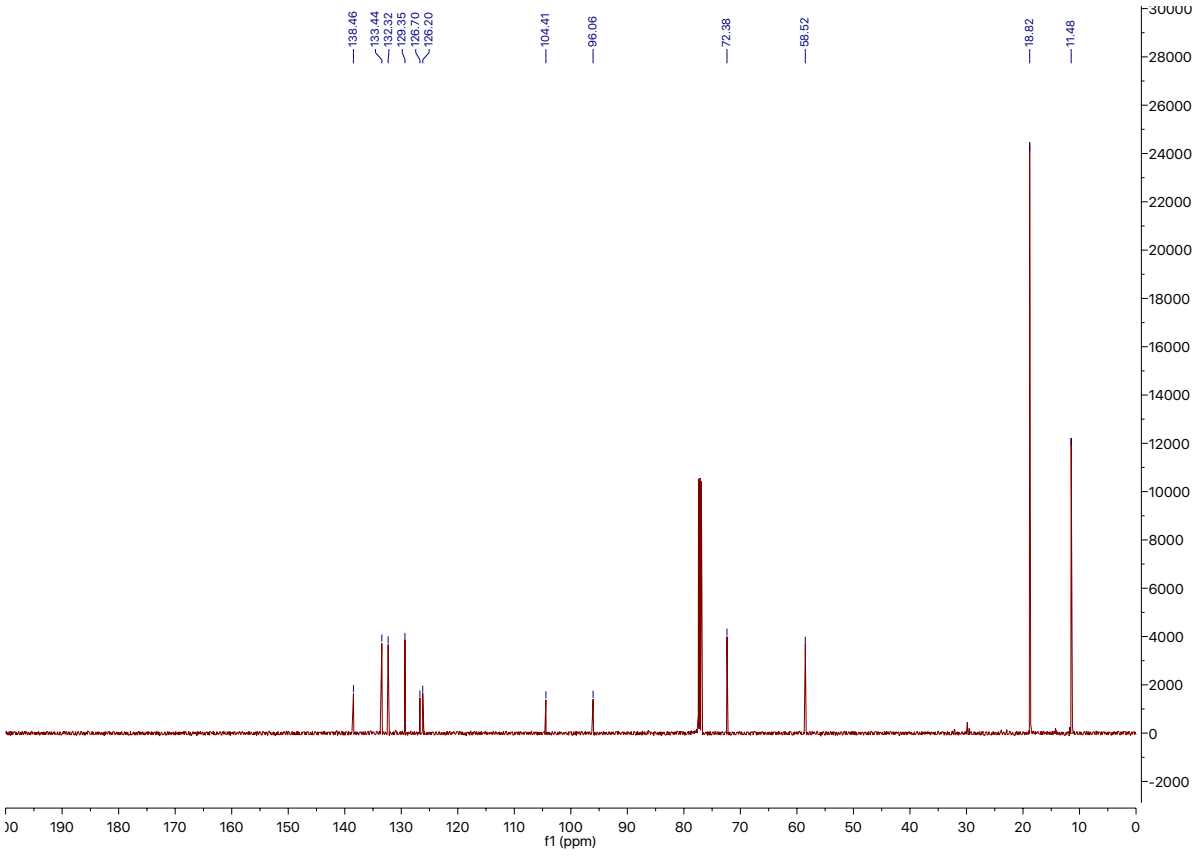
***((3-Chloro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane* (5i)**



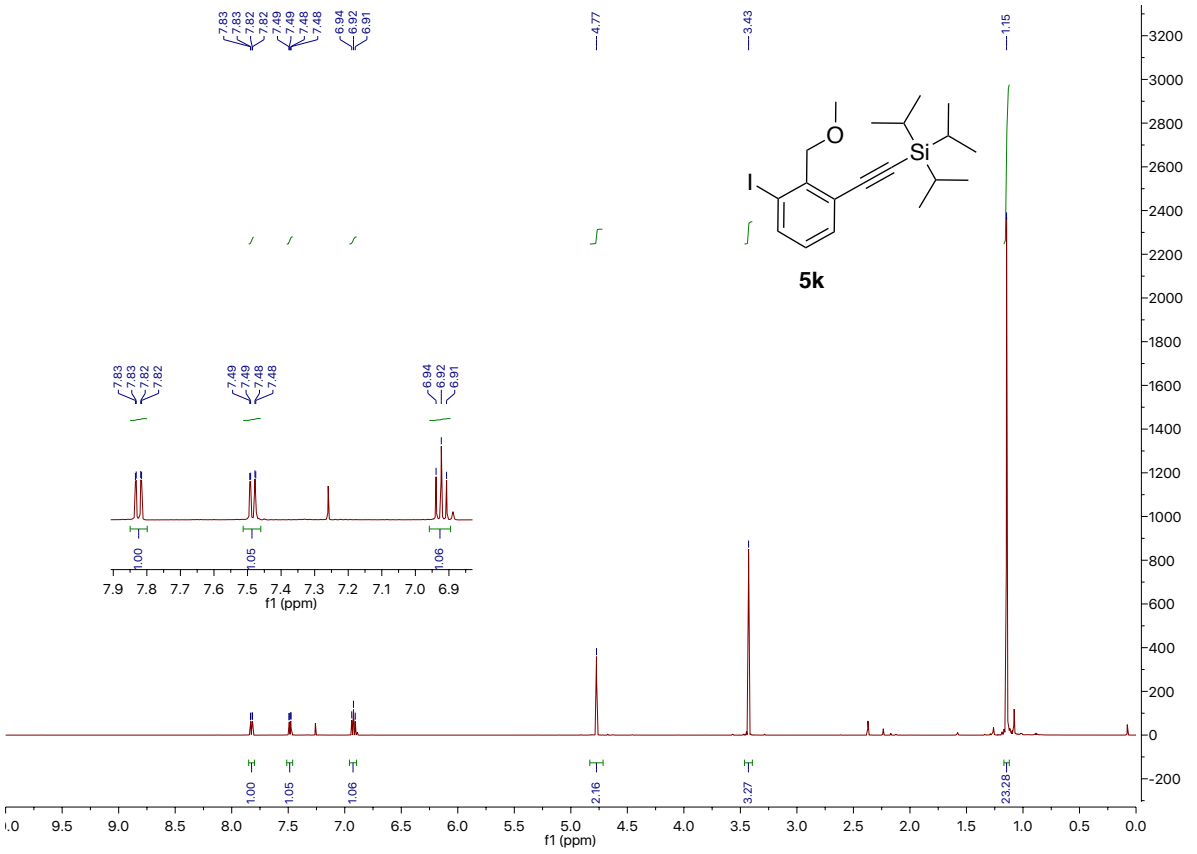


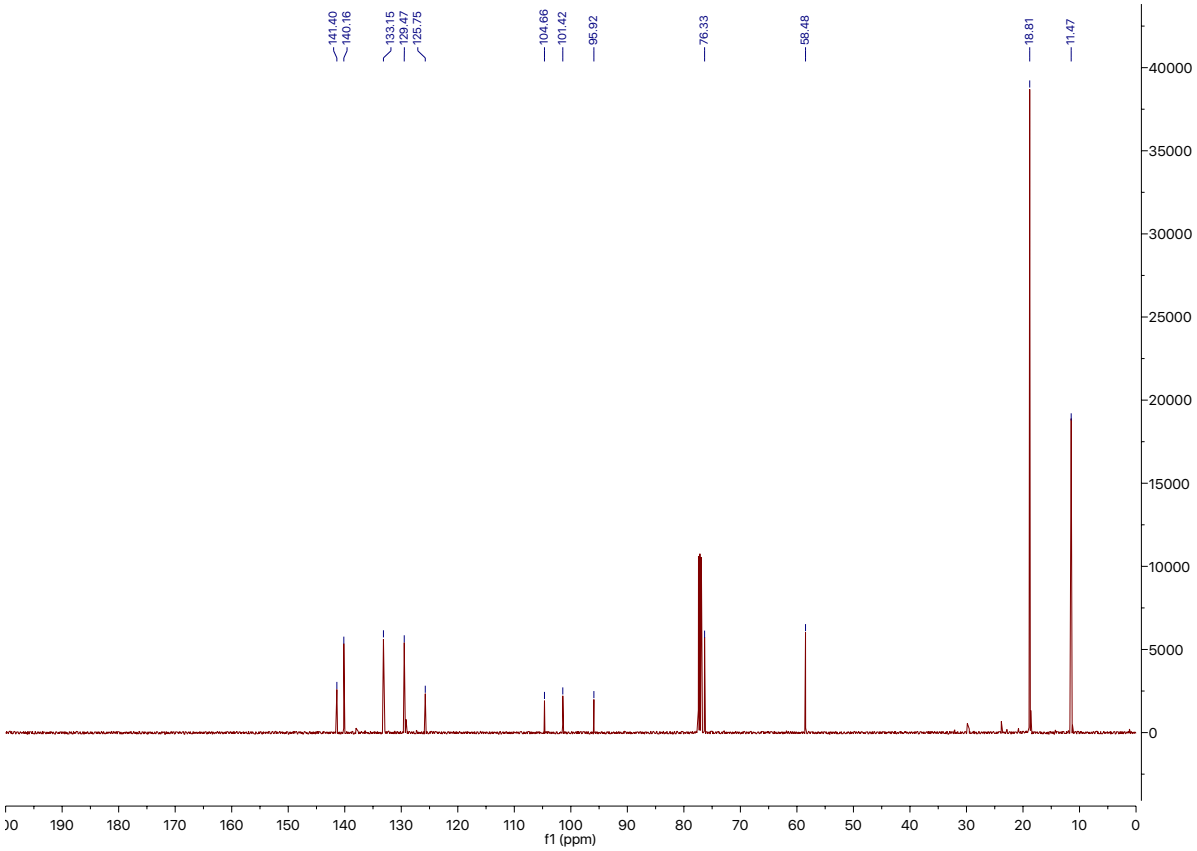
***((3-Bromo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane* (5j)**



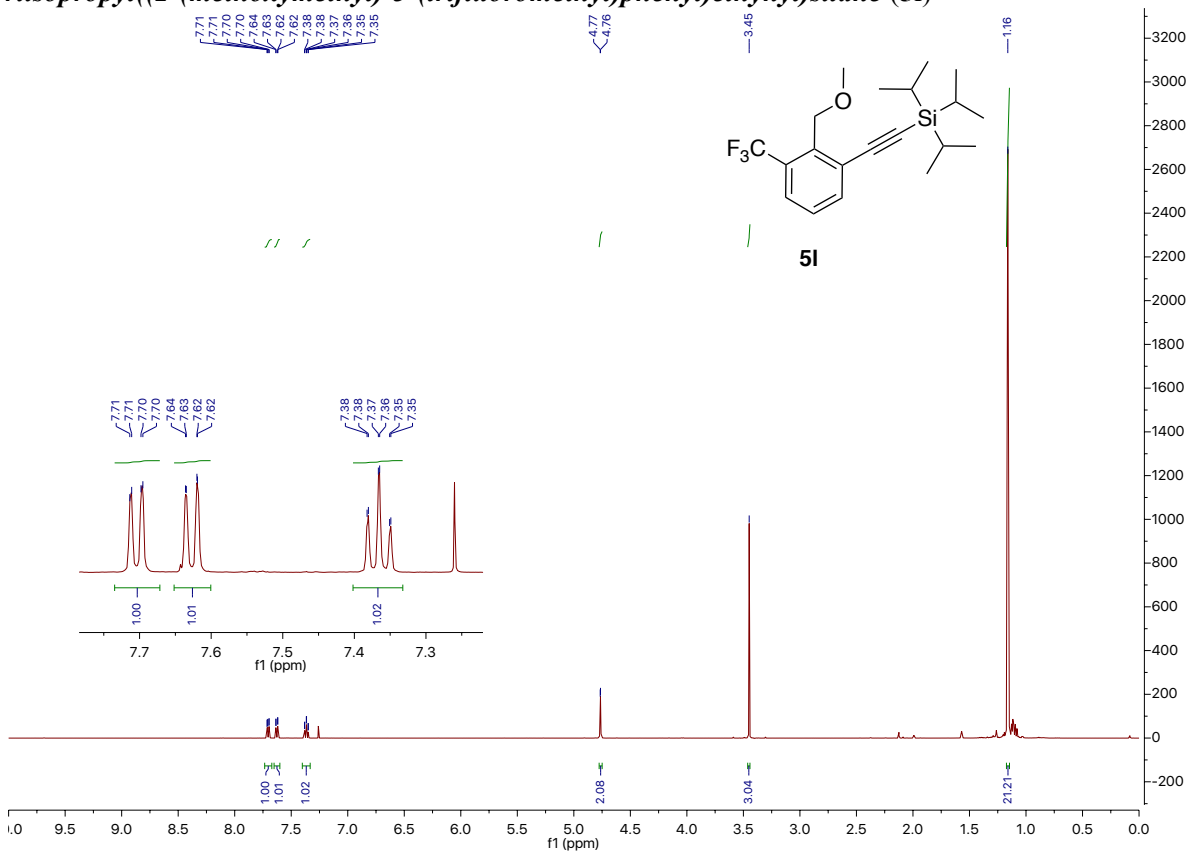


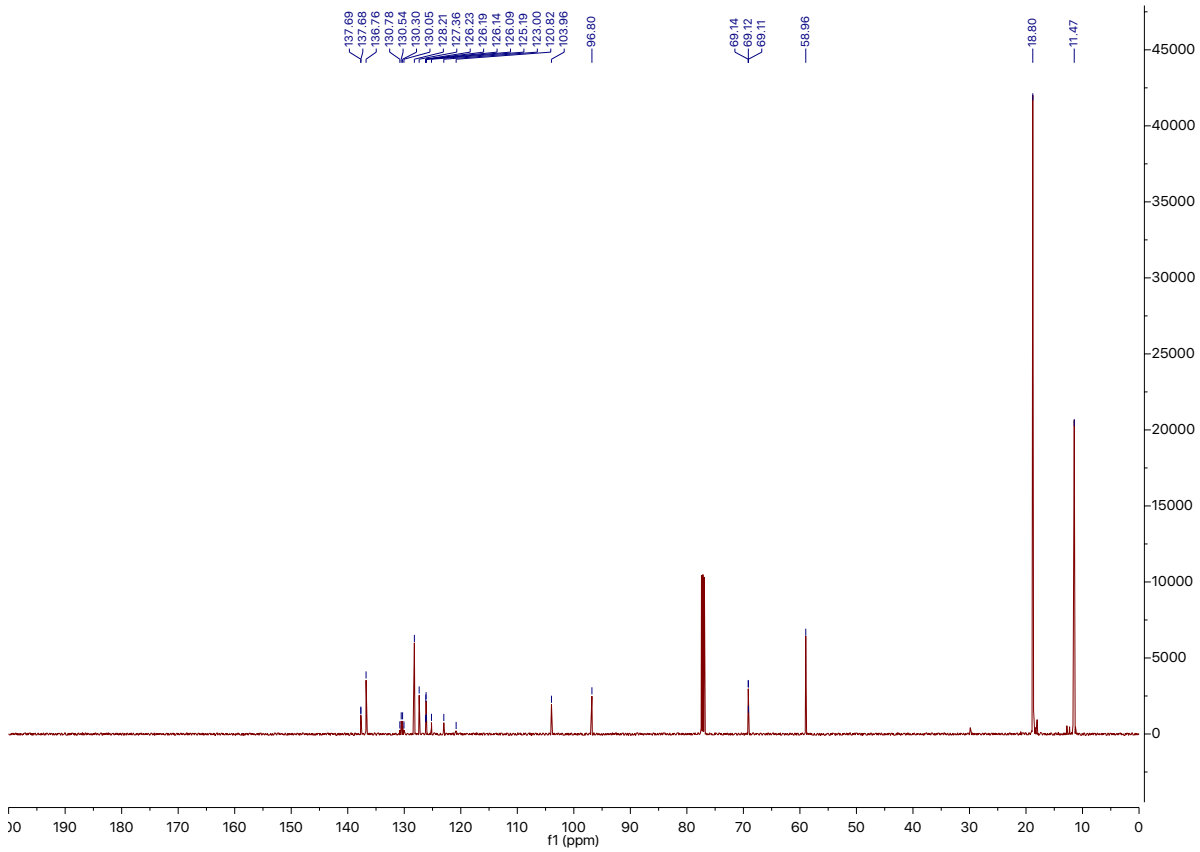
((3-Iodo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5k**)



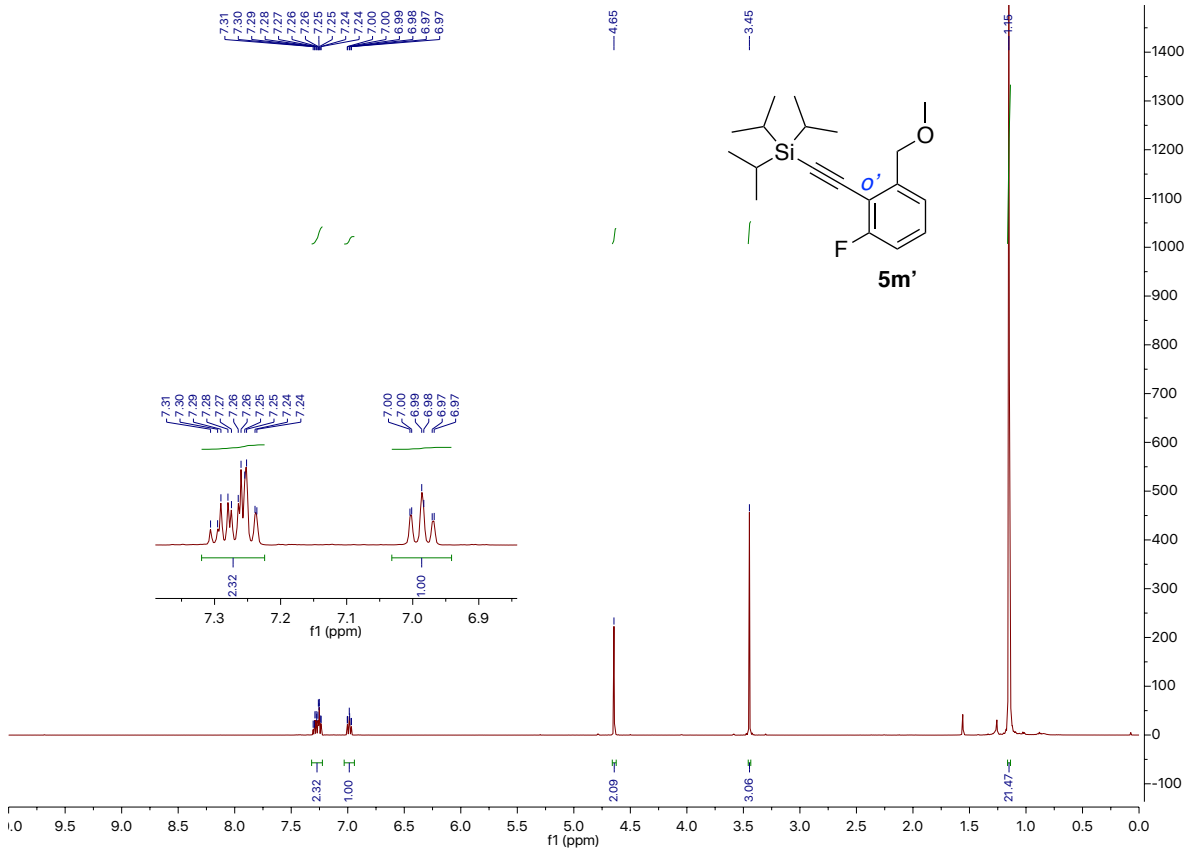


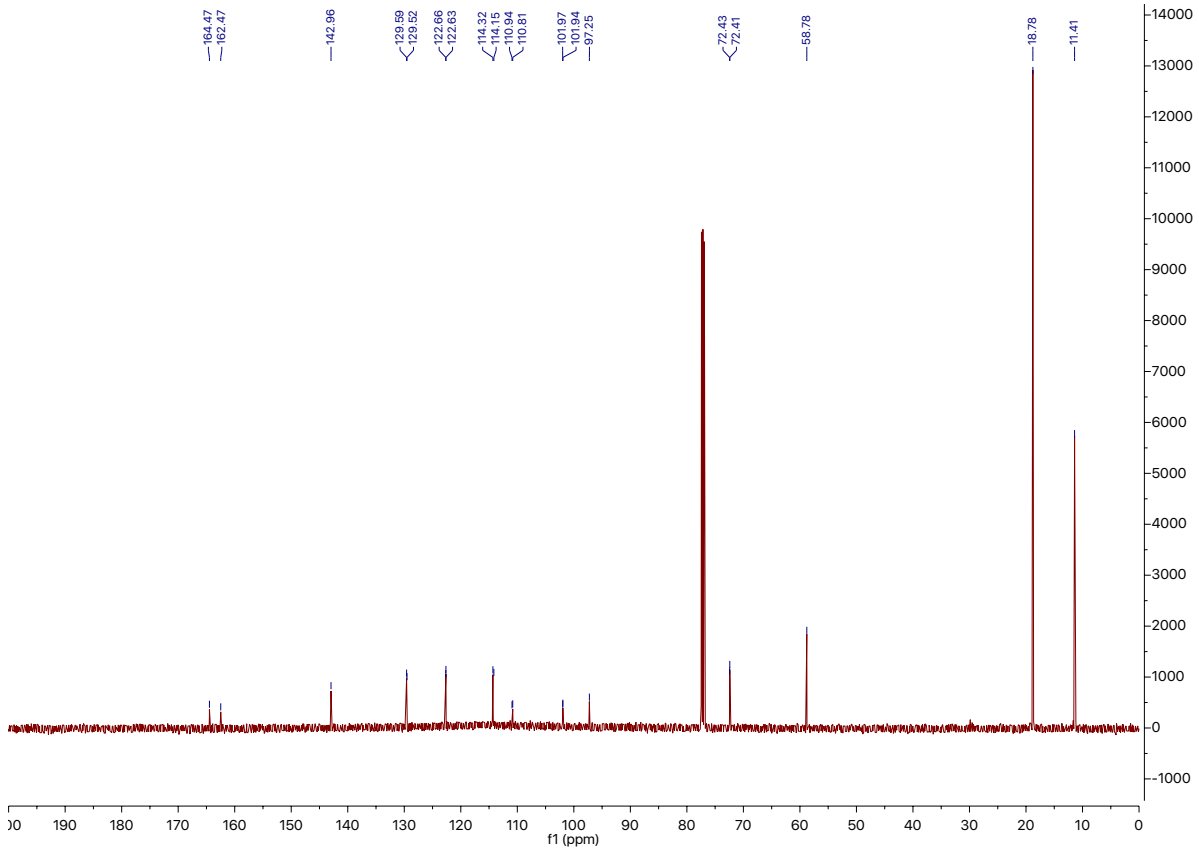
***Triisopropyl((2-(methoxymethyl)-3-(trifluoromethyl)phenyl)ethynyl)silane* (5l)**



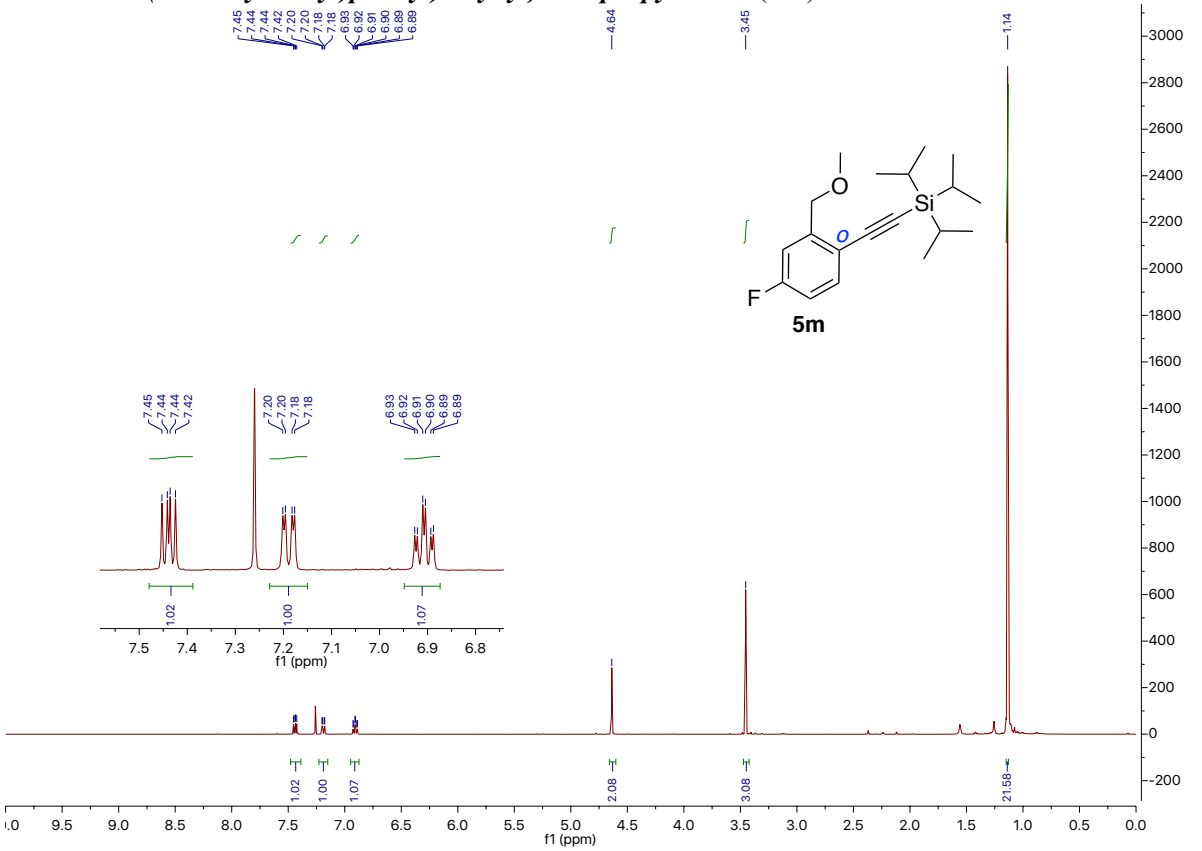


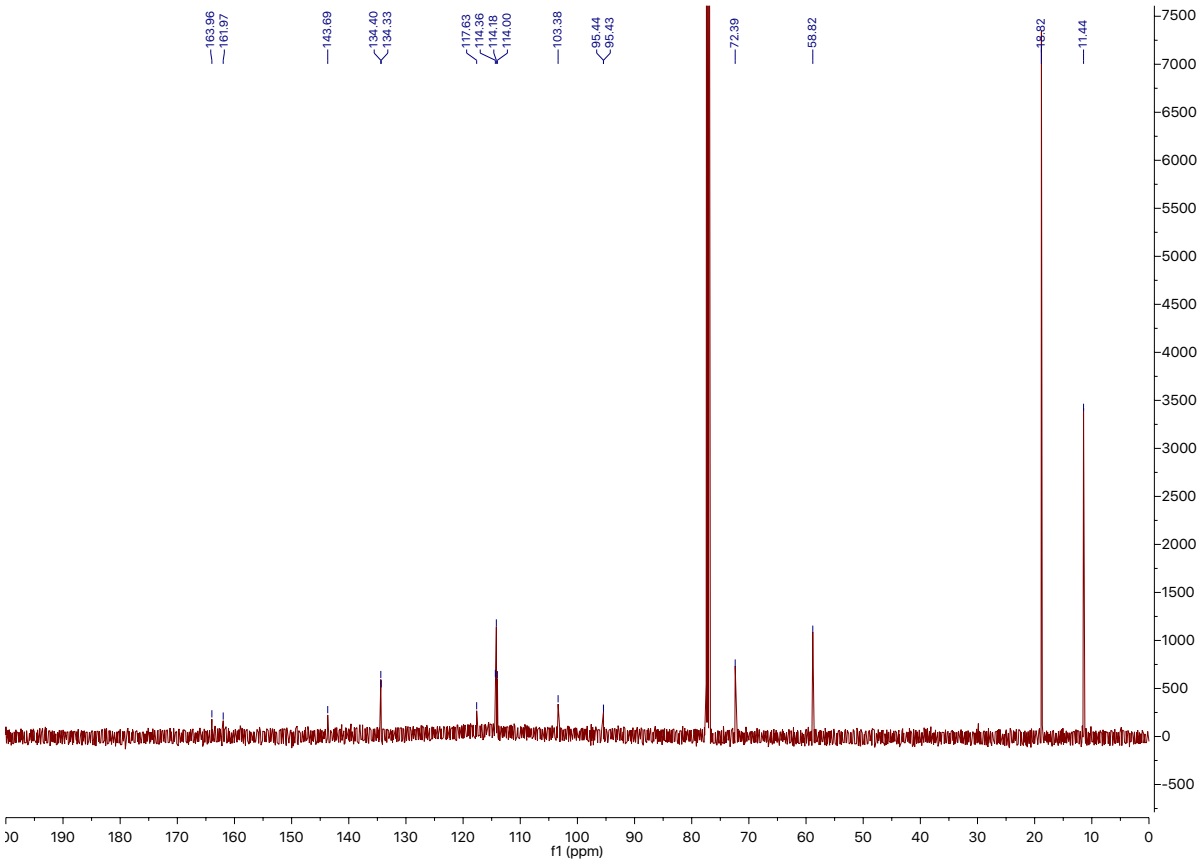
((2-Fluoro-6-(methoxymethyl)phenyl)ethynyl)triisopropylsilane **(5m')**



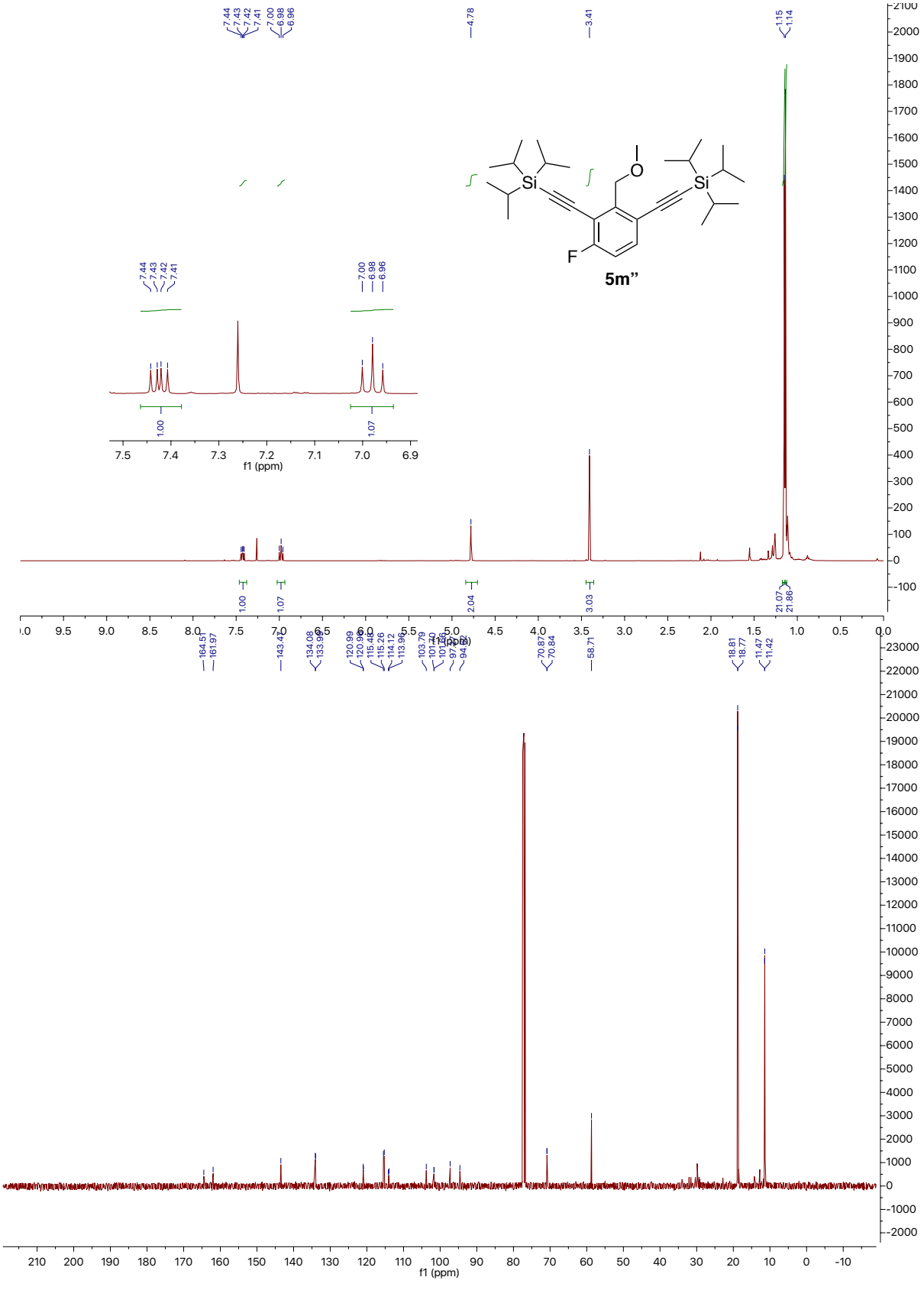


***((4-Fluoro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane* (5m)**

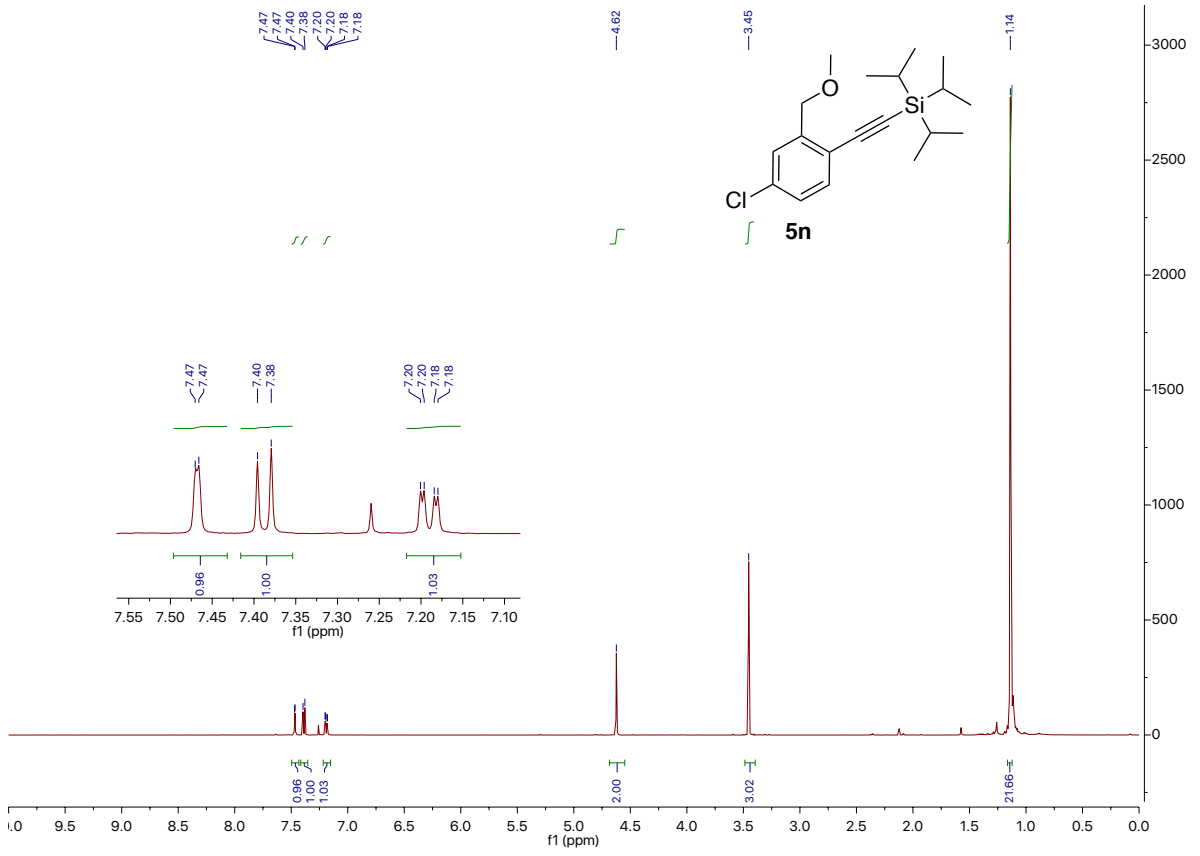


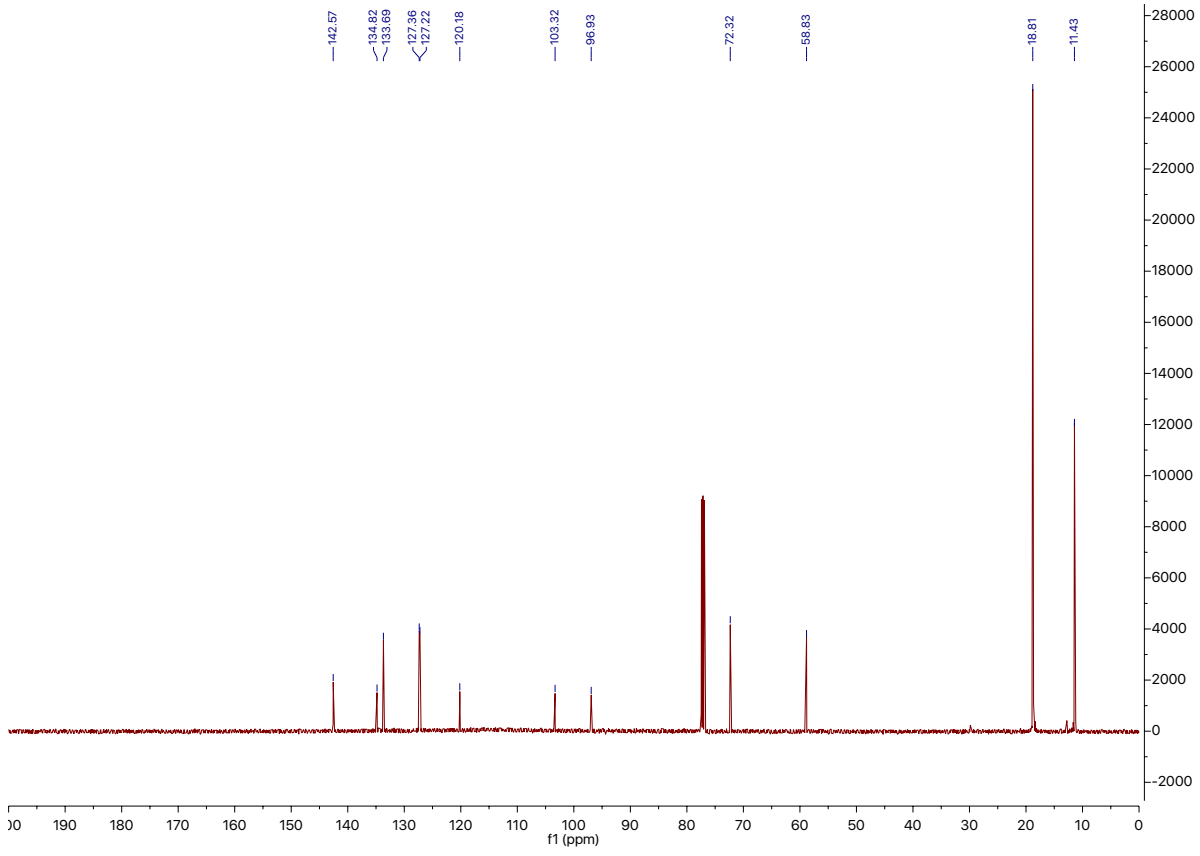


***((4-Fluoro-2-(methoxymethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane)*(5m")**

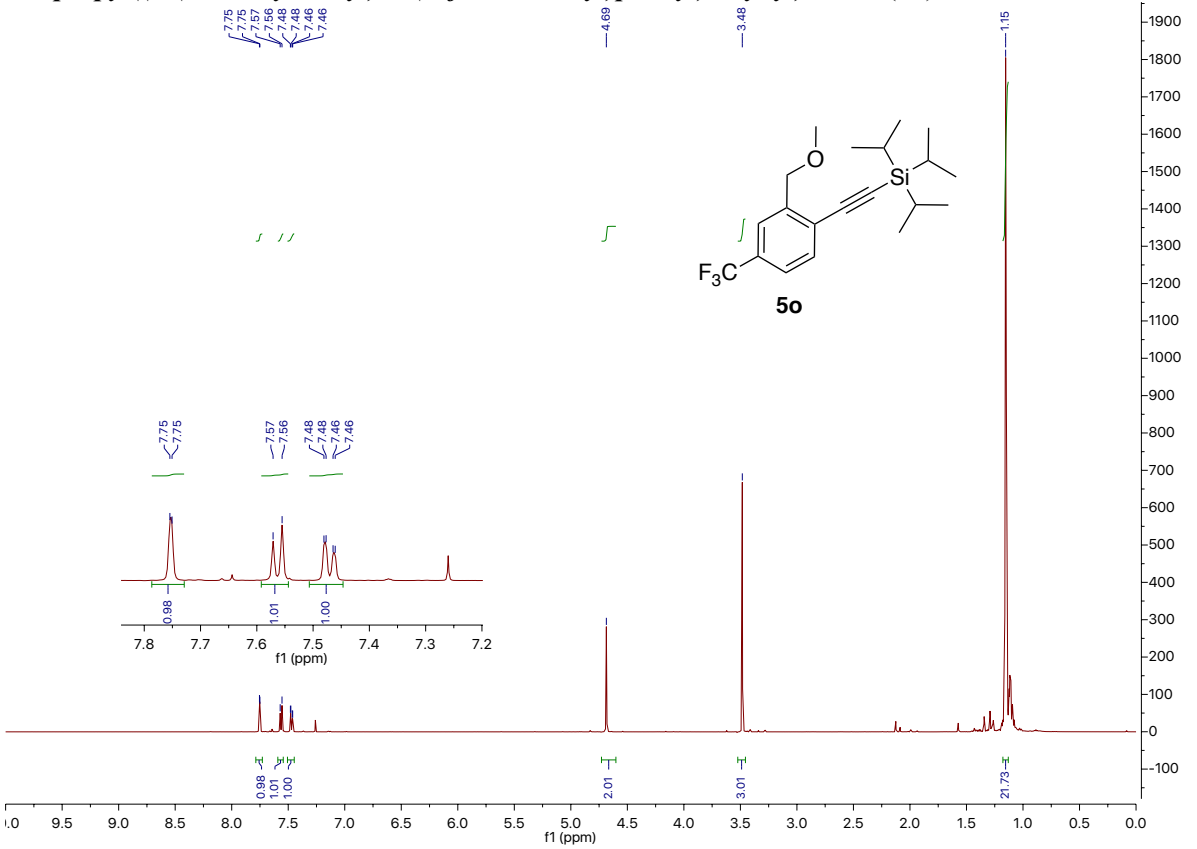


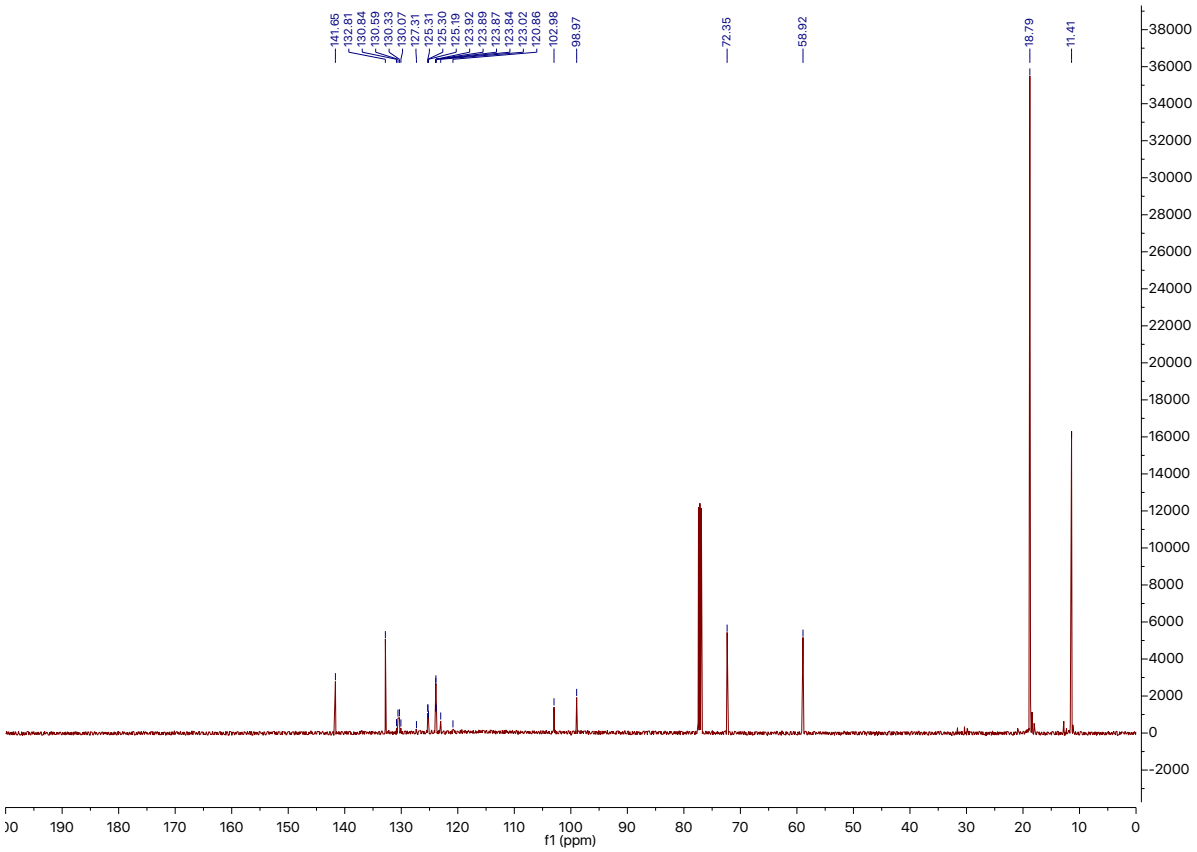
((4-Chloro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane **(5n)**



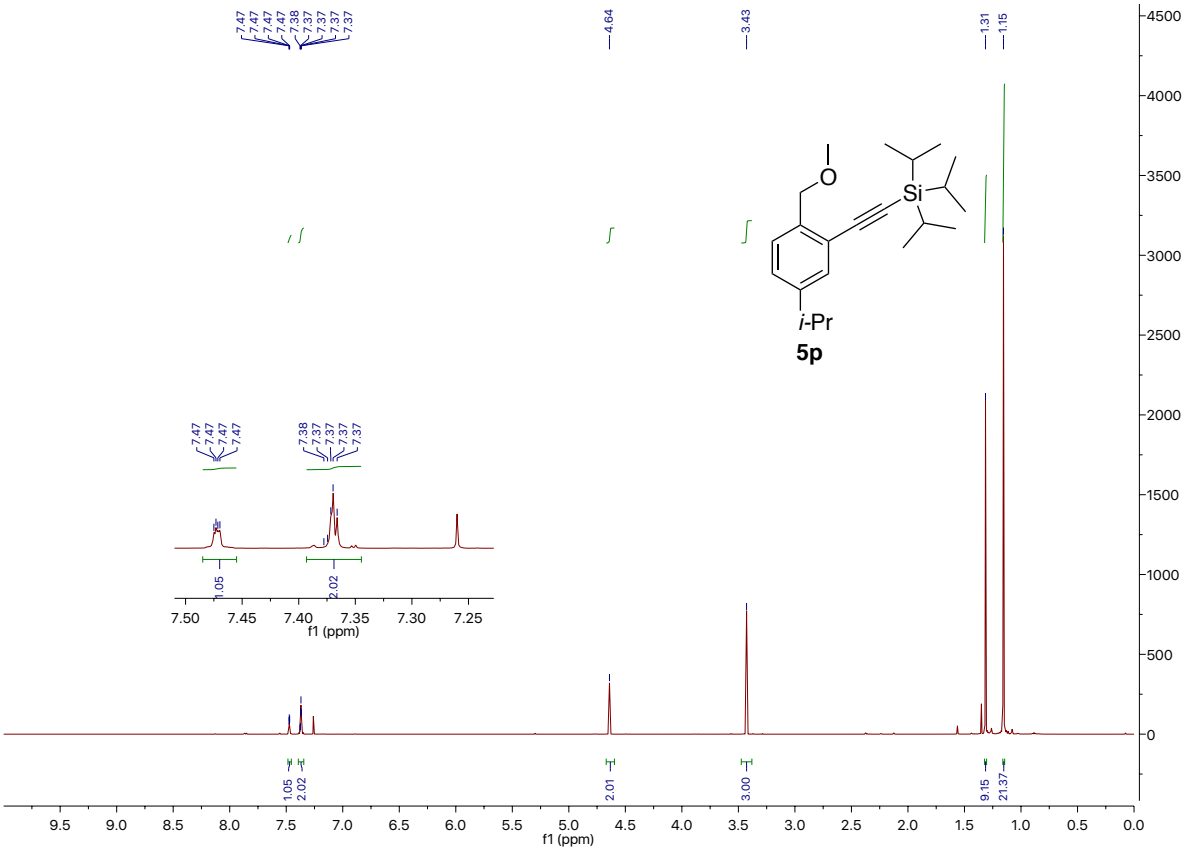


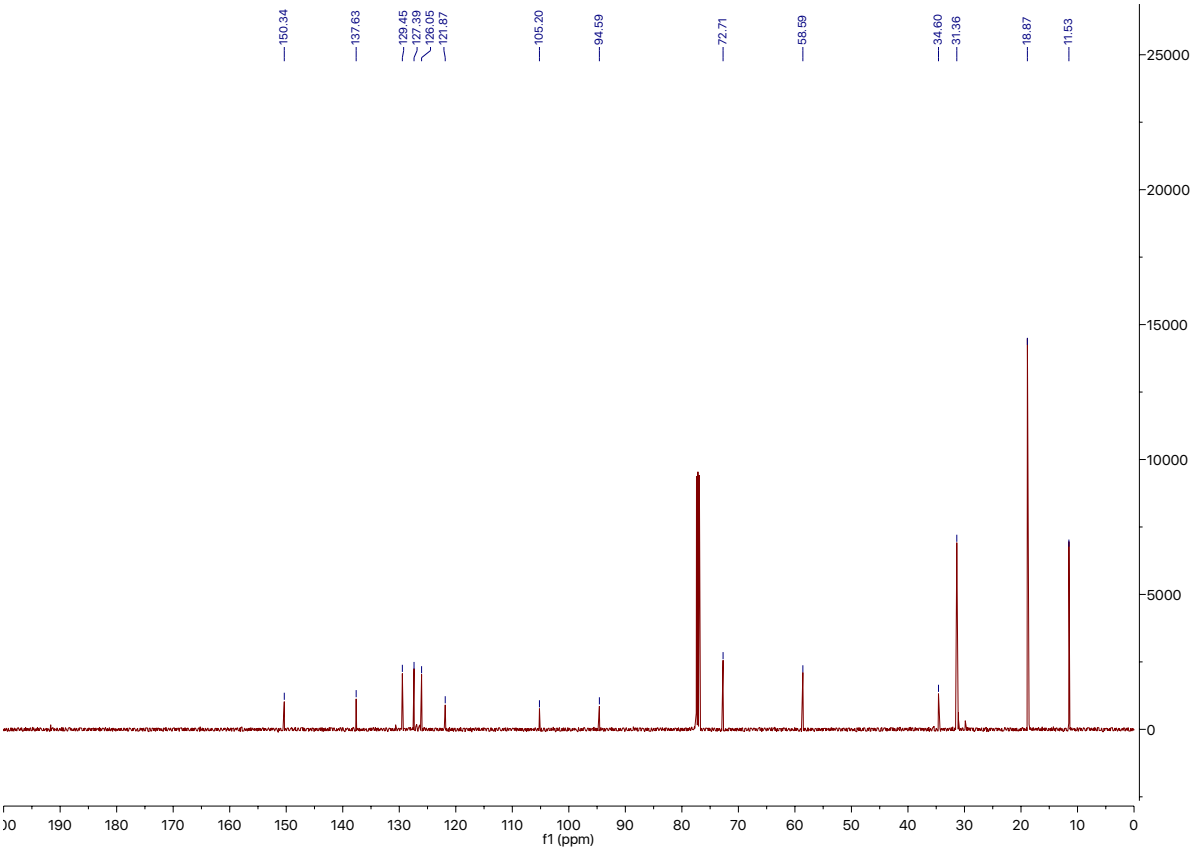
***Triisopropyl((2-(methoxymethyl)-4-(trifluoromethyl)phenyl)ethynyl)silane* (5o)**



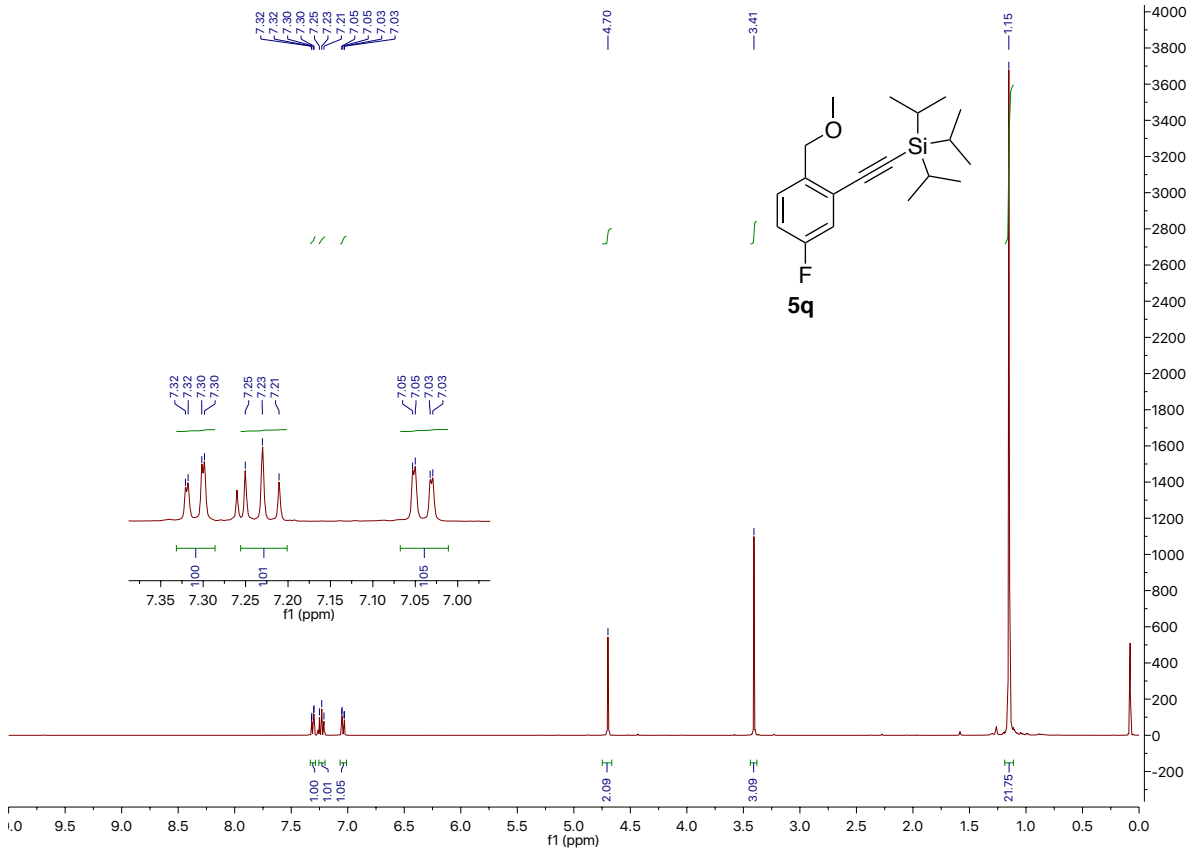


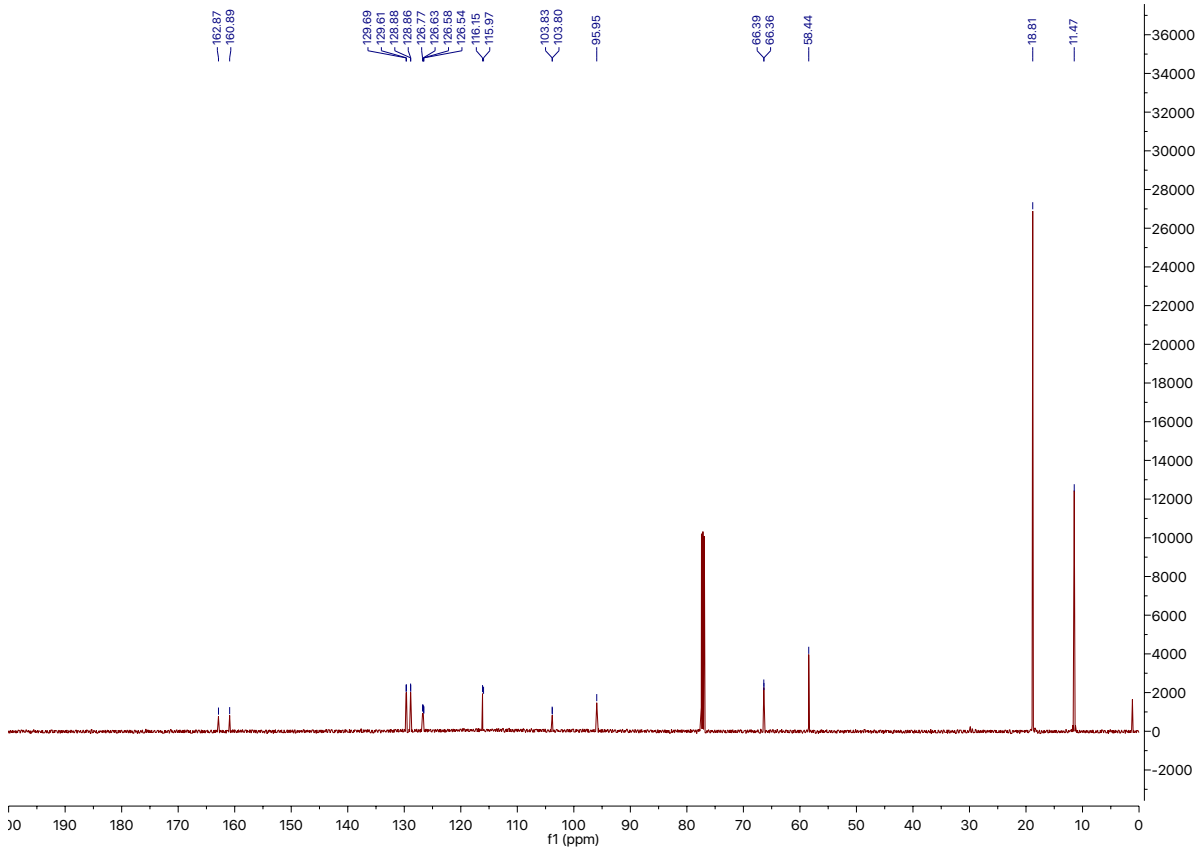
Triisopropyl((5-isopropyl-2-(methoxymethyl)phenyl)ethynyl)silane (**5p**)



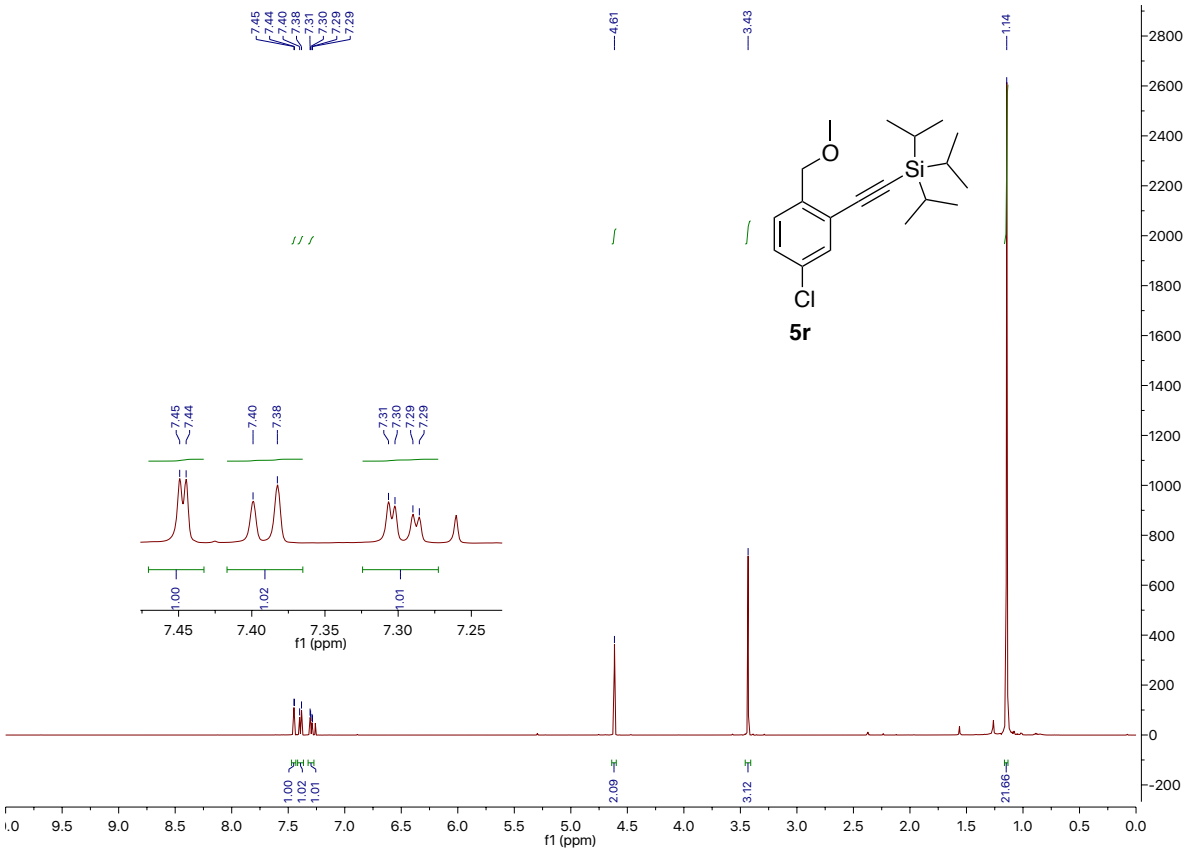


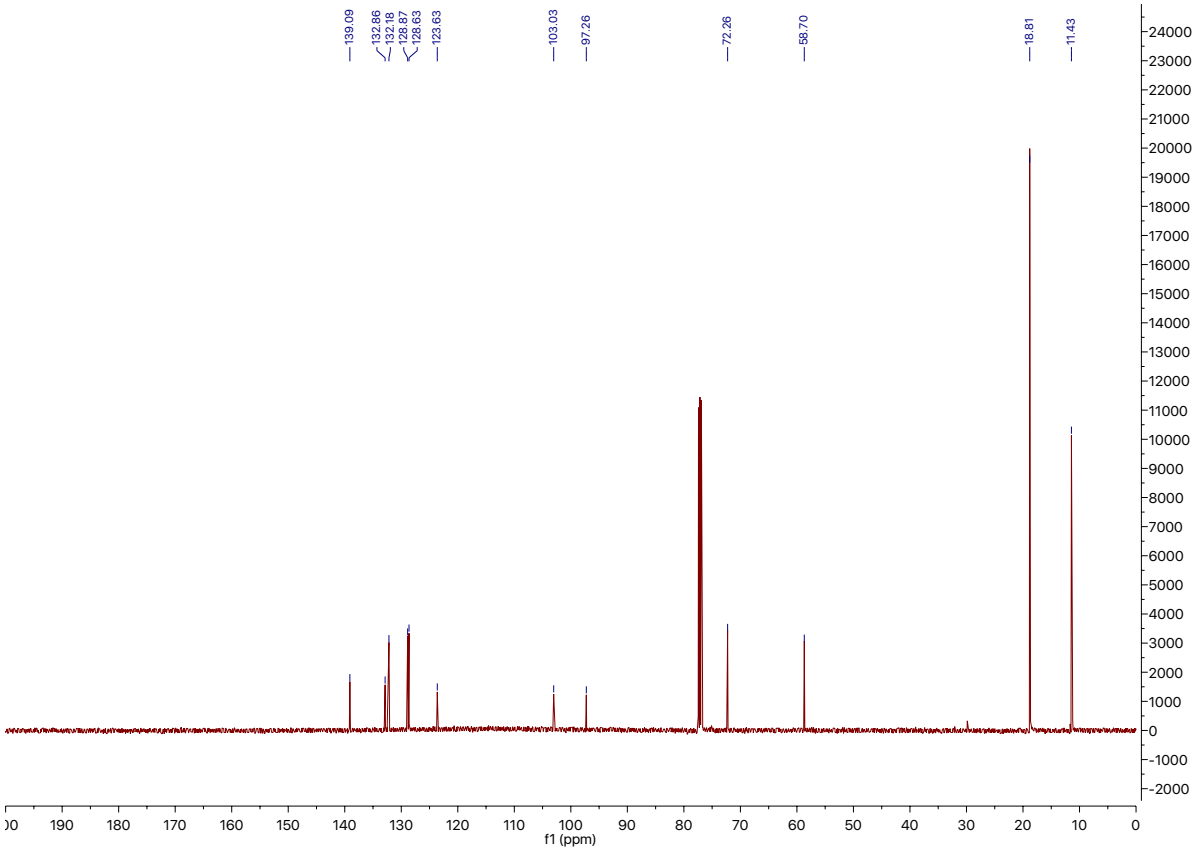
***((5-Fluoro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane* (5q)**



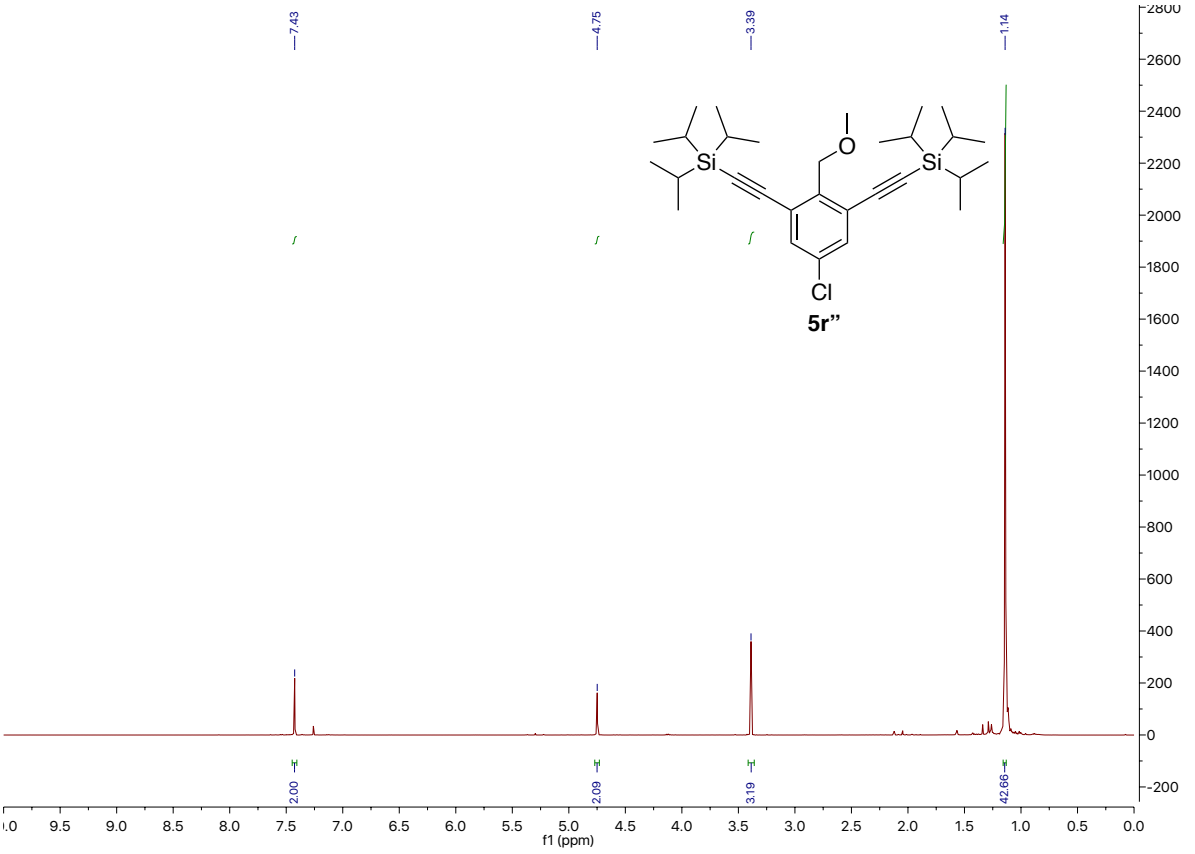


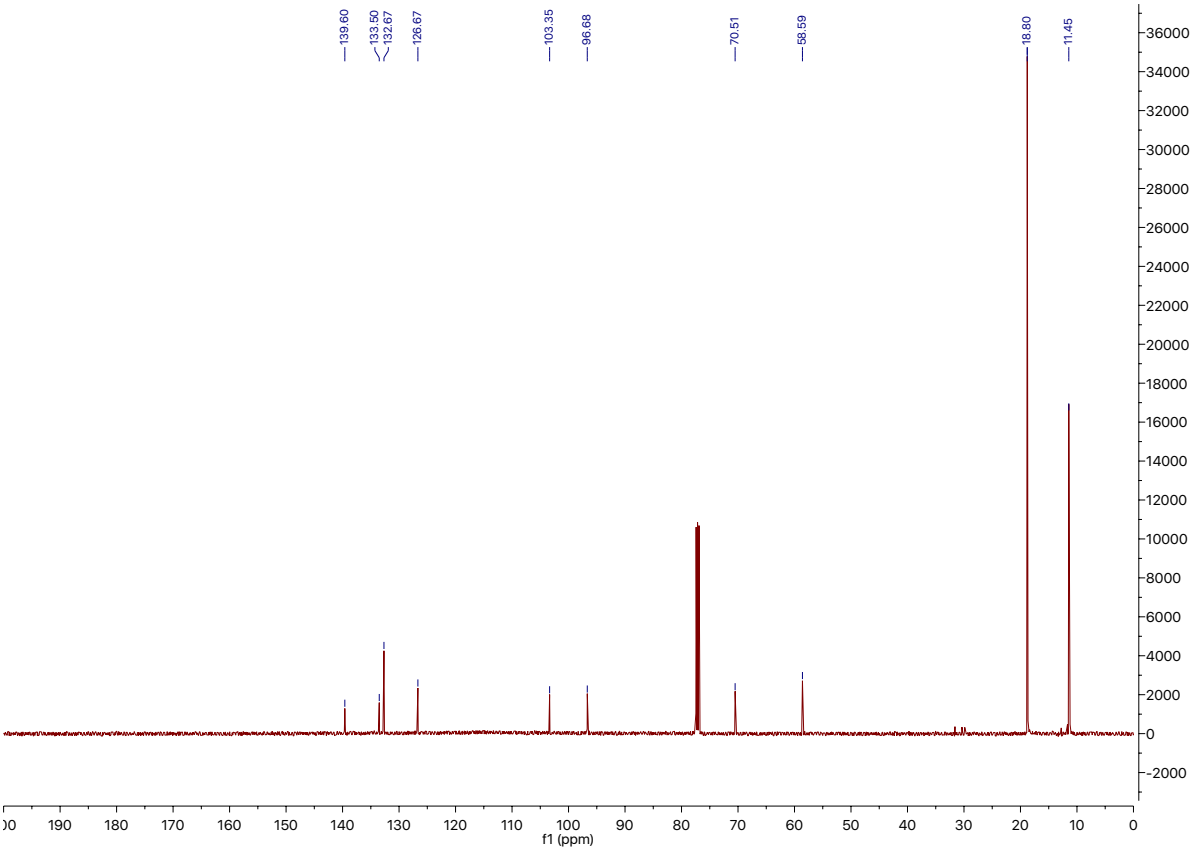
((5-Chloro-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5r**)



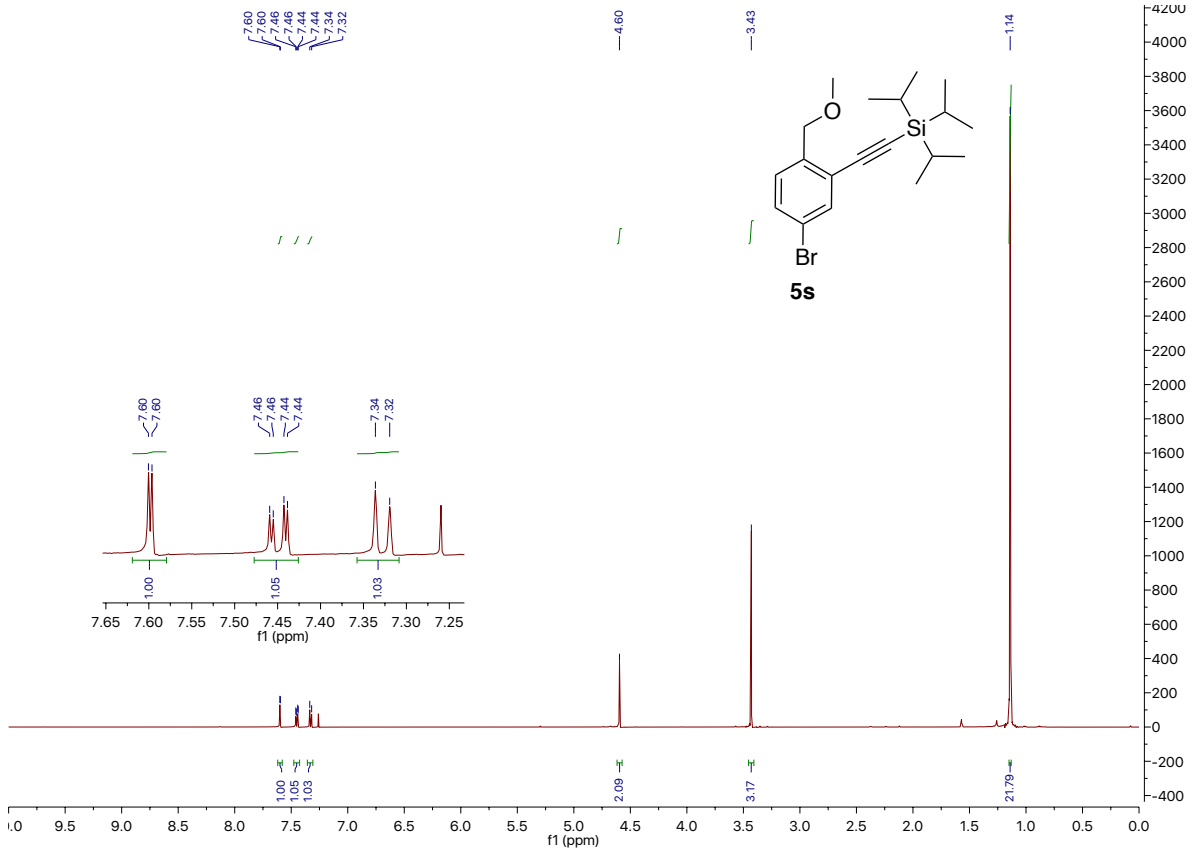


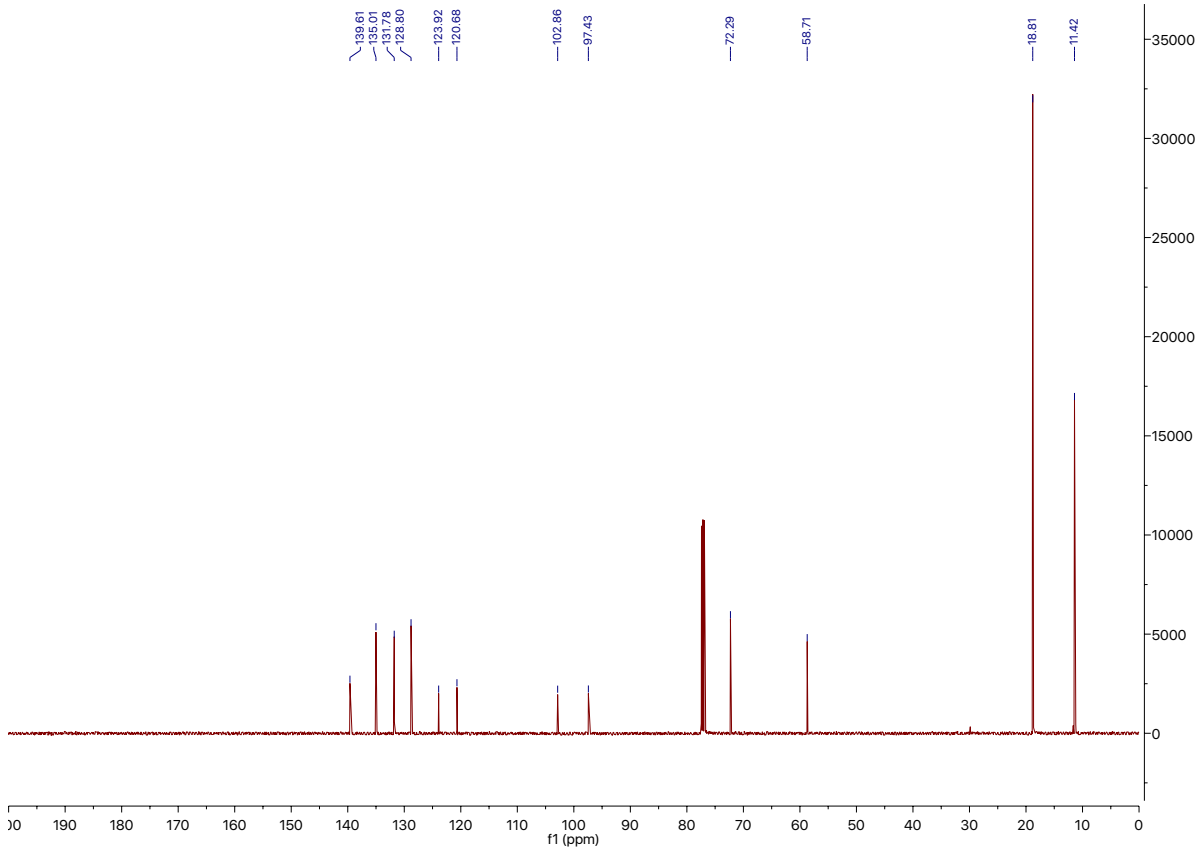
***((5-Chloro-2-(methoxymethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane)*(5r")**



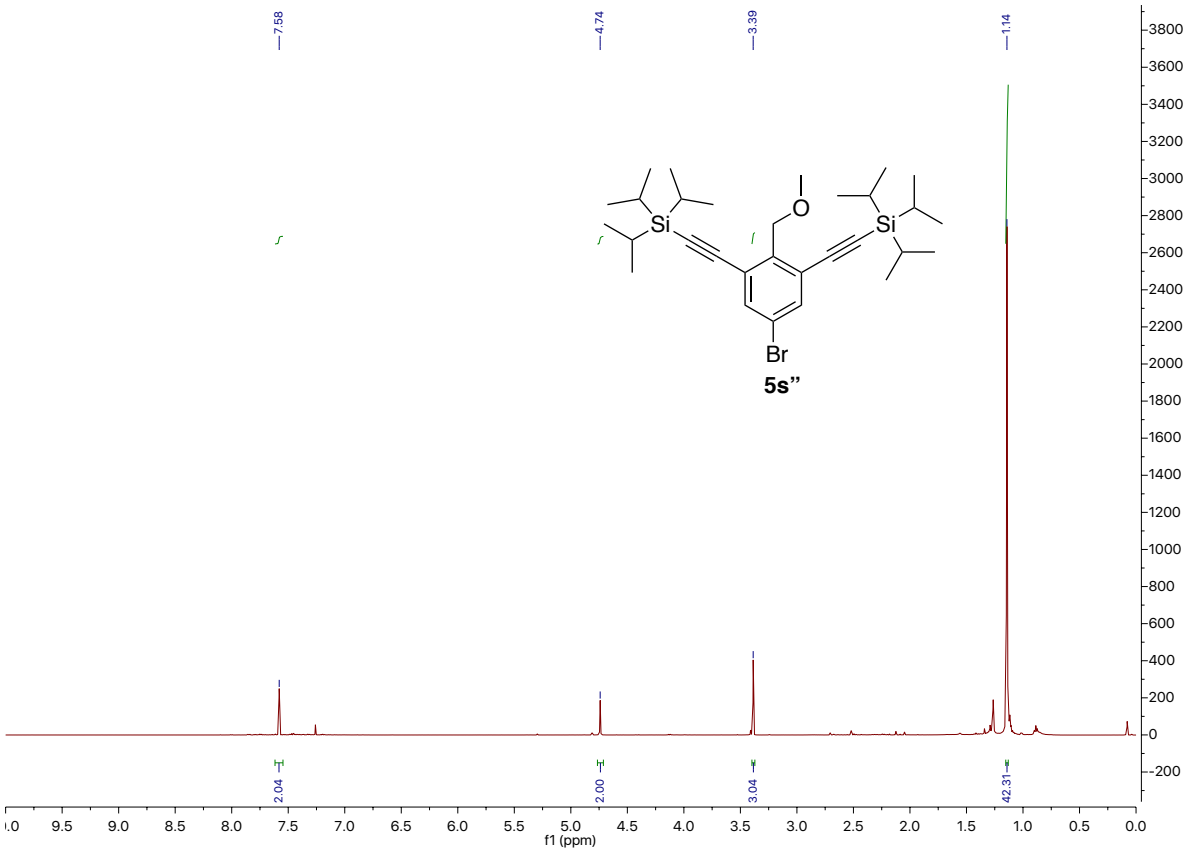


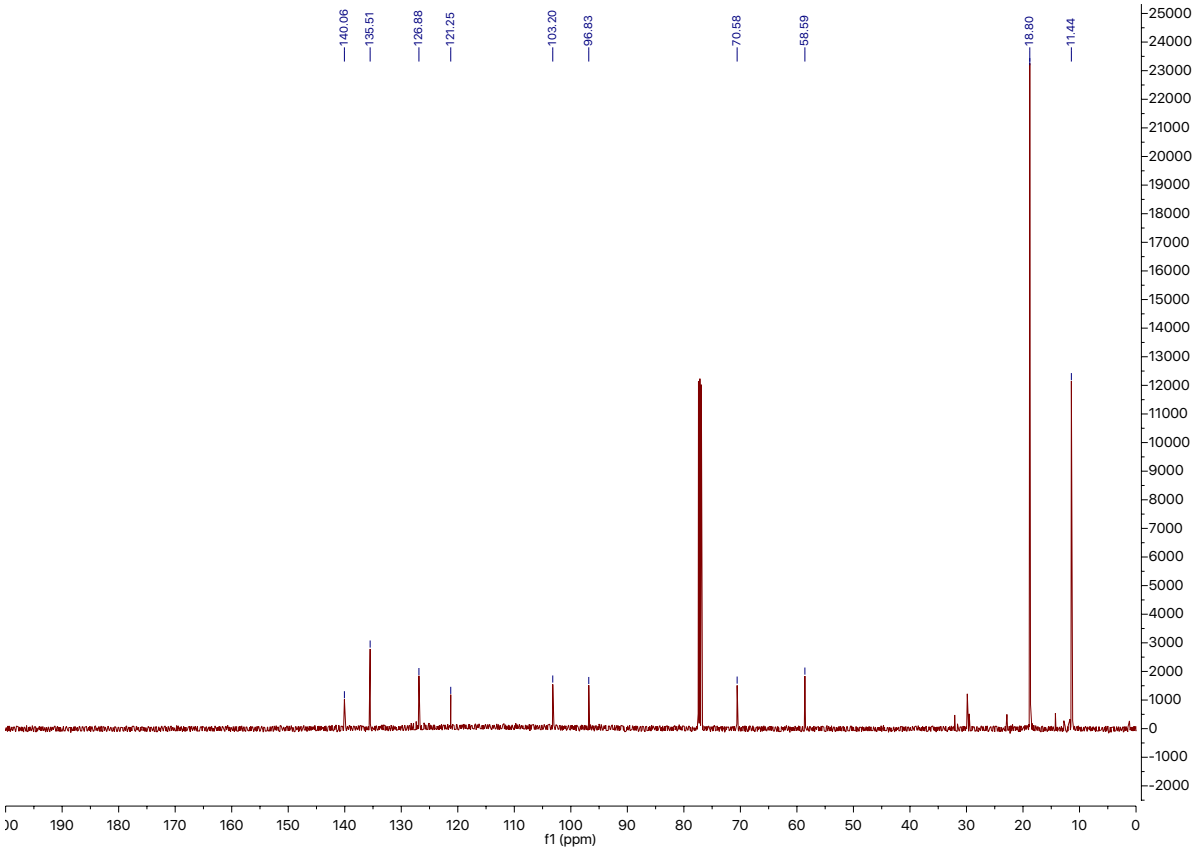
((5-Bromo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane (**5s**)



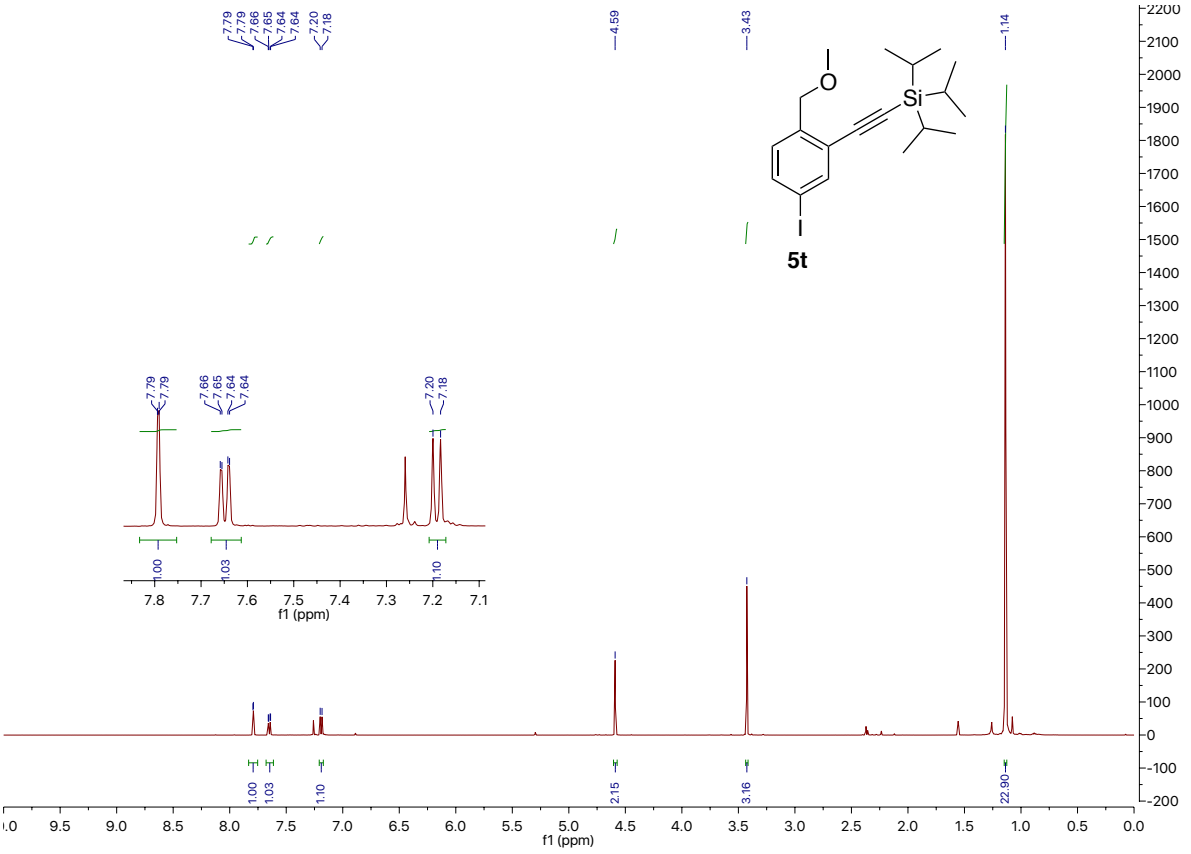


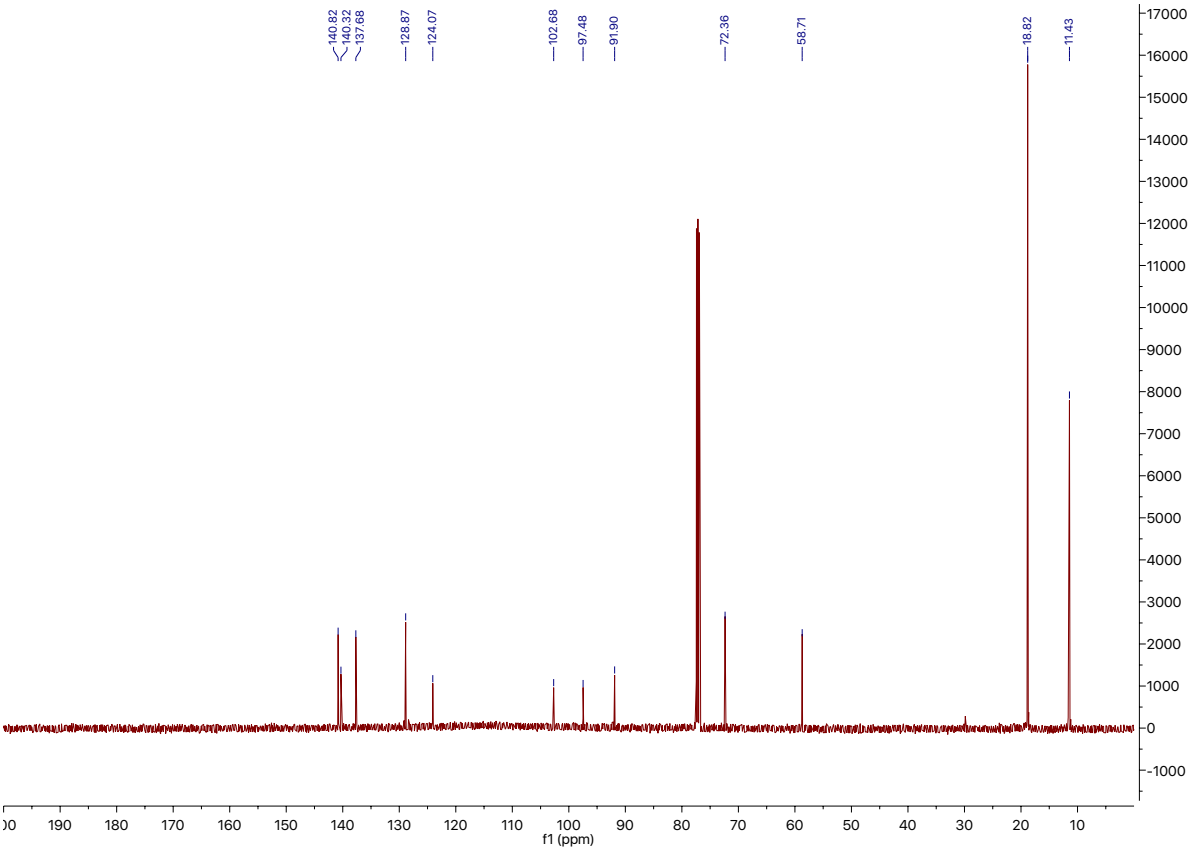
((5-Bromo-2-(methoxymethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) **(5s")**



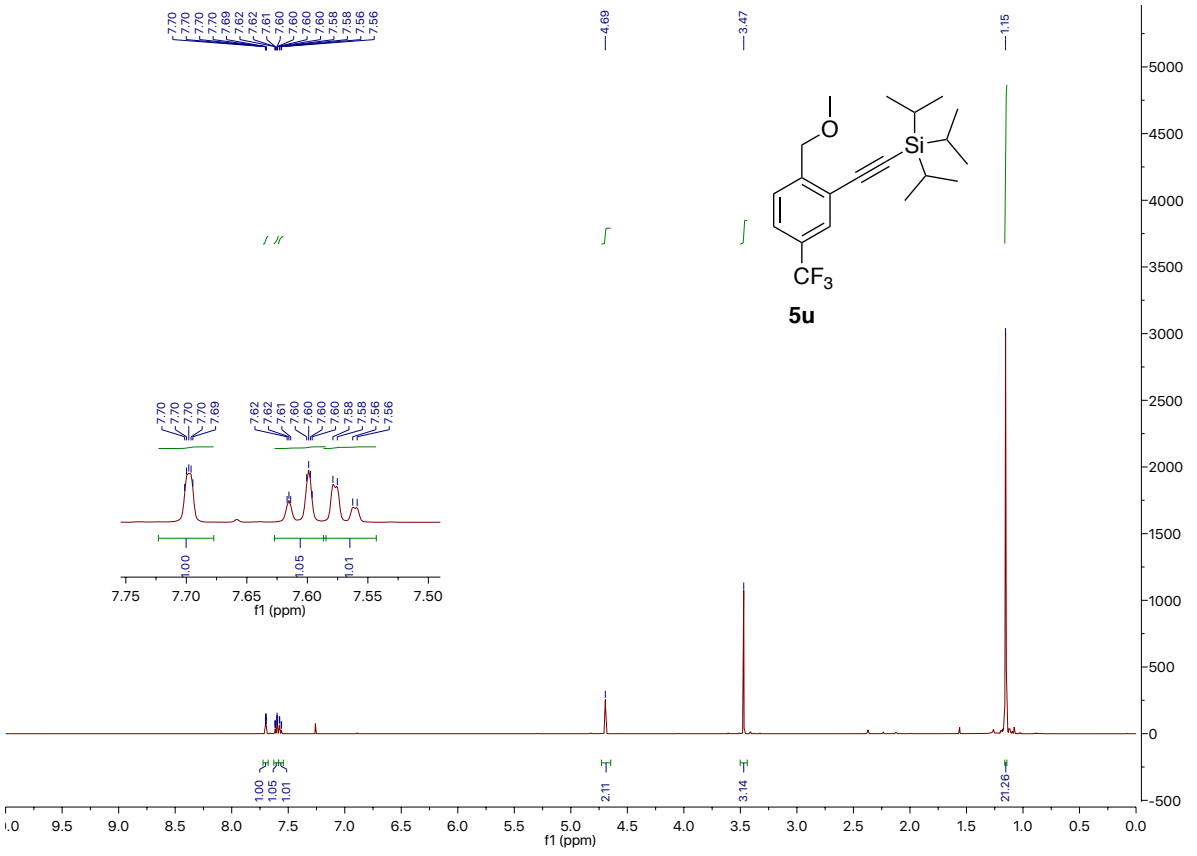


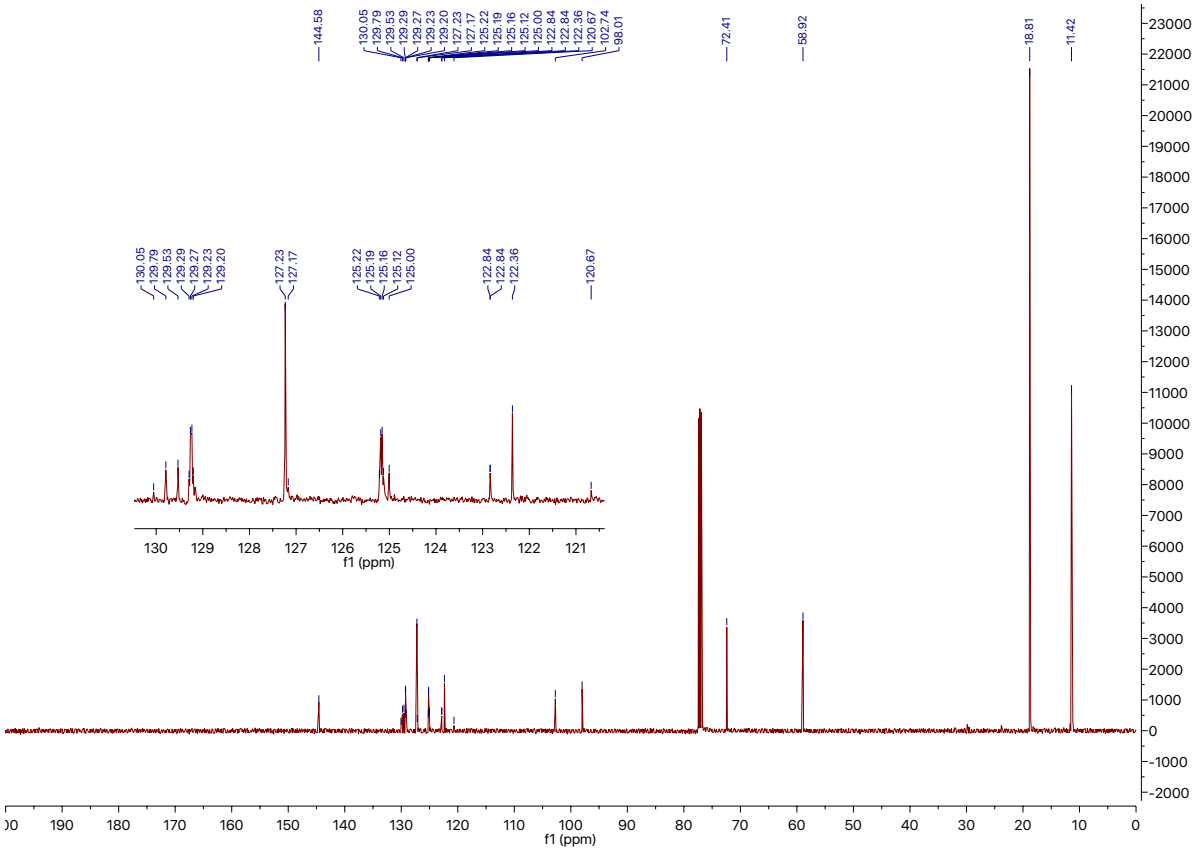
***((5-Iodo-2-(methoxymethyl)phenyl)ethynyl)triisopropylsilane* (5t)**



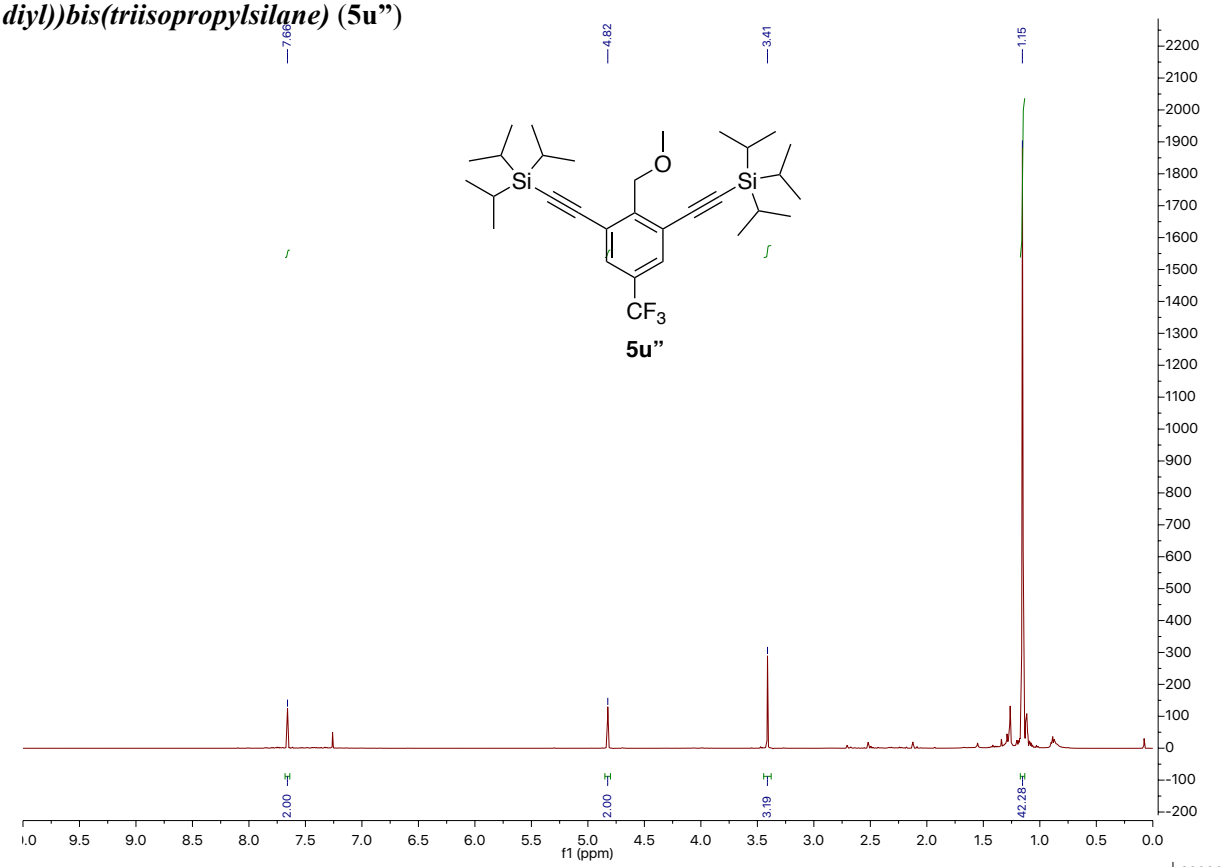


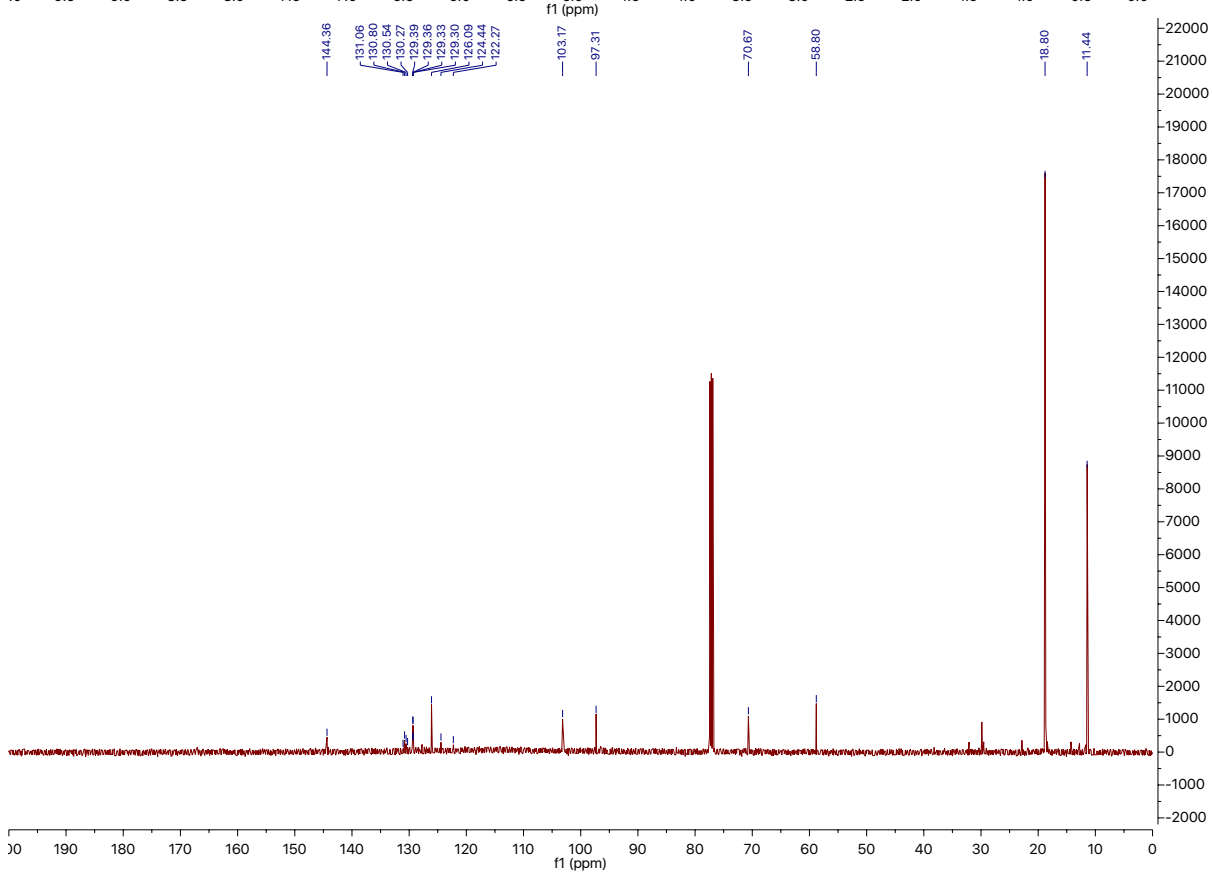
***Triisopropyl((2-(methoxymethyl)-5-(trifluoromethyl)phenyl)ethynyl)silane* (5u)**



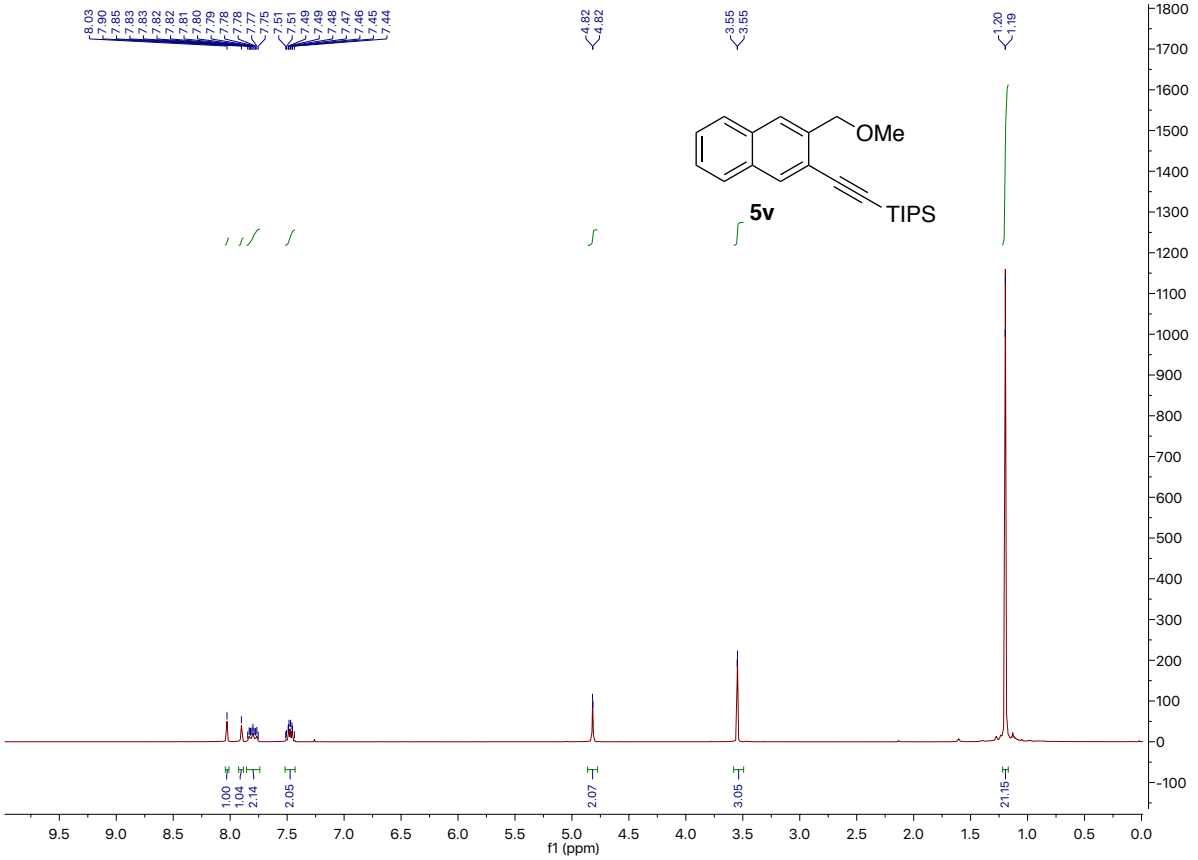


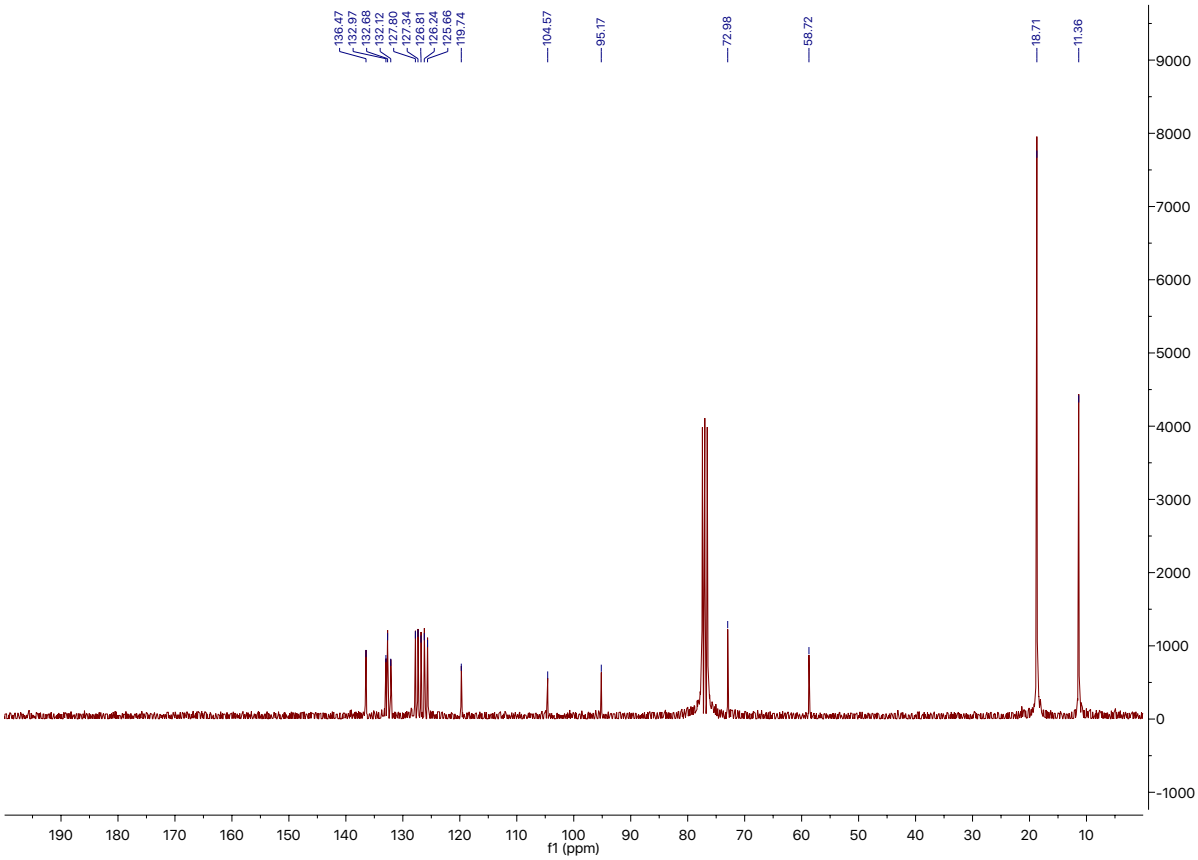
((2-(Methoxymethyl)-5-(trifluoromethyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) **(5u")**



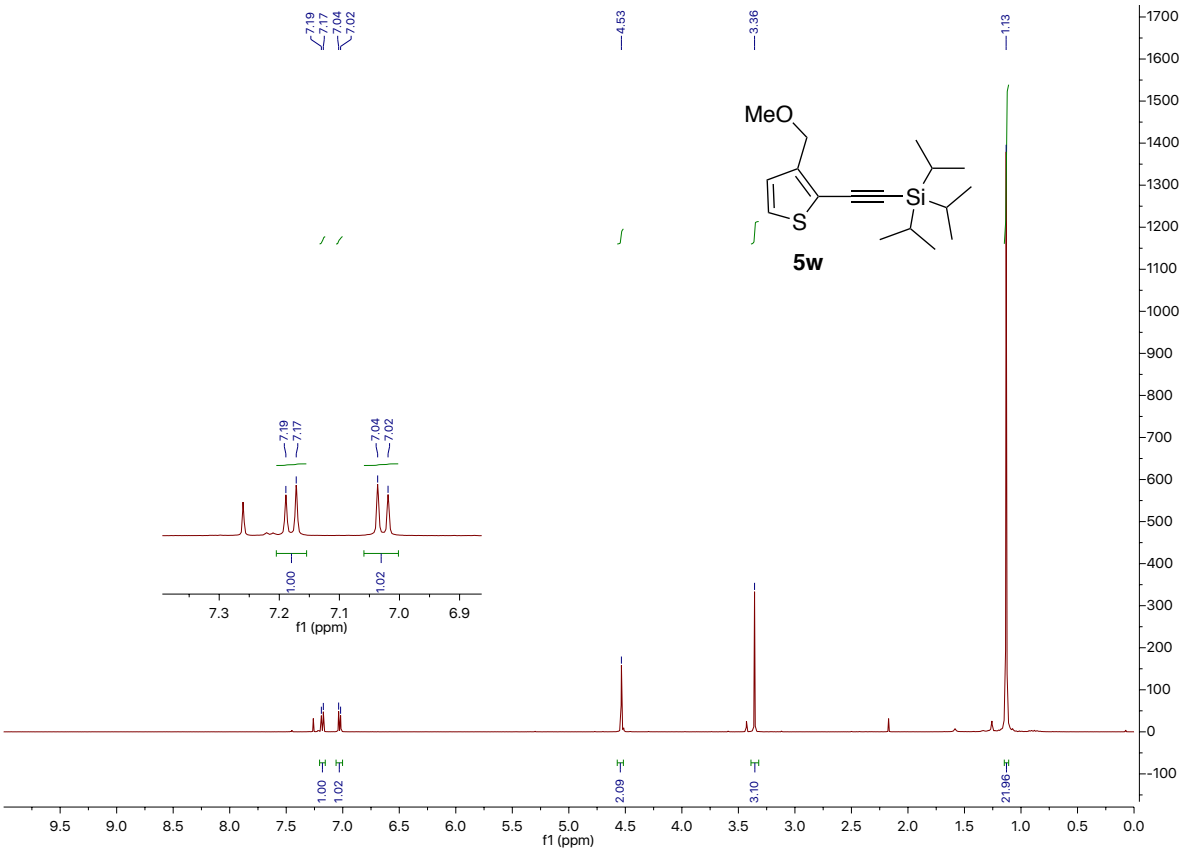


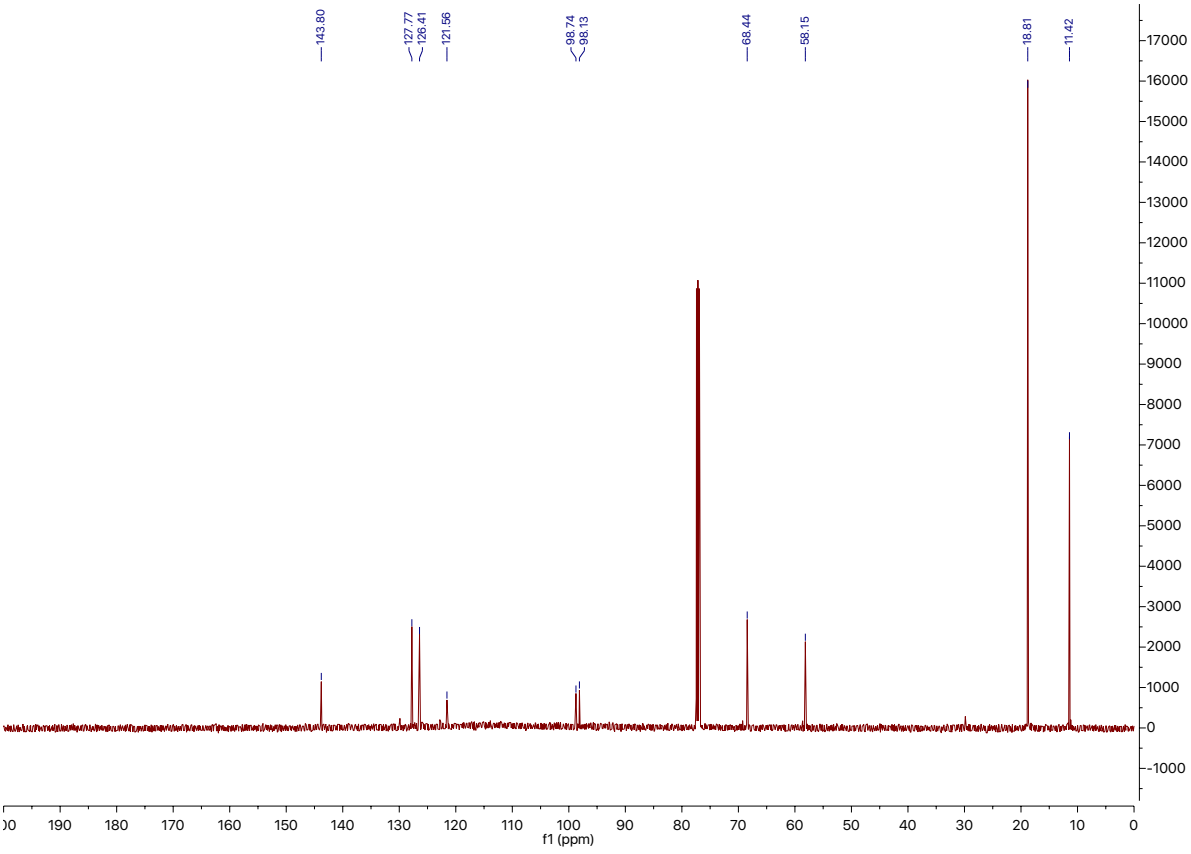
***Triisopropyl((3-(methoxymethyl)naphthalen-2-yl)ethynyl)silane* (5v)**



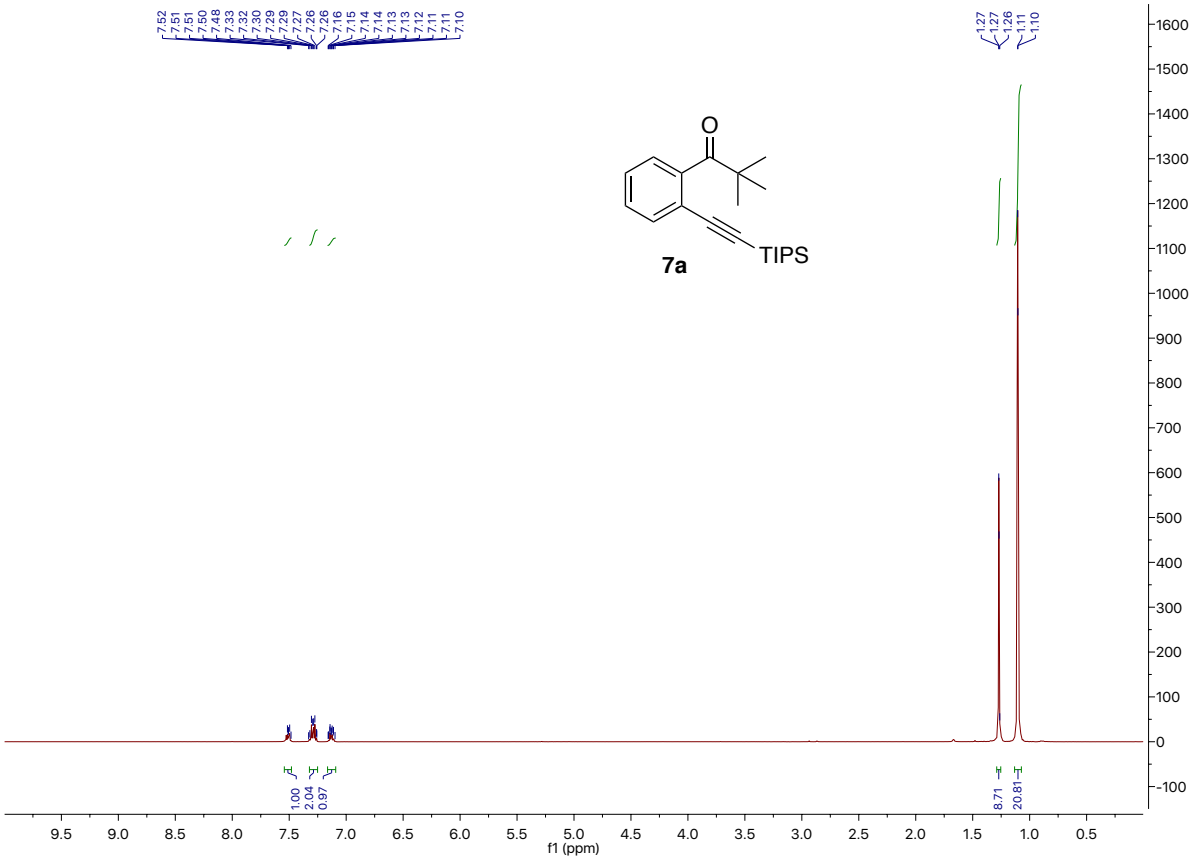


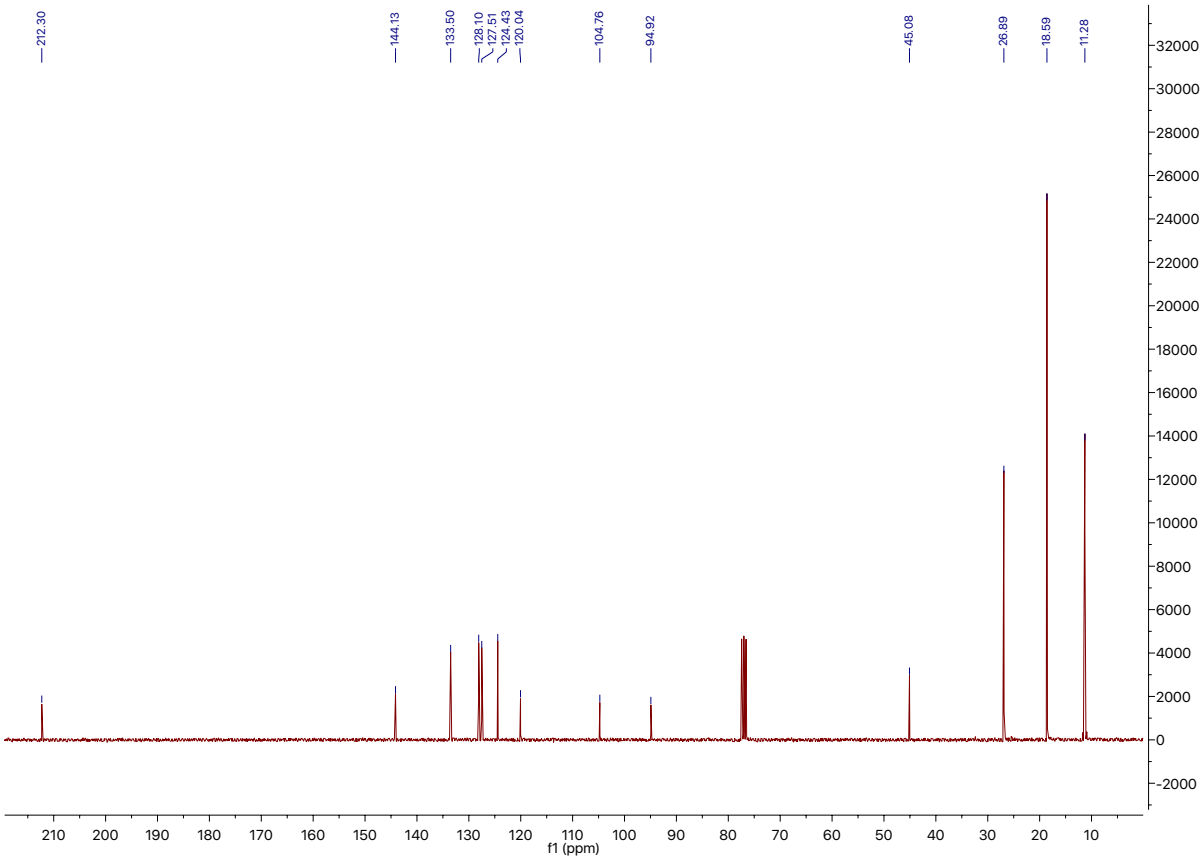
Triisopropyl((3-(methoxymethyl)thiophen-2-yl)ethynyl)silane **(5w)**



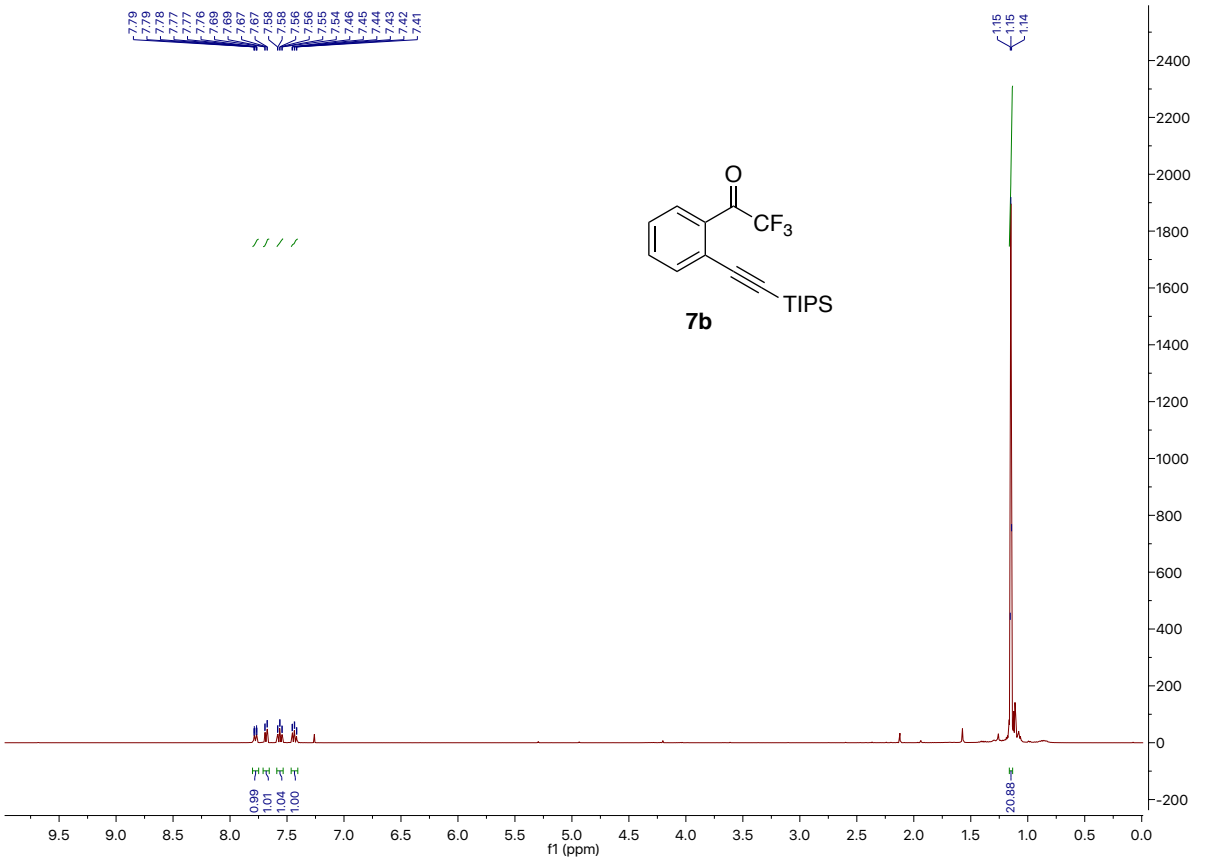


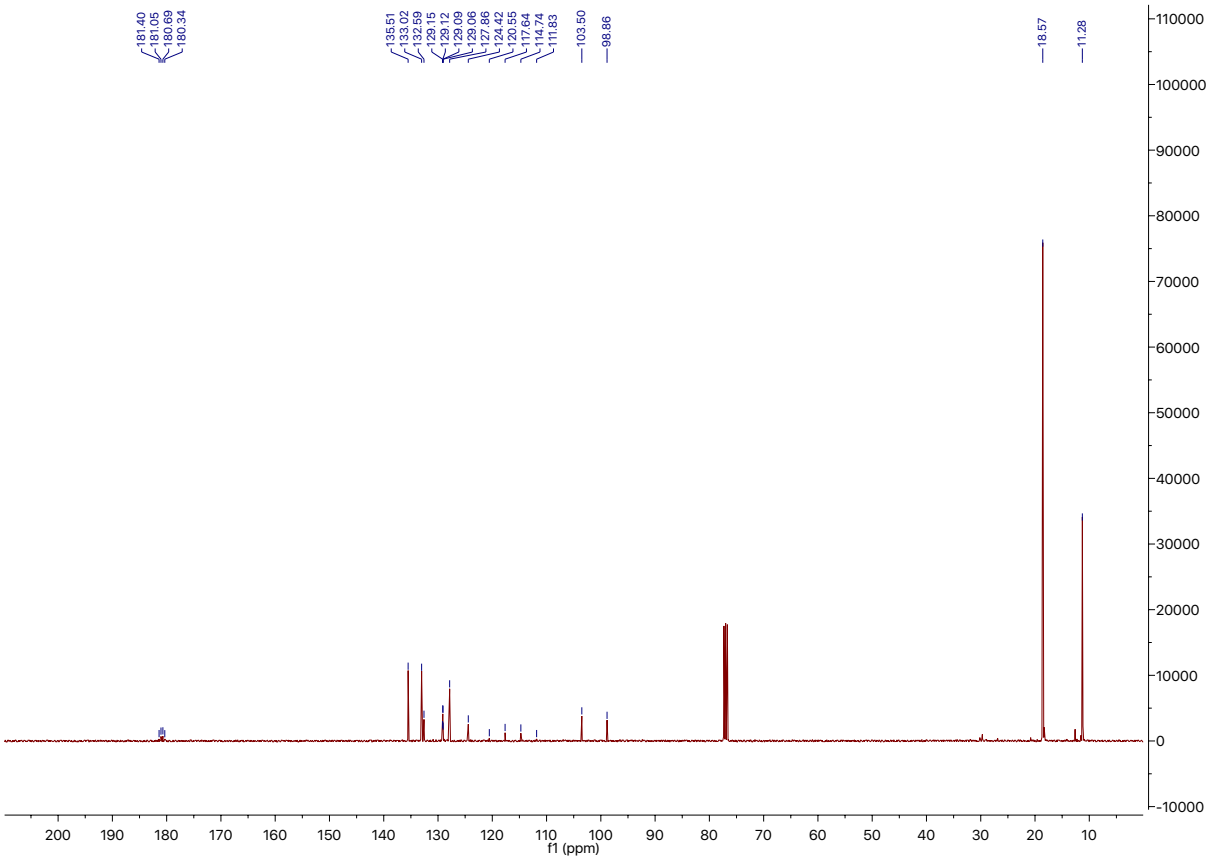
2,2-Dimethyl-1-(2-((triisopropylsilyl)ethynyl)phenyl)propan-1-one (**7a**)



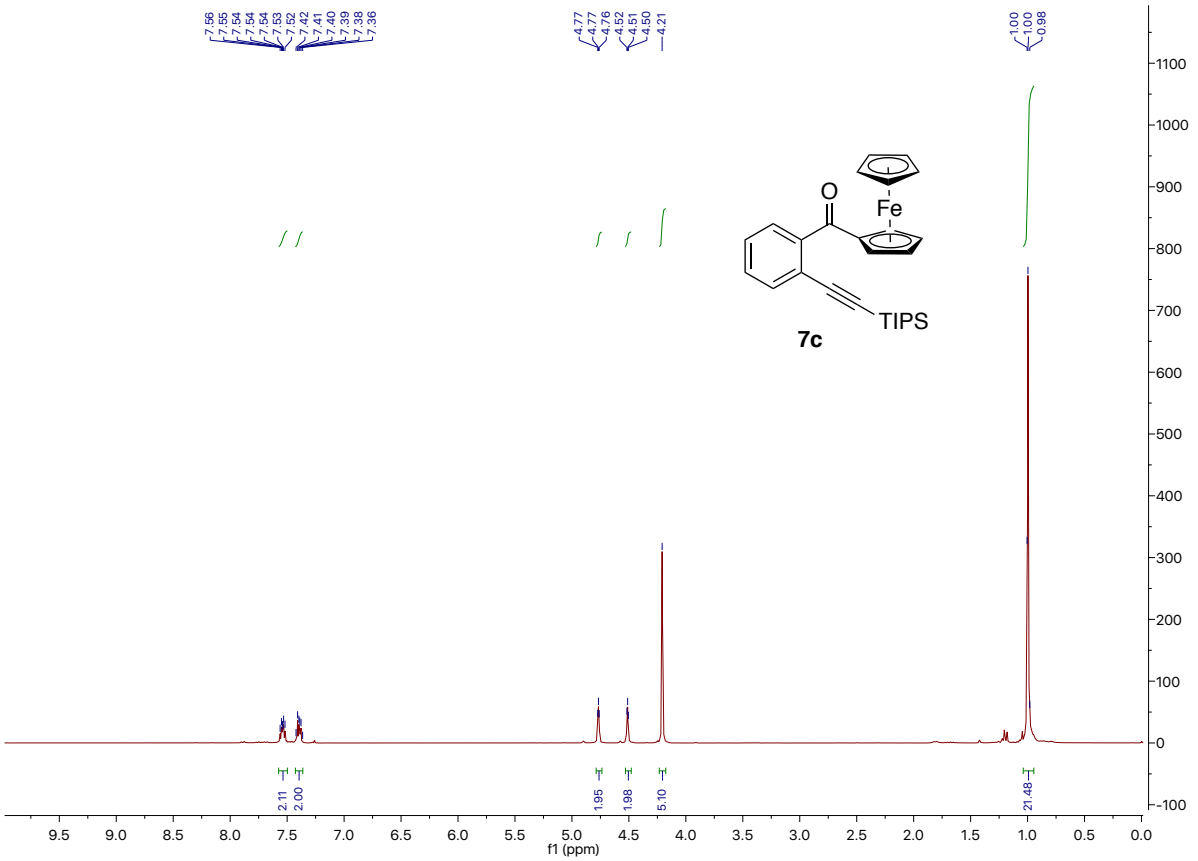


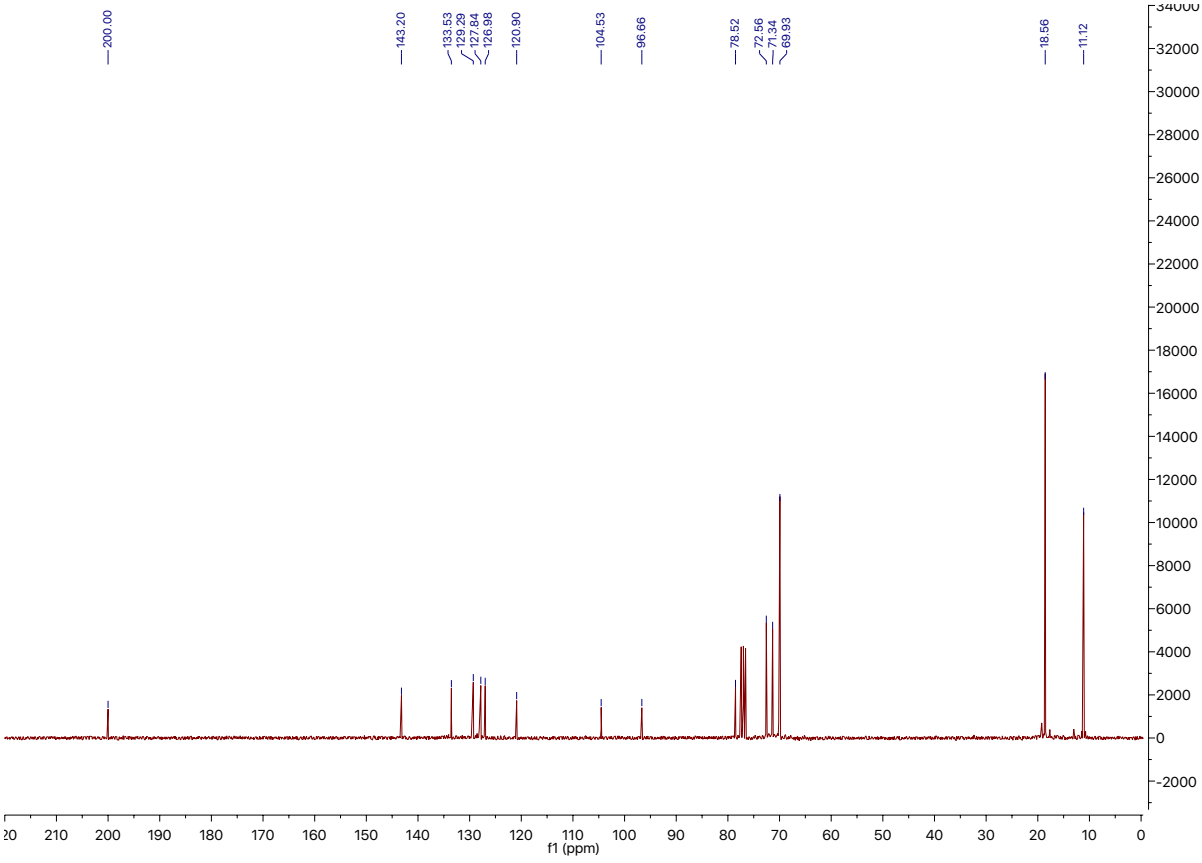
2,2,2-Trifluoro-1-(2-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7b**)



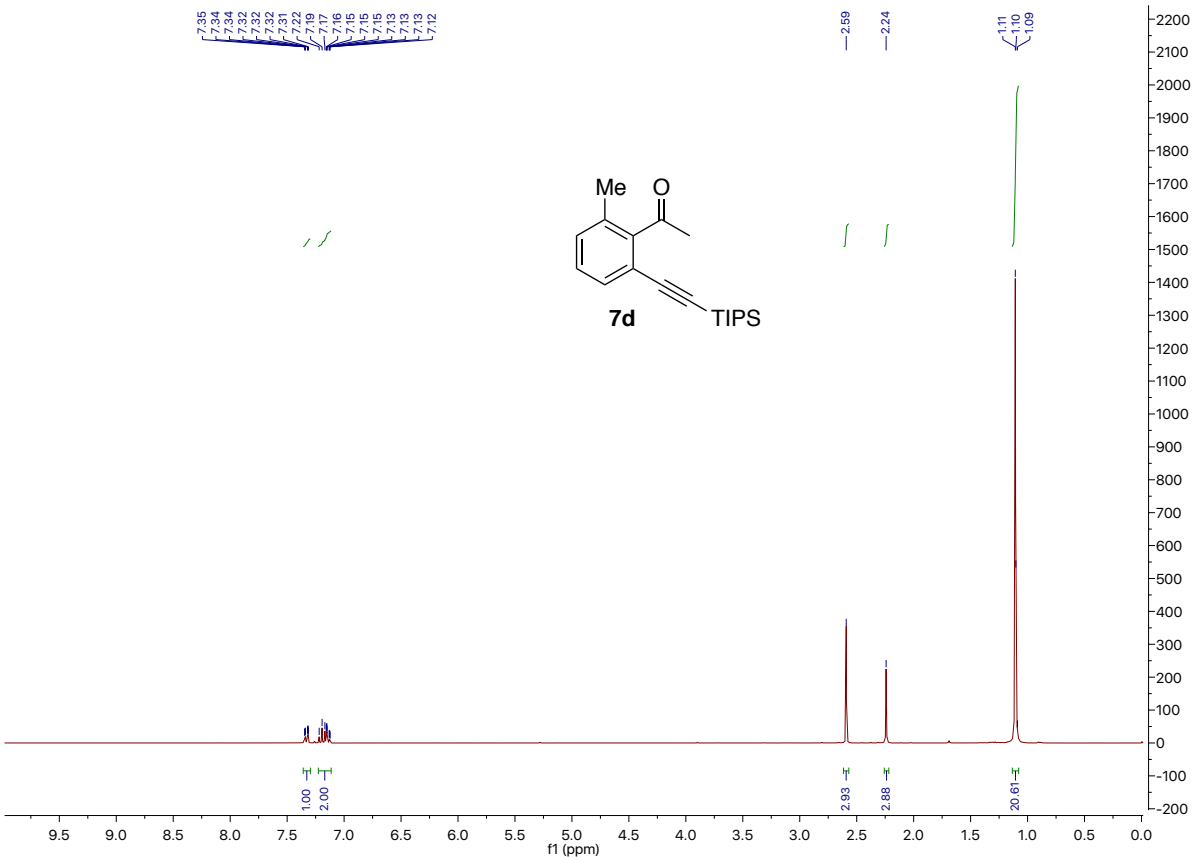


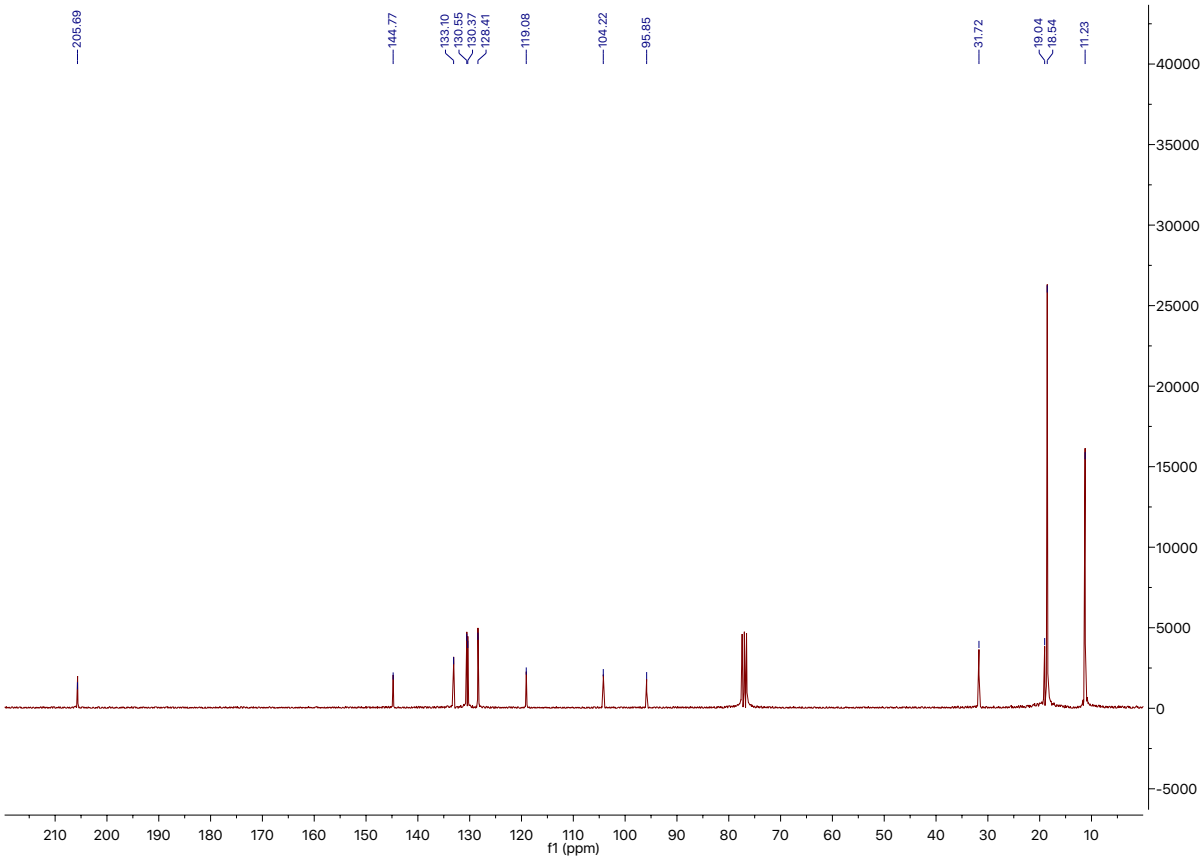
***2-((Triisopropylsilyl)ethynyl)benzoyl ferrocene* (7c)**



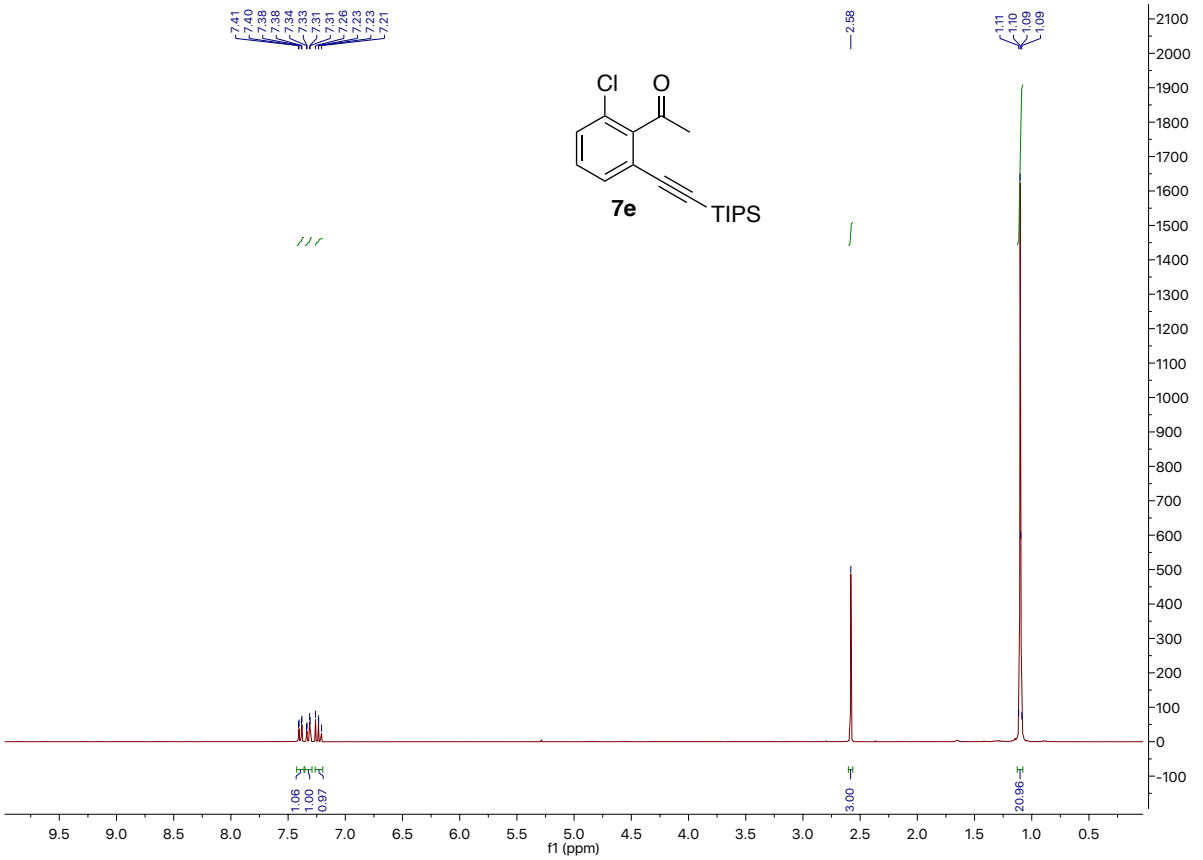


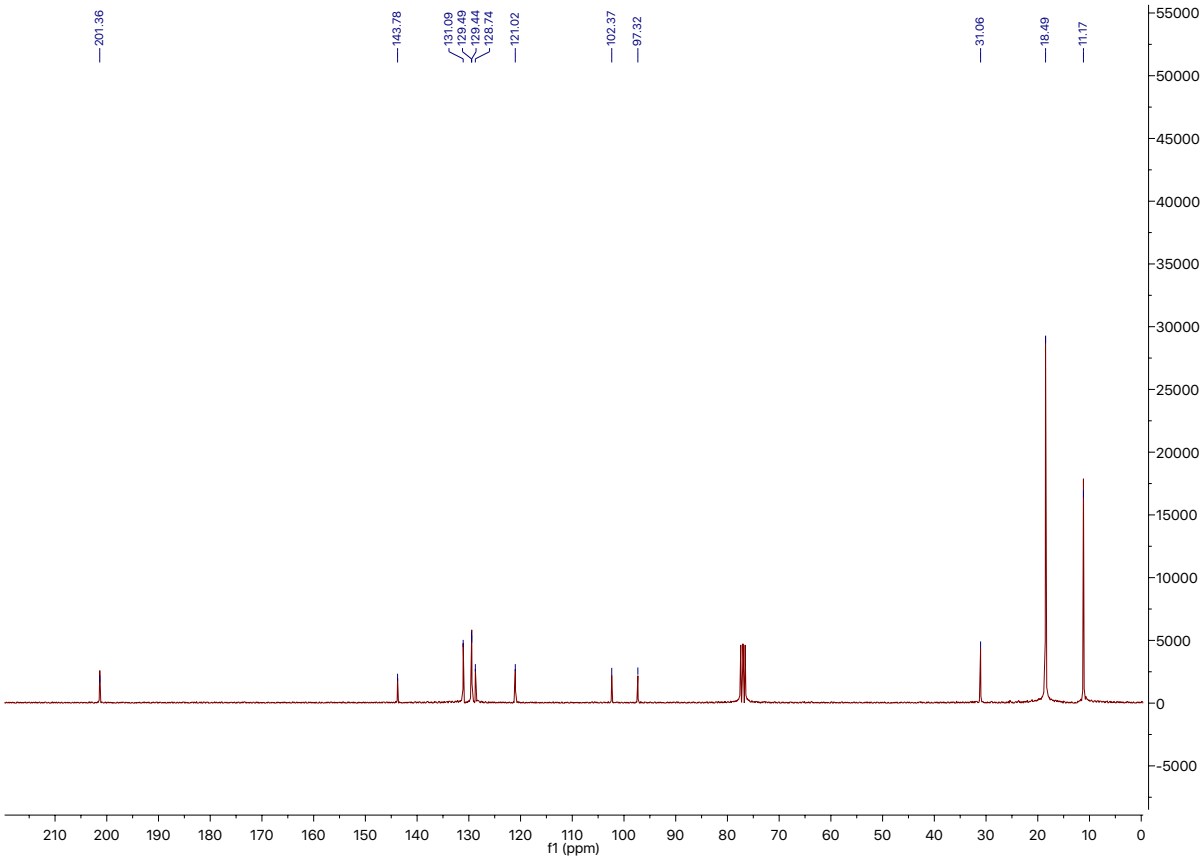
1-(2-Methyl-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7d**)



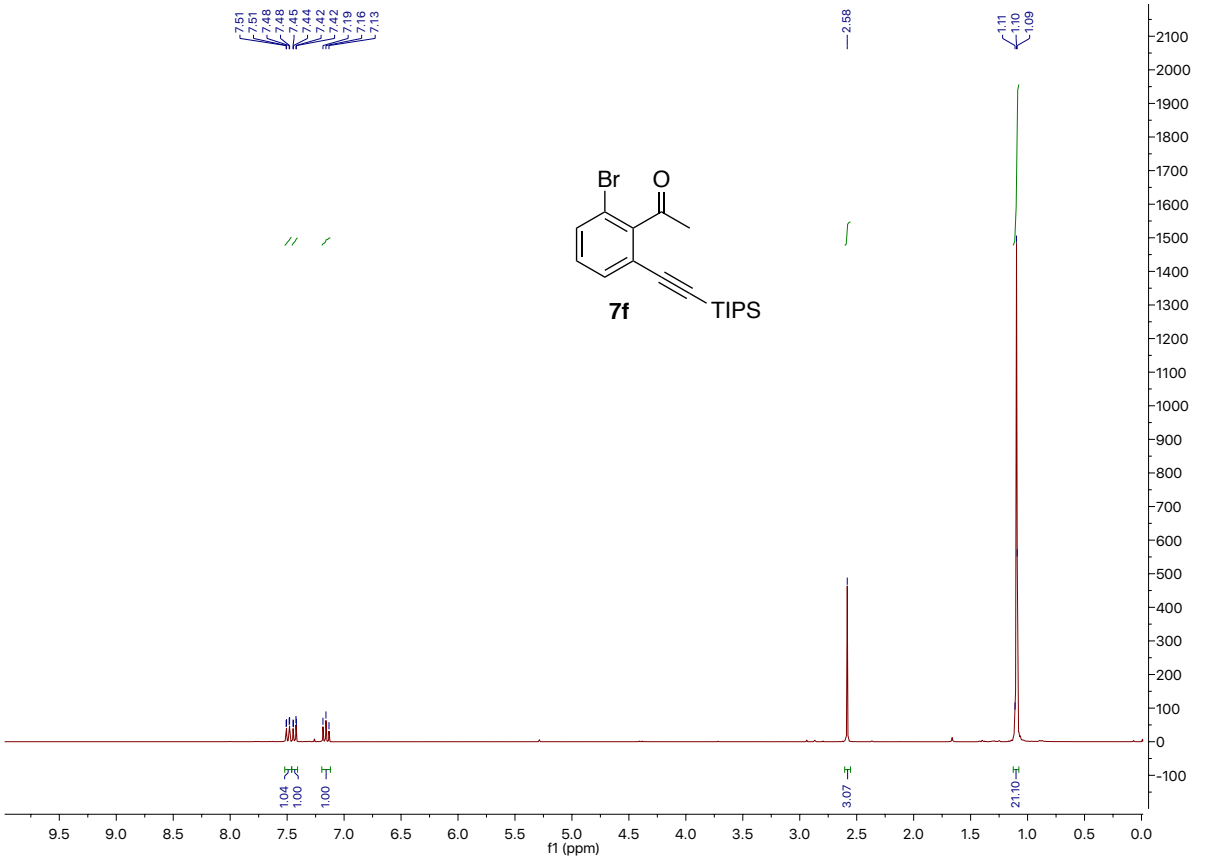


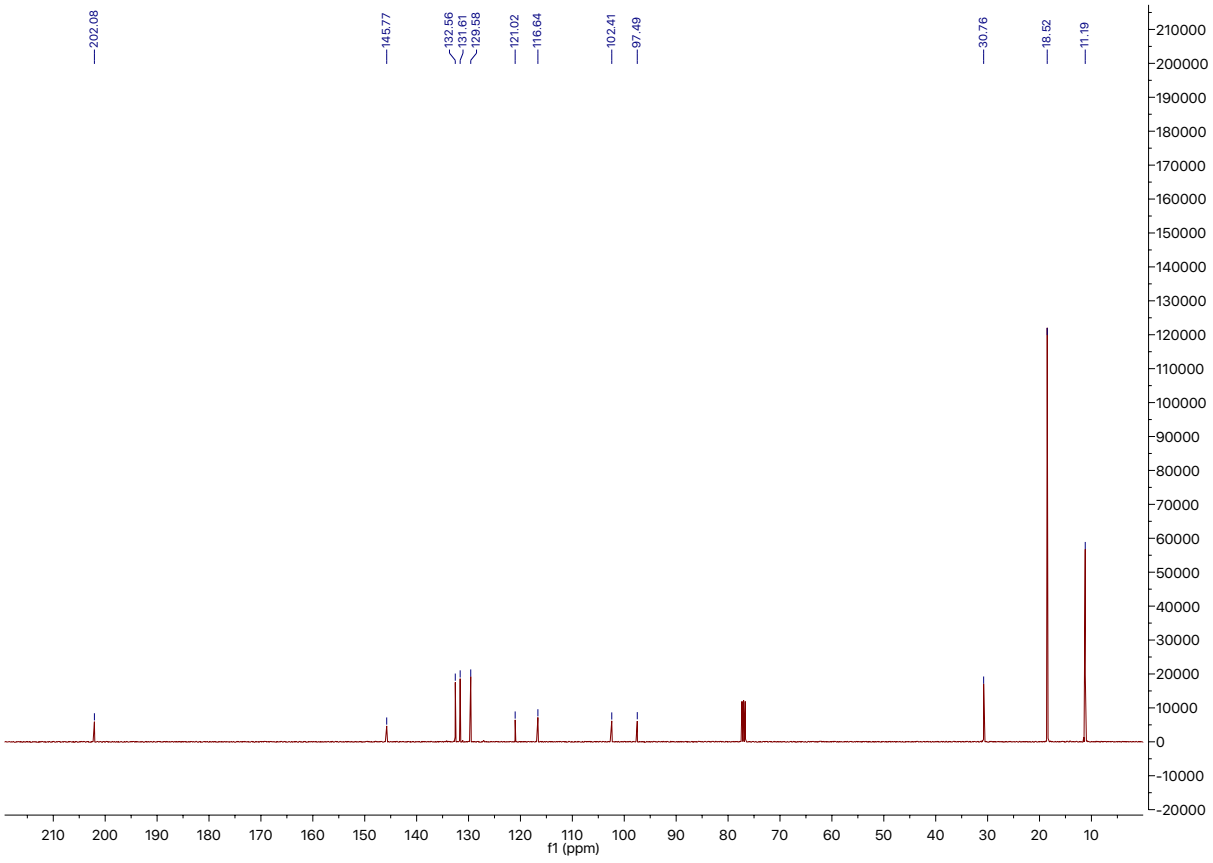
1-(2-Chloro-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one **(7e)**



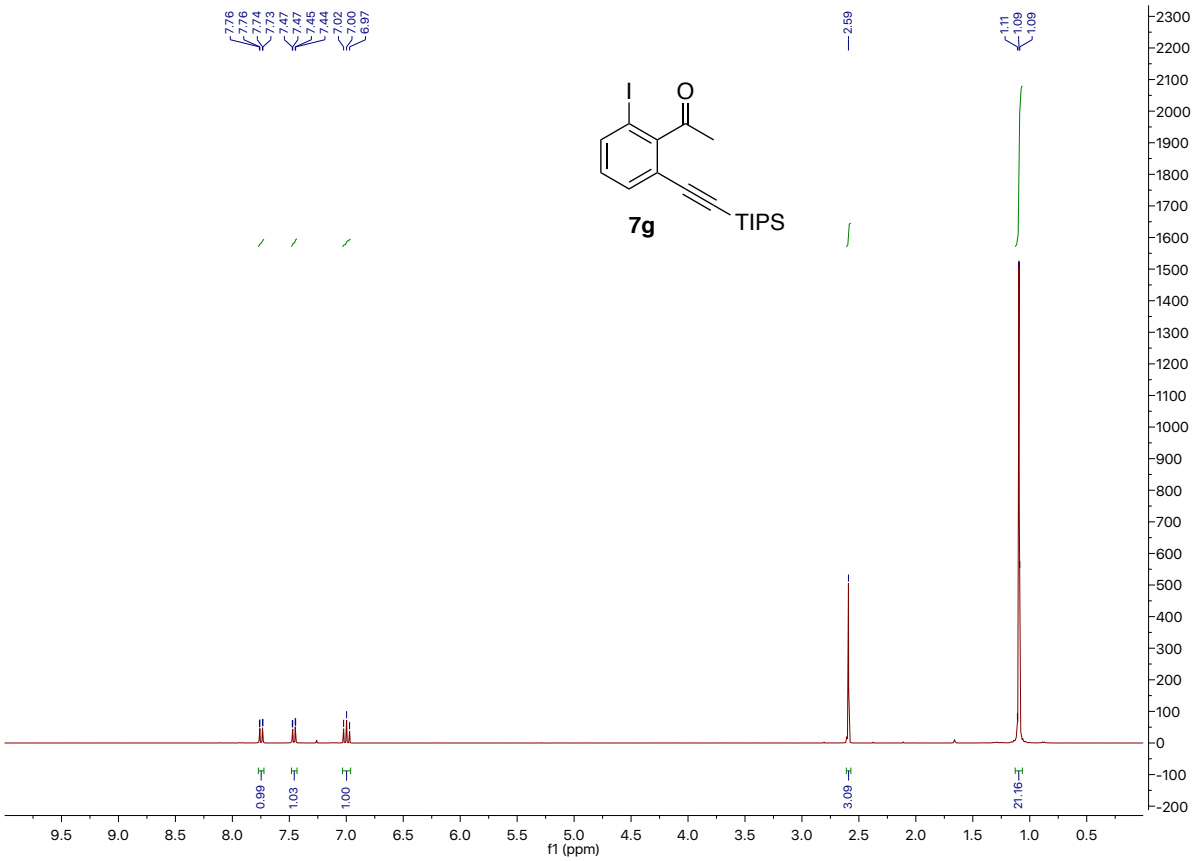


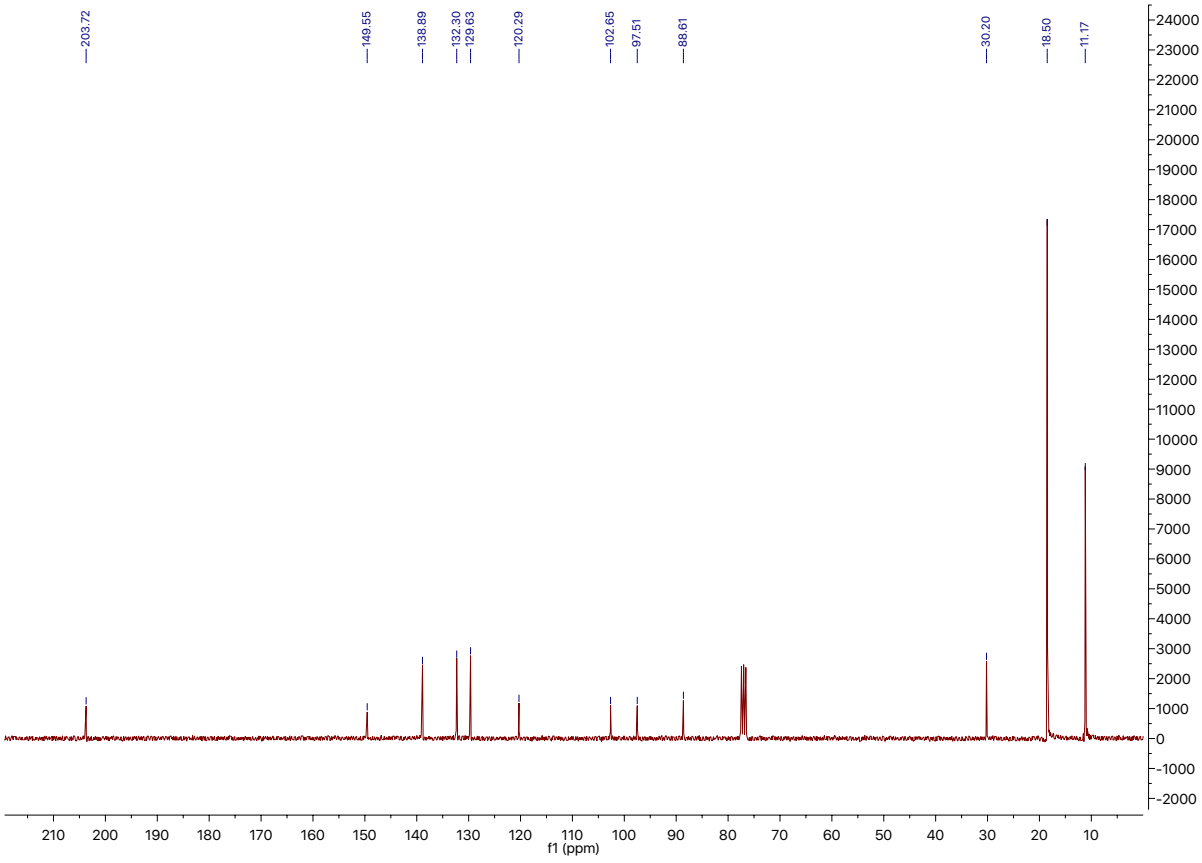
***1-(2-Bromo-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one* (7f)**



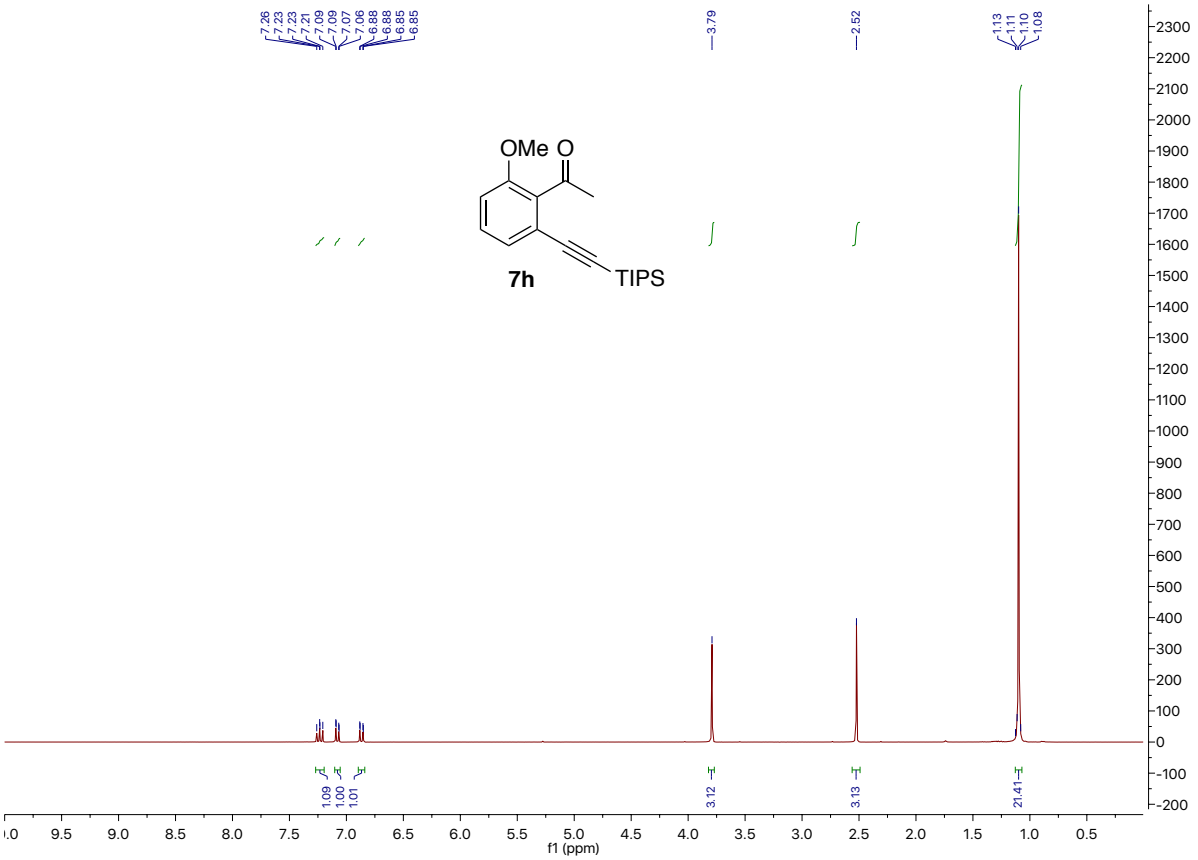


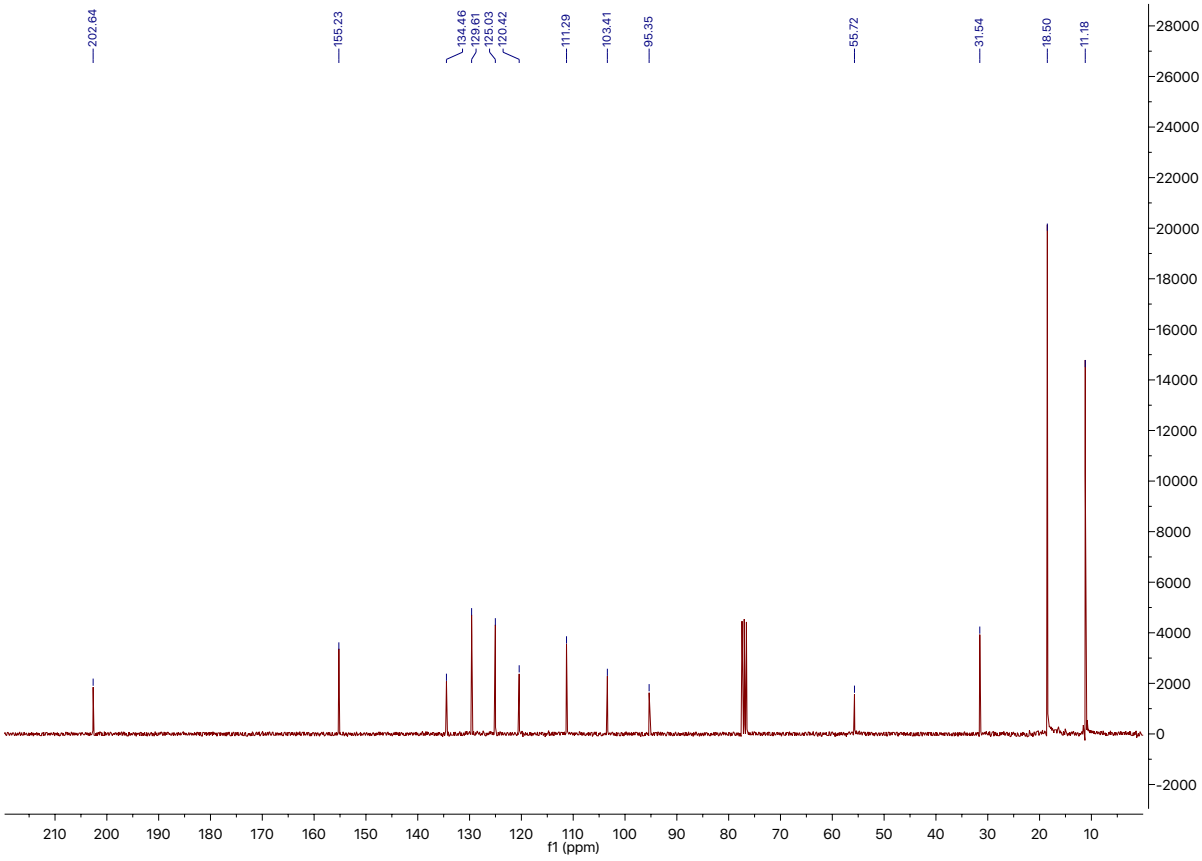
***1-(2-Iodo-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one* (7g)**



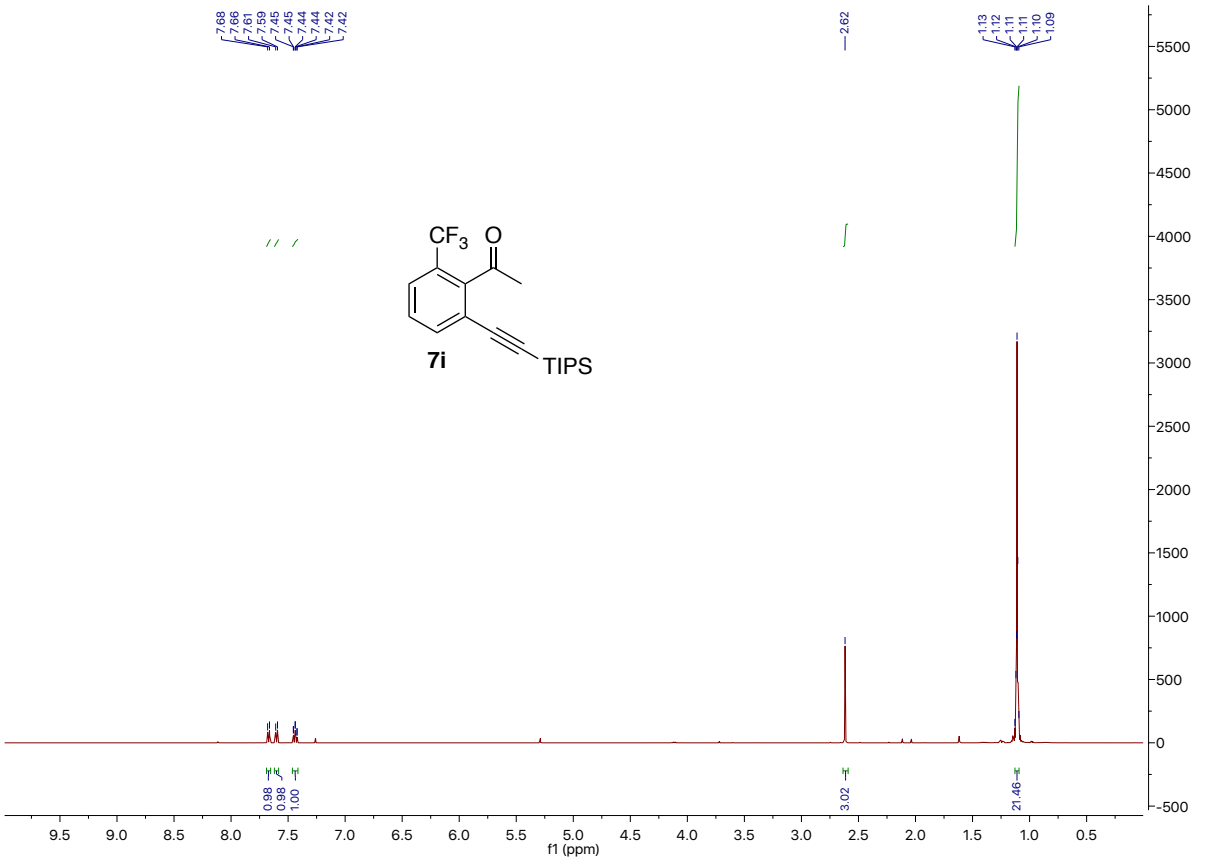


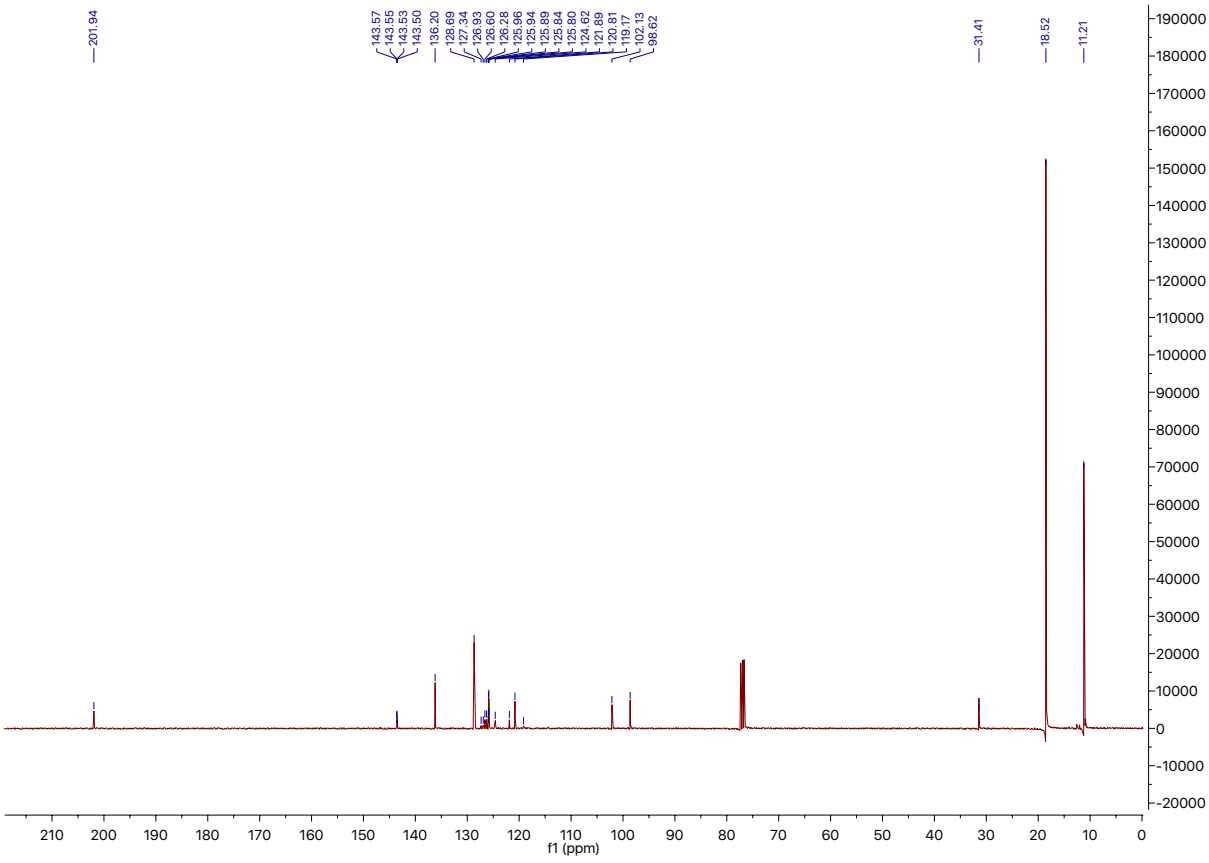
1-(2-Methoxy-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7h**)



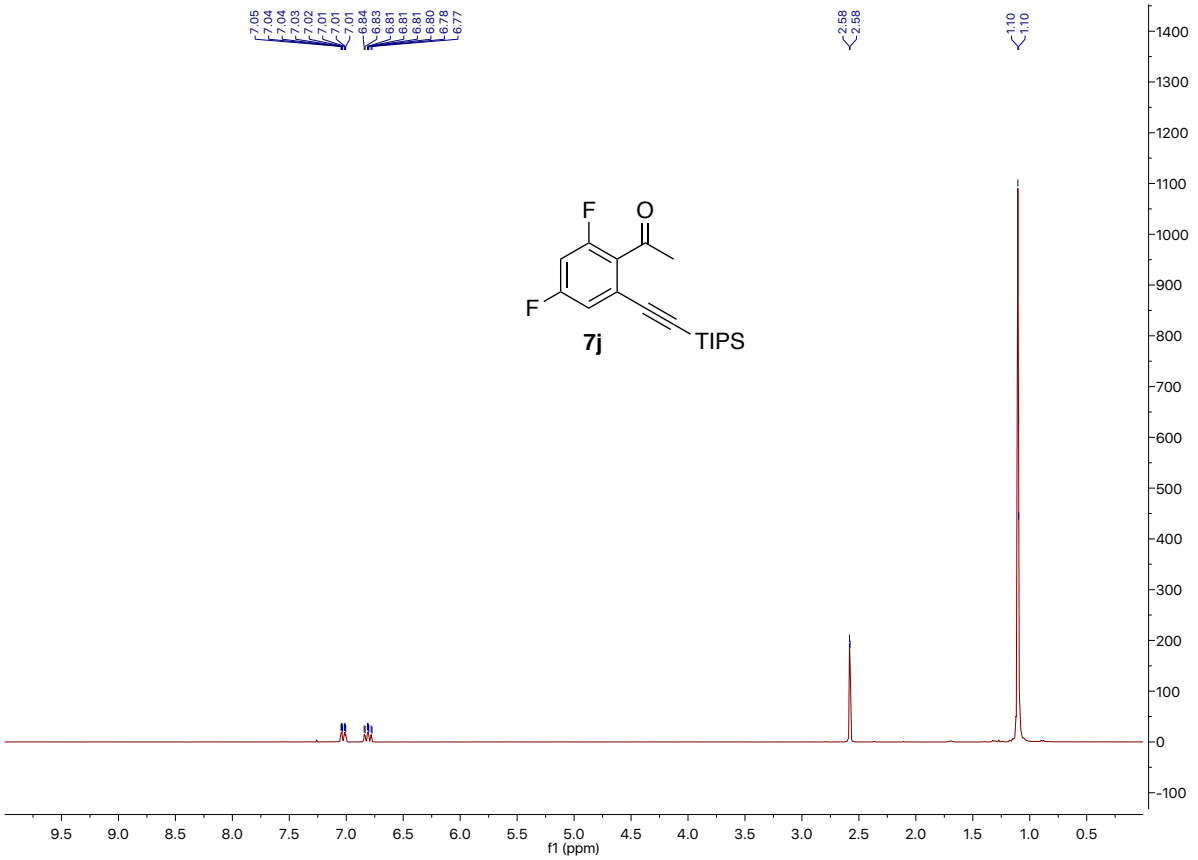


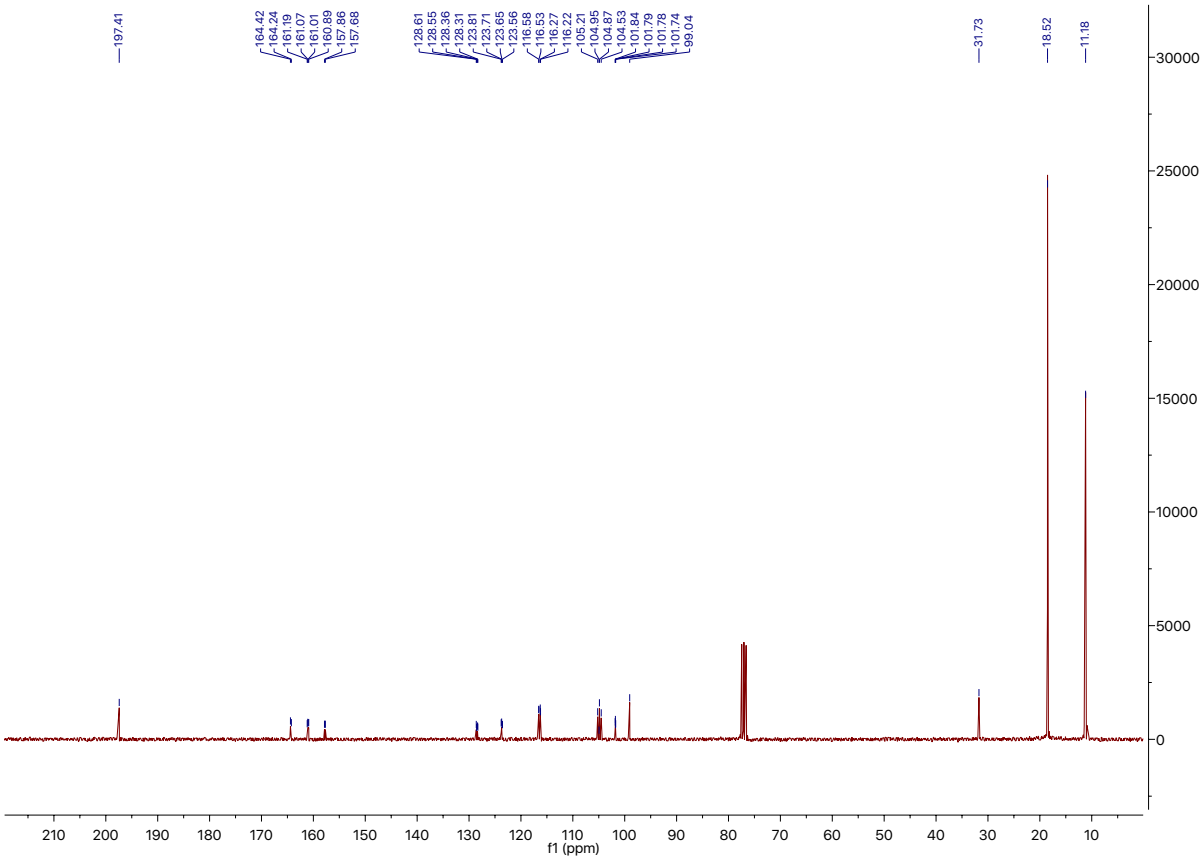
1-(2-(Trifluoromethyl)-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7i**)



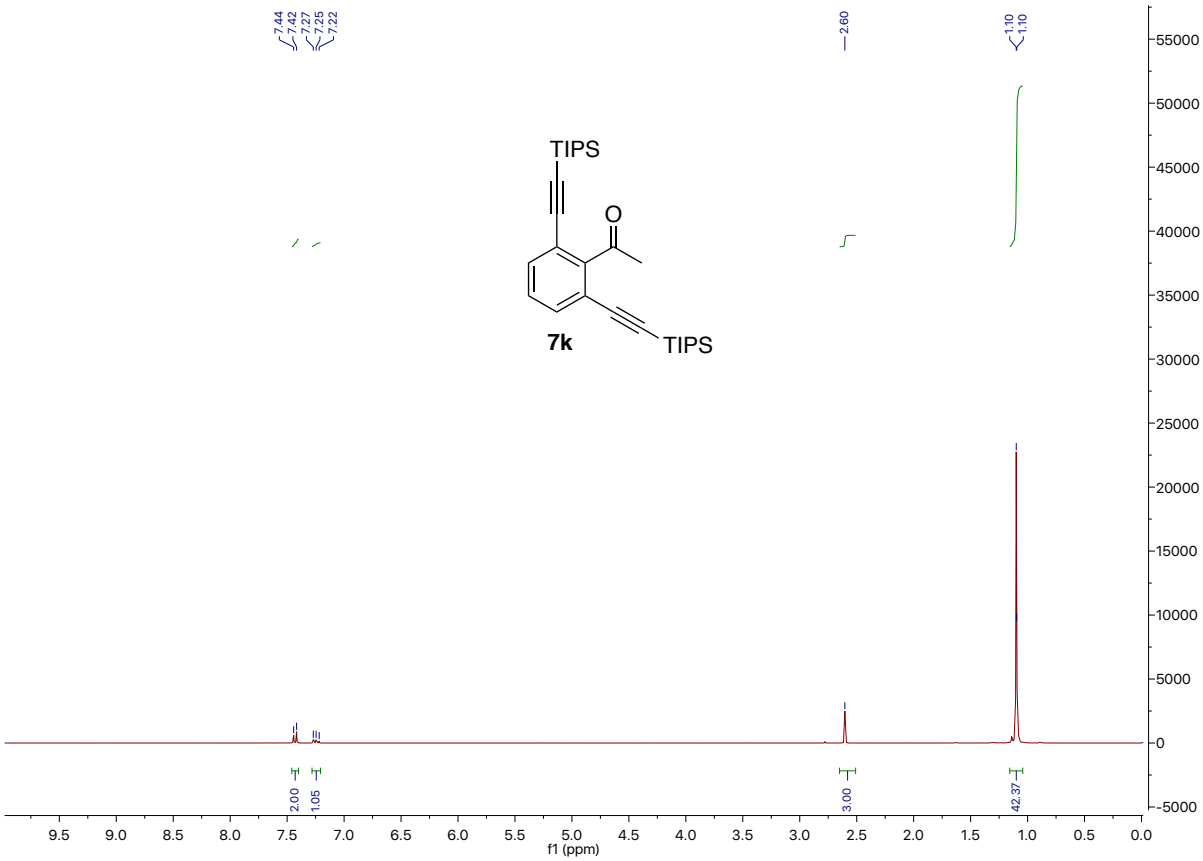


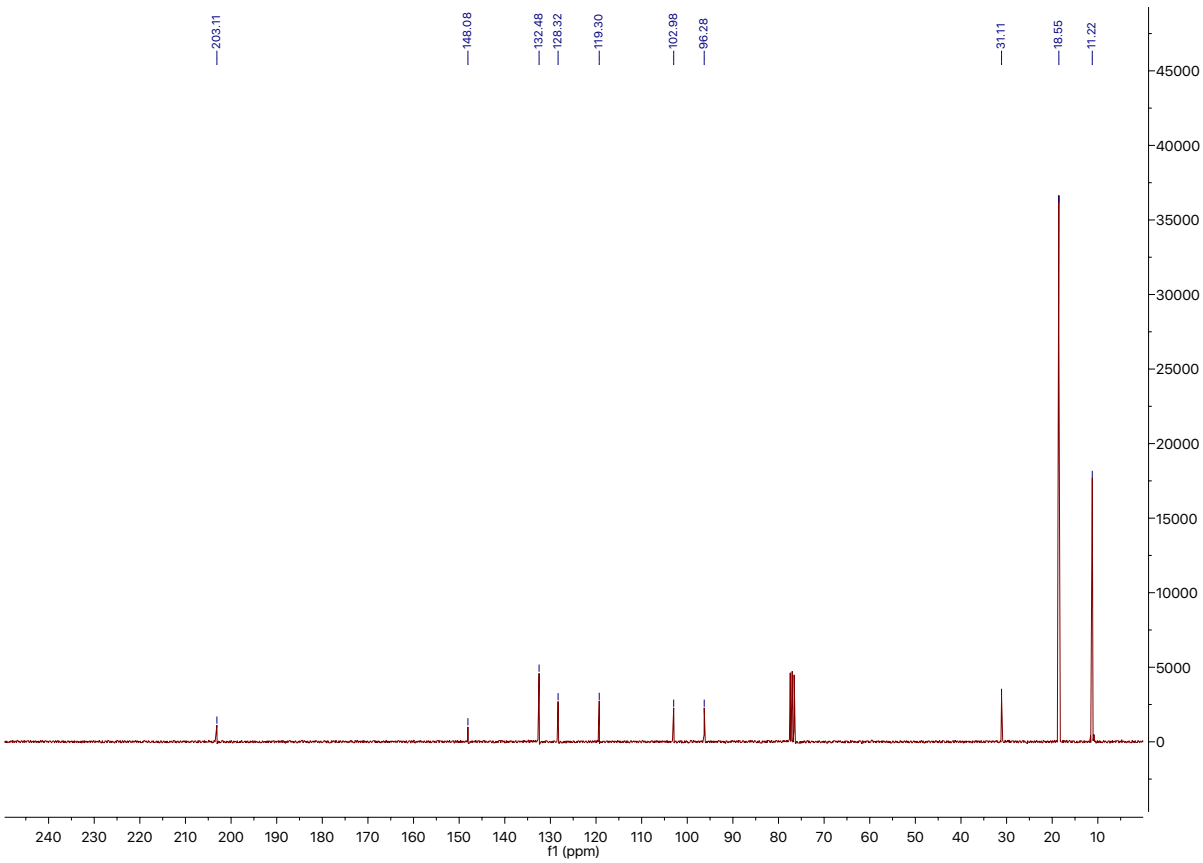
1-(2,4-Difluoro-6-((triisopropylsilyl)ethynyl)phenyl)ethan-1-one (**7j**)



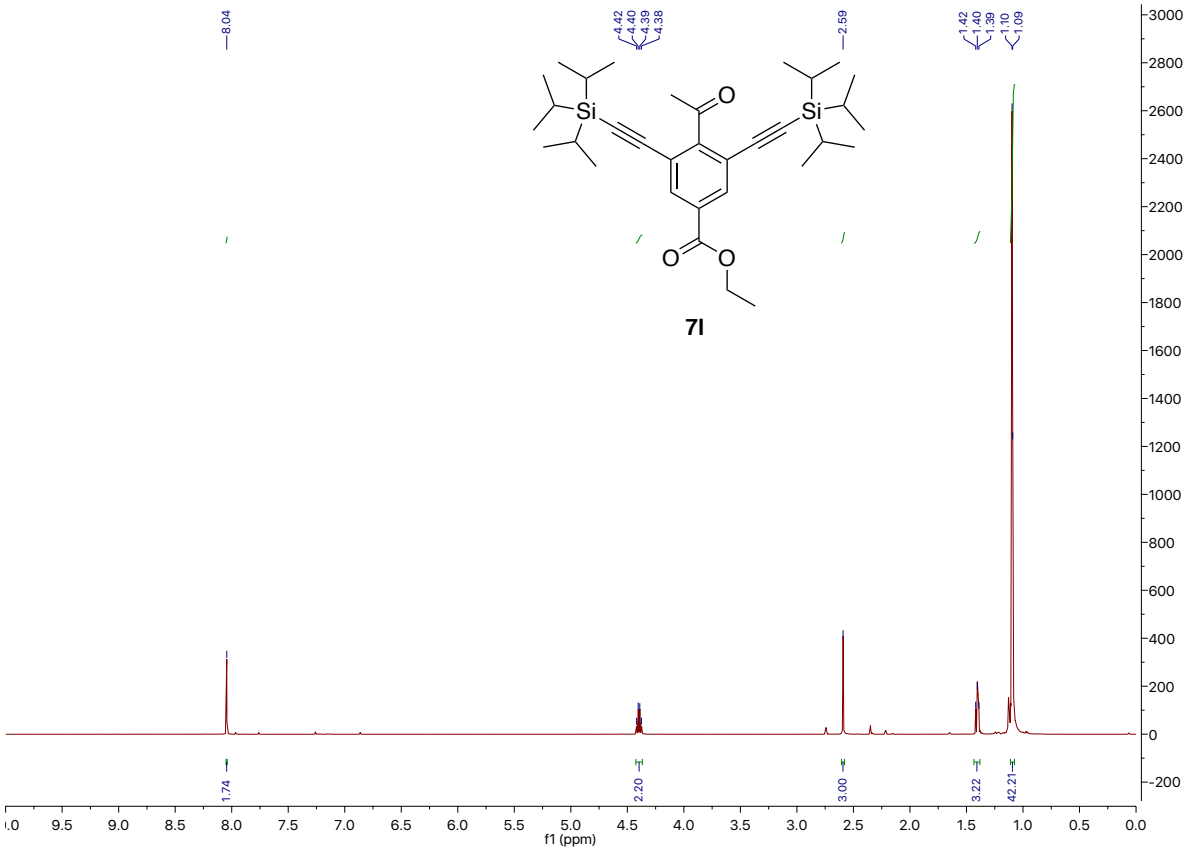


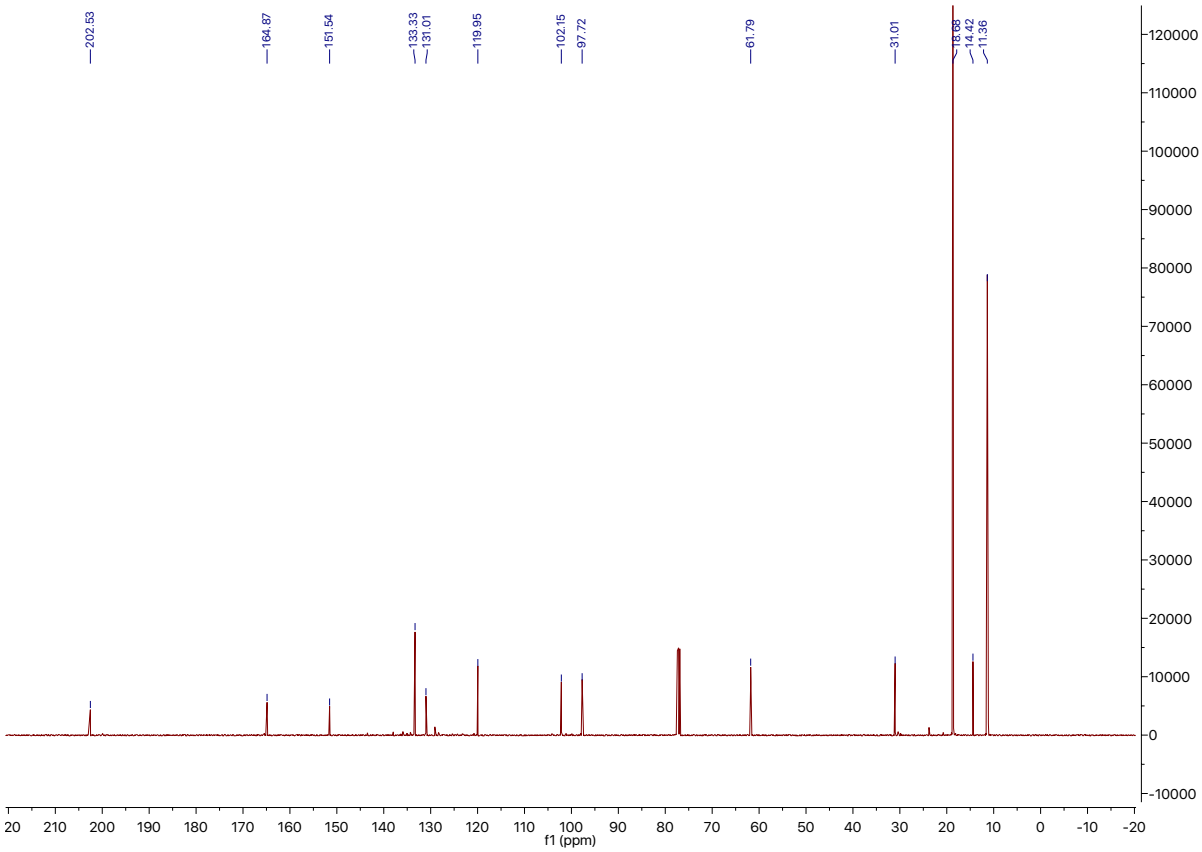
1-*(2,6-Bis((triisopropylsilyl)ethynyl)phenyl)ethan-1-one* (**7k**)



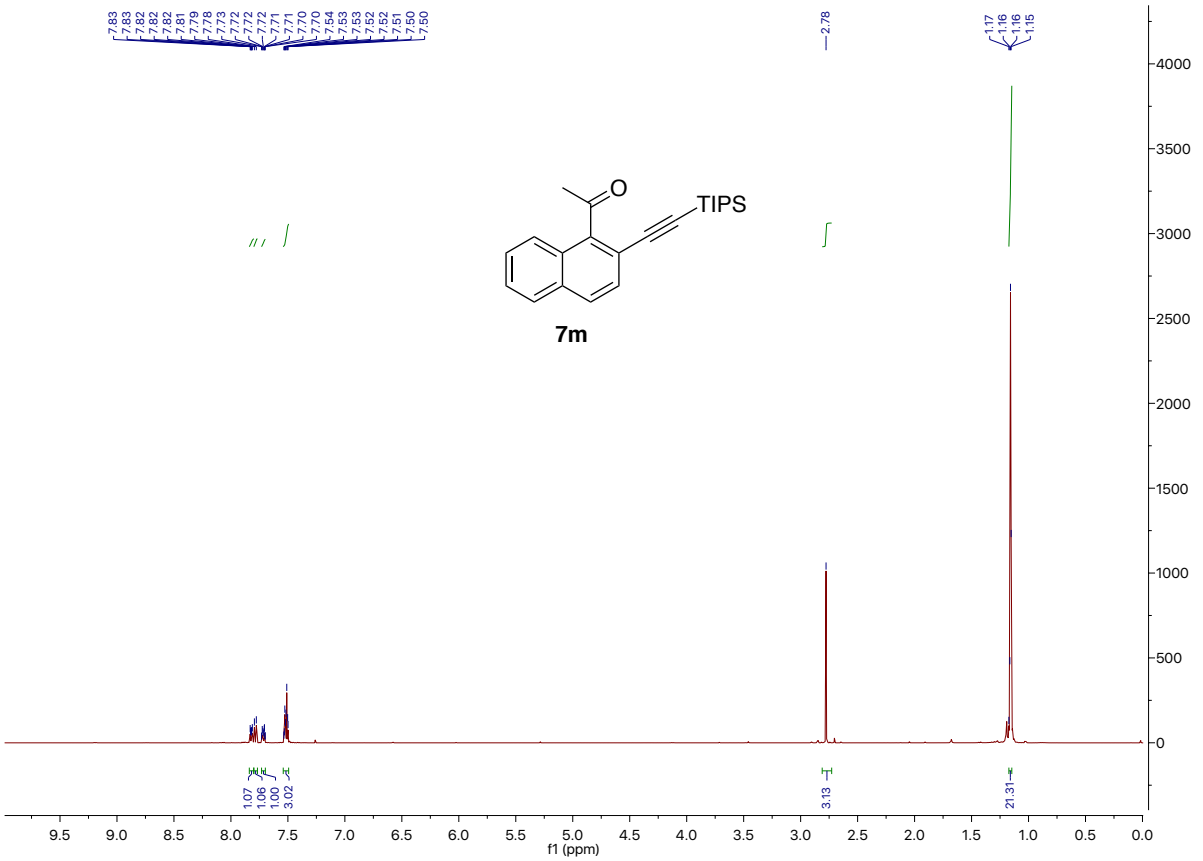


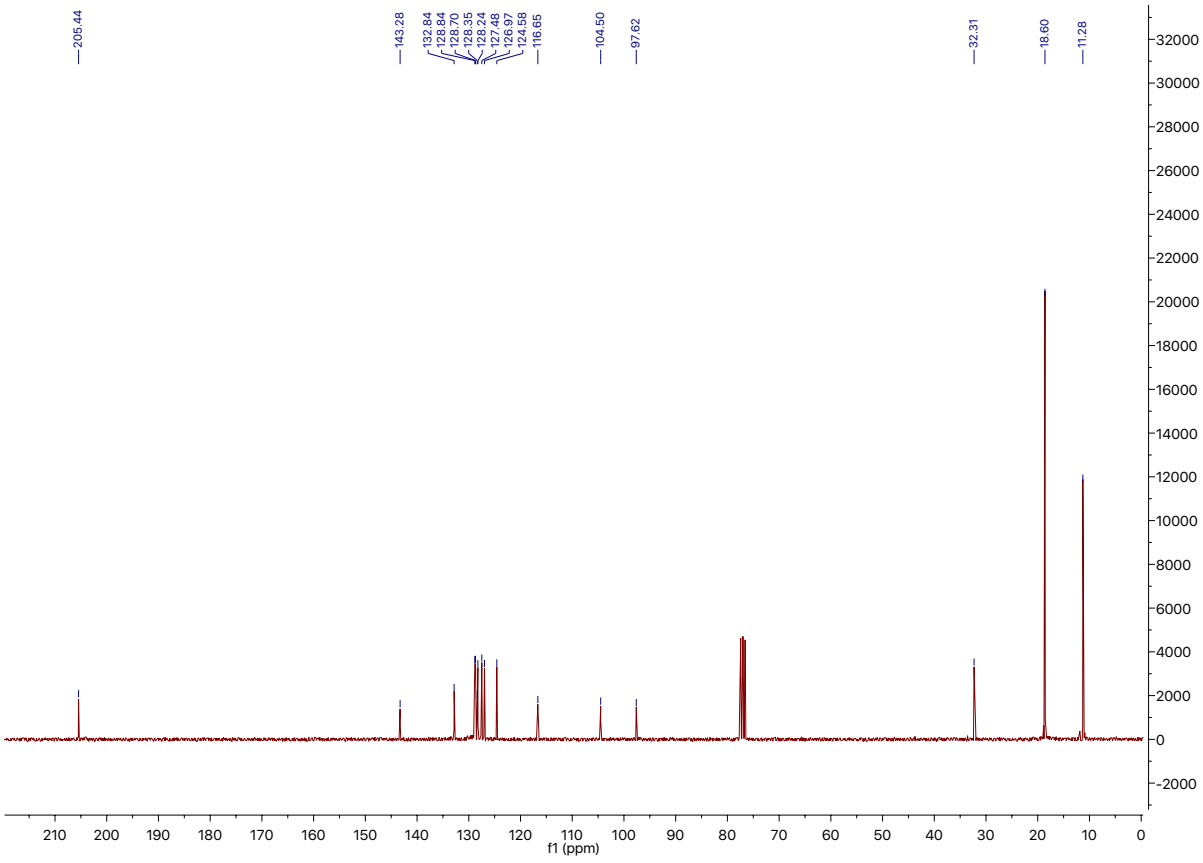
Ethyl 4-acetyl-3,5-bis((triisopropylsilyl)ethynyl)benzoate **(7l)**



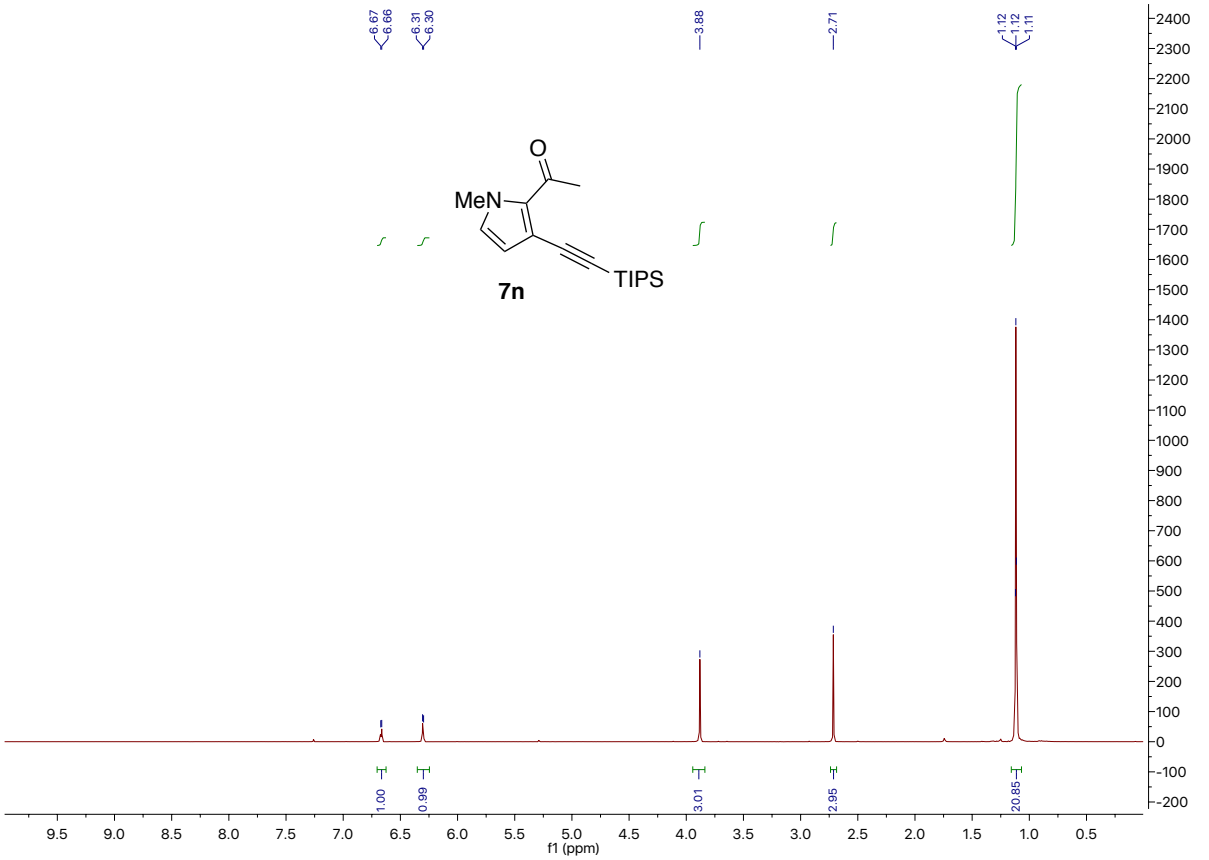


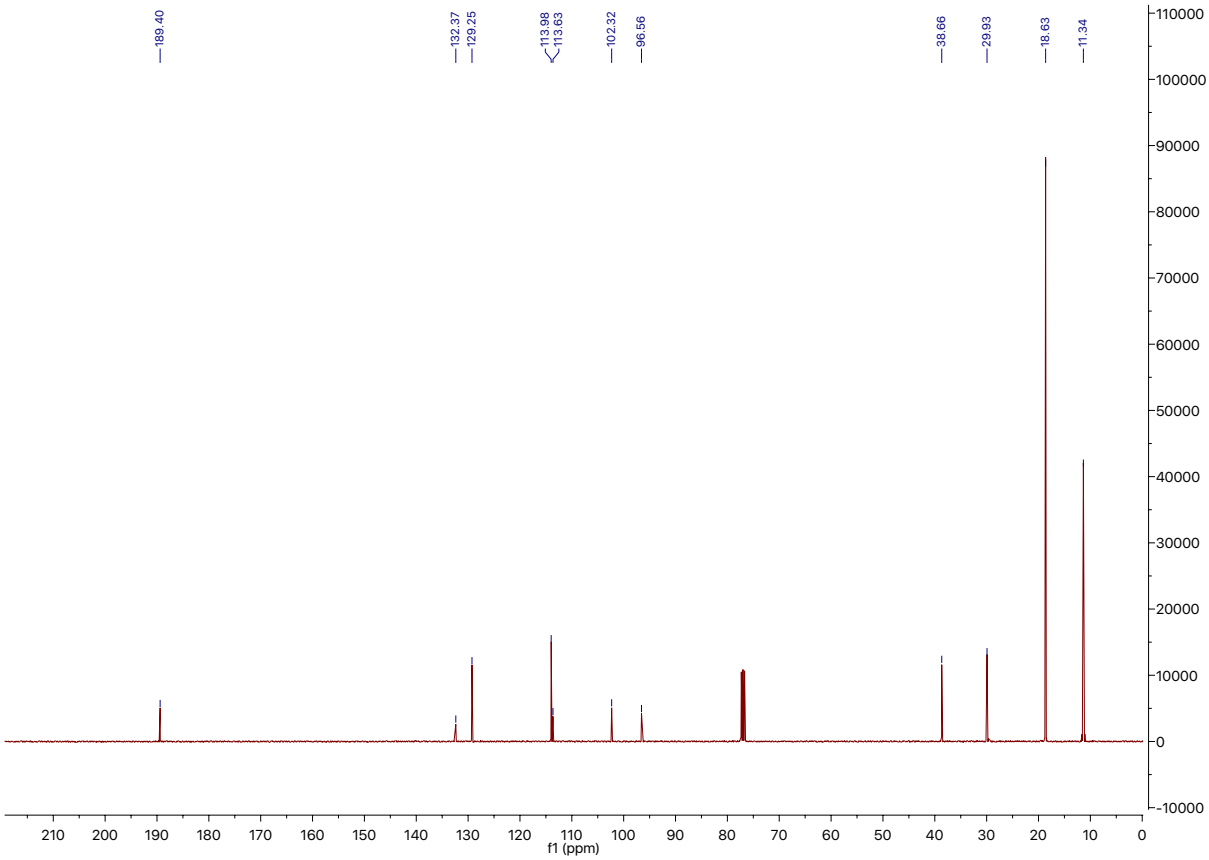
1-(2-((Triisopropylsilyl)ethynyl)naphthalen-1-yl)ethan-1-one (**7m**)



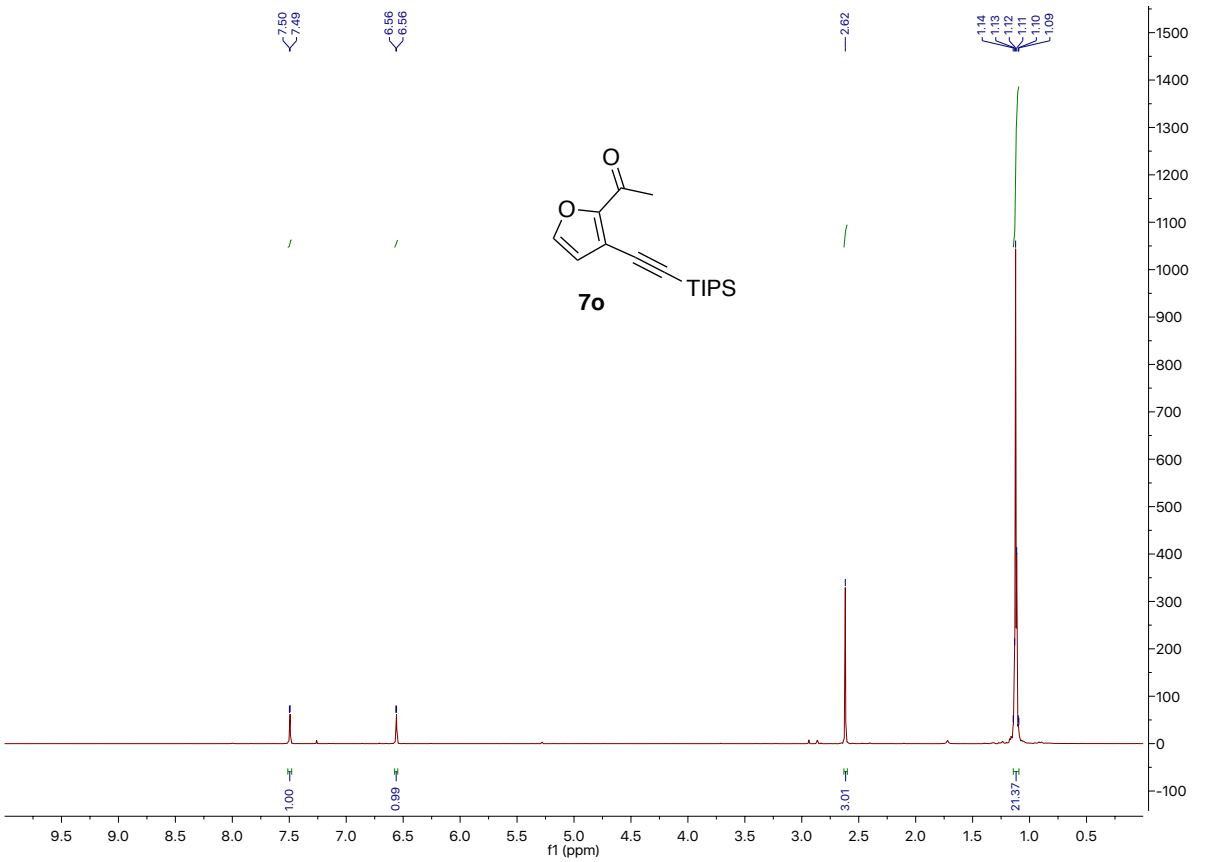


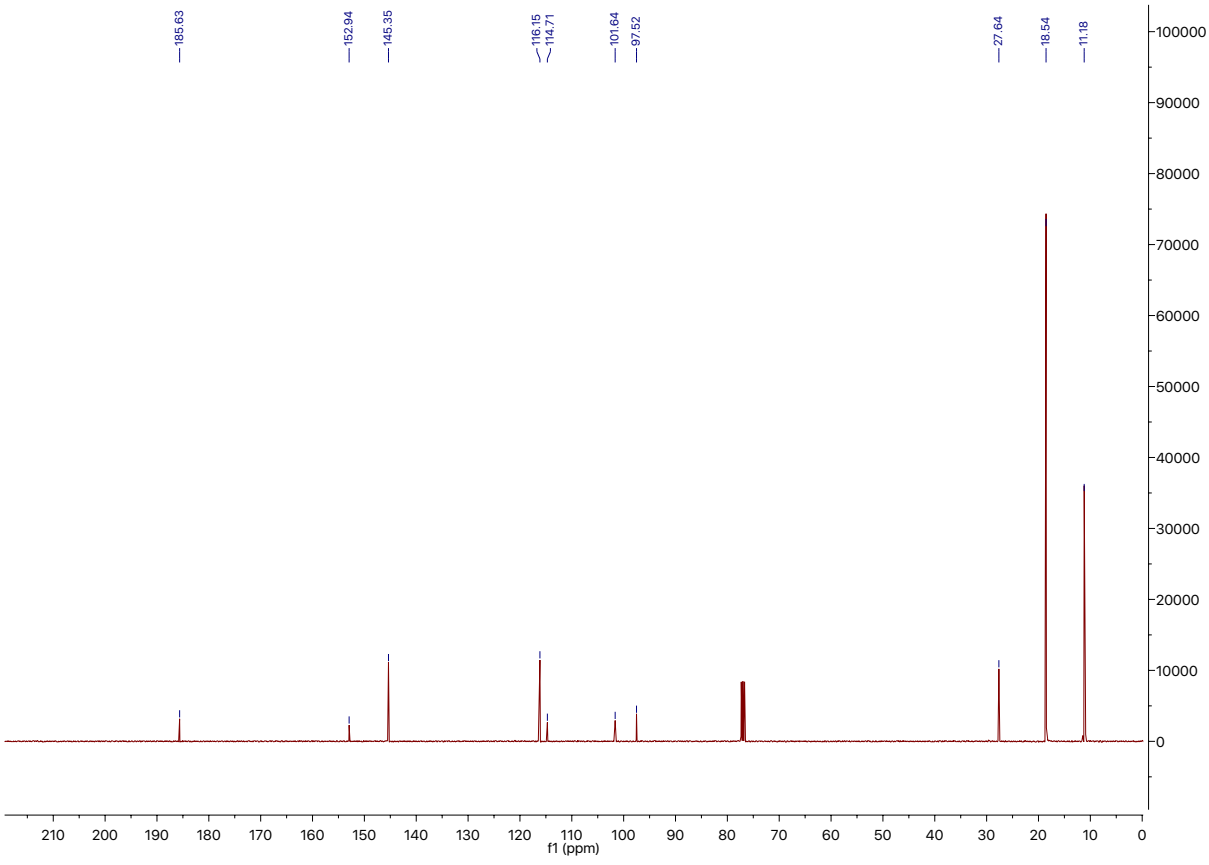
1-(1-Methyl-3-((triisopropylsilyl)ethynyl)-1H-pyrrol-2-yl)ethan-1-one (**7n**)



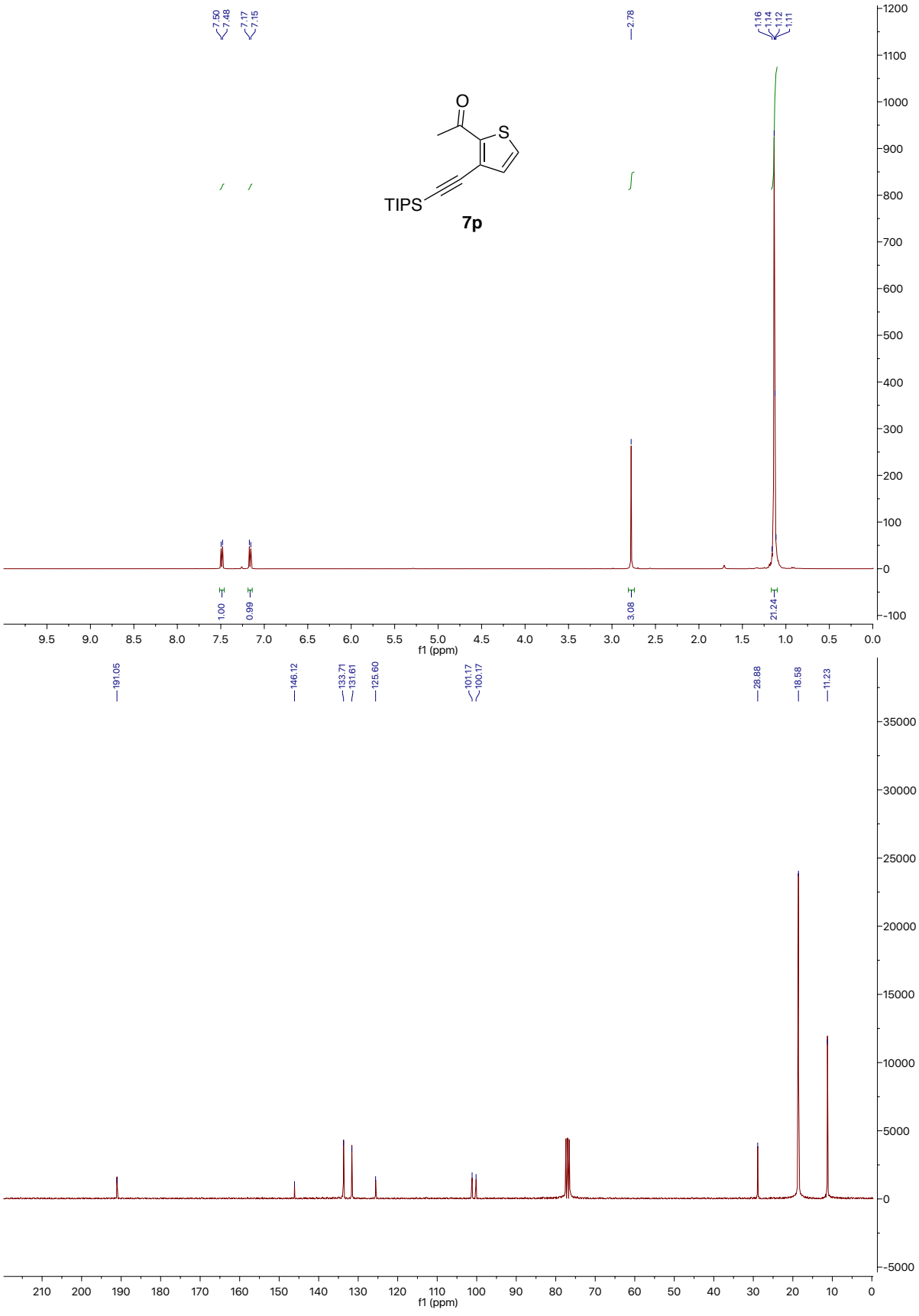


***1-(3-((Triisopropylsilyl)ethynyl)furan-2-yl)ethan-1-one* (7o)**

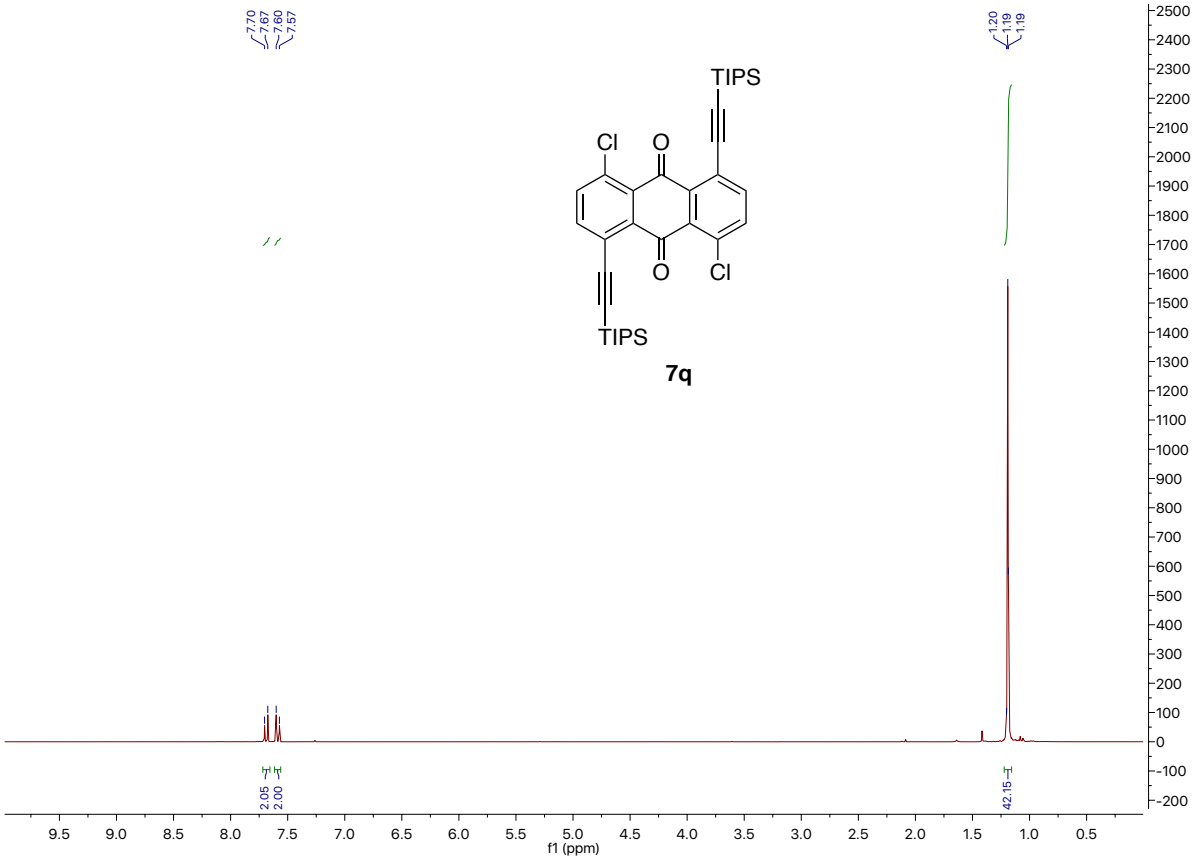


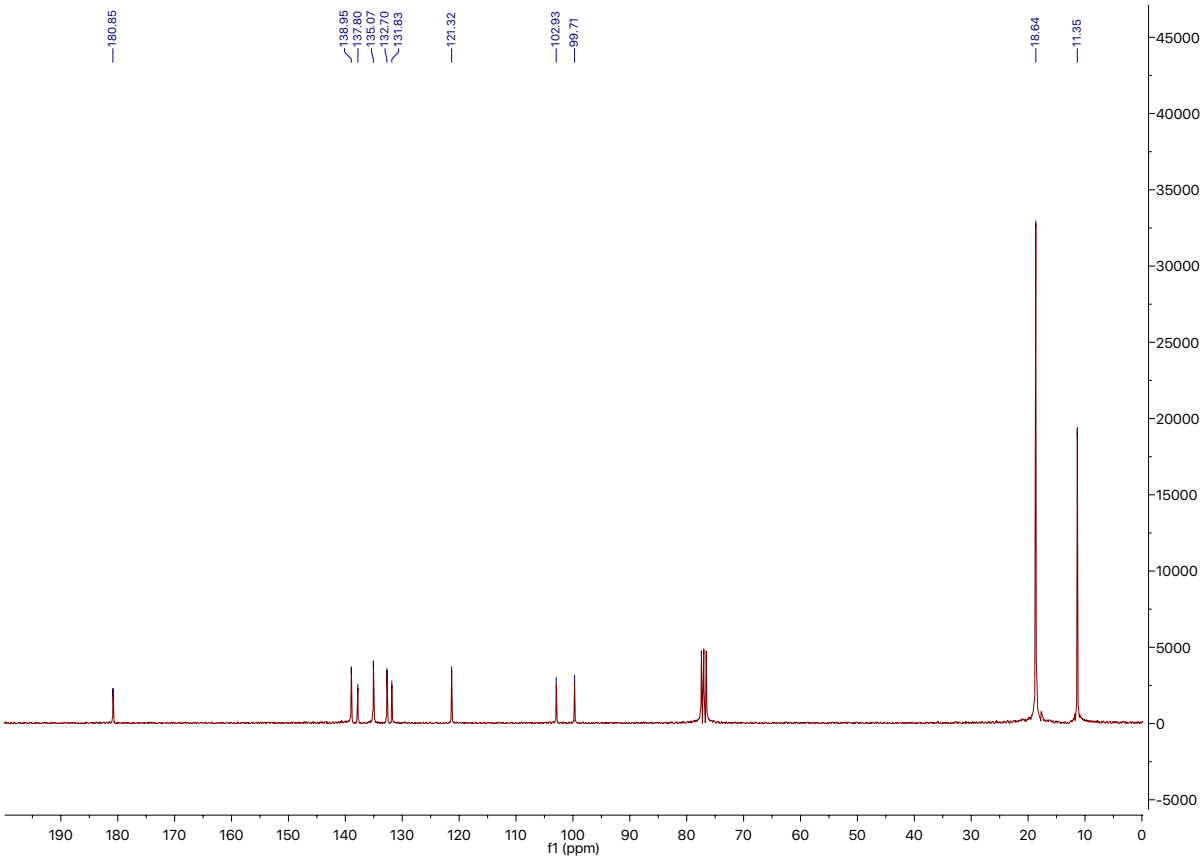


1-(3-((Triisopropylsilyl)ethynyl)thiophen-2-yl)ethan-1-one **(7p)**

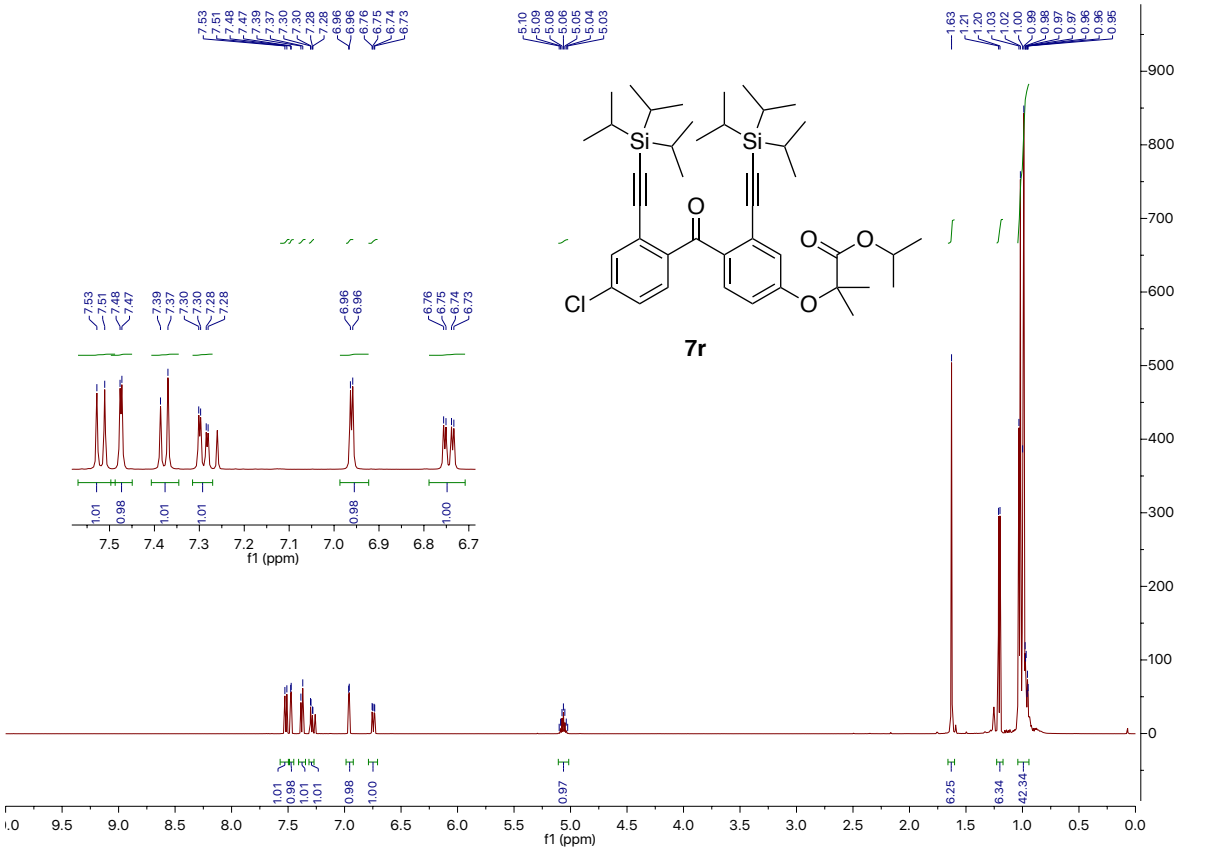


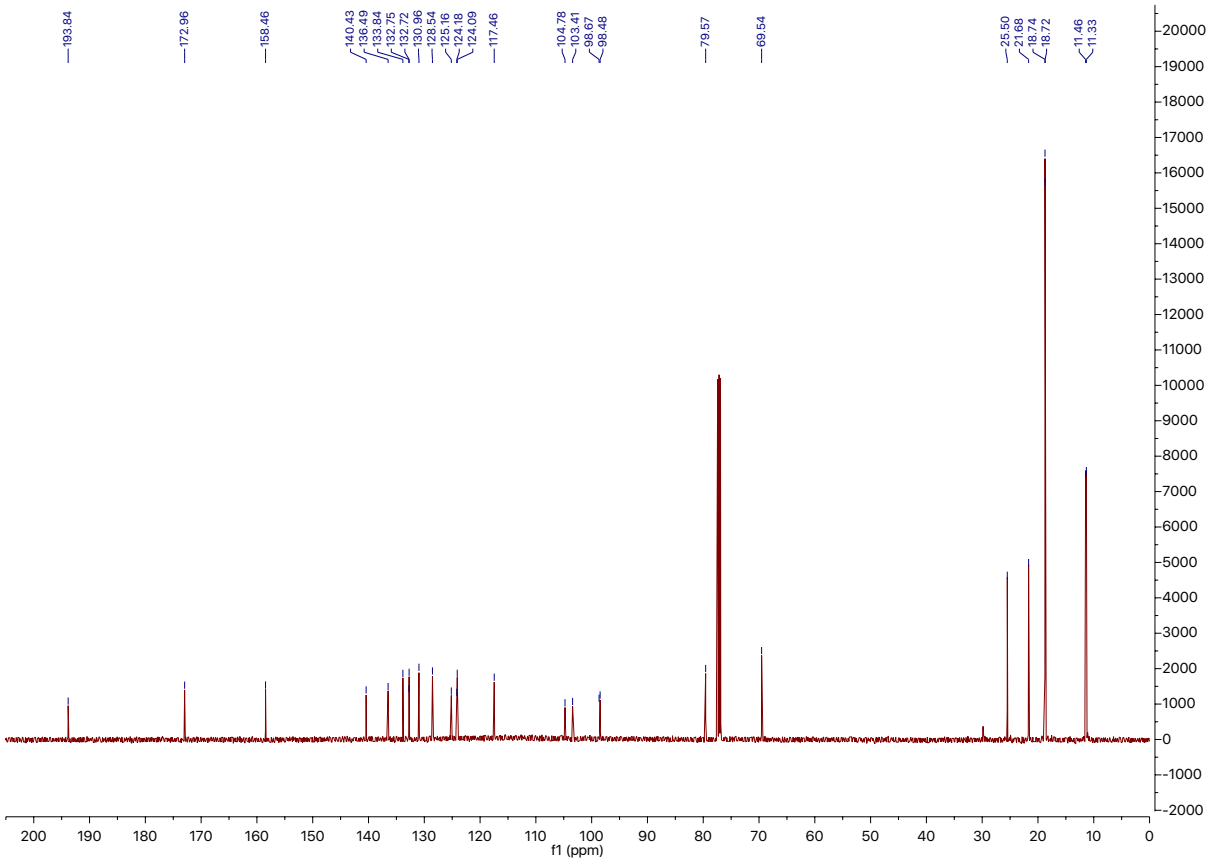
1,5-Dichloro-4,8-bis((triisopropylsilyl)ethynyl)anthracene-9,10-dione (**7q**)



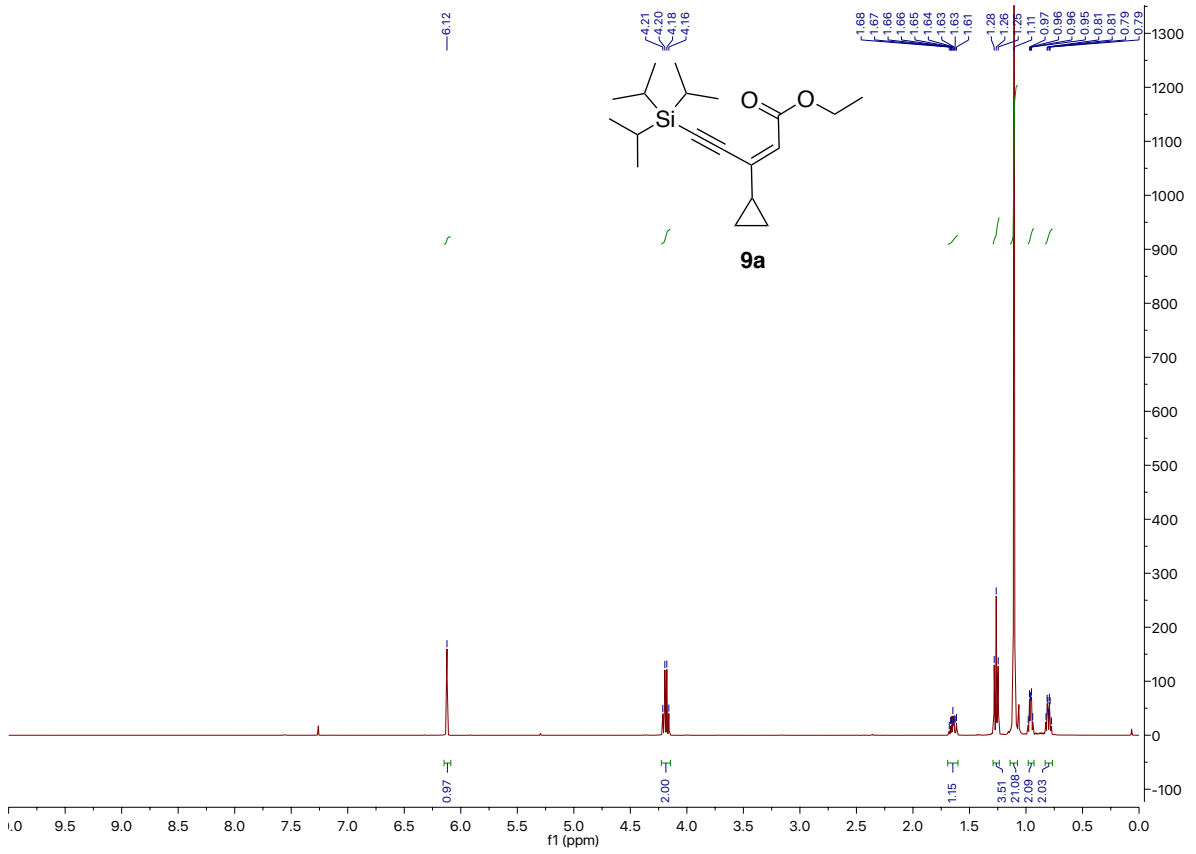


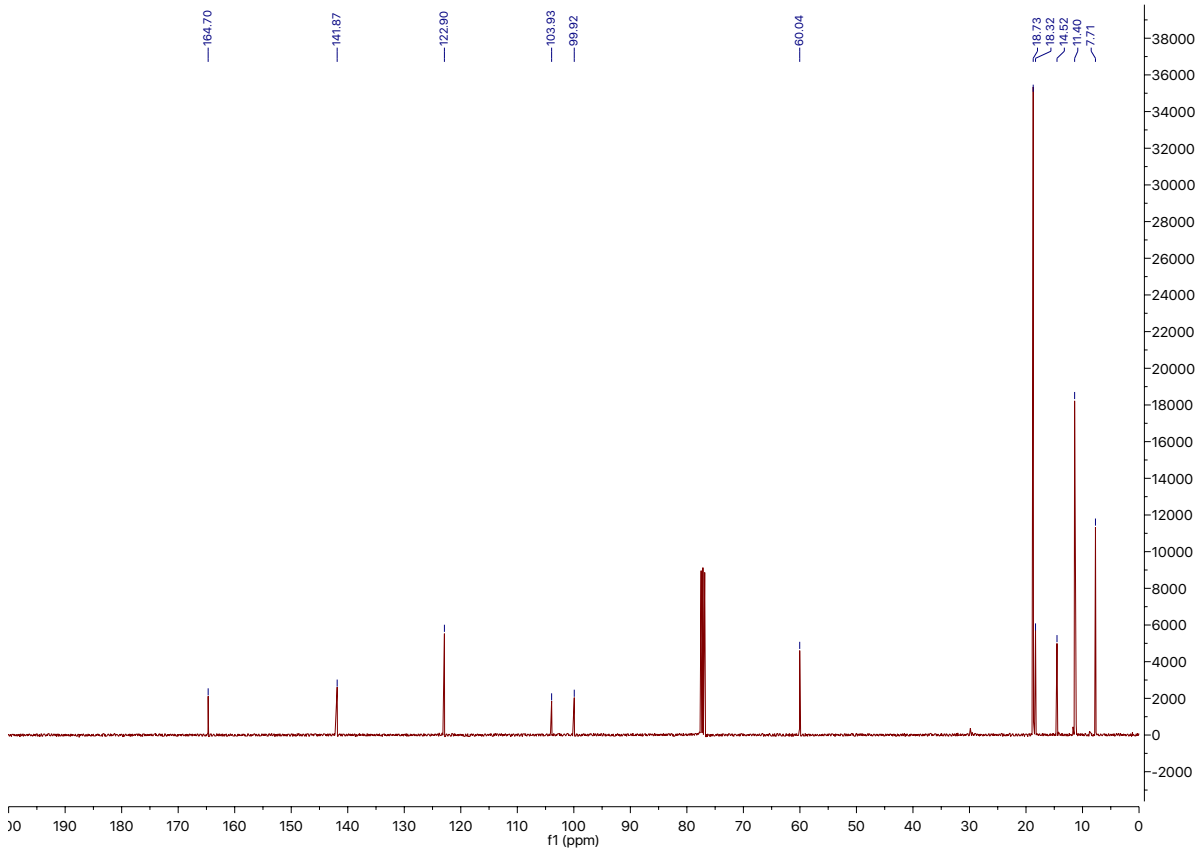
Isopropyl 2-(4-(4-chloro-2-((triisopropylsilyl)ethynyl)benzoyl)-3-((triisopropylsilyl)ethynyl) phenoxy) -2-methylpropanoate (**7r**)



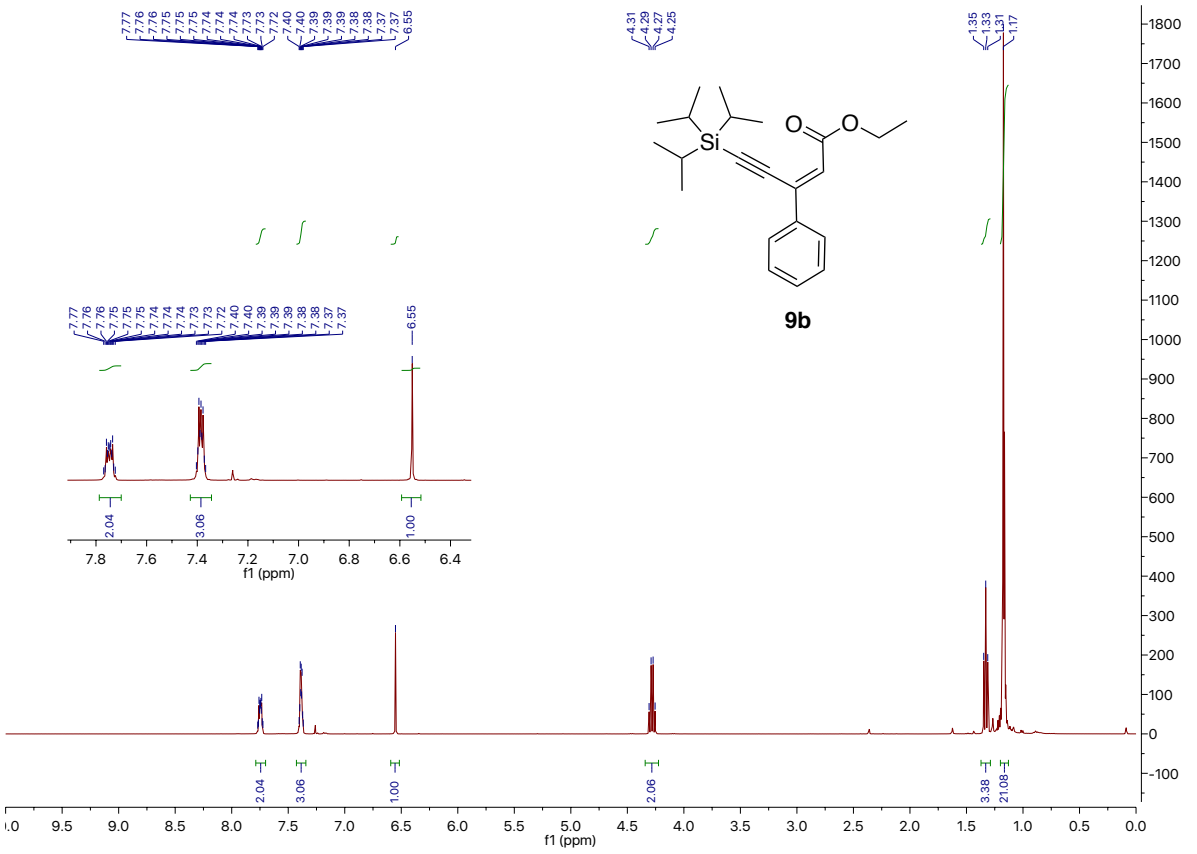


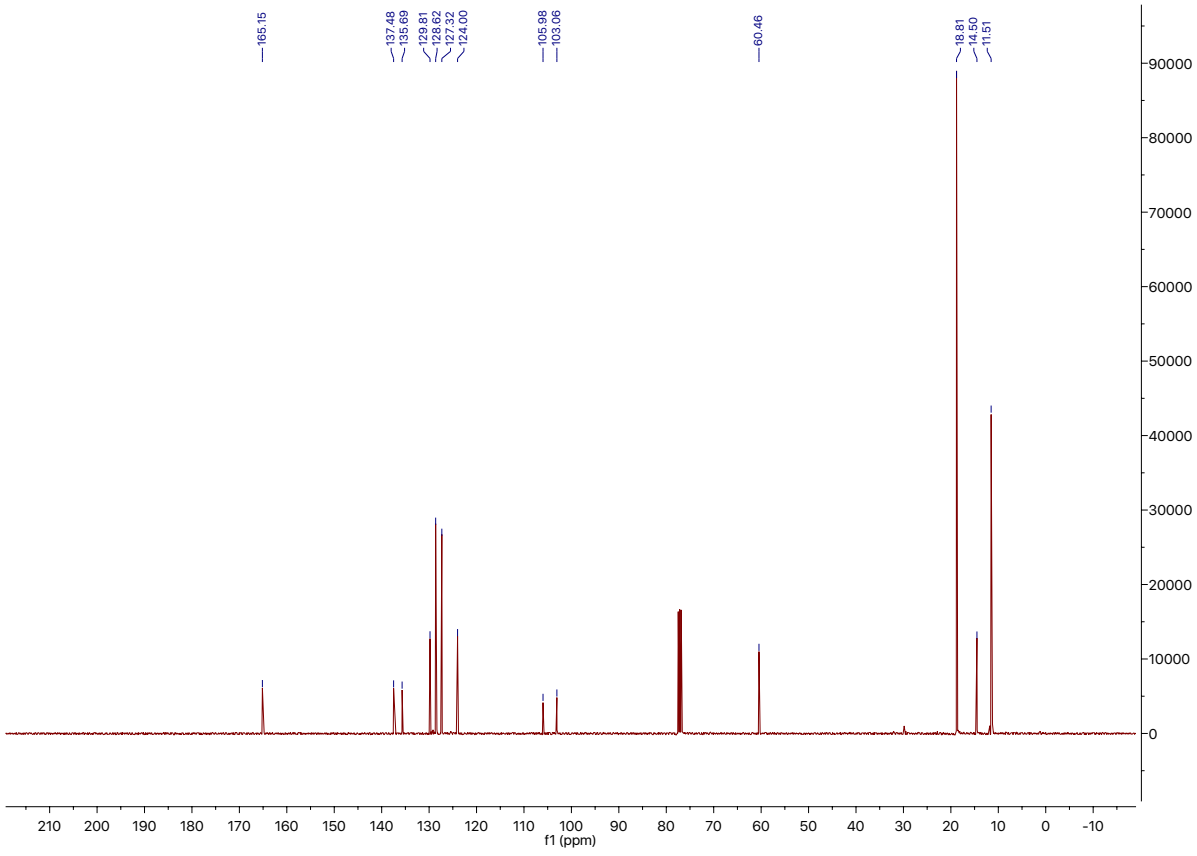
Ethyl (Z)-3-cyclopropyl-5-(triisopropylsilyl)pent-2-en-4-ynoate **(9a)**



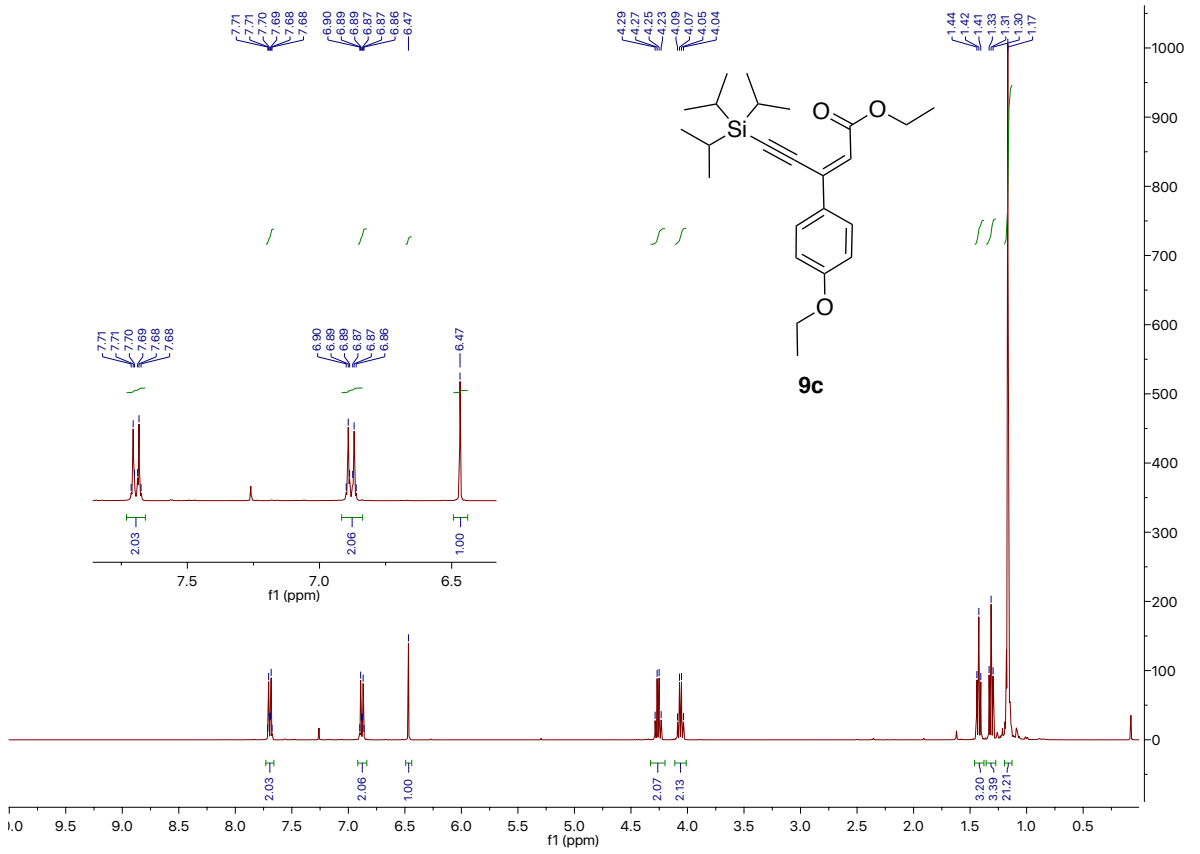


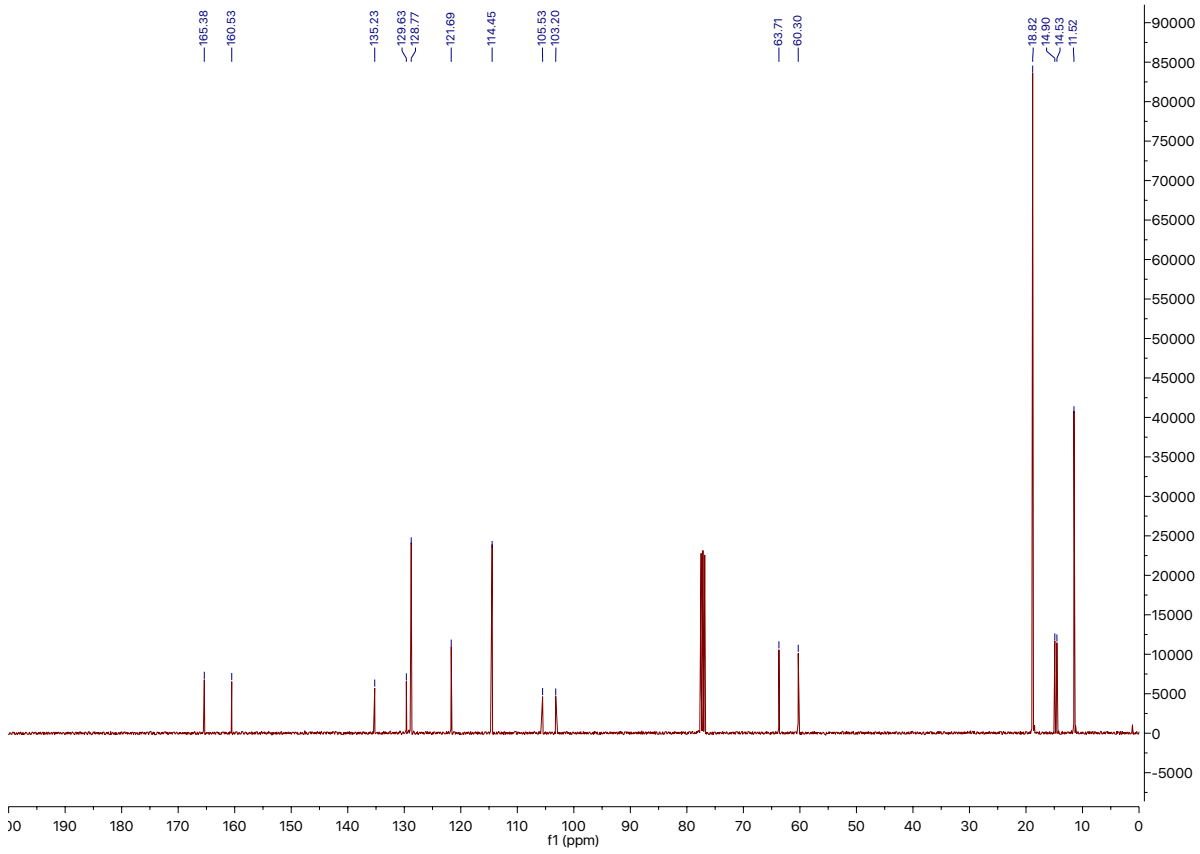
Ethyl (Z)-3-phenyl-5-(triisopropylsilyl)pent-2-en-4-ynoate (**9b**)



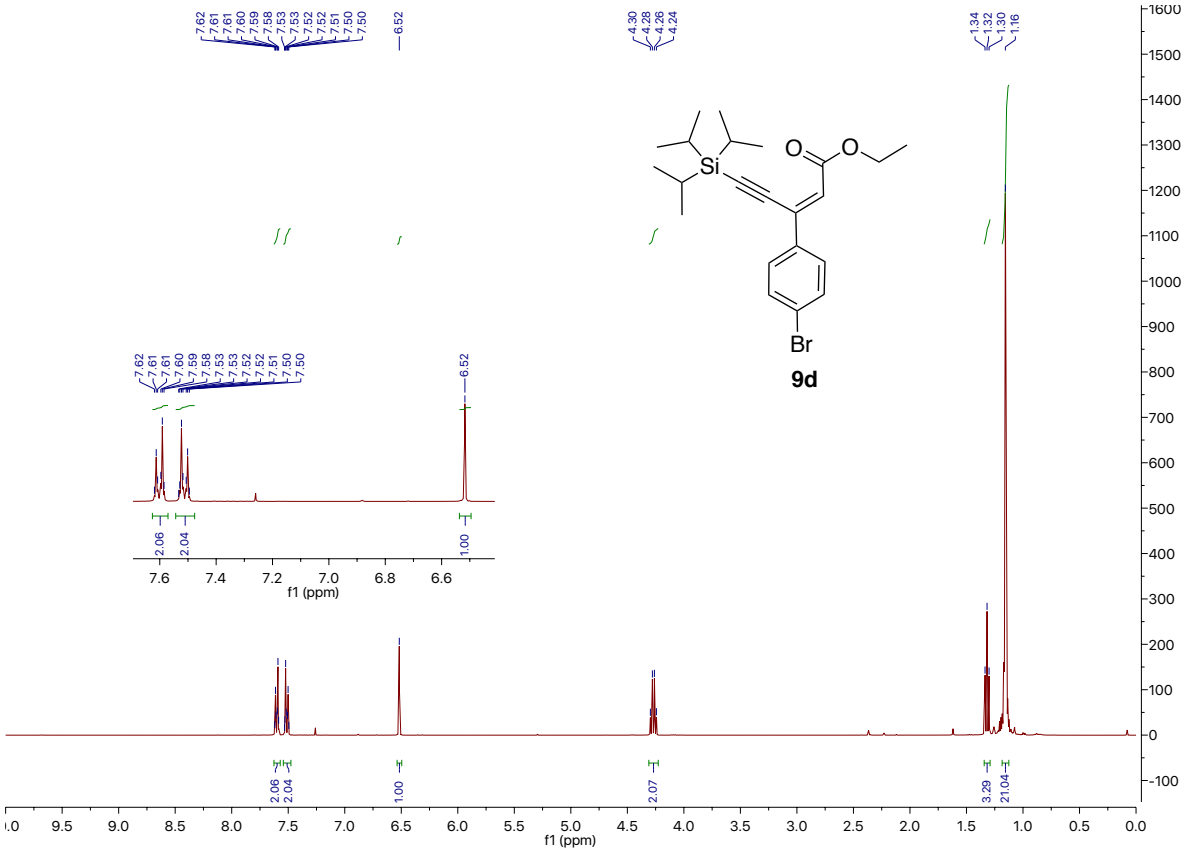


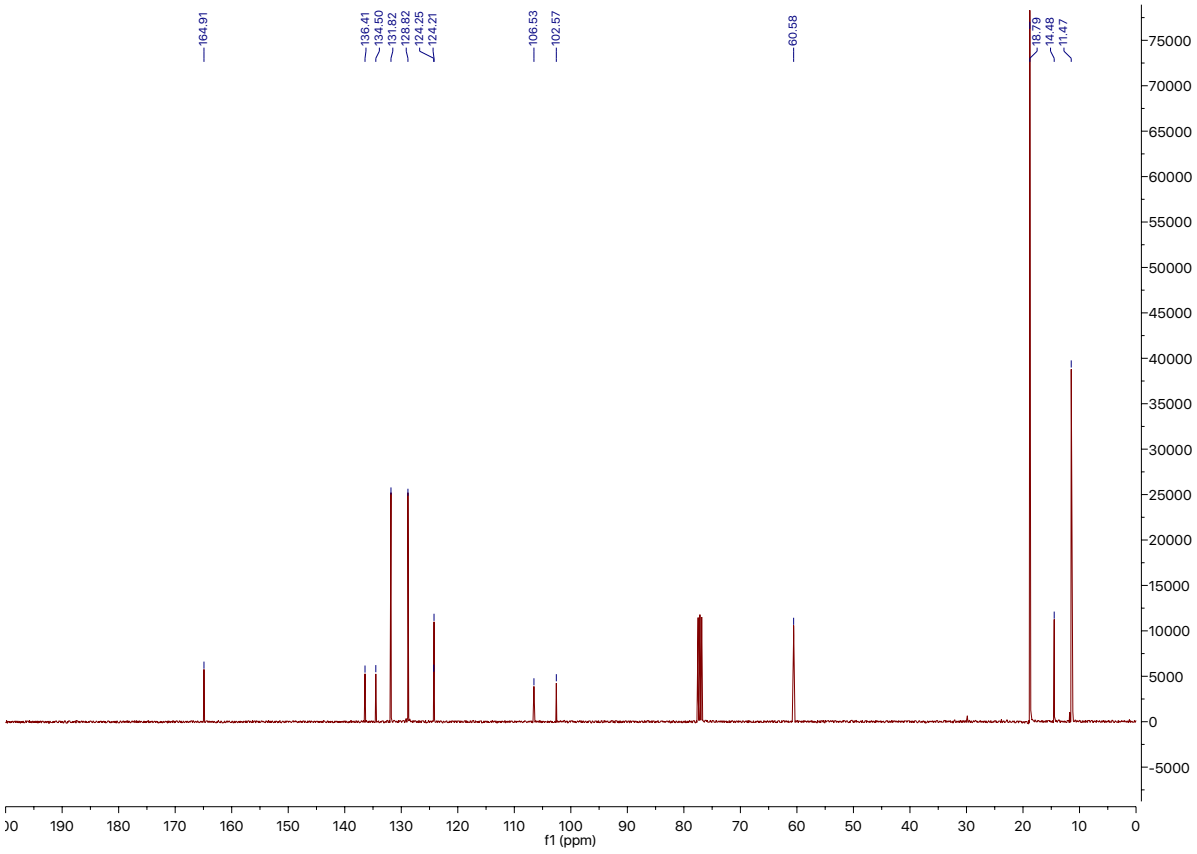
Ethyl (Z)-3-(4-ethoxyphenyl)-5-(triisopropylsilyl)pent-2-en-4-ynoate **(9c)**



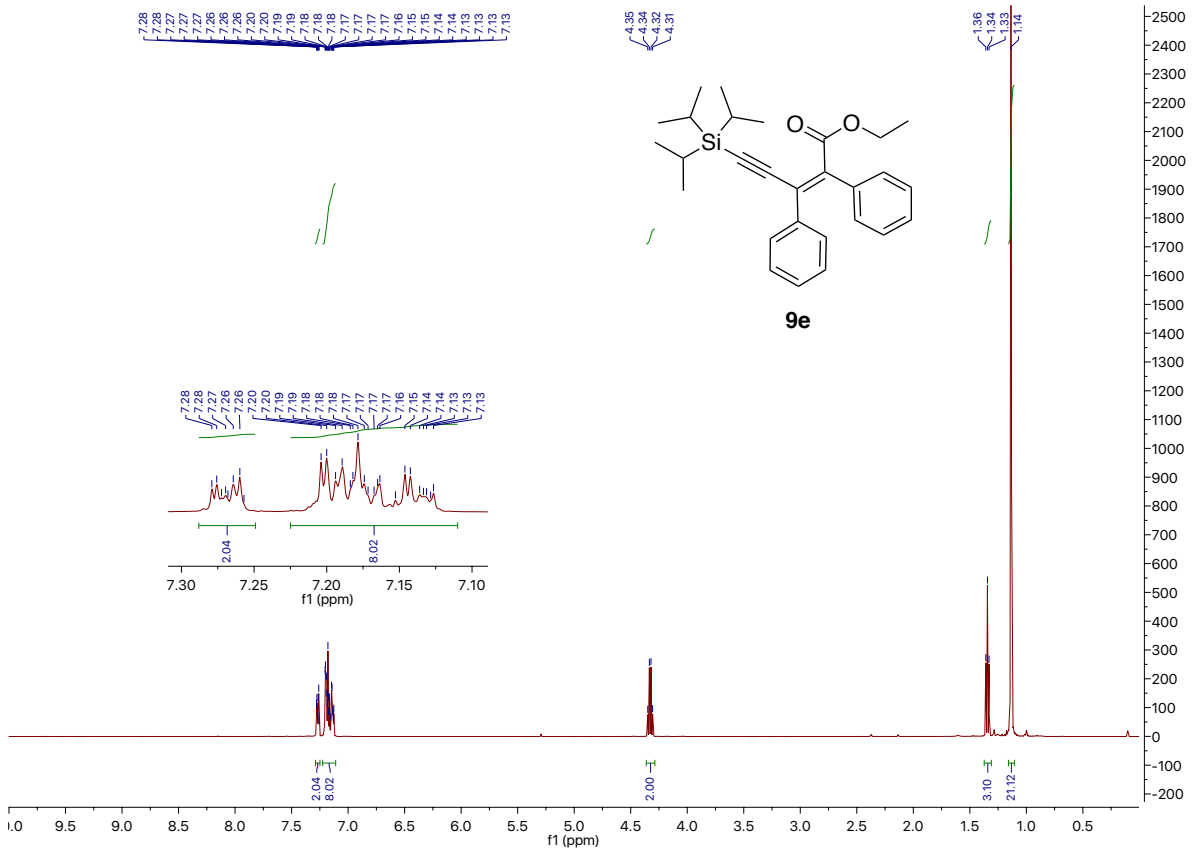


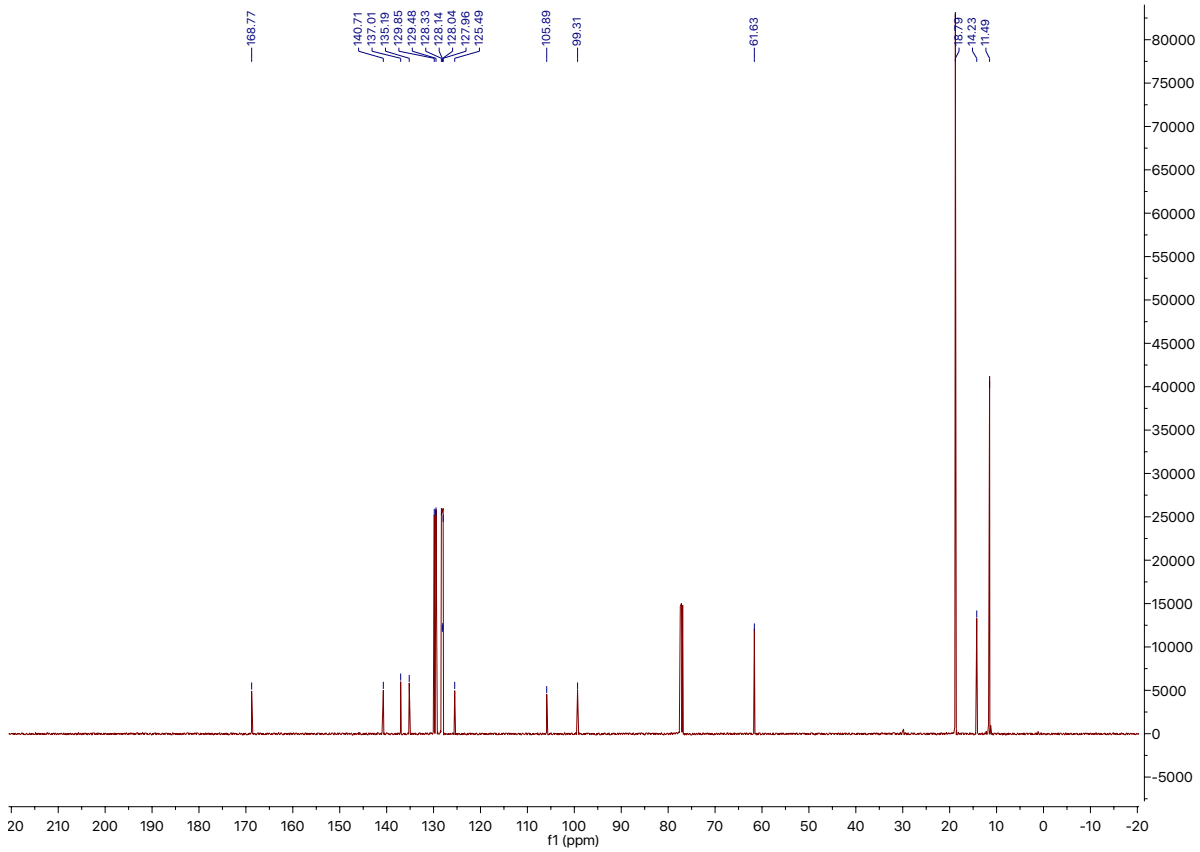
***Ethyl (Z)-3-(4-bromophenyl)-5-(triisopropylsilyl)pent-2-en-4-ynoate* (9d)**



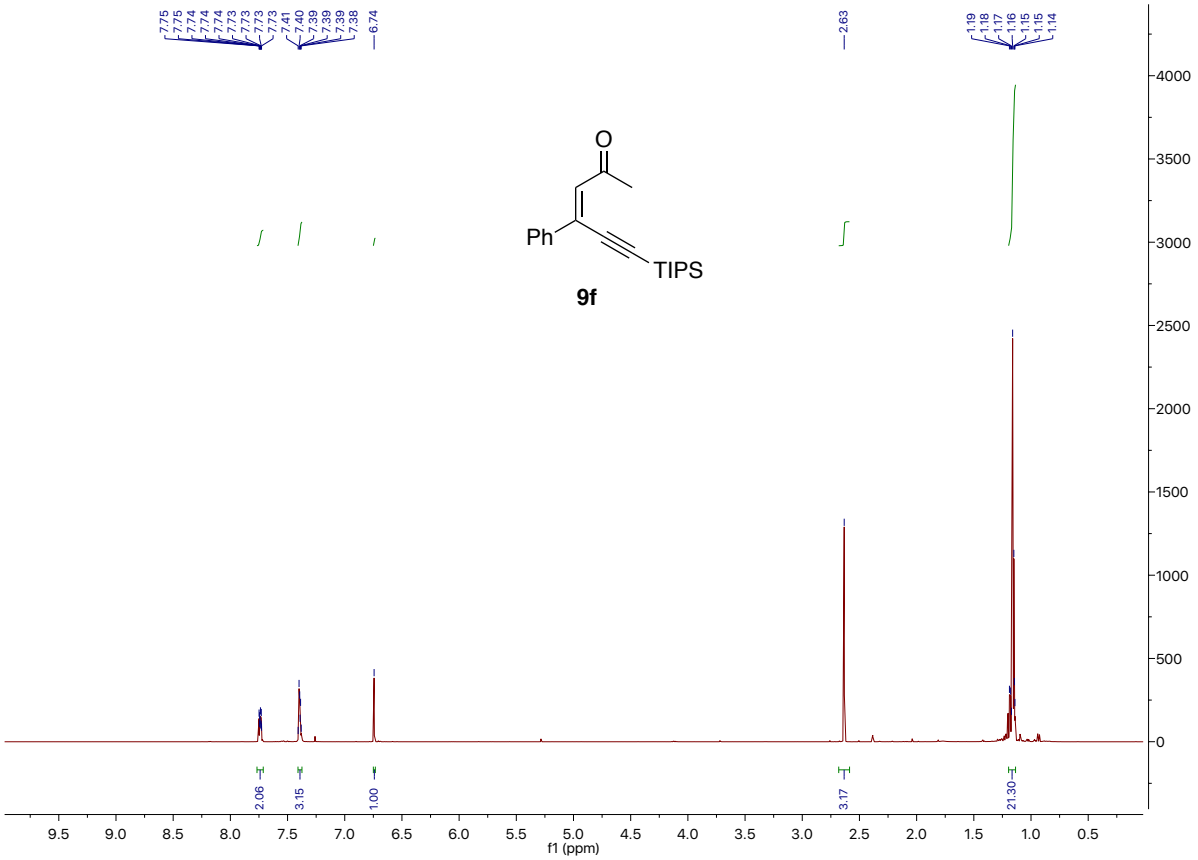


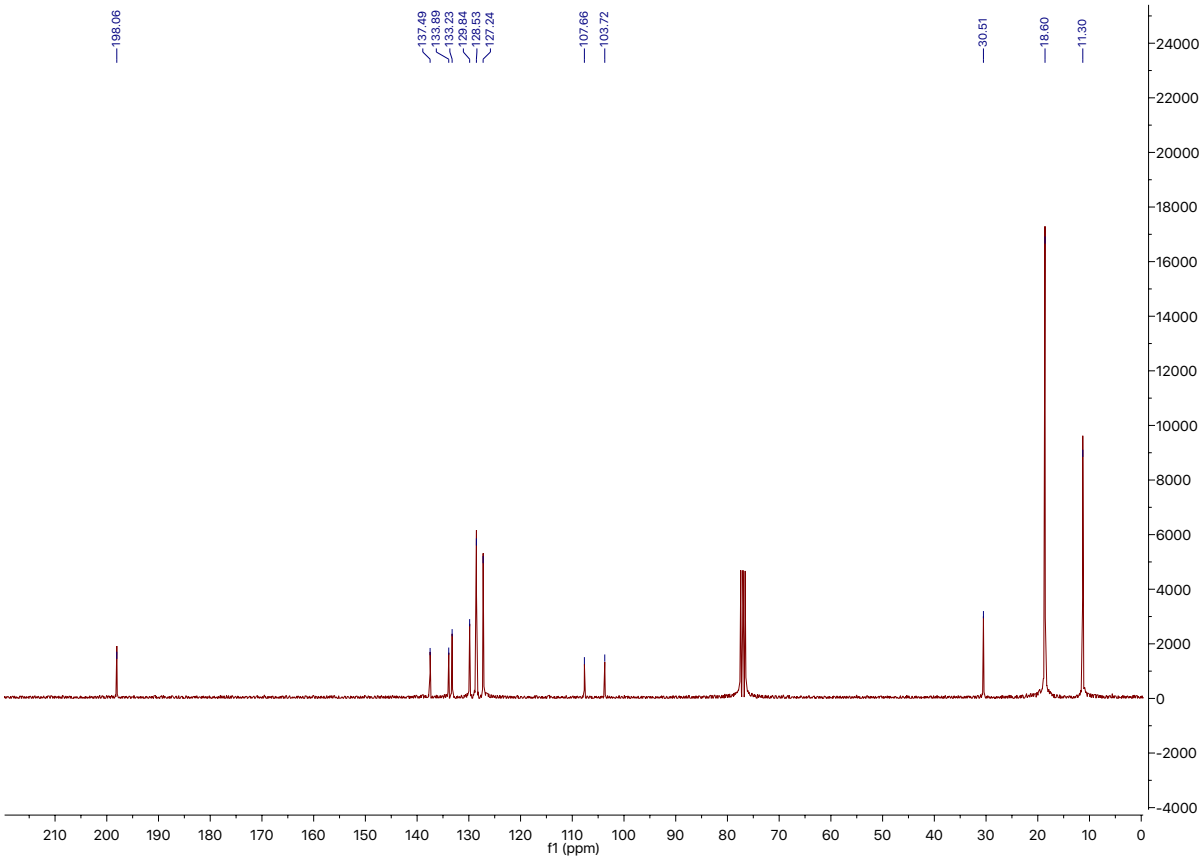
Ethyl (Z)-2,3-diphenyl-5-(triisopropylsilyl)pent-2-en-4-ynoate **(9e)**



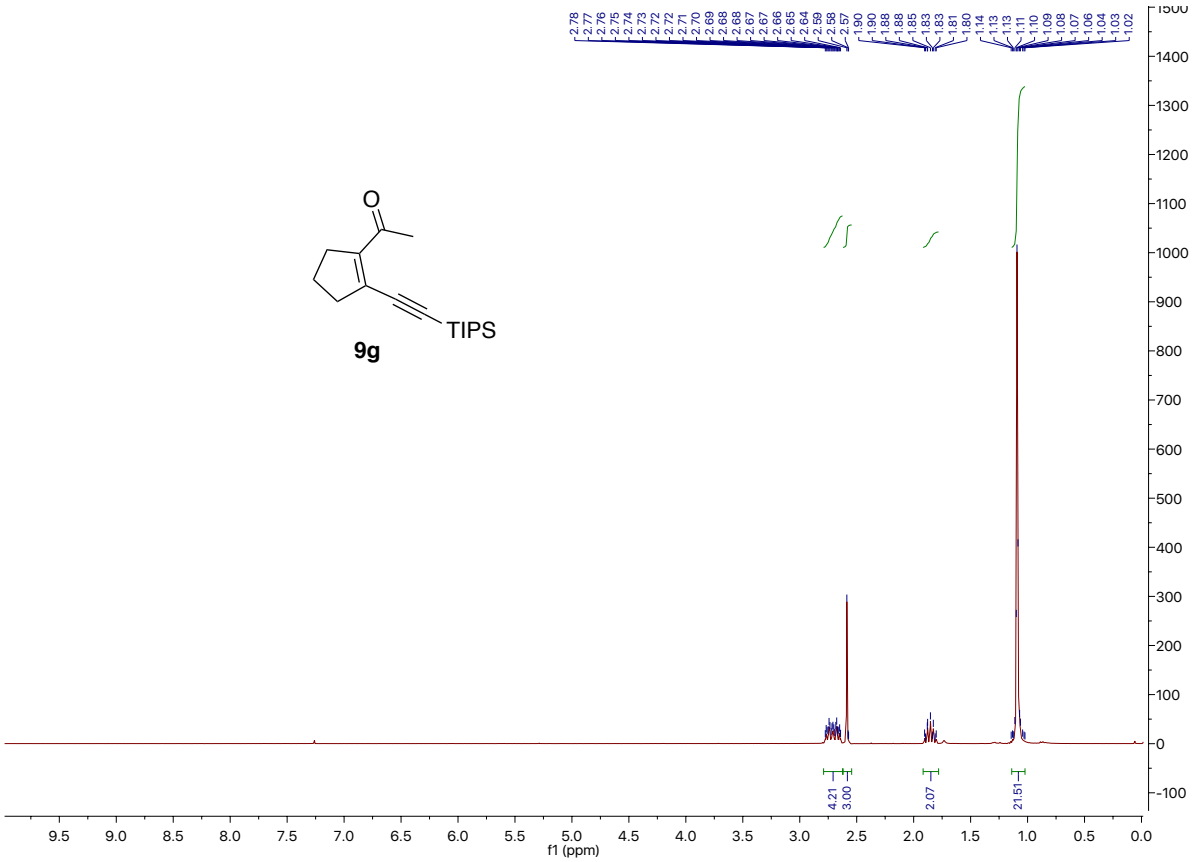


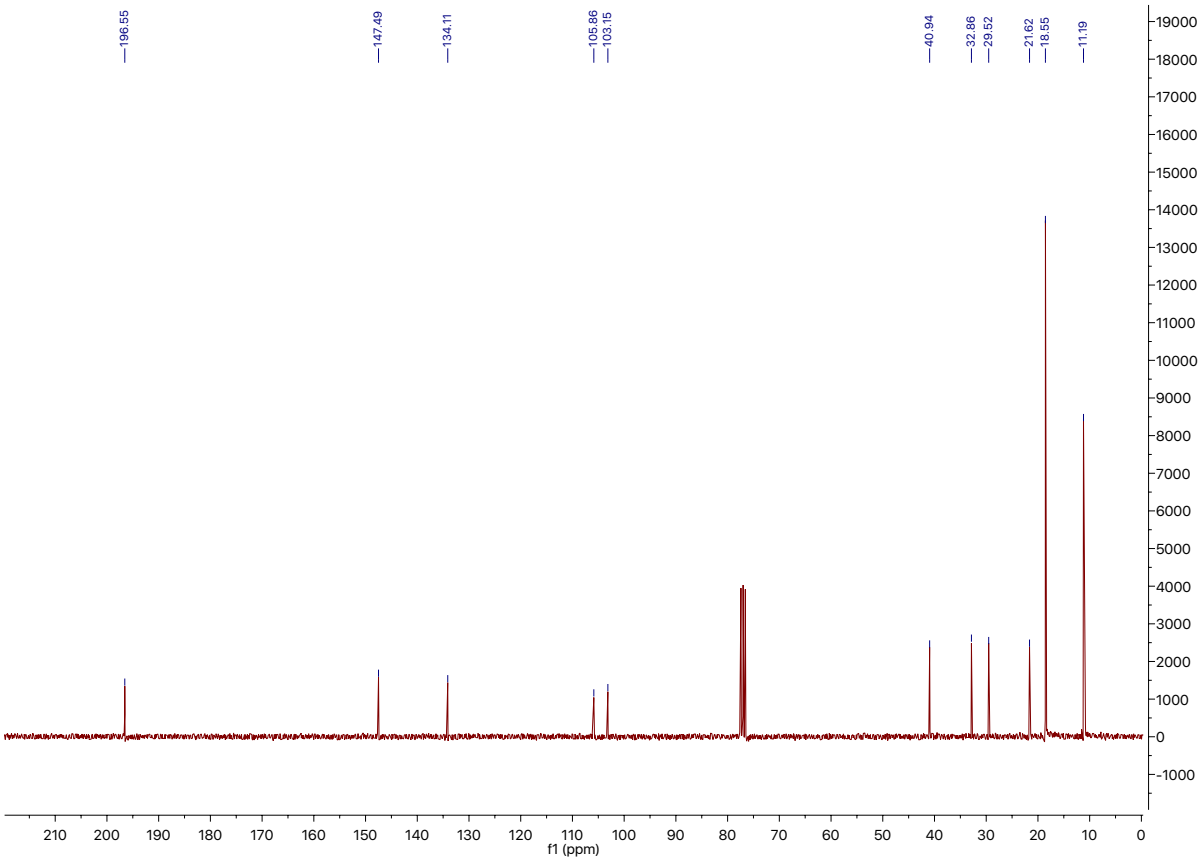
***(Z)-4-Phenyl-6-(triisopropylsilyl)hex-3-en-5-yn-2-one* (9f)**



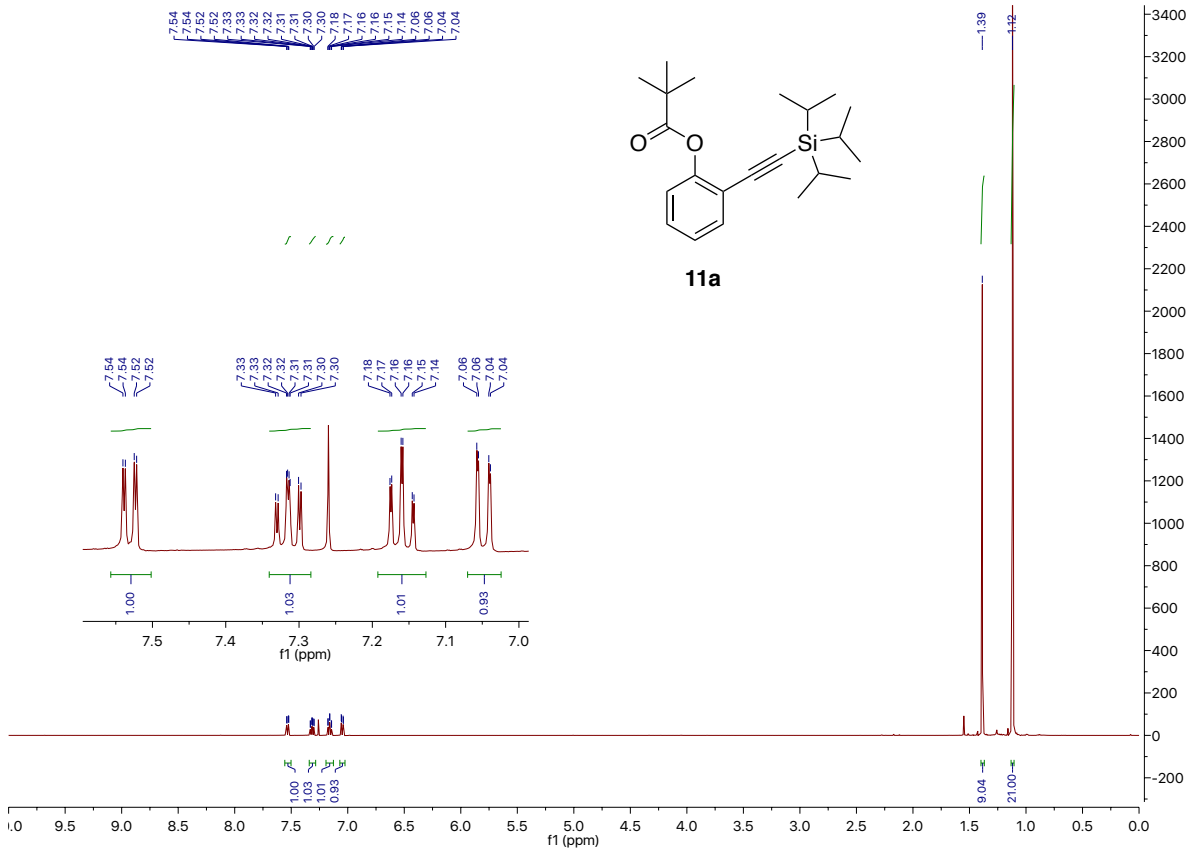


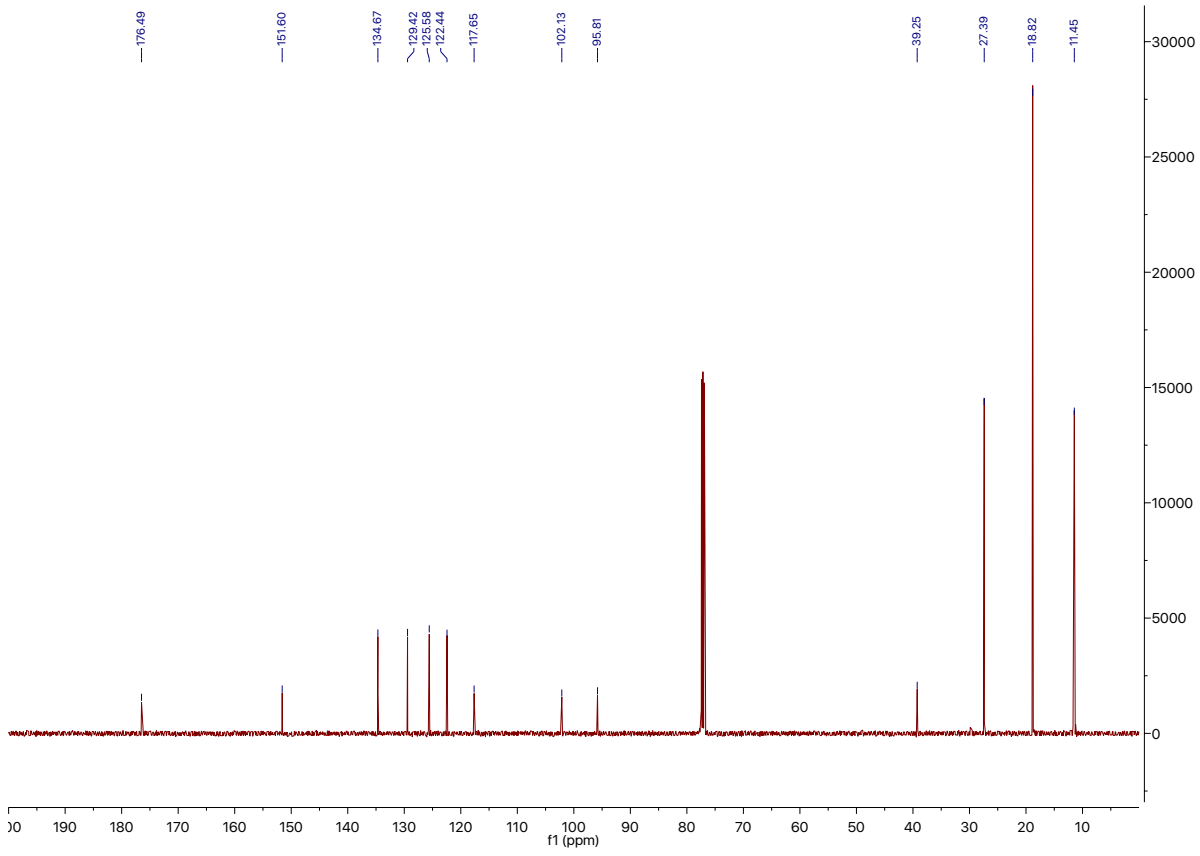
***1-(2-((Triisopropylsilyl)ethynyl)cyclopent-1-en-1-yl)ethan-1-one* (9g)**



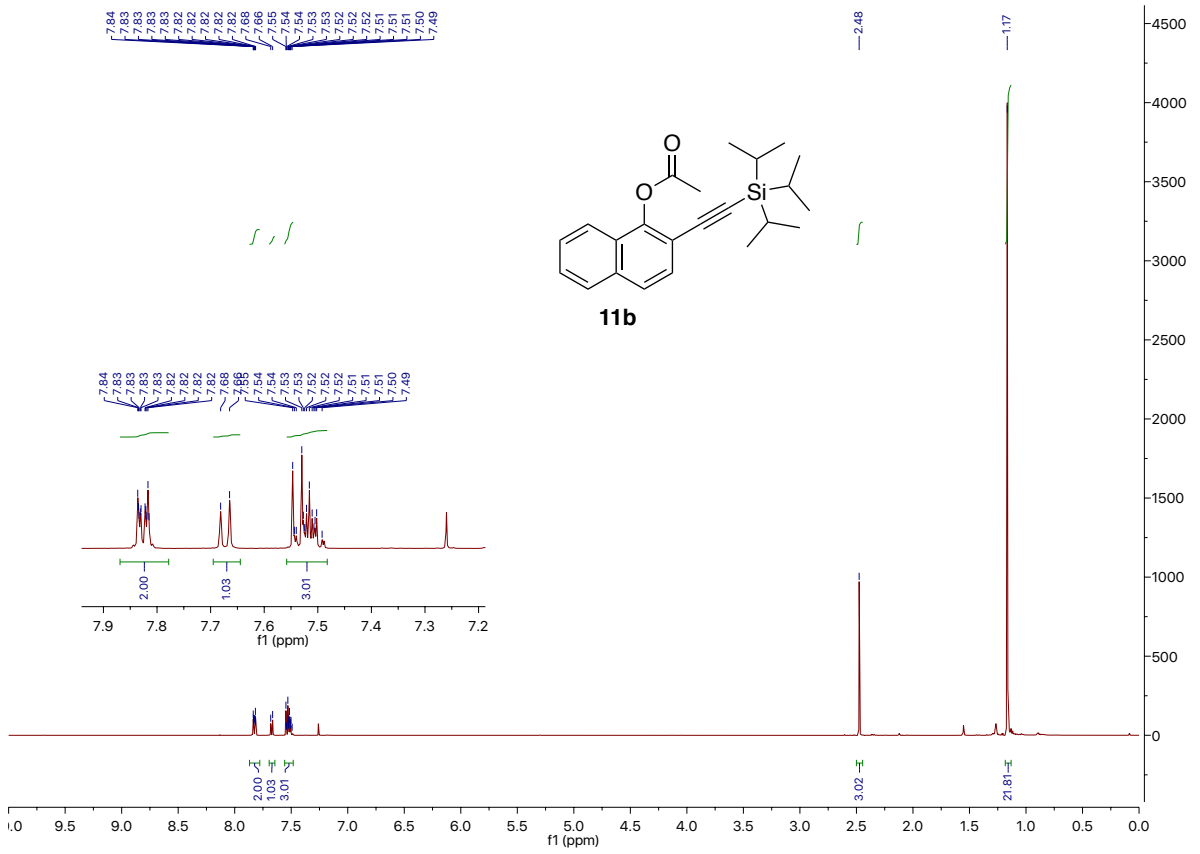


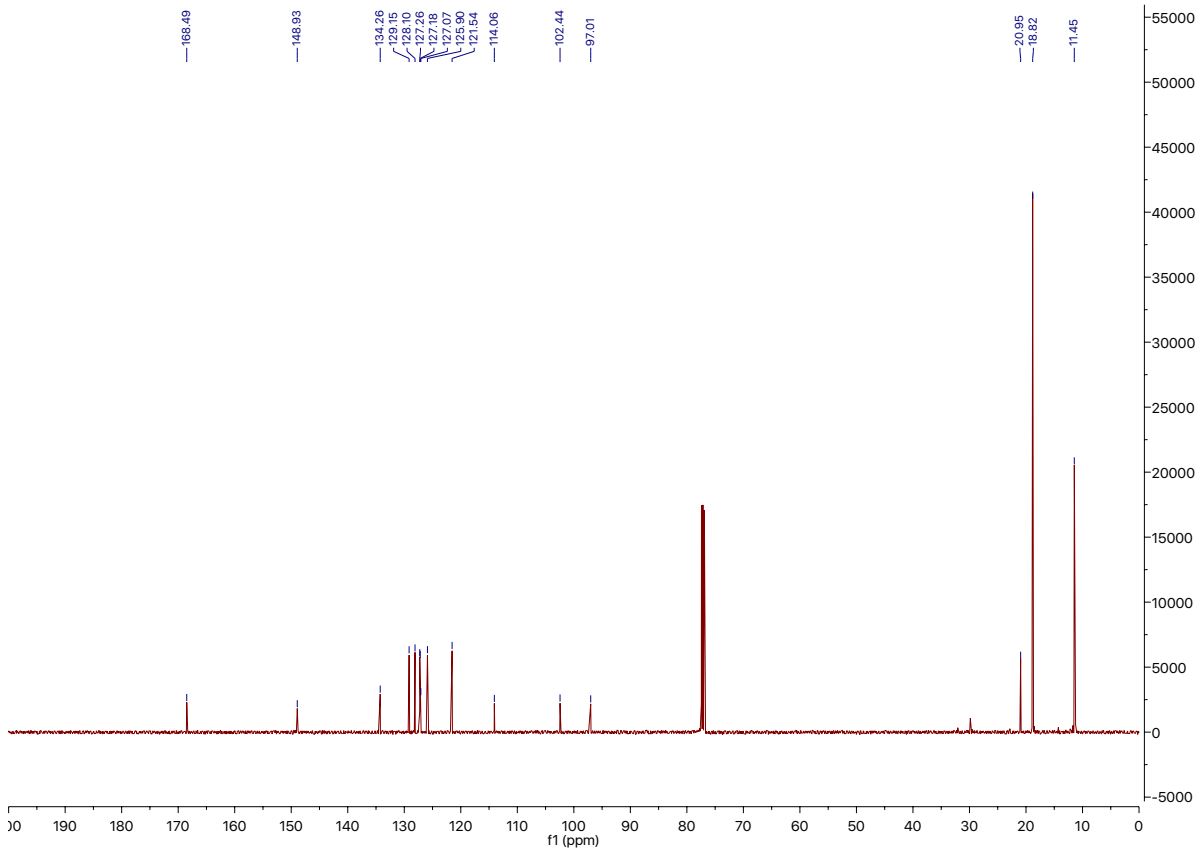
***2-((Triisopropylsilyl)ethynyl)phenyl pivalate* (11a)**



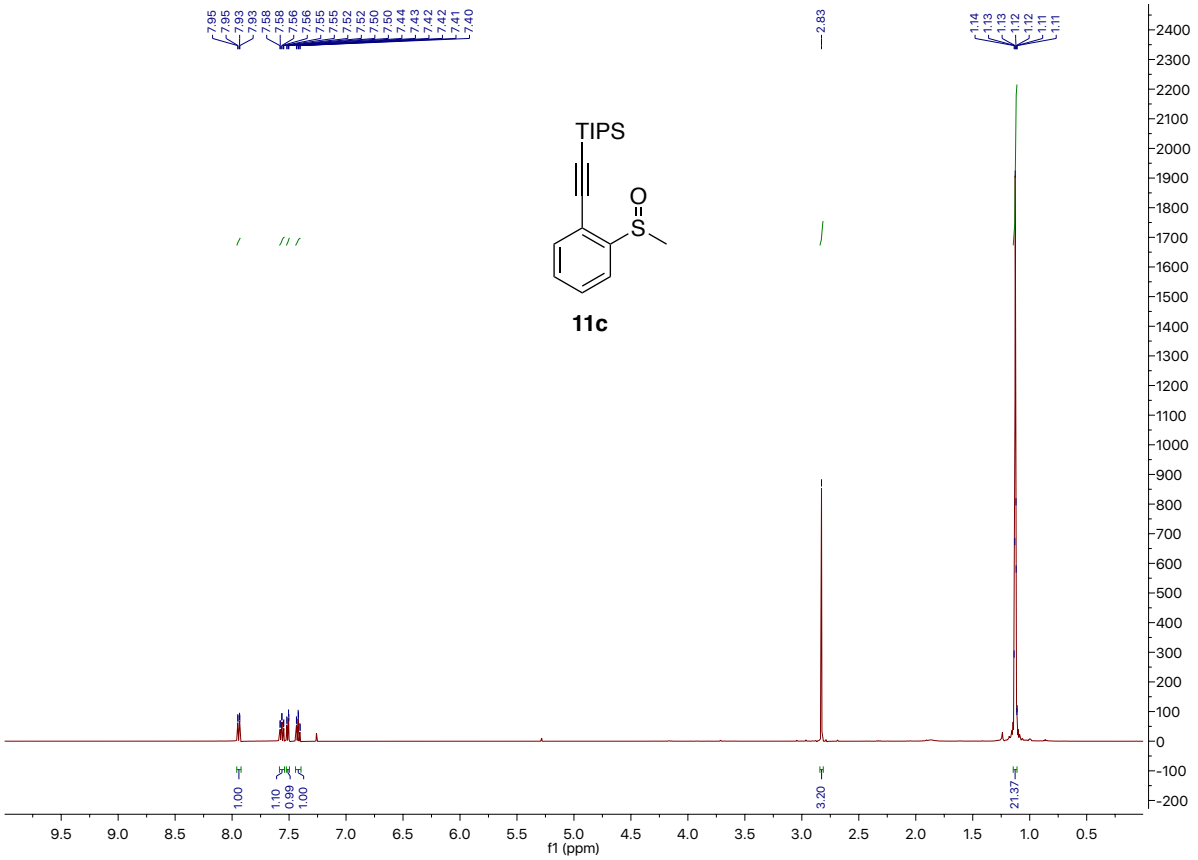


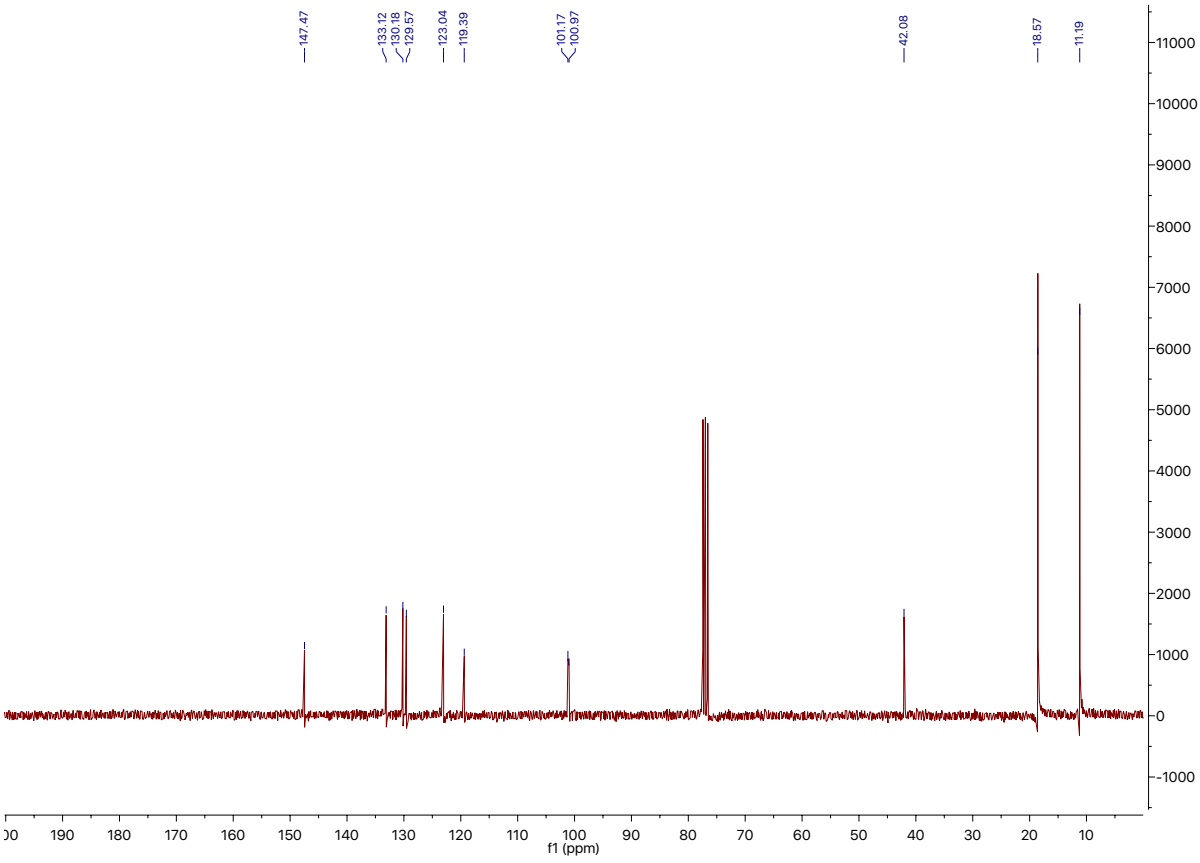
***2-((Triisopropylsilyl)ethynyl)naphthalen-1-yl acetate* (11b)**



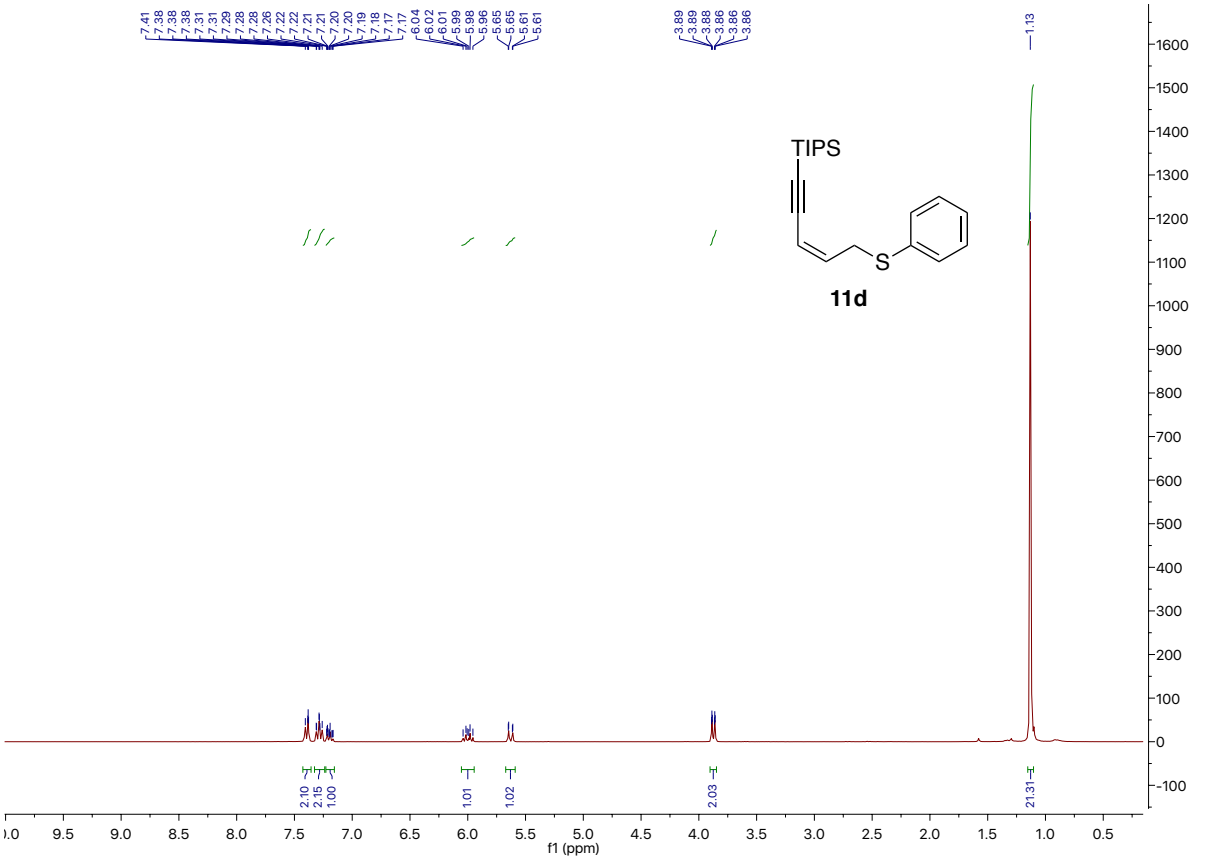


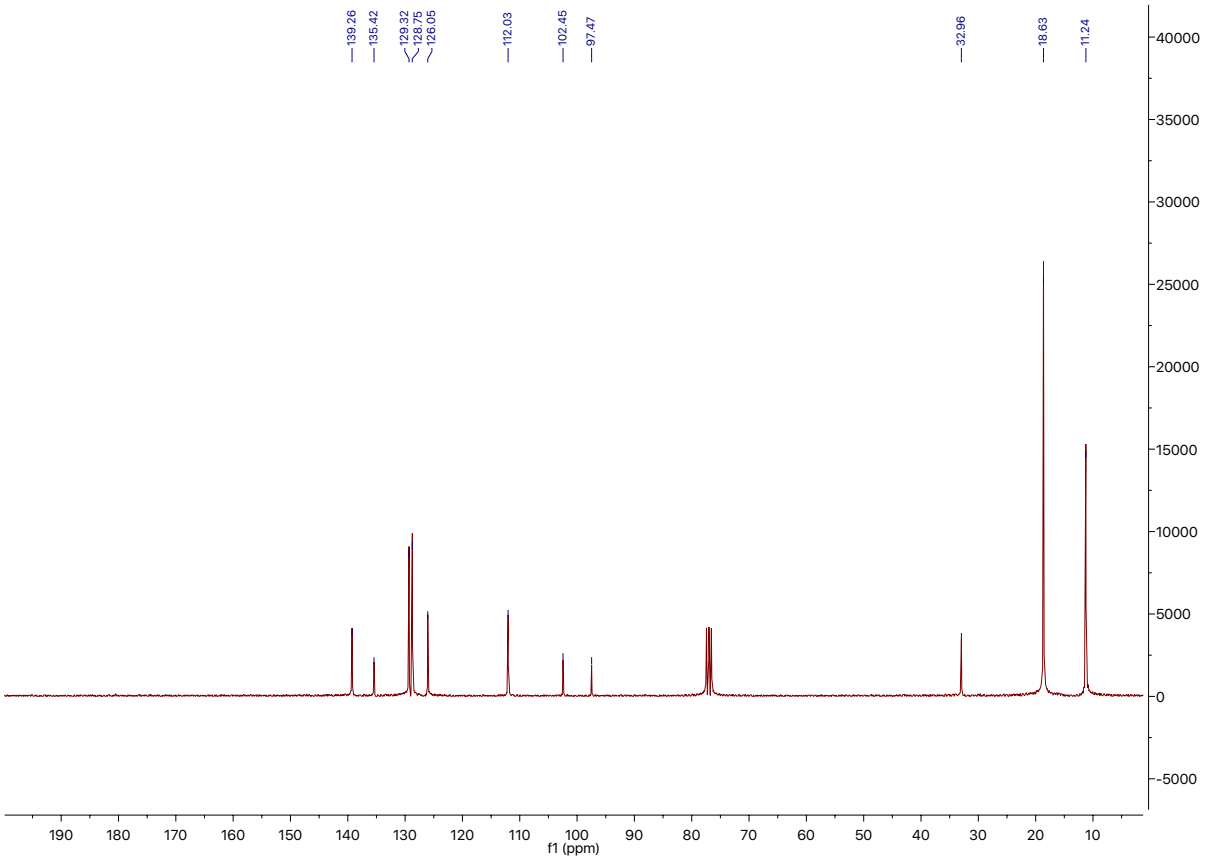
***Triisopropyl((2-(methylsulfinyl)phenyl)ethynyl)silane* (11c)**



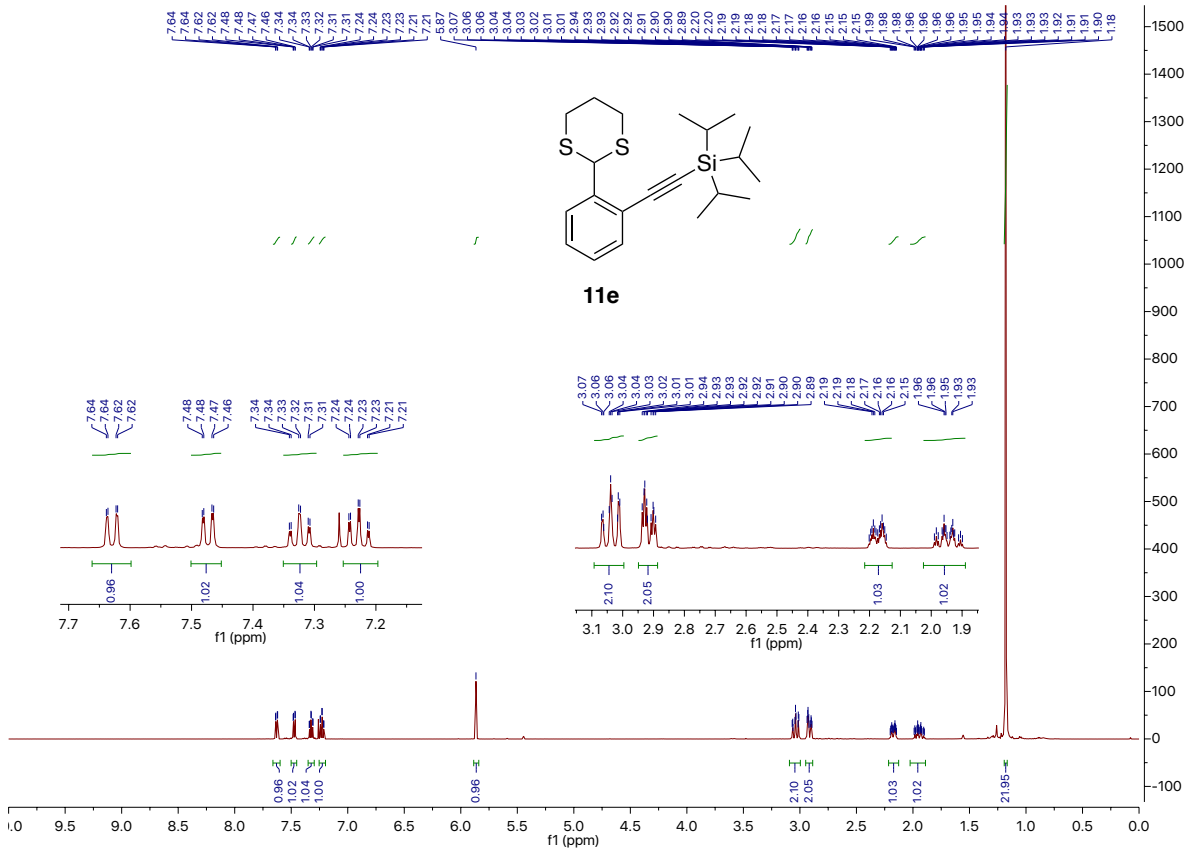


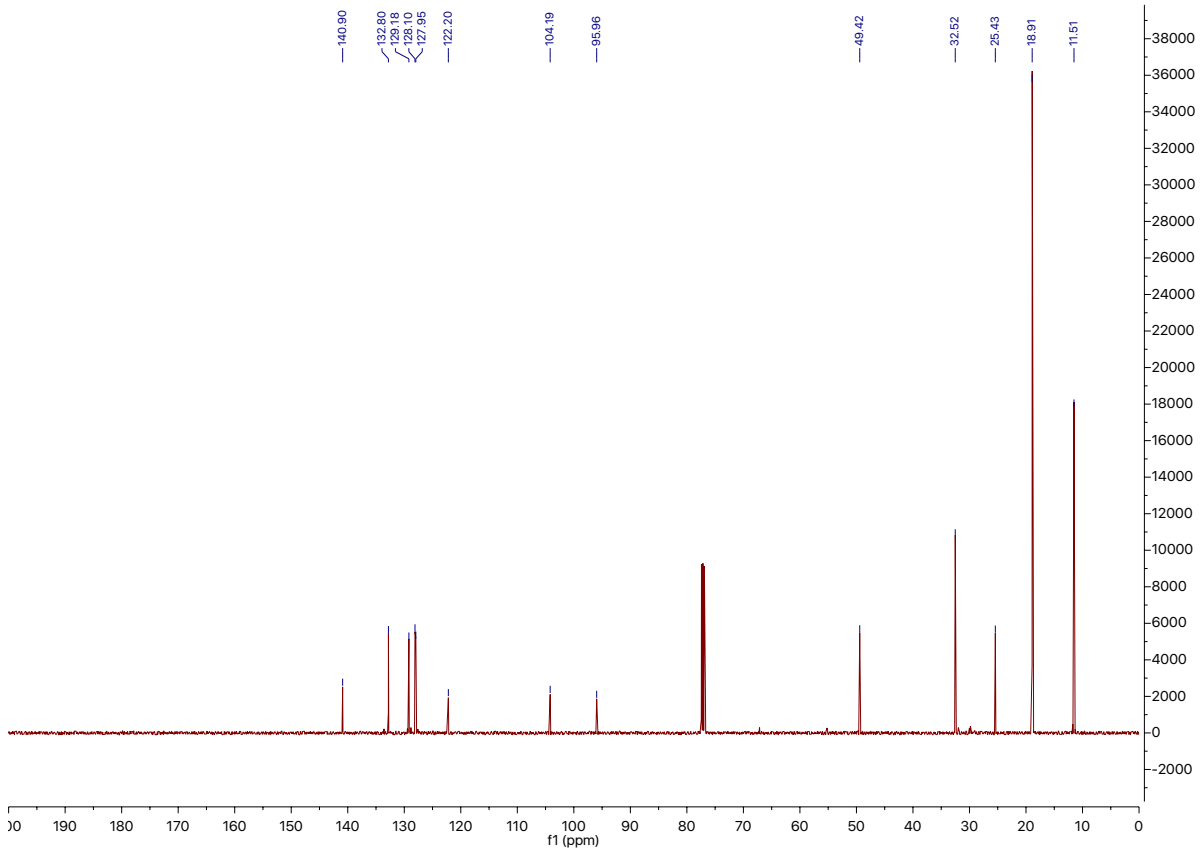
***(Z)-Triisopropyl(5-(phenylthio)pent-3-en-1-yn-1-yl)silane* (11d)**



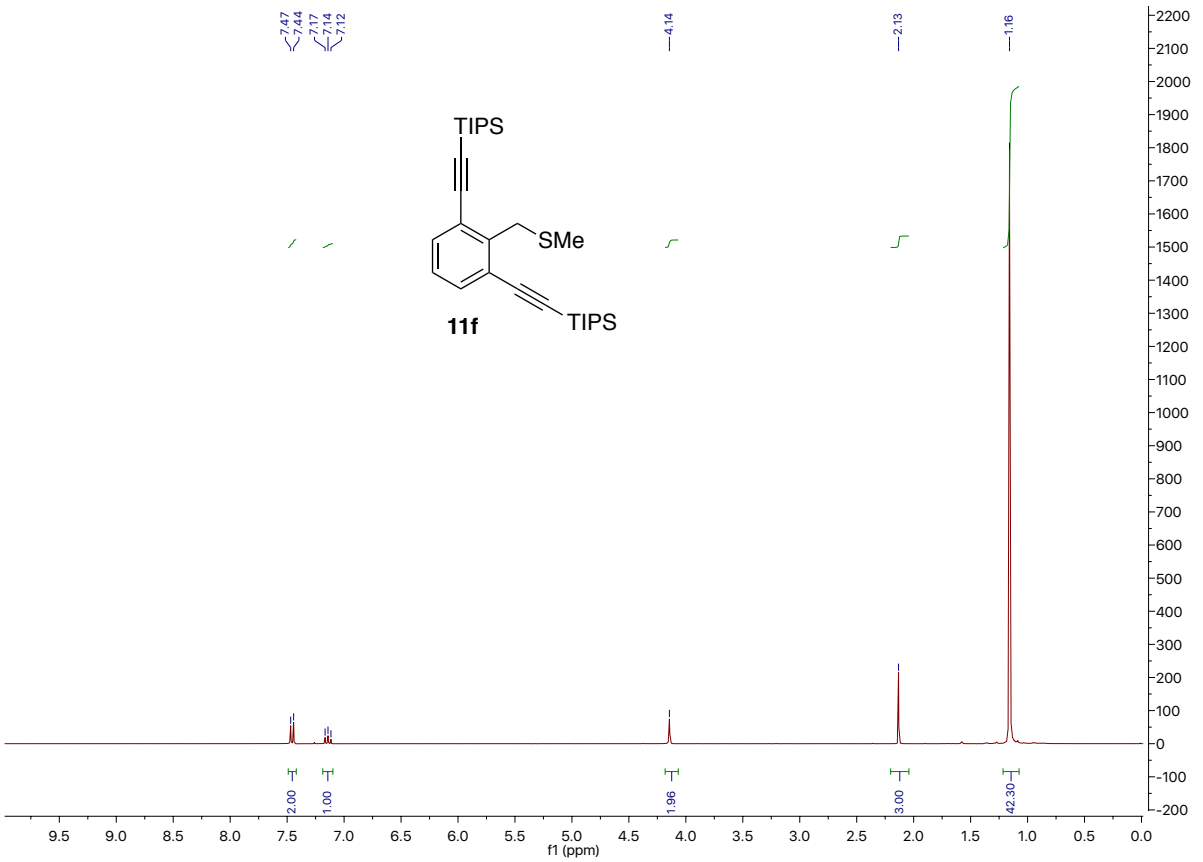


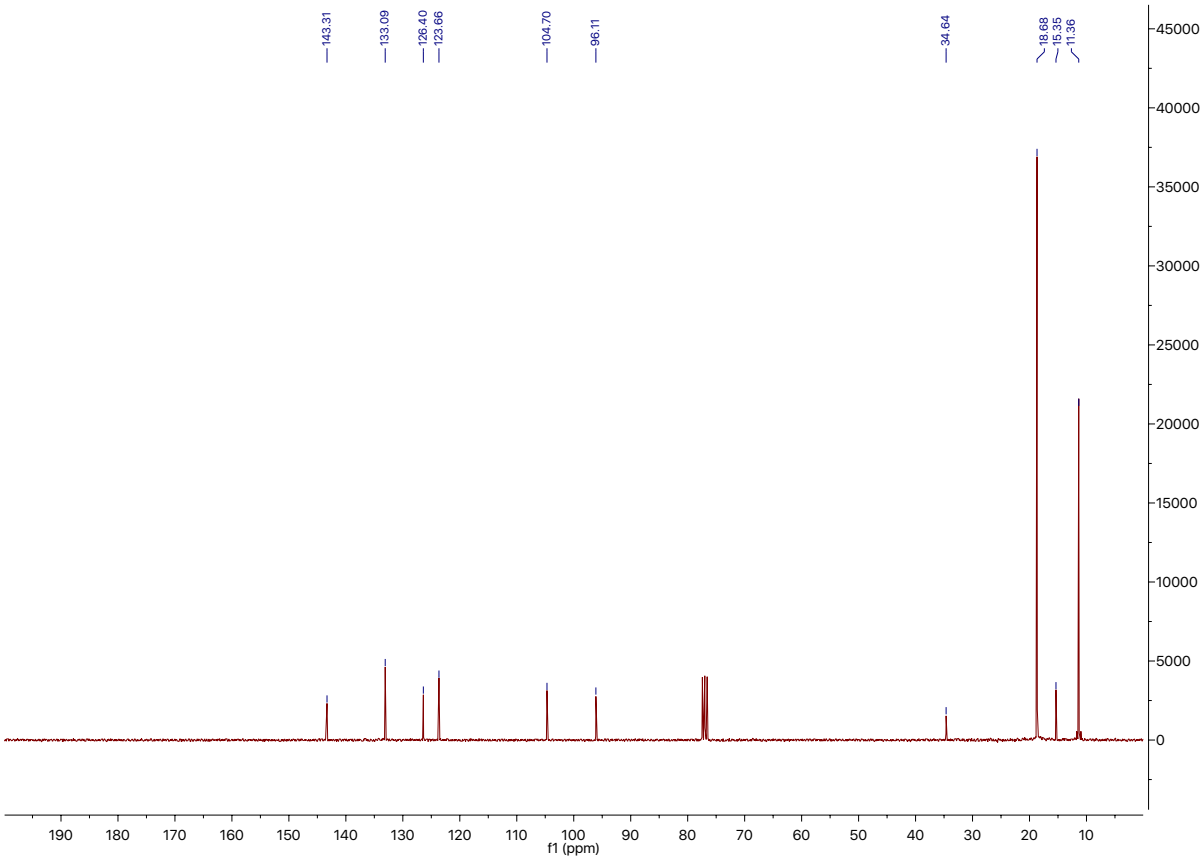
***((2-(1,3-Dithian-2-yl)phenyl)ethynyl)triisopropylsilane* (11e)**



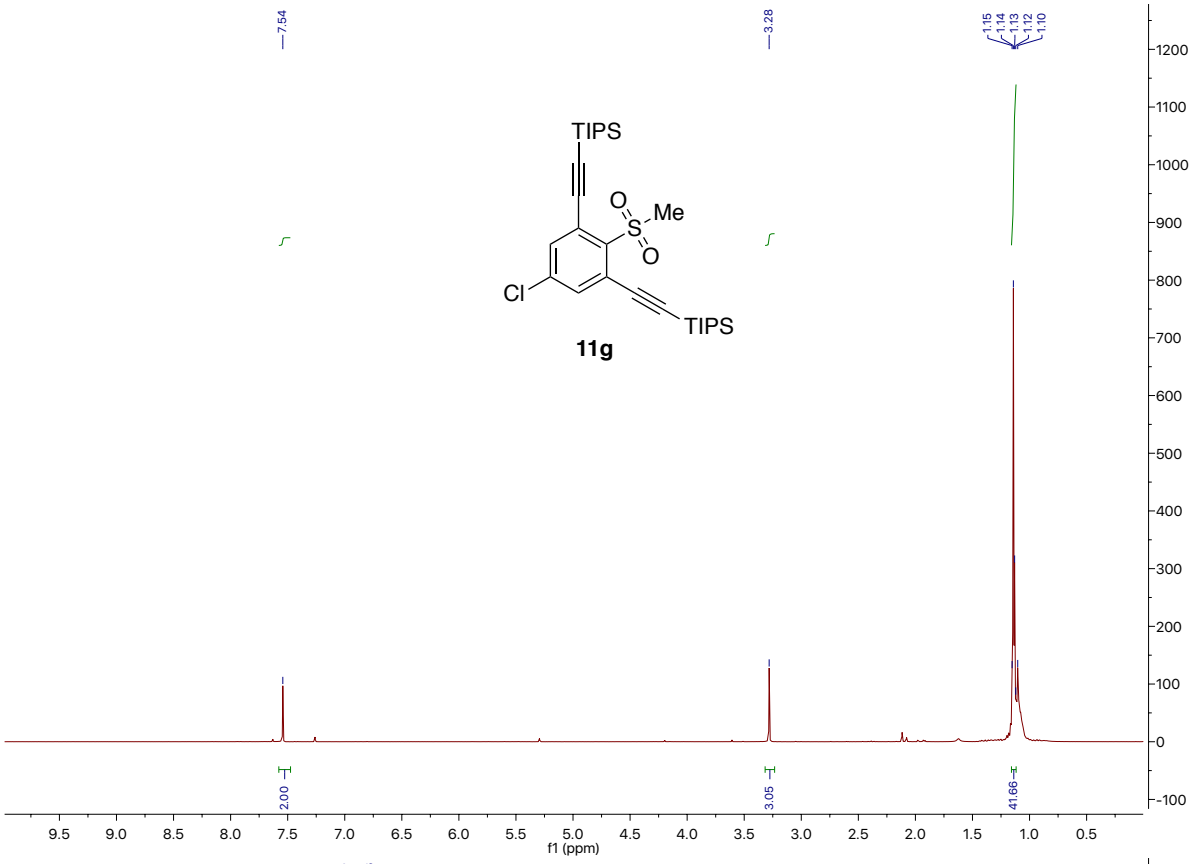


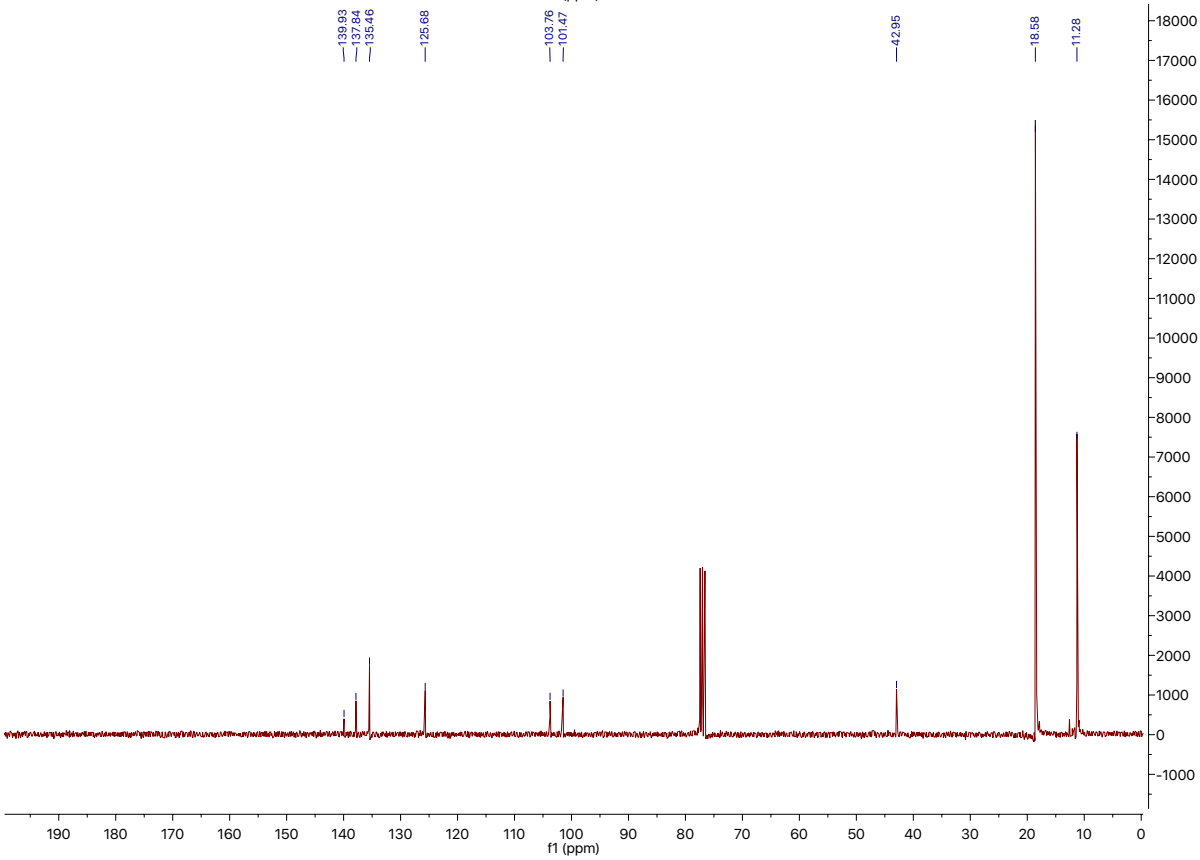
((2-((Methylthio)methyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) **(11f)**



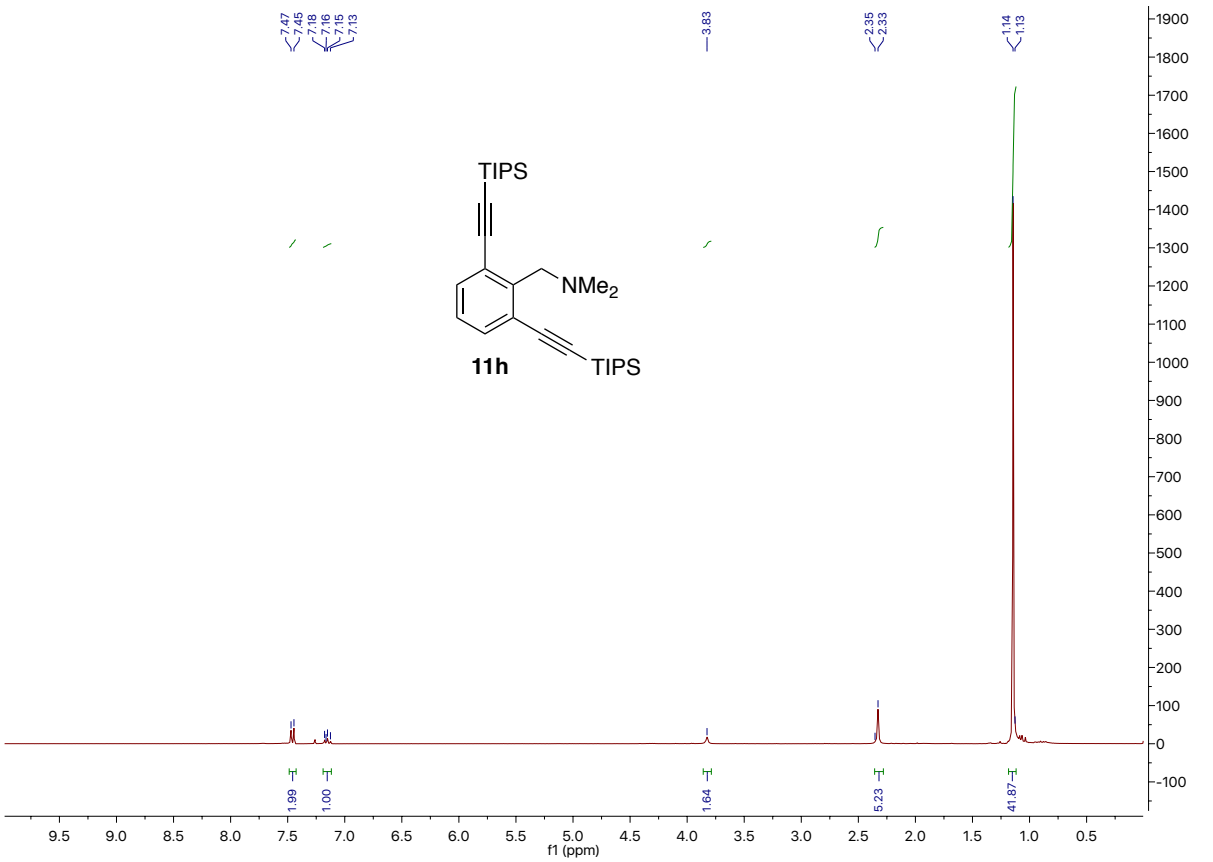


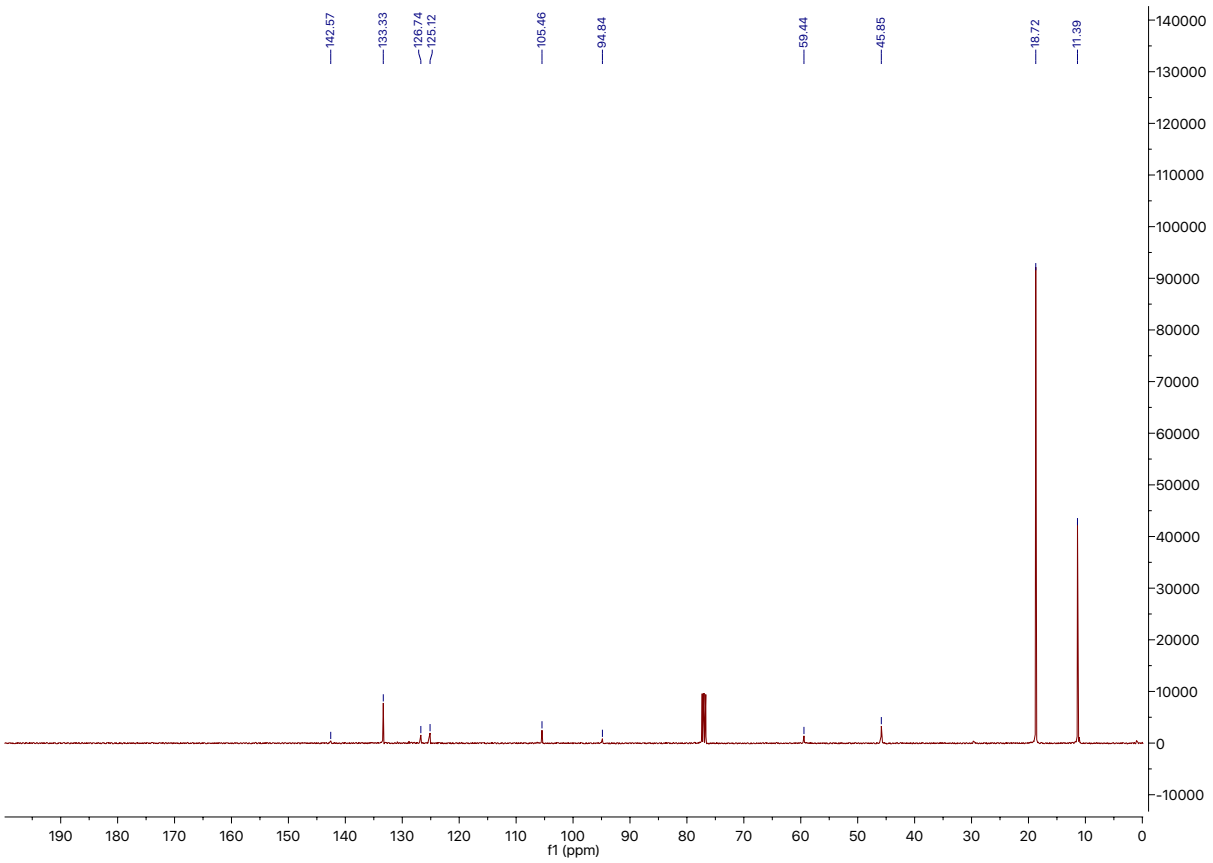
((5-Chloro-2-(methylsulfonyl)-1,3-phenylene)bis(ethyne-2,1-diyl))bis(triisopropylsilane) **(11g)**



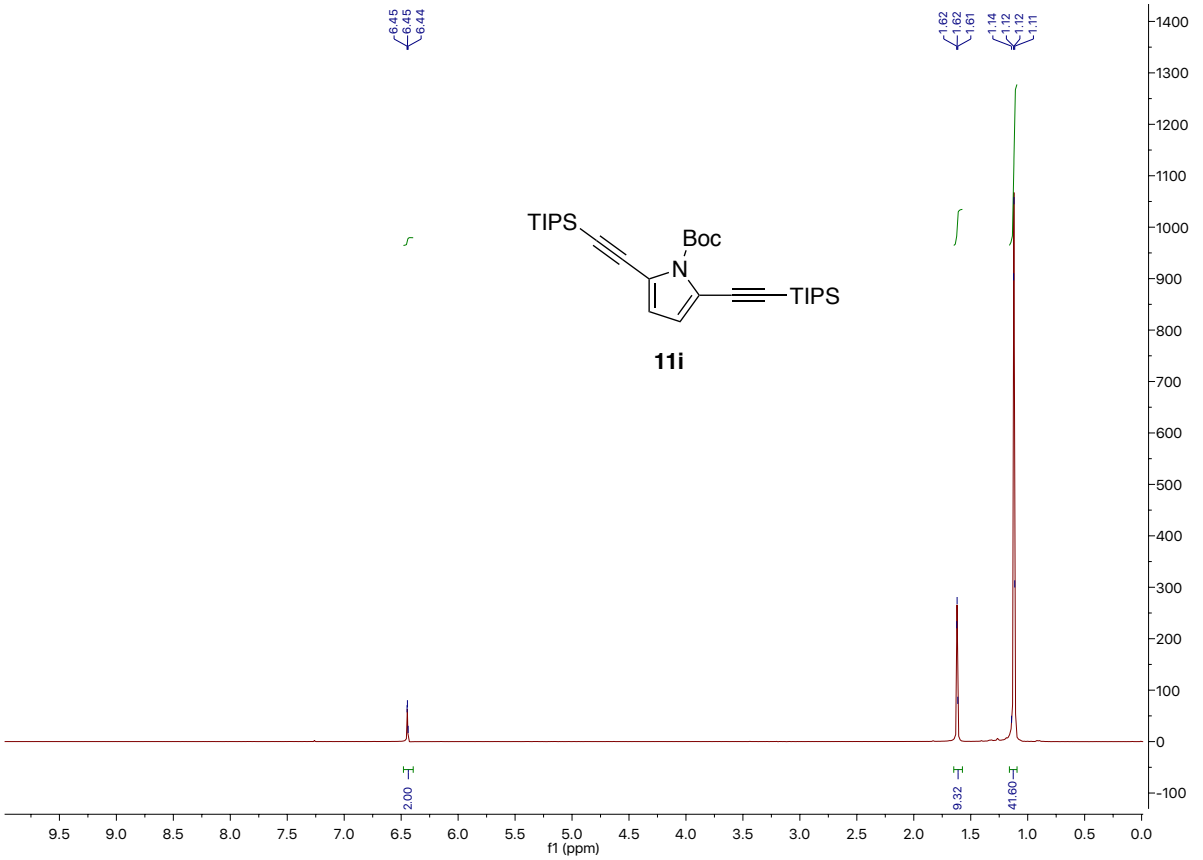


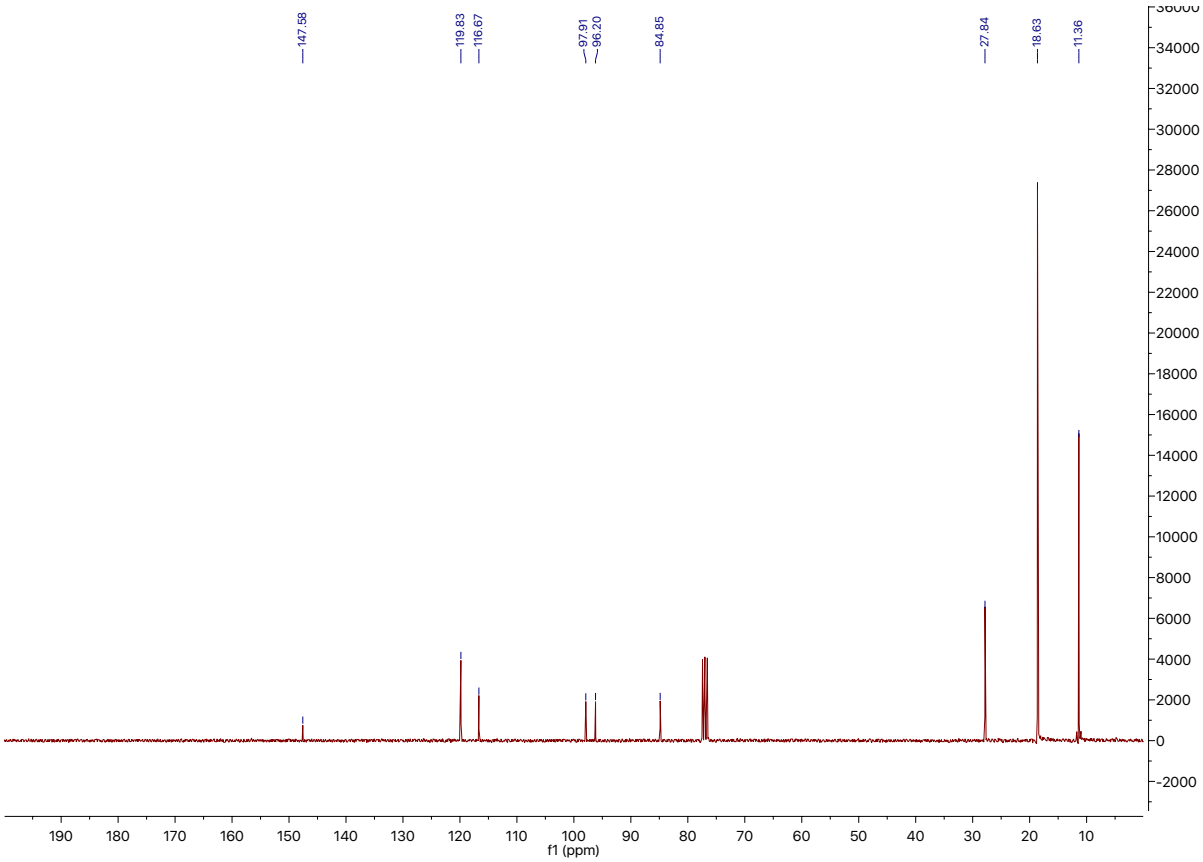
***1-(2,6-Bis((triisopropylsilyl)ethynyl)phenyl)-N,N-dimethylmethanamine* (11h)**





***Tert-butyl 2,5-bis((triisopropylsilyl)ethynyl)-1H-pyrrole-1-carboxylate* (11i)**



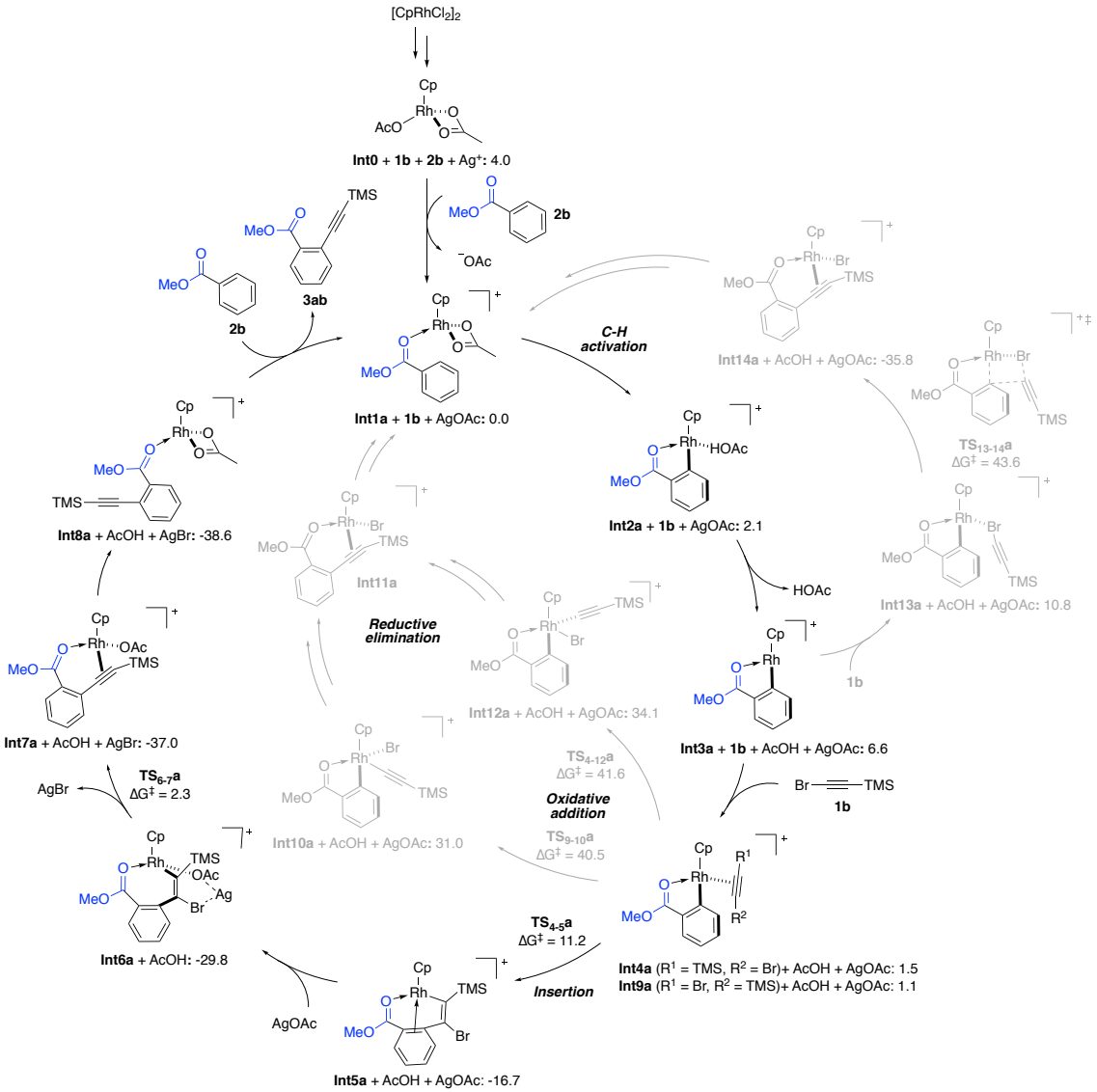


7) DFT Mechanistic Studies

7.1. Computational methods

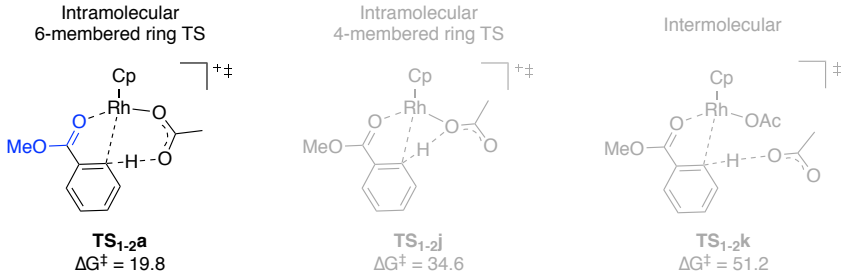
Calculations were performed by means of the Gaussian 09 suite of programs.[4] DFT was applied using wB97XD.[5] Rh, Ag, K and Br atoms were described by ECP with the LANL2DZ basis set.[6] Polarization functions were added for Rh (ζ_f= 1.35), Ag (ζ_f= 1.611), K (ζ_d= 1.000) and Br (ζ_d= 0.428).[7] The 6-31G(d) basis set[8] was employed for all remaining atoms (C, H, O, Si and F). Full geometry optimizations were carried out in 1,2-dichloroethane, through an implicit solvent SMD.[9] The stationary points were characterized by vibrational analysis. Transition states were identified by the presence of one imaginary frequency while minima by a full set of real frequencies. The connectivity of the transition states was confirmed by relaxing each transition state towards both the reactant and the product. Reported energies are potential energies (E) and free energies (G) in solution, computed at 298 K and 1 atm. Mulliken charges[10] were calculated at the same level of theory.

7.2. Mechanism of the Rh-Catalyzed *ortho*-Alkynylation of Methyl Benzoate



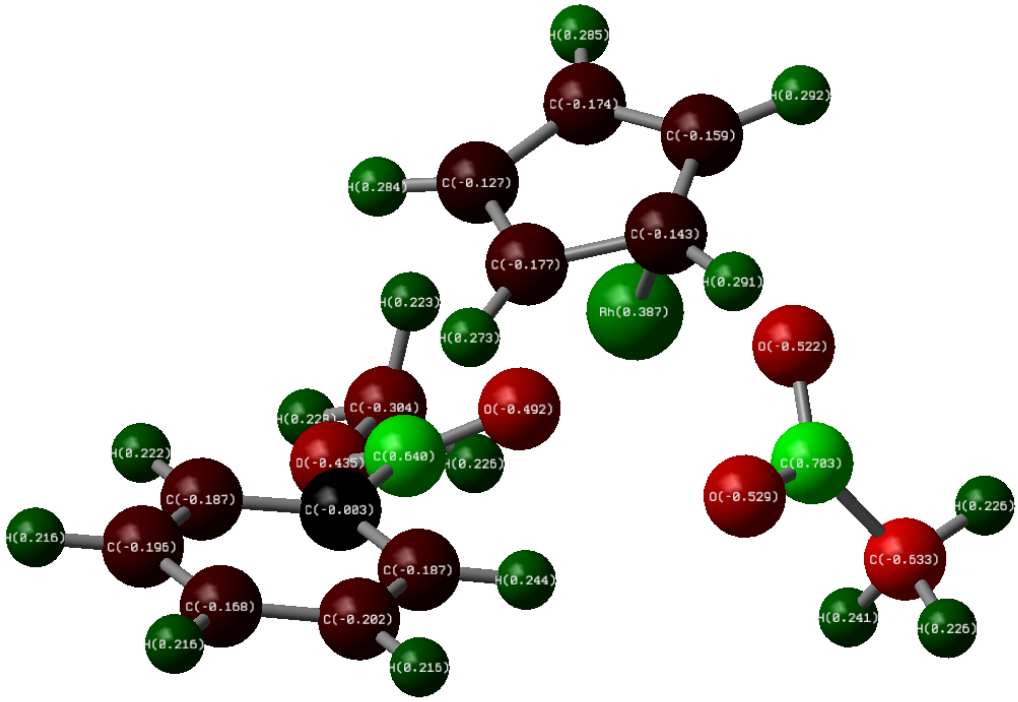
[a] Free energies in kcal/mol.

Scheme S7.2.1- Rh-catalyzed *ortho*-alkynylation of methyl benzoate.[a]



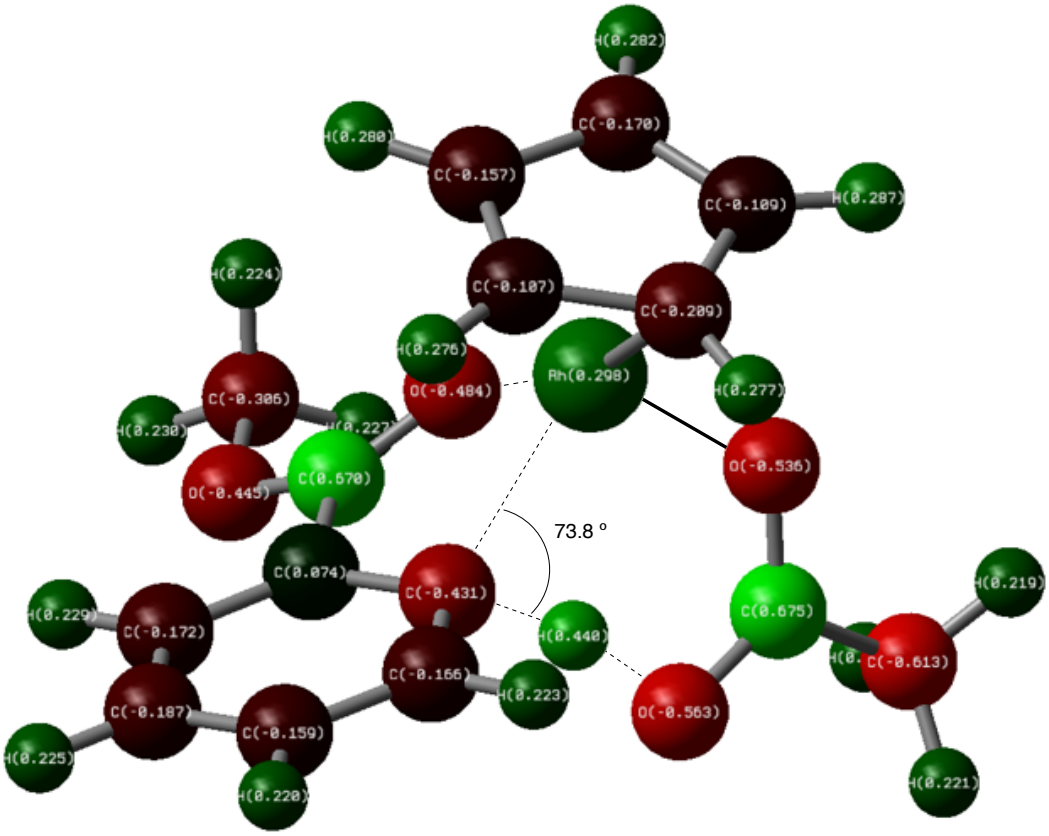
[a] Free energies in kcal/mol.

Scheme S7.2.2 - Acetate-assisted C-H activation of methyl benzoate.[a]



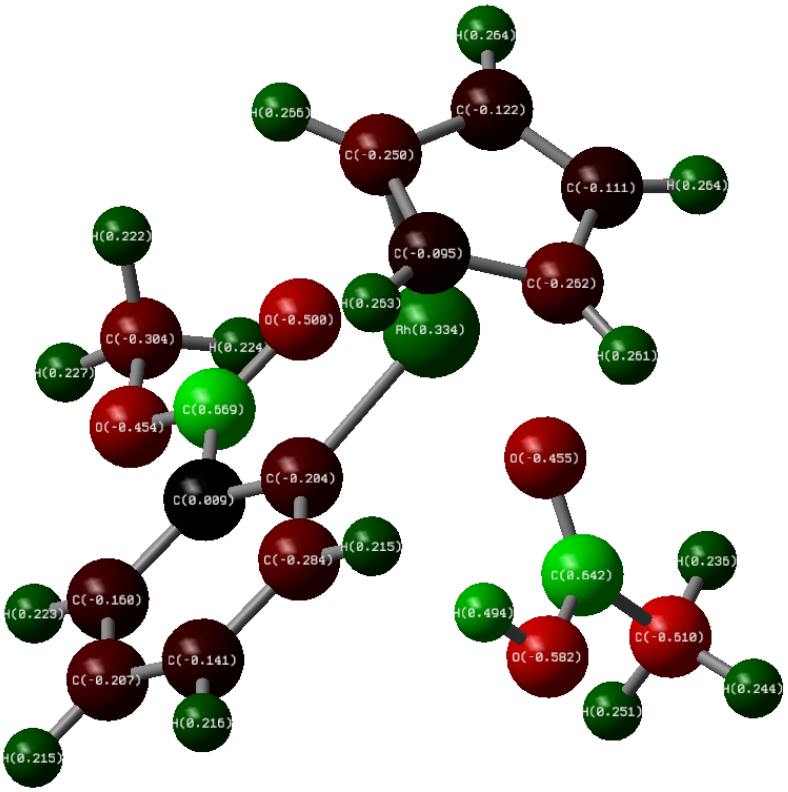
[a] Colored atoms by charge: from more positive in green to more negative in red.

Figure S7.2.1- Mulliken atomic charges on Int1a[a]



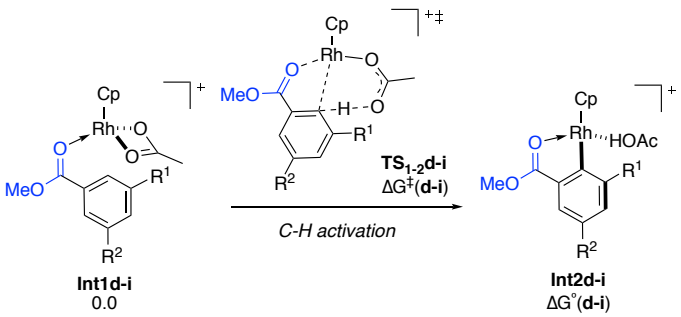
[a] Colored atoms by charge: from more positive in green to more negative in red.

Figure S7.2.2- Mulliken atomic charges on $TS_{1\text{-}2}$a[a]



[a] Colored atoms by charge: from more positive in green to more negative in red.

Figure S7.2.3-Mulliken atomic charges on Int2a[a]

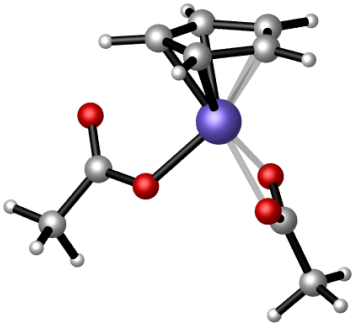


Entry	R^1	R^2	$TS_{1\text{-}2}$d-i	$\Delta G^{\ddagger}$ (d-i)	Int2d-i	ΔG° (d-i)
1	H	OMe	$TS_{1\text{-}2}$**d**	17.2	**Int2d**	2.9
2	H	Me	$TS_{1\text{-}2}$**e**	18.9	**Int2e**	3.3
3	H	Br	$TS_{1\text{-}2}$**f**	20.8	**Int2f**	3.1
4	H	CF_3	$TS_{1\text{-}2}$**g**	21.5	**Int2g**	3.4
5	H	F	$TS_{1\text{-}2}$**h**	19.5	**Int2h**	2.5
6	F	H	$TS_{1\text{-}2}$**i**	17.8	**Int2i**	2.7

[a] Free energies in kcal/mol.

Table S7.2.1- Acetate-assisted C-H activation of substituted methyl benzoates[a]

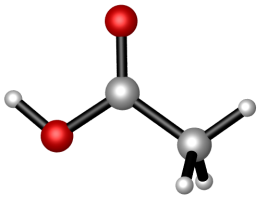
Int0



E = -759.835759 Hartrees
G = -759.689661 Hartrees

6	2.283685	-3.478474	1.806403
1	3.339915	-3.262176	1.876079
6	1.371126	-2.904016	0.877140
1	1.635122	-2.218751	0.084607
6	0.098215	-3.510413	1.072353
1	-0.797072	-3.317623	0.496750
6	1.544581	-4.394129	2.640964
1	1.960984	-5.009570	3.427469
6	0.208419	-4.417520	2.189833
1	-0.581736	-5.052174	2.568908
45	1.514357	-5.035002	0.566852
8	2.107713	-5.012355	-1.392354
6	3.069611	-4.230541	-1.782050
8	3.676290	-3.425049	-1.079617
6	3.410440	-4.419865	-3.251254
1	3.852251	-5.411886	-3.396689
1	2.505532	-4.370309	-3.864526
1	4.122505	-3.660136	-3.580005
8	2.676035	-6.850182	0.630600
8	0.614870	-6.898994	-0.070721
6	1.720242	-7.496727	0.100287
6	1.910288	-8.911448	-0.351835
1	0.957858	-9.445552	-0.352916
1	2.303484	-8.898306	-1.374803
1	2.632893	-9.424087	0.287053

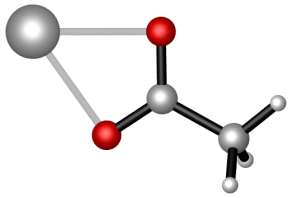
AcOH



E = -229.014845 Hartrees
G = -228.979969 Hartrees

6	0.109757	-0.842062	-0.660169
1	0.705436	-1.659712	-1.079057
1	-0.172305	-0.147587	-1.451981
1	-0.787886	-1.281913	-0.213802
6	0.902411	-0.121136	0.390822
8	1.212131	1.049233	0.369645
8	1.250381	-0.937895	1.400097
1	1.756280	-0.406719	2.041368

AgOAc



E = -374.200558 Hartrees
G = -374.182650 Hartrees

6	0.092255	-0.865802	-0.689164
1	0.668266	-1.714190	-1.072454
1	-0.161764	-0.194654	-1.511790
1	-0.828603	-1.269608	-0.254531
6	0.889778	-0.152432	0.389023
8	1.306088	-0.848963	1.359134
8	1.098720	1.086484	0.274714
47	2.348071	1.044324	2.314410

AgBr

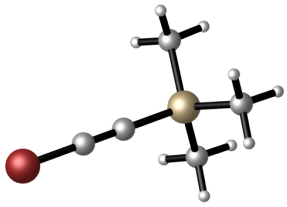
E = -159.009364 Hartrees
G = -159.034547 Hartrees

47	-1.018886	1.131621	0.000000
35	1.508516	1.131621	0.000000

Ag^+

E = -145.614434 Hartrees
G = -145.631040 Hartrees

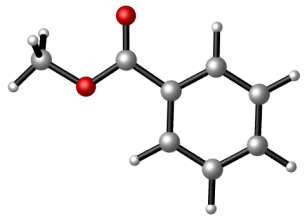
(Bromoethynyl)trimethylsilane (1b)



E = -498.509006 Hartrees
G = -498.423476 Hartrees

6	-2.312030	-0.244284	-0.001118
6	-1.096463	-0.241889	0.000717
35	-4.118071	-0.246785	-0.002924
14	0.759521	-0.239095	0.001337
6	1.331808	1.547469	-0.061550
1	0.975276	2.112279	0.807488
1	2.428049	1.595116	-0.067295
1	0.968728	2.050477	-0.965239
6	1.330437	-1.082498	1.576956
1	0.958418	-2.111974	1.635778
1	2.426454	-1.118386	1.614092
1	0.982217	-0.546413	2.467413
6	1.331290	-1.185587	-1.514619
1	0.969711	-0.719248	-2.438291
1	2.427457	-1.209709	-1.557128
1	0.973305	-2.221541	-1.495616

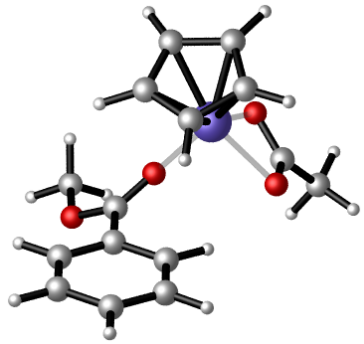
2b



E = -459.980113 Hartrees
G = -459.868594 Hartrees

6	0.909464	-0.640936	-0.213899
6	2.247297	-0.682639	-0.604321
6	3.041161	0.455306	-0.500139
6	2.494316	1.641909	-0.002072
6	1.152674	1.680993	0.387626
6	0.362783	0.541526	0.283504
1	0.292911	-1.531306	-0.297022
1	2.673007	-1.602620	-0.993412
1	4.081867	0.423893	-0.803687
1	0.740126	2.608421	0.771382
1	-0.679120	0.575814	0.587227
6	3.295462	2.892612	0.122647
8	2.849418	3.950984	0.516794
8	4.568962	2.726656	-0.248337
6	5.395990	3.891246	-0.182254
1	5.430892	4.283556	0.837190
1	6.387959	3.564618	-0.494471
1	5.023949	4.664305	-0.859625

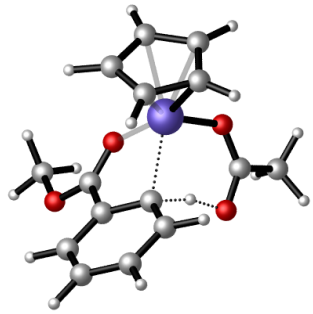
Int1a



E = -991.249669 Hartrees
G = -991.013054 Hartrees

6	2.783836	-4.013830	2.077772
1	3.735608	-4.428073	2.384121
6	2.585678	-3.058693	1.051690
1	3.361806	-2.606937	0.448017
6	1.171311	-2.848429	0.902673
1	0.697763	-2.183330	0.193675
6	1.492812	-4.431630	2.556347
1	1.303483	-5.166554	3.326882
6	0.505399	-3.673556	1.847369
1	-0.566603	-3.787361	1.945147
45	1.631848	-4.920920	0.509069
8	2.321821	-6.966166	0.491525
8	0.251530	-6.491909	0.043758
6	1.166811	-7.369903	0.148099
6	0.888124	-8.813432	-0.110275
1	-0.024180	-8.927788	-0.698296
1	1.734879	-9.277836	-0.621172
1	0.753548	-9.319662	0.852349
6	0.182445	-5.106443	-2.929914
6	-0.602868	-5.919658	-3.753779
6	-0.324201	-3.898493	-2.441677
6	-1.898018	-5.527105	-4.070971
1	-0.206664	-6.855621	-4.132473
6	-1.615456	-3.506736	-2.770426
1	0.303088	-3.264875	-1.824939
6	-2.403821	-4.323798	-3.580223
1	-2.514285	-6.159960	-4.701471
1	-2.006904	-2.565130	-2.398346
1	-3.415649	-4.020576	-3.832113
8	2.189056	-5.033423	-1.603070
6	1.555116	-5.500067	-2.559667
8	2.095464	-6.391304	-3.354838
6	3.406153	-6.881135	-3.009205
1	3.418400	-7.225014	-1.973449
1	3.590662	-7.704972	-3.696520
1	4.145973	-6.091331	-3.152791

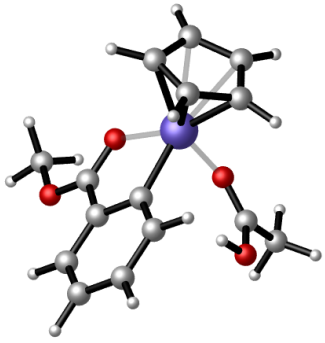
$TS_{1\text{-}2}a$



E = -991.213896 Hartrees
G = -990.981500 Hartrees

8	-1.397831	1.121233	0.697958
6	-1.993502	0.194695	0.085796
8	-1.402400	-0.816536	-0.405811
6	1.815708	1.665014	-0.268941
6	1.209841	0.862375	0.722060
6	2.844434	2.552444	0.026925
6	1.686920	0.970579	2.032903
6	3.303924	2.631362	1.340902
6	2.730090	1.843781	2.338249
1	-0.093591	0.821966	0.687391
1	3.293577	3.158987	-0.752791
1	1.221813	0.386414	2.821721
1	4.112029	3.312669	1.587181
1	3.093236	1.918776	3.358697
45	0.672485	-1.047422	-0.291731
6	2.460244	-2.177855	-0.782634
1	3.246015	-1.781833	-1.412479
6	1.293821	-2.899794	-1.238802
1	1.060909	-3.145522	-2.266222
6	0.505138	-3.206063	-0.104986
1	-0.463275	-3.688545	-0.119243
6	2.373625	-2.042747	0.620476
1	3.078344	-1.519760	1.252597
6	1.132117	-2.632291	1.049769
1	0.765513	-2.683790	2.065823
6	-3.479362	0.294093	-0.116168
1	-3.921396	-0.695198	-0.245534
1	-3.943558	0.815307	0.723206
1	-3.660457	0.877889	-1.025942
8	0.688035	0.412184	-1.926270
6	1.308233	1.448297	-1.635310
8	1.539741	2.392861	-2.504768
6	1.076688	2.182584	-3.854734
1	1.355673	3.085909	-4.393697
1	1.570173	1.308614	-4.283938
1	-0.006339	2.048459	-3.860110

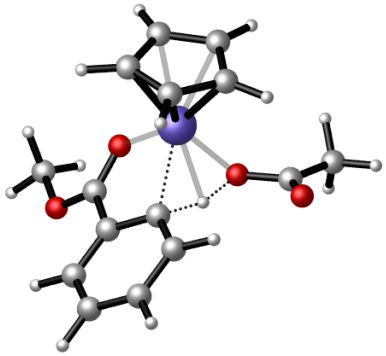
Int2a



E = -991.246363 Hartrees
G = -991.009660 Hartrees

8	-1.275119	0.796877	1.534742
6	-1.764548	0.349627	0.399567
8	-1.102160	-0.285808	-0.423656
6	1.841609	1.661627	-0.439327
6	1.659419	0.587825	0.451685
6	2.320328	2.903176	-0.016392
6	1.979317	0.791063	1.795772
6	2.627555	3.086290	1.326542
6	2.455149	2.034019	2.225157
1	-0.314713	0.609466	1.579609
1	2.450077	3.710393	-0.730613
1	1.860290	-0.010095	2.521029
1	3.002966	4.043385	1.673553
1	2.697147	2.177629	3.274332
45	0.928736	-1.087324	-0.416331
6	2.497252	-2.502056	-0.698172
1	3.425266	-2.256000	-1.197501
6	1.354784	-3.164977	-1.311212
1	1.257468	-3.400514	-2.362710
6	0.379320	-3.323809	-0.337071
1	-0.621695	-3.706552	-0.487316
6	2.239401	-2.379605	0.697879
1	2.914391	-1.967608	1.435334
6	0.886404	-2.768495	0.910655
1	0.365228	-2.771507	1.858859
6	-3.199327	0.690123	0.178737
1	-3.578817	0.168630	-0.699297
1	-3.784889	0.426251	1.063920
1	-3.286170	1.771961	0.031443
8	1.114962	0.209121	-2.139844
6	1.489809	1.353038	-1.826551
8	1.583742	2.318497	-2.702161
6	1.222033	2.019227	-4.064623
1	1.348815	2.956578	-4.603109
1	1.885789	1.251764	-4.467350
1	0.183596	1.686117	-4.112036

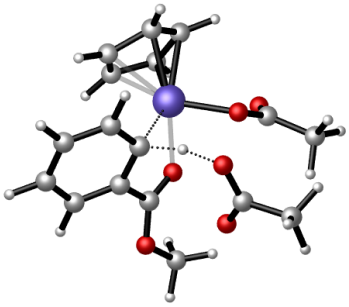
$TS_{1\text{-}2}j$



E = -991.191243 Hartrees
G = -990.957960 Hartrees

6	3.071380	-4.298899	1.745085
1	4.138254	-4.148911	1.840830
6	2.186616	-3.563172	0.872818
1	2.488605	-2.803090	0.164685
6	0.895627	-4.098973	1.013375
1	0.022883	-3.819055	0.437926
6	2.285692	-5.231098	2.485618
1	2.658445	-5.939088	3.213768
6	0.949751	-5.161585	1.992599
1	0.115416	-5.767306	2.320258
45	2.230931	-5.718996	0.390055
6	1.988033	-8.644855	0.054034
6	3.954470	-8.248581	1.398888
6	1.954778	-9.977318	0.443214
6	3.922801	-9.584396	1.802956
1	4.748361	-7.588870	1.734111
6	2.930695	-10.43977	1.328036
1	1.181427	-10.64487	0.077704
1	4.677422	-9.961710	2.485935
1	2.914952	-11.47785	1.644288
8	3.676789	-5.968184	-1.266550
8	5.576665	-5.656487	-0.102058
6	4.889760	-5.427783	-1.078372
6	5.298518	-4.529869	-2.215559
1	4.561489	-3.728337	-2.330958
1	6.285097	-4.103250	-2.028764
1	5.311487	-5.099846	-3.150021
6	2.987183	-7.762588	0.517688
1	3.518201	-6.956370	-0.408932
8	0.906661	-6.796432	-0.950197
6	0.982775	-8.031450	-0.833598
8	0.192818	-8.841339	-1.478492
6	-0.807167	-8.252285	-2.337690
1	-0.322711	-7.674461	-3.126526
1	-1.352034	-9.095339	-2.757361
1	-1.470716	-7.615610	-1.749802

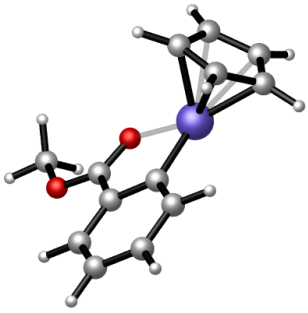
$TS_{1\text{-}2}k$



E = -1219.760091 Hartrees
G = -1219.483103 Hartrees

6	2.781472	-4.277391	2.263082
1	3.777558	-4.072619	2.631070
6	1.964956	-3.395655	1.490145
1	2.262628	-2.433656	1.097077
6	0.749573	-4.069707	1.192145
1	-0.045493	-3.691635	0.565087
6	2.008985	-5.470584	2.520964
1	2.355961	-6.339401	3.063691
6	0.772155	-5.350130	1.861462
1	-0.001106	-6.105185	1.813773
45	2.385471	-5.186374	0.377493
6	2.563572	-8.015851	-0.282508
6	4.270354	-7.646469	1.367393
6	2.301181	-9.280393	0.232545
6	4.004429	-8.901447	1.910132
1	5.061252	-7.032808	1.790864
6	3.025983	-9.717339	1.341261
1	1.530568	-9.907709	-0.204940
1	4.565622	-9.253387	2.770890
1	2.825423	-10.69750	1.763062
8	3.481578	-4.255180	-1.062663
6	2.865313	-3.430238	-1.853686
8	1.734988	-2.976914	-1.686491
6	3.692472	-3.082442	-3.078523
1	3.269043	-2.219314	-3.597040
1	4.733390	-2.884052	-2.808257
1	3.683948	-3.947931	-3.751153
8	5.339789	-6.351056	-1.461368
8	3.781093	-6.853551	-3.001836
6	4.910597	-6.465642	-2.661155
6	5.927359	-6.077729	-3.733055
1	6.176875	-5.015312	-3.633212
1	6.856769	-6.641972	-3.599509
1	5.530379	-6.259564	-4.735095
6	3.552974	-7.168269	0.260497
1	4.249140	-6.525550	-0.547689
8	1.464564	-6.200288	-1.310934
6	1.747574	-7.405631	-1.353264
8	1.277041	-8.208042	-2.269580
6	0.568064	-7.586877	-3.355631
1	0.308714	-8.398715	-4.033368
1	-0.333987	-7.092876	-2.987735
1	1.227206	-6.868100	-3.844609

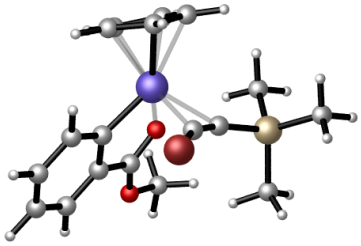
Int3a



E = -762.203068 Hartrees
G = -762.022642 Hartrees

6	2.838701	-4.294050	2.183149
1	3.855717	-4.178106	2.535117
6	2.201904	-3.470500	1.158643
1	2.698360	-2.702937	0.579673
6	0.904579	-3.918693	0.989507
1	0.191633	-3.573596	0.252755
6	1.870613	-5.175755	2.715813
1	2.009721	-5.883155	3.521659
6	0.702353	-5.052075	1.887323
1	-0.221108	-5.604225	2.004836
45	2.274604	-5.747307	0.701653
6	2.206621	-8.584975	0.180476
6	3.436901	-8.154544	2.201343
6	2.441217	-9.957165	0.290627
6	3.682767	-9.525190	2.311884
1	3.834772	-7.477687	2.951872
6	3.184524	-10.42471	1.367935
1	2.054336	-10.64290	-0.456843
1	4.267958	-9.896427	3.148575
1	3.378543	-11.48715	1.473802
6	2.692393	-7.665907	1.129184
8	1.376987	-6.723796	-0.999272
6	1.480243	-7.965842	-0.929944
8	0.959845	-8.753253	-1.829697
6	0.226038	-8.142535	-2.910548
1	-0.149109	-8.974311	-3.503639
1	-0.601103	-7.552439	-2.511565
1	0.890035	-7.514286	-3.506944

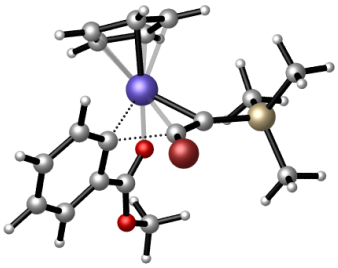
Int4a



E = -1260.747432 Hartrees
G = -1260.454187 Hartrees

6	2.240562	-3.249840	1.507444
1	3.186429	-2.759984	1.317429
6	0.955016	-2.838002	0.976430
1	0.799037	-2.051823	0.250294
6	-0.008749	-3.706401	1.483491
1	-1.057584	-3.725163	1.217970
6	2.020569	-4.305208	2.441948
1	2.778242	-4.801717	3.032203
6	0.649019	-4.663590	2.356844
1	0.158164	-5.449235	2.915738
45	1.567761	-4.987982	0.412598
6	2.640849	-6.699373	0.618904
6	2.022597	-7.831300	0.060434
6	3.873907	-6.862110	1.245760
6	2.615708	-9.097556	0.108816
6	4.464145	-8.124326	1.303669
1	4.387800	-6.013171	1.685959
6	3.844867	-9.240095	0.734372
1	2.114398	-9.951532	-0.336073
1	5.424515	-8.239236	1.798360
1	4.321655	-10.21336	0.785363
6	1.897470	-4.477464	-1.760705
6	3.021617	-4.667325	-1.261083
35	4.846147	-4.710254	-1.292670
14	0.490315	-4.120640	-2.954583
6	-1.104839	-3.893818	-2.004226
1	-1.034596	-3.064486	-1.291619
1	-1.916460	-3.663452	-2.705949
1	-1.374267	-4.801576	-1.455661
6	0.993687	-2.538483	-3.826705
1	1.954834	-2.653407	-4.340623
1	0.241367	-2.261364	-4.575403
1	1.083272	-1.707688	-3.117065
6	0.429768	-5.588632	-4.120071
1	0.497039	-6.535870	-3.573952
1	-0.506249	-5.590912	-4.691886
1	1.260457	-5.557620	-4.834704
8	0.237317	-6.416152	-0.476389
6	0.717895	-7.566678	-0.528436
8	0.071473	-8.554879	-1.084955
6	-1.249404	-8.283019	-1.596358
1	-1.208815	-7.505319	-2.360833
1	-1.585504	-9.224120	-2.027429
1	-1.908010	-7.979958	-0.779802

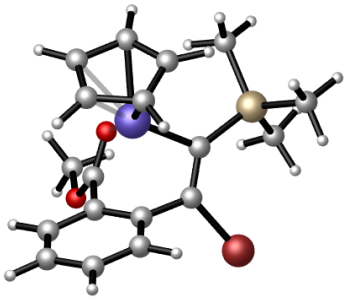
$TS_{4\text{-}5}a$



E = -1260.727359 Hartrees
G = -1260.436304 Hartrees

6	2.191843	-3.259400	1.365127
1	3.154990	-2.829941	1.121400
6	0.928849	-2.864298	0.801011
1	0.786878	-2.142310	0.008114
6	-0.056449	-3.689264	1.368644
1	-1.107559	-3.702524	1.112184
6	1.938945	-4.223168	2.408074
1	2.690896	-4.698290	3.023312
6	0.571360	-4.526674	2.380766
1	0.061313	-5.256640	2.995219
45	1.412834	-5.008350	0.374498
6	2.738030	-6.642108	0.273346
6	2.061079	-7.855973	0.048239
6	3.994798	-6.677952	0.884504
6	2.648295	-9.082372	0.367179
6	4.557322	-7.896730	1.243522
1	4.537704	-5.755507	1.065084
6	3.899978	-9.099181	0.966566
1	2.112040	-10.00578	0.173804
1	5.526104	-7.912701	1.733253
1	4.363398	-10.04441	1.228831
6	1.640390	-4.877270	-1.691389
6	2.718232	-5.467620	-1.351766
35	4.423562	-5.653480	-2.101533
14	0.513057	-4.046055	-2.933670
6	-1.191645	-3.880966	-2.174784
1	-1.190663	-3.150062	-1.358336
1	-1.911123	-3.536886	-2.928170
1	-1.547058	-4.838167	-1.777817
6	1.271992	-2.367307	-3.286065
1	2.264231	-2.469095	-3.740518
1	0.640557	-1.791876	-3.974120
1	1.379610	-1.783655	-2.364073
6	0.503020	-5.156181	-4.444688
1	0.125521	-6.155947	-4.200510
1	-0.142041	-4.735974	-5.226211
1	1.510163	-5.267901	-4.862965
8	0.088739	-6.638665	-0.314441
6	0.681906	-7.724791	-0.419662
8	0.116118	-8.789929	-0.923941
6	-1.263506	-8.676907	-1.324800
1	-1.362467	-7.931225	-2.115733
1	-1.533900	-9.664024	-1.694908
1	-1.882324	-8.405358	-0.466933

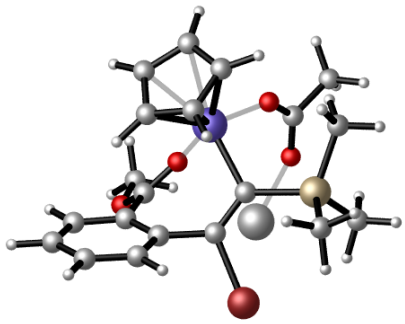
Int5a



E = -1260.775909 Hartrees
G = -1260.483099 Hartrees

6	2.167892	-3.735739	1.509968
1	3.210916	-3.489355	1.360466
6	1.061674	-3.138519	0.847260
1	1.103449	-2.383721	0.073930
6	-0.108959	-3.814139	1.310727
1	-1.120755	-3.638139	0.969466
6	1.651127	-4.643562	2.527641
1	2.261638	-5.248726	3.185377
6	0.269078	-4.685501	2.414345
1	-0.407654	-5.316495	2.974478
45	1.167645	-5.240430	0.379525
6	2.929870	-6.757717	-0.578691
6	2.064479	-7.729017	-0.014779
6	4.211217	-6.607334	-0.014529
6	2.490986	-8.534541	1.050310
6	4.613513	-7.387542	1.055723
1	4.889567	-5.876685	-0.444129
6	3.756343	-8.358853	1.584107
1	1.818606	-9.283051	1.456828
1	5.603584	-7.251824	1.478556
1	4.081282	-8.978714	2.413199
6	1.552145	-5.045308	-1.622602
6	2.511988	-5.947452	-1.762811
35	3.478667	-6.347041	-3.401303
14	0.641736	-3.921561	-2.832548
6	-1.026286	-3.479077	-2.084477
1	-0.939520	-2.748600	-1.272823
1	-1.673190	-3.037526	-2.853001
1	-1.535410	-4.368106	-1.694066
6	1.687993	-2.380348	-3.089617
1	2.660727	-2.632356	-3.527998
1	1.185662	-1.679963	-3.768307
1	1.870697	-1.855916	-2.143884
6	0.341696	-4.820865	-4.457637
1	-0.105062	-5.808699	-4.292511
1	-0.355123	-4.238066	-5.073567
1	1.261533	-4.959885	-5.033490
8	-0.115087	-6.896898	-0.415277
6	0.655286	-7.859494	-0.483789
8	0.306576	-9.039158	-0.906985
6	-1.070489	-9.213893	-1.312621
1	-1.289594	-8.560037	-2.158554
1	-1.149415	-10.25959	-1.602166
1	-1.734413	-8.992274	-0.475302

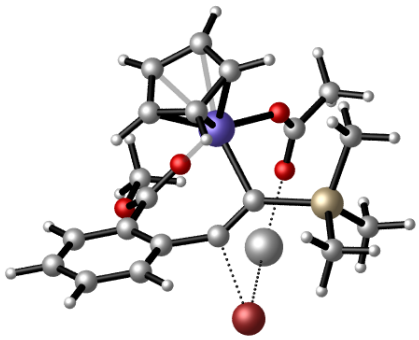
Int6a



E = -1635.024754 Hartrees
G = -1634.686713 Hartrees

6	-2.746980	-0.076634	0.554040
6	-4.616526	-1.830320	1.731899
6	-1.817601	0.849064	-0.168987
6	-0.662891	0.572661	-0.805381
6	-2.464798	-0.726644	1.769522
1	-3.166816	-2.060859	3.301672
6	-3.405029	-1.578026	2.359794
6	-3.981313	-0.333371	-0.051070
6	-4.897559	-1.210180	0.517126
1	-5.333259	-2.506624	2.185456
1	-5.837865	-1.401470	0.009966
1	-4.225032	0.157946	-0.987733
6	0.550541	-2.483581	-1.989539
6	-0.857492	-2.281856	-1.863384
6	0.989157	-3.313672	-0.882486
1	-1.493035	-1.742105	-2.552574
1	2.008514	-3.628569	-0.703836
6	-1.246851	-2.823157	-0.608046
1	-2.246915	-2.825746	-0.195861
6	-0.098036	-3.507759	-0.038439
1	-0.083763	-4.007435	0.921501
1	1.170334	-2.178608	-2.820038
14	0.081408	1.586498	-2.265140
35	-2.715518	2.625702	-0.407863
6	1.394021	0.600119	-3.174155
1	0.947299	-0.200377	-3.773893
1	2.145839	0.171279	-2.506170
1	1.899285	1.279178	-3.873551
6	-1.290566	1.915524	-3.516893
1	-1.875371	2.812092	-3.293297
1	-1.985852	1.069821	-3.586819
1	-0.835502	2.050575	-4.506689
6	0.874446	3.193521	-1.680921
1	1.182356	3.767382	-2.565260
1	1.776509	3.004748	-1.086164
1	0.198585	3.834421	-1.101917
8	2.151936	-0.367046	-0.172027
6	2.798926	0.569789	0.387207
8	2.341469	1.493097	1.106339
47	0.163115	1.944486	1.158173
6	4.286893	0.586411	0.098893
1	4.444174	1.127923	-0.841877
1	4.829850	1.108486	0.889507
1	4.677251	-0.426161	-0.024995
45	0.188477	-1.238626	-0.295455
8	-0.064256	-0.649414	1.810070
6	-1.143147	-0.621107	2.418956
8	-1.183781	-0.515958	3.722265
6	0.077091	-0.491736	4.424633
1	0.652200	0.388178	4.128449
1	-0.187630	-0.439236	5.478747
1	0.641866	-1.401020	4.211121

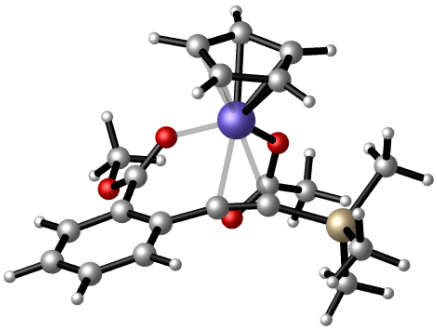
$TS_{6\text{-}7}a$



E = -1635.019263 Hartrees
G = -1634.683017 Hartrees

6	-2.726190	-0.165673	0.486142
6	-4.727484	-1.577698	1.847561
6	-1.724436	0.597177	-0.266624
6	-0.674132	0.472172	-1.007875
6	-2.466489	-0.732962	1.747297
1	-3.263243	-1.855479	3.398593
6	-3.473021	-1.422674	2.426242
6	-3.992870	-0.325172	-0.079945
6	-4.982999	-1.033305	0.591121
1	-5.502404	-2.122840	2.376034
1	-5.958733	-1.153880	0.131789
1	-4.200409	0.123536	-1.046078
6	0.627653	-2.605240	-2.090985
6	-0.789366	-2.523917	-1.908722
6	1.183908	-3.308436	-0.956197
1	-1.496478	-2.071754	-2.591243
1	2.234813	-3.508953	-0.796003
6	-1.082629	-3.041037	-0.617943
1	-2.060064	-3.086031	-0.156508
6	0.145961	-3.564004	-0.054436
1	0.247230	-4.004354	0.928874
1	1.180289	-2.285284	-2.962328
14	0.089561	1.549550	-2.382015
35	-2.450391	2.786751	0.073464
6	1.307626	0.535734	-3.382713
1	0.809713	-0.276648	-3.923432
1	2.096413	0.114532	-2.751882
1	1.777252	1.186556	-4.131549
6	-1.346152	2.033191	-3.494404
1	-2.061634	2.685033	-2.982899
1	-1.884758	1.144334	-3.844998
1	-0.971413	2.565704	-4.377678
6	0.973281	3.071728	-1.720439
1	1.440526	3.583339	-2.572674
1	1.773190	2.823662	-1.013990
1	0.292597	3.788997	-1.248280
8	2.051397	-0.268099	-0.266658
6	2.566472	0.600754	0.506868
8	1.976051	1.398750	1.272409
47	-0.045753	2.303804	1.246121
6	4.078724	0.689549	0.431477
1	4.347173	1.270880	-0.458769
1	4.482938	1.194502	1.310821
1	4.522960	-0.303414	0.327169
45	0.220268	-1.342842	-0.423928
8	-0.064441	-0.775548	1.685148
6	-1.109385	-0.678698	2.333521
8	-1.088070	-0.530148	3.636256
6	0.208483	-0.537029	4.269823
1	0.836499	0.249212	3.846639
1	0.009956	-0.350386	5.323267
1	0.683372	-1.510739	4.132631

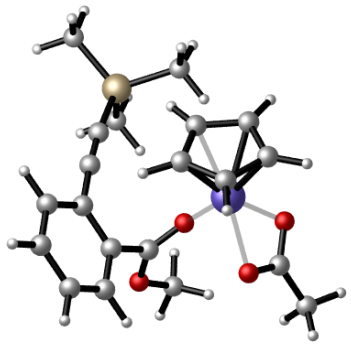
Int7a



E = -1476.006275 Hartrees
G = -1475.663590 Hartrees

6	-2.498453	-0.346424	0.514935
6	-4.551793	-0.516666	2.405076
6	-1.482439	-0.162611	-0.482032
6	-0.782491	0.213711	-1.427313
6	-2.201628	-0.667629	1.853188
1	-3.005199	-0.978737	3.821812
6	-3.234255	-0.737483	2.790130
6	-3.827705	-0.117527	0.140111
6	-4.847401	-0.209756	1.079744
1	-5.345042	-0.585009	3.142061
1	-5.874238	-0.034850	0.775420
1	-4.048359	0.138724	-0.890765
6	1.415474	-2.807652	-1.980161
6	0.086268	-2.608871	-2.451502
6	1.341787	-3.535279	-0.754208
1	-0.197536	-2.061928	-3.339944
1	2.175330	-3.832668	-0.132451
6	-0.820511	-3.275086	-1.552121
1	-1.898359	-3.297150	-1.634034
6	-0.045017	-3.845137	-0.519305
1	-0.434324	-4.350323	0.355509
1	2.310498	-2.393224	-2.424367
14	0.008036	1.298895	-2.744331
6	1.597295	0.521752	-3.353526
1	1.410983	-0.381141	-3.946125
1	2.248903	0.263719	-2.512384
1	2.128530	1.234758	-3.996215
6	-1.269894	1.434721	-4.110215
1	-2.224391	1.813813	-3.727073
1	-1.453558	0.465966	-4.589255
1	-0.920188	2.129864	-4.883725
6	0.299661	2.947541	-1.900801
1	0.911383	3.600741	-2.535132
1	0.809482	2.825772	-0.939432
1	-0.652377	3.456217	-1.709040
8	1.821933	-0.369149	-0.162291
6	1.748167	0.682674	0.606731
8	0.771659	1.051138	1.252661
6	3.045269	1.473272	0.609997
1	3.899691	0.814568	0.791361
1	3.188244	1.938162	-0.372158
1	3.008854	2.253516	1.372751
45	0.283576	-1.682212	-0.513106
8	0.017776	-1.600410	1.621738
6	-0.825141	-0.997087	2.292905
8	-0.588115	-0.678982	3.538238
6	0.720085	-0.979176	4.059897
1	1.475591	-0.472199	3.457972
1	0.712355	-0.594000	5.078006
1	0.888276	-2.057976	4.057977

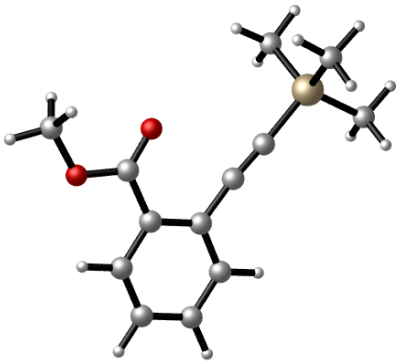
Int8a



E = -1476.005955 Hartrees
G = -1475.666163 Hartrees

6	2.662110	-2.903660	0.478349
1	3.727460	-2.740827	0.577236
6	1.879378	-2.606592	-0.662418
1	2.237129	-2.174439	-1.586892
6	0.536612	-3.055453	-0.416408
1	-0.296872	-2.985822	-1.101424
6	1.818857	-3.566494	1.437951
1	2.124541	-3.943162	2.404794
6	0.499541	-3.620354	0.887150
1	-0.355782	-4.100502	1.344714
45	1.872871	-4.750385	-0.311588
8	3.363750	-6.226628	0.130077
8	1.256667	-6.754254	0.105384
6	2.470041	-7.123300	0.229359
6	2.820698	-8.557289	0.451528
1	2.025699	-9.059534	1.006769
1	2.926604	-9.051501	-0.520935
1	3.769900	-8.638776	0.984959
6	-0.080721	-5.304554	-3.171138
6	-1.252357	-5.962692	-2.808800
6	-0.117220	-3.981346	-3.653094
6	-2.472128	-5.296721	-2.892357
1	-1.207699	-6.985146	-2.446750
6	-1.354452	-3.334769	-3.754921
6	-2.520390	-3.987869	-3.367208
1	-3.383911	-5.804780	-2.595873
1	-1.392609	-2.320812	-4.139106
1	-3.472769	-3.473207	-3.444224
6	1.099897	-3.329779	-4.030693
6	2.179350	-2.846820	-4.316823
14	3.905172	-2.276703	-4.677646
6	4.796024	-2.130876	-3.028851
1	5.853718	-1.889291	-3.192557
1	4.368236	-1.341653	-2.399632
1	4.753171	-3.076112	-2.473968
6	4.705238	-3.600870	-5.740603
1	4.175651	-3.727111	-6.691887
1	5.745772	-3.336928	-5.967200
1	4.711816	-4.568266	-5.224861
6	3.831412	-0.629836	-5.572084
1	3.313278	0.130916	-4.976775
1	4.844543	-0.261951	-5.776289
1	3.309671	-0.723206	-6.531606
8	2.141611	-5.642235	-2.290806
6	1.228455	-5.998895	-3.039380
8	1.343966	-7.046484	-3.810877
6	2.566385	-7.807893	-3.713857
1	2.426290	-8.653073	-4.384615
1	3.410814	-7.195728	-4.035095
1	2.713057	-8.146530	-2.686476

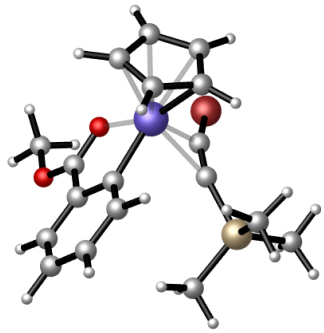
3ab



E = -944.731447 Hartrees
G = -944.521070 Hartrees

6	1.166194	-0.609356	-0.332398
6	2.550197	-0.517564	-0.270328
6	3.188182	0.728417	-0.162091
6	2.399130	1.898831	-0.118418
6	1.007032	1.787024	-0.186178
6	0.390441	0.546572	-0.291058
1	0.694893	-1.583741	-0.415677
1	3.159513	-1.414945	-0.306910
1	0.404526	2.686934	-0.152564
1	-0.692005	0.483257	-0.340382
6	4.621261	0.719244	-0.121613
6	5.830505	0.580665	-0.109802
14	7.672042	0.451426	-0.092168
6	8.342390	1.488303	-1.508135
1	8.036757	2.536726	-1.412422
1	9.439235	1.457590	-1.520833
1	7.984992	1.119380	-2.476806
6	8.294262	1.096297	1.558993
1	7.852940	0.543907	2.396800
1	9.384260	0.987871	1.623692
1	8.053953	2.157660	1.690845
6	8.139103	-1.355148	-0.312859
1	7.760314	-1.754514	-1.261180
1	9.230106	-1.472862	-0.312789
1	7.735901	-1.973240	0.497997
6	3.029739	3.246317	0.013731
8	4.204121	3.449846	0.232766
8	2.135813	4.231764	-0.134224
6	2.646427	5.560144	0.001718
1	3.401657	5.761998	-0.762136
1	1.788790	6.218602	-0.134340
1	3.082516	5.706676	0.993226

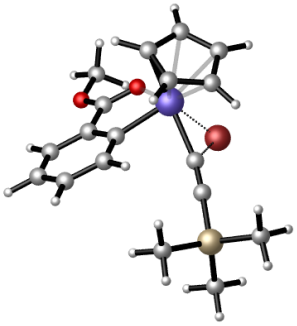
Int9a



E = -1260.745639 Hartrees
G = -1260.454738 Hartrees

45	0.518141	1.216712	0.114761
6	0.080638	3.123635	-0.456080
6	0.431569	4.316008	0.174919
6	-0.613235	3.202382	-1.674937
6	0.086476	5.539821	-0.399049
1	0.970200	4.312121	1.116030
6	-0.979382	4.426458	-2.244615
6	-0.626458	5.601540	-1.598729
1	0.372731	6.459540	0.103361
1	-1.520650	4.447653	-3.185371
1	-0.893380	6.561674	-2.027746
6	1.812253	0.981250	1.838610
1	1.520781	1.284832	2.835373
6	2.495963	1.788648	0.883218
6	1.693759	-0.356249	1.295233
1	2.767864	2.827274	1.005961
6	2.646638	1.016008	-0.299186
1	1.239890	-1.200043	1.797032
6	2.184490	-0.329905	-0.011990
1	3.104177	1.344194	-1.222881
1	2.168337	-1.149056	-0.719396
35	-1.967092	-1.318770	0.233981
6	-1.381745	0.335674	0.734571
6	-1.440478	1.448403	1.291578
14	-2.143308	2.762518	2.432671
6	-3.442660	1.817390	3.402219
1	-3.927311	2.475920	4.133680
1	-4.220217	1.419599	2.739818
1	-2.998953	0.976440	3.947570
6	-2.933568	4.108275	1.399668
1	-3.530426	4.763646	2.046656
1	-2.196645	4.725990	0.878611
1	-3.608731	3.676674	0.651493
6	-0.777734	3.362581	3.565403
1	-0.435995	2.551494	4.219034
1	0.086629	3.753831	3.020974
1	-1.156051	4.165705	4.210065
8	-0.402888	0.871212	-1.789842
6	-0.853197	1.913134	-2.307938
8	-1.524645	1.890712	-3.426818
6	-1.733855	0.609561	-4.053605
1	-2.334398	-0.029281	-3.403386
1	-2.270346	0.827782	-4.975060
1	-0.774287	0.136836	-4.270640

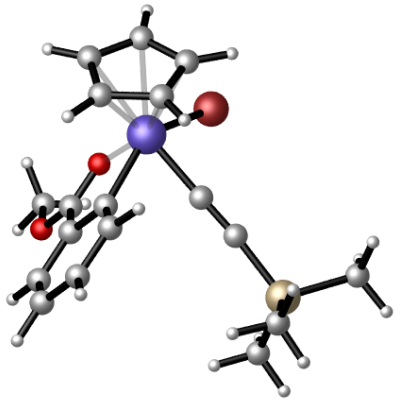
$TS_{9\text{-}10}a$



E = -1260.677441 Hartrees
G = -1260.390234 Hartrees

45	0.525555	1.037719	-0.345019
6	-0.231079	2.838329	-0.971503
6	-0.292806	4.020917	-0.247378
6	-0.668974	2.828145	-2.302753
6	-0.786235	5.172575	-0.858894
1	0.014385	4.053429	0.791650
6	-1.181689	3.979815	-2.910824
6	-1.235363	5.156966	-2.182078
1	-0.827709	6.096126	-0.288584
1	-1.524801	3.940343	-3.939933
1	-1.626358	6.061451	-2.635737
6	1.877732	0.792969	1.376612
1	1.499303	0.744307	2.388825
6	2.204354	1.990729	0.669047
6	2.213334	-0.341575	0.549515
1	2.108421	2.998536	1.046877
6	2.588091	1.605591	-0.645338
1	2.081712	-1.380516	0.818892
6	2.625772	0.151297	-0.688232
1	2.880811	2.269765	-1.447798
1	2.868059	-0.437569	-1.563851
35	-1.397259	-0.581995	0.158504
6	-0.921254	1.357057	1.120405
6	-1.412944	1.968782	2.061390
14	-2.150923	2.965290	3.426155
6	-4.015088	2.746308	3.371891
1	-4.494503	3.339016	4.161055
1	-4.425632	3.074176	2.409595
1	-4.297470	1.697648	3.520310
6	-1.698338	4.771223	3.163078
1	-2.143083	5.389008	3.953745
1	-0.613439	4.927972	3.190540
1	-2.072859	5.142119	2.201768
6	-1.444382	2.338139	5.050024
1	-1.655008	1.272090	5.194490
1	-0.357752	2.478339	5.095064
1	-1.885351	2.883452	5.893747
8	-0.006419	0.588633	-2.360168
6	-0.524635	1.547659	-2.973323
8	-0.934701	1.434574	-4.201831
6	-0.779207	0.150727	-4.846299
1	-1.322973	-0.613695	-4.288786
1	-1.206825	0.280340	-5.838308
1	0.280327	-0.102673	-4.912815

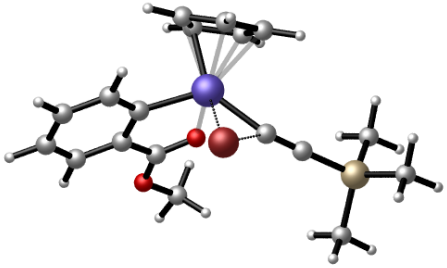
Int10a



E = -1260.696418 Hartrees
G = -1260.407151 Hartrees

45	0.953735	1.062989	-0.162649
6	0.208819	2.917377	-0.836447
6	0.499015	4.184096	-0.351818
6	-0.671798	2.764406	-1.910864
6	-0.090554	5.289162	-0.962339
1	1.154328	4.335567	0.497097
6	-1.269120	3.878243	-2.511554
6	-0.973432	5.144165	-2.034817
1	0.138448	6.279846	-0.581662
1	-1.960299	3.735600	-3.336037
1	-1.428630	6.017796	-2.488264
6	2.728339	0.621059	1.023005
1	2.649227	0.173233	2.003955
6	2.689418	2.006556	0.737616
6	2.933044	-0.087156	-0.232145
1	2.571357	2.797110	1.465665
6	2.844044	2.156496	-0.688210
1	3.001257	-1.160103	-0.344203
6	3.020495	0.860620	-1.262331
1	2.876971	3.092256	-1.227890
1	3.126051	0.649133	-2.318081
35	0.138895	-1.185185	0.766693
6	-0.384850	1.745123	1.122467
6	-1.176175	2.182249	1.942750
14	-2.399999	2.953504	3.084548
6	-4.065377	2.971354	2.213603
1	-4.829188	3.438962	2.847410
1	-4.016262	3.534536	1.274116
1	-4.401057	1.954286	1.979125
6	-1.819267	4.708789	3.430836
1	-2.541664	5.241754	4.061491
1	-0.853620	4.715336	3.950187
1	-1.705505	5.274980	2.498424
6	-2.488138	1.951923	4.670492
1	-2.785110	0.916189	4.467440
1	-1.519332	1.928508	5.183369
1	-3.222769	2.382537	5.362342
8	-0.325338	0.462909	-1.726249
6	-0.922066	1.392540	-2.311726
8	-1.764176	1.167410	-3.272839
6	-2.014452	-0.209271	-3.640005
1	-2.394538	-0.756948	-2.776385
1	-2.764776	-0.158339	-4.426105
1	-1.095157	-0.664859	-4.011084

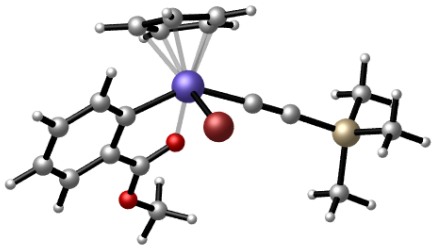
$TS_{4\text{-}12}a$



E = -1260.675950 Hartrees
G = -1260.387830 Hartrees

45	0.576612	0.861971	-1.125680
6	0.826720	2.813687	-0.556042
6	2.019794	3.405375	-0.166547
6	-0.352481	3.567098	-0.565240
6	2.021000	4.753779	0.193492
1	2.944184	2.837724	-0.132174
6	-0.350948	4.915735	-0.196076
6	0.846256	5.508645	0.176932
1	2.955214	5.219674	0.492740
1	-1.278584	5.479240	-0.199299
1	0.868930	6.555084	0.462059
6	-0.388820	-0.584761	-0.015265
6	-1.229429	-1.467632	0.095283
14	-2.537481	-2.766336	0.147381
6	-2.998012	-3.202706	-1.621881
1	-3.776002	-3.976261	-1.636262
1	-2.133509	-3.587500	-2.175788
1	-3.383897	-2.328154	-2.158884
6	-4.017576	-2.055568	1.058932
1	-4.396056	-1.154980	0.561428
1	-3.762830	-1.790875	2.091791
1	-4.832670	-2.789103	1.091624
6	-1.848638	-4.270384	1.036418
1	-0.953623	-4.656343	0.534702
1	-2.594681	-5.074484	1.055975
1	-1.581240	-4.035282	2.073193
35	1.059648	0.411894	1.360054
6	2.446995	-0.058088	-1.865395
1	3.264639	-0.326299	-1.208717
6	2.279762	1.196469	-2.517606
6	1.399445	-0.950423	-2.313856
1	2.926908	2.056677	-2.423653
6	1.046698	1.140366	-3.224133
1	1.268571	-1.974435	-1.993444
6	0.535248	-0.217234	-3.130899
1	0.602610	1.944115	-3.797196
1	-0.396138	-0.566040	-3.556733
8	-1.436430	1.606097	-1.235698
6	-1.539596	2.816246	-0.946127
8	-2.684364	3.433809	-0.965299
6	-3.856808	2.661205	-1.305074
1	-4.680629	3.370768	-1.266096
1	-3.751222	2.246037	-2.308707
1	-3.996877	1.863269	-0.573864

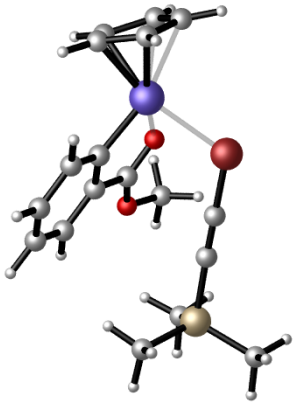
Int12a



E = -1260.690983 Hartrees
G = -1260.402271 Hartrees

45	0.476825	0.838448	-1.116341
6	0.927616	2.815331	-0.514104
6	2.166052	3.341768	-0.178910
6	-0.210690	3.623304	-0.454933
6	2.250926	4.681394	0.197588
1	3.067677	2.740899	-0.196398
6	-0.121522	4.965782	-0.067513
6	1.117094	5.495203	0.252361
1	3.222615	5.092985	0.453247
1	-1.021864	5.569873	-0.018715
1	1.206209	6.534175	0.550665
6	-0.697180	-0.720441	-0.658023
6	-1.478818	-1.632983	-0.447813
14	-2.690567	-2.969367	-0.057980
6	-3.071409	-3.910107	-1.640634
1	-3.791801	-4.714114	-1.444395
1	-2.168583	-4.367470	-2.062598
1	-3.505129	-3.251327	-2.402371
6	-4.245237	-2.158294	0.616752
1	-4.675881	-1.457708	-0.108760
1	-4.036554	-1.602730	1.538608
1	-5.006165	-2.914843	0.845677
6	-1.922817	-4.113098	1.219127
1	-1.015893	-4.591829	0.831138
1	-2.627578	-4.906604	1.497113
1	-1.652295	-3.568926	2.131555
35	1.026809	0.525459	1.335060
6	2.491992	0.539736	-1.889102
1	3.366211	0.672720	-1.266453
6	1.890582	1.530777	-2.734931
6	1.748396	-0.670636	-2.028667
1	2.235109	2.544386	-2.881218
6	0.765869	0.933710	-3.374291
1	1.952674	-1.605515	-1.524685
6	0.678880	-0.422283	-2.959396
1	0.072450	1.438321	-4.034647
1	-0.071495	-1.134894	-3.270515
8	-1.445652	1.744324	-1.086761
6	-1.457867	2.954910	-0.774845
8	-2.562149	3.635661	-0.726390
6	-3.794691	2.941694	-1.028123
1	-4.574601	3.690441	-0.906343
1	-3.768971	2.573992	-2.055162
1	-3.934682	2.116750	-0.327906

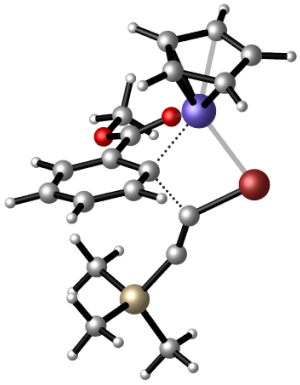
Int13a



E = -1260.725162 Hartrees
G = -1260.439357 Hartrees

6	-0.099662	-3.560439	2.794017
1	0.487767	-2.728796	3.161849
6	-1.110024	-3.485491	1.741570
1	-1.340250	-2.605101	1.155315
6	-1.650165	-4.751334	1.573928
1	-2.367732	-5.051677	0.822261
6	-0.119216	-4.868172	3.337929
1	0.484041	-5.234397	4.157053
6	-0.985353	-5.652442	2.508467
1	-1.204147	-6.704902	2.633485
45	0.612318	-4.961751	1.314742
6	2.267401	-6.005930	1.806754
6	2.562802	-7.060408	0.926495
6	3.120382	-5.783943	2.885310
6	3.671992	-7.890486	1.109555
6	4.232593	-6.606617	3.070778
1	2.929900	-4.973096	3.582328
6	4.506594	-7.660224	2.195021
1	3.876842	-8.693989	0.408416
1	4.895025	-6.424690	3.912443
1	5.373359	-8.292198	2.359147
6	3.257969	-4.396265	-1.080292
6	4.037317	-5.143209	-1.636805
14	5.320243	-6.205067	-2.478924
35	2.117675	-3.279506	-0.234502
6	6.561096	-6.704870	-1.167202
1	6.077046	-7.243072	-0.344597
1	7.325890	-7.362289	-1.598762
1	7.067821	-5.829656	-0.744737
6	4.463765	-7.695644	-3.224372
1	4.045208	-8.349450	-2.452510
1	3.657857	-7.399493	-3.905216
1	5.188792	-8.281403	-3.803434
6	6.104914	-5.137625	-3.805355
1	5.366594	-4.807680	-4.545039
1	6.576944	-4.246777	-3.375663
1	6.880329	-5.705275	-4.334684
8	0.707152	-6.336761	-0.316867
6	1.658216	-7.139888	-0.216734
8	1.886458	-8.049375	-1.122728
6	1.051925	-8.041220	-2.297936
1	1.434891	-8.843030	-2.925925
1	0.013514	-8.232519	-2.020939
1	1.139524	-7.078239	-2.804178

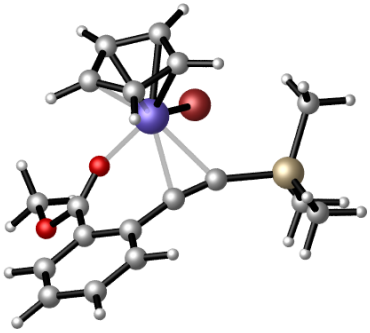
$TS_{13\text{-}14}$a



E = -1260.657483 Hartrees
G = -1260.369805 Hartrees

6	0.257636	-3.696145	2.755015
1	0.881947	-2.873212	3.076950
6	-0.938666	-3.586329	1.942370
1	-1.311552	-2.675752	1.491921
6	-1.460567	-4.871168	1.758160
1	-2.307602	-5.136054	1.139302
6	0.398112	-5.060990	3.144301
1	1.188488	-5.470080	3.759053
6	-0.603081	-5.807001	2.459784
1	-0.743185	-6.878877	2.507855
45	0.643579	-4.853988	0.999785
6	2.597243	-5.667392	0.881123
6	2.391242	-7.022290	0.465824
6	3.524021	-5.444459	1.933556
6	3.190394	-8.054683	0.919867
6	4.305567	-6.484634	2.408632
1	3.660885	-4.437716	2.317598
6	4.167045	-7.774540	1.881659
1	3.048975	-9.067854	0.557195
1	5.039936	-6.300140	3.186389
1	4.801987	-8.575381	2.246559
6	3.141597	-4.699198	-0.552689
6	4.074851	-4.980450	-1.332313
14	5.431662	-5.988423	-2.056996
35	1.821957	-3.224272	-0.583650
6	6.764656	-6.250496	-0.754775
1	6.384889	-6.840583	0.086953
1	7.621099	-6.783989	-1.186395
1	7.132448	-5.296269	-0.359032
6	4.681106	-7.628642	-2.595431
1	4.273355	-8.180728	-1.741947
1	3.872499	-7.480375	-3.320847
1	5.443988	-8.258664	-3.070395
6	6.165340	-5.101485	-3.543931
1	5.410410	-4.927147	-4.319803
1	6.587895	-4.130036	-3.261124
1	6.970948	-5.700034	-3.987792
8	0.475747	-6.263817	-0.664294
6	1.325441	-7.165155	-0.529847
8	1.330631	-8.242690	-1.263529
6	0.295995	-8.373776	-2.260471
1	0.457542	-9.350630	-2.711938
1	-0.686663	-8.323793	-1.788400
1	0.400211	-7.583857	-3.006789

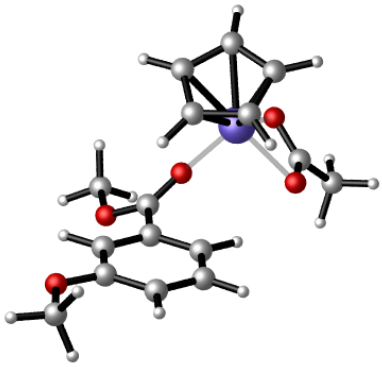
Int14a



E = -1260.804724 Hartrees
G = -1260.513573 Hartrees

6	2.026229	-3.230320	0.355573
1	2.945512	-2.715964	0.112469
6	0.809806	-3.168848	-0.387049
1	0.665306	-2.639556	-1.318834
6	-0.138363	-4.027186	0.245486
1	-1.146791	-4.223816	-0.092537
6	1.797926	-4.058702	1.512189
1	2.530302	-4.310259	2.267438
6	0.473031	-4.544502	1.442449
1	0.020316	-5.247862	2.129552
45	1.567087	-5.197823	-0.341320
6	3.212728	-7.382812	1.335093
6	2.099103	-8.242365	1.408081
6	4.185909	-7.428587	2.337766
6	1.984413	-9.136148	2.472514
6	4.052391	-8.315997	3.400912
1	5.045751	-6.770178	2.271996
6	2.954470	-9.168821	3.469106
1	1.130241	-9.801714	2.524021
1	4.812748	-8.341184	4.174734
1	2.852061	-9.863849	4.295744
6	3.418558	-6.486989	0.229838
6	3.843597	-5.781495	-0.690885
14	5.033390	-5.042260	-1.946316
35	1.321558	-5.377064	-2.858096
6	6.678544	-5.068509	-1.040400
1	6.965367	-6.090780	-0.767360
1	7.468481	-4.658939	-1.682373
1	6.646038	-4.467791	-0.123880
6	5.066876	-6.173172	-3.436393
1	5.313297	-7.201639	-3.148217
1	4.099466	-6.183142	-3.947841
1	5.828872	-5.830320	-4.147637
6	4.534760	-3.289012	-2.367298
1	3.510139	-3.240886	-2.749947
1	4.622288	-2.623528	-1.500997
1	5.204317	-2.901377	-3.145775
8	0.772777	-7.229845	-0.341626
6	1.046024	-8.201742	0.368010
8	0.380181	-9.323823	0.252024
6	-0.685322	-9.364606	-0.718922
1	-1.105121	-10.36516	-0.634290
1	-1.436670	-8.609324	-0.481768
1	-0.280387	-9.196902	-1.718172

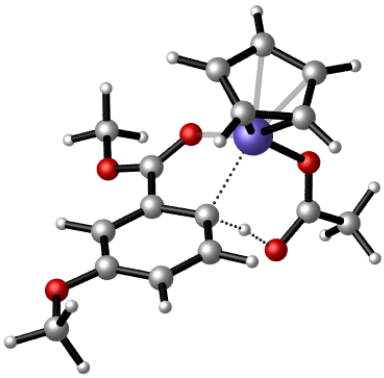
Int1d



E =-1105.739099 Hartrees
G =-1105.471243 Hartrees

8	-1.471826	-0.326713	0.476217
6	-2.204330	-0.528507	-0.545259
8	-1.692106	-1.188286	-1.502015
6	1.905164	1.804881	0.040118
6	1.184209	1.522862	1.206839
6	3.219153	2.258927	0.099644
6	1.808296	1.697918	2.433085
6	3.843471	2.413518	1.342567
6	3.132558	2.130372	2.513346
1	0.152270	1.192991	1.148903
1	3.778335	2.482594	-0.802534
1	3.593318	2.249495	3.487163
45	0.201793	-1.237037	-0.516011
6	1.996487	-2.239827	-1.152733
1	2.516386	-1.993530	-2.069055
6	0.950798	-3.188859	-1.016388
1	0.508798	-3.762629	-1.820892
6	0.482189	-3.149929	0.338480
1	-0.324181	-3.739173	0.753677
6	2.221266	-1.641139	0.136829
1	2.936539	-0.860450	0.358257
6	1.306887	-2.213302	1.053028
1	1.183516	-1.924026	2.088604
6	-3.601278	-0.007054	-0.605171
1	-4.055398	-0.223188	-1.573136
1	-4.191191	-0.471852	0.191335
1	-3.593424	1.072630	-0.428246
8	0.440991	0.691927	-1.518230
6	1.264680	1.583068	-1.275358
8	1.637494	2.429064	-2.202803
6	1.092062	2.251885	-3.525124
1	1.568026	3.019811	-4.132157
1	1.334532	1.256619	-3.902764
1	0.010488	2.396278	-3.502357
1	1.262192	1.497655	3.349726
8	5.124471	2.835766	1.304499
6	5.799148	3.041387	2.536215
1	6.800123	3.385787	2.273741
1	5.299341	3.806716	3.141089
1	5.876627	2.109744	3.108990

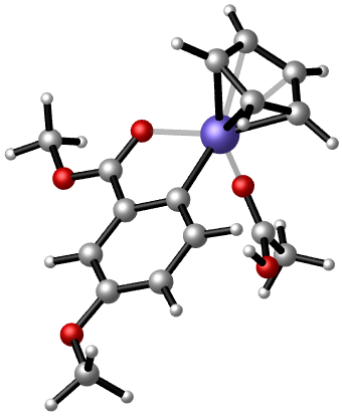
$TS_{1\text{-}2}$d



E =-1105.705687 Hartrees
G =-1105.443791 Hartrees

8	-1.438346	1.189031	0.636929
6	-2.021106	0.223703	0.071145
8	-1.421146	-0.802159	-0.371288
6	1.802369	1.635037	-0.242431
6	1.153880	0.824676	0.724754
6	2.828688	2.500164	0.071827
6	1.621262	0.925921	2.042786
6	3.267936	2.574445	1.407212
6	2.660346	1.781826	2.391584
1	-0.140563	0.896743	0.678822
1	3.315075	3.112276	-0.680365
1	2.982153	1.836613	3.425168
45	0.659520	-1.055917	-0.286394
6	2.466909	-2.169476	-0.721172
1	3.288677	-1.754541	-1.289704
6	1.341542	-2.897554	-1.264896
1	1.169163	-3.108896	-2.311781
6	0.489818	-3.238873	-0.195084
1	-0.470130	-3.730717	-0.281304
6	2.302378	-2.087026	0.681428
1	2.967515	-1.583849	1.370026
6	1.041784	-2.691192	1.015094
1	0.618277	-2.782663	2.006010
6	-3.515016	0.288448	-0.091031
1	-3.897749	-0.609269	-0.577443
1	-3.979397	0.406183	0.892865
1	-3.772268	1.170433	-0.685801
8	0.695059	0.408404	-1.928641
6	1.321868	1.434757	-1.624551
8	1.584593	2.380402	-2.483063
6	1.154276	2.179057	-3.845481
1	1.455659	3.081307	-4.373948
1	1.650864	1.301884	-4.264431
1	0.070635	2.054775	-3.879724
1	1.141405	0.341630	2.822995
8	4.270168	3.431027	1.632401
6	4.777155	3.564249	2.956141
1	5.570229	4.309430	2.894140
1	3.999606	3.916955	3.641958
1	5.192632	2.616963	3.316582

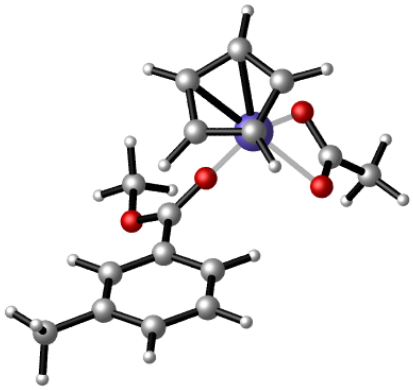
Int2d



E =-1105.733910 Hartrees
G =-1105.466640 Hartrees

8	-1.045926	0.757434	1.654815
6	-1.623712	0.442262	0.516242
8	-1.040250	-0.137032	-0.402638
6	2.041645	1.503703	-0.432097
6	1.809816	0.410120	0.424855
6	2.610845	2.692110	0.008363
6	2.194606	0.552124	1.756058
6	2.975208	2.816557	1.352769
6	2.765365	1.742194	2.222788
1	-0.092734	0.531307	1.612414
1	2.781491	3.521710	-0.670305
1	3.043817	1.813135	3.268261
45	0.903672	-1.160152	-0.475447
6	2.297449	-2.723641	-0.848887
1	3.236718	-2.559798	-1.360741
6	1.074229	-3.227723	-1.458496
1	0.929666	-3.407895	-2.515444
6	0.108542	-3.319843	-0.465787
1	-0.932518	-3.579484	-0.606628
6	2.082451	-2.625079	0.556817
1	2.812560	-2.316946	1.292386
6	0.699046	-2.871803	0.788092
1	0.200228	-2.855500	1.748088
6	-3.058069	0.841341	0.430438
1	-3.469322	0.561052	-0.538648
1	-3.615674	0.345164	1.231422
1	-3.148273	1.920884	0.582900
8	1.183224	0.162204	-2.163798
6	1.643266	1.266331	-1.823602
8	1.796435	2.247818	-2.671703
6	1.403725	2.012303	-4.038007
1	1.628380	2.939540	-4.561839
1	1.979379	1.184380	-4.455734
1	0.335216	1.793721	-4.086246
1	2.051034	-0.260935	2.463553
8	3.520988	3.999648	1.707786
6	3.936286	4.169062	3.053487
1	4.352823	5.175311	3.113205
1	3.091650	4.087233	3.748009
1	4.709635	3.441391	3.326234

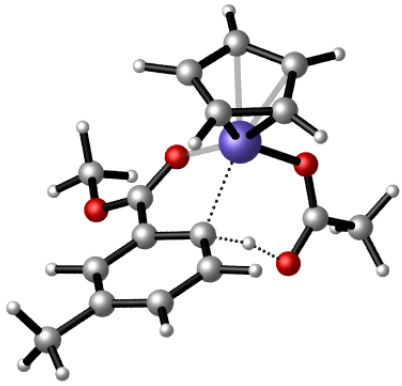
Int1e



E =-1030.558347 Hartrees
G =-1030.294924 Hartrees

8	-1.520555	-0.356275	0.640505
6	-2.263011	-0.586591	-0.366988
8	-1.763634	-1.278872	-1.308223
6	1.818582	1.883140	-0.014225
6	1.202195	1.603283	1.207641
6	3.097754	2.447918	-0.055381
6	1.882136	1.885524	2.387080
6	3.789761	2.718663	1.123964
6	3.162940	2.429198	2.342581
1	0.198780	1.189424	1.232742
1	3.561854	2.661995	-1.013483
1	3.688411	2.639673	3.270885
45	0.148103	-1.274099	-0.354838
6	2.185138	-1.617618	0.272519
1	2.888752	-0.816400	0.454488
6	1.952110	-2.265977	-0.991252
1	2.451666	-2.041450	-1.924279
6	0.925448	-3.227487	-0.805423
1	0.481532	-3.836960	-1.582141
6	1.297254	-2.176321	1.222957
1	1.186171	-1.854356	2.250369
6	0.480518	-3.153472	0.555622
1	-0.307253	-3.742922	1.004790
6	-3.642178	-0.024719	-0.459595
1	-4.270625	-0.655505	-1.091510
1	-4.080224	0.077407	0.535446
1	-3.578509	0.970749	-0.913722
8	0.302207	0.631856	-1.407583
6	1.109788	1.558890	-1.268449
8	1.392657	2.355738	-2.270572
6	0.770721	2.070171	-3.538785
1	1.183344	2.803103	-4.229781
1	1.016597	1.055950	-3.859581
1	-0.311187	2.187711	-3.456333
1	1.409392	1.685751	3.343649
6	5.169741	3.322329	1.097794
1	5.870613	2.727024	1.693011
1	5.557703	3.390238	0.077327
1	5.158739	4.332631	1.522839

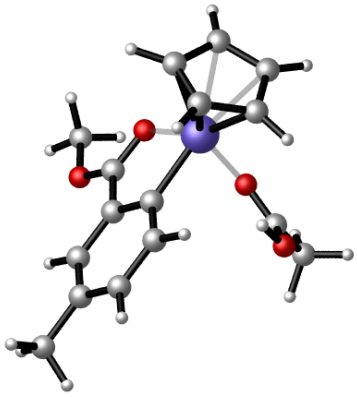
$TS_{1\text{-}2}e$



E =-1030.522412 Hartrees
G =-1030.264837 Hartrees

8	-1.407145	1.132639	0.696569
6	-1.997423	0.196737	0.093178
8	-1.401580	-0.814438	-0.391632
6	1.807944	1.664220	-0.264058
6	1.198881	0.852265	0.719215
6	2.832469	2.549541	0.036198
6	1.683469	0.959860	2.027237
6	3.309583	2.639627	1.351036
6	2.722835	1.835112	2.333514
1	-0.102444	0.839987	0.690930
1	3.277006	3.160962	-0.744065
1	3.081433	1.906045	3.356958
45	0.675297	-1.044592	-0.294440
6	2.465503	-2.167379	-0.789664
1	3.249606	-1.766974	-1.418836
6	1.305257	-2.898959	-1.246858
1	1.075045	-3.145575	-2.274644
6	0.517281	-3.208563	-0.115009
1	-0.448017	-3.697210	-0.129876
6	2.378559	-2.034774	0.614082
1	3.080178	-1.508627	1.247083
6	1.139776	-2.630510	1.041388
1	0.773306	-2.686670	2.057246
6	-3.484711	0.285192	-0.105539
1	-3.920191	-0.707223	-0.233220
1	-3.950657	0.803568	0.734710
1	-3.672491	0.867487	-1.014937
8	0.683477	0.419379	-1.928301
6	1.302003	1.454985	-1.632734
8	1.532869	2.403687	-2.498151
6	1.070508	2.197874	-3.848945
1	1.348421	3.103468	-4.384651
1	1.565194	1.326131	-4.281348
1	-0.012346	2.062251	-3.855317
1	1.224232	0.374254	2.818630
6	4.441820	3.571906	1.681509
1	5.391611	3.163992	1.314973
1	4.300030	4.546872	1.204075
1	4.534042	3.722793	2.760564

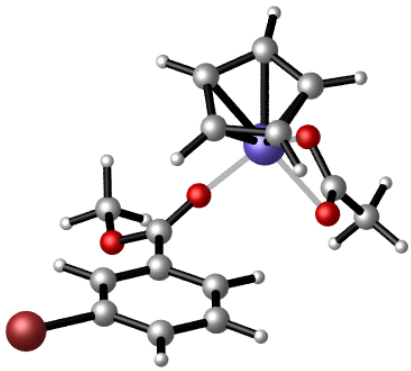
Int2e



E =-1030.554765 Hartrees
G =-1030.289636 Hartrees

8	-1.198478	0.070217	1.839746
6	-1.592487	0.317242	0.608224
8	-0.953382	-0.028690	-0.387699
6	2.029089	1.557058	-0.513141
6	1.805624	0.493779	0.375249
6	2.556239	2.781747	-0.092252
6	2.145255	0.689300	1.713797
6	2.883384	2.973916	1.246434
6	2.670938	1.909870	2.134802
1	-0.328751	-0.376251	1.821931
1	2.706860	3.581268	-0.812570
1	2.922334	2.043968	3.184607
45	0.933516	-1.118644	-0.479712
6	2.342199	-2.673204	-0.842468
1	3.276715	-2.504792	-1.361451
6	1.119842	-3.193831	-1.440310
1	0.970618	-3.382265	-2.495151
6	0.161355	-3.288581	-0.441272
1	-0.877202	-3.562846	-0.572363
6	2.135211	-2.565702	0.563490
1	2.865551	-2.242459	1.292522
6	0.757286	-2.831078	0.806529
1	0.268651	-2.829080	1.772443
6	-2.883981	1.055331	0.517917
1	-3.152615	1.211123	-0.526203
1	-3.667006	0.486798	1.028877
1	-2.783335	2.018365	1.027994
8	1.202033	0.145156	-2.198484
6	1.652959	1.265492	-1.894992
8	1.808685	2.211910	-2.783027
6	1.427519	1.917748	-4.140832
1	1.663002	2.819304	-4.703660
1	2.001652	1.068972	-4.516953
1	0.358160	1.703457	-4.190280
1	2.001255	-0.103579	2.443990
6	3.461239	4.276175	1.737022
1	4.513063	4.154299	2.021283
1	3.410473	5.049753	0.965092
1	2.924361	4.638097	2.620543

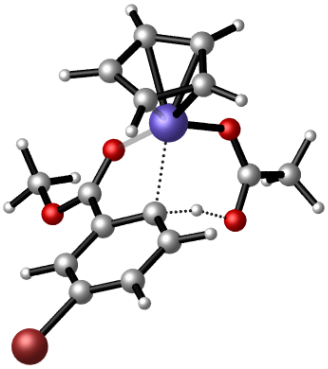
Int1f



E =-1003.827036 Hartrees
G =-1003.603556 Hartrees

8	-1.449499	-0.370409	0.466152
6	-2.175438	-0.560035	-0.561830
8	-1.665340	-1.232164	-1.512164
6	1.864988	1.821085	0.054719
6	1.178995	1.488803	1.225184
6	3.159927	2.343356	0.105990
6	1.798470	1.670954	2.455355
6	3.764280	2.497981	1.347500
6	3.098362	2.166880	2.525331
1	0.163745	1.108846	1.172051
1	3.682524	2.603471	-0.807698
1	3.581090	2.297082	3.487813
45	0.224706	-1.280364	-0.527581
6	2.017393	-2.279395	-1.176294
1	2.530385	-2.034391	-2.096829
6	0.975274	-3.231152	-1.030087
1	0.528099	-3.807153	-1.830129
6	0.516599	-3.190256	0.327735
1	-0.285835	-3.779850	0.750072
6	2.251025	-1.678634	0.110966
1	2.966939	-0.896788	0.325620
6	1.344569	-2.250111	1.034795
1	1.229111	-1.961194	2.071413
6	-3.543738	0.024073	-0.668197
1	-4.175573	-0.598323	-1.305194
1	-3.989952	0.135570	0.322021
1	-3.459429	1.016480	-1.125847
8	0.437978	0.665721	-1.507699
6	1.217883	1.591573	-1.258280
8	1.538126	2.475203	-2.168641
6	0.988731	2.300258	-3.491000
1	1.412576	3.110373	-4.081196
1	1.286291	1.330765	-3.895072
1	-0.098932	2.379152	-3.453138
1	1.269101	1.428402	3.370874
35	5.547789	3.180549	1.438217

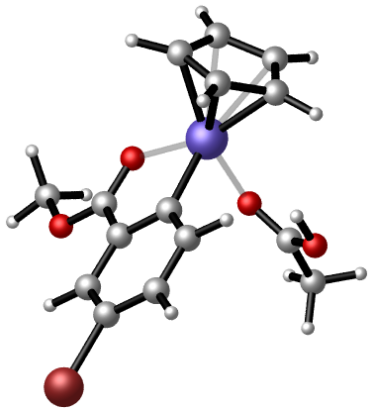
$TS_{1\text{-}2}$f



E =-1003.789525 Hartrees
G =-1003.570464 Hartrees

8	-1.406629	1.114222	0.694850
6	-1.997969	0.185967	0.080979
8	-1.401951	-0.822331	-0.411856
6	1.813474	1.667480	-0.265625
6	1.200495	0.876974	0.727121
6	2.853196	2.546055	0.014292
6	1.682643	0.989800	2.035443
6	3.307869	2.615289	1.329064
6	2.736279	1.846933	2.342059
1	-0.102026	0.823867	0.686825
1	3.305019	3.142117	-0.770741
1	3.102036	1.920007	3.360540
45	0.670964	-1.048725	-0.287728
6	2.460567	-2.176091	-0.778314
1	3.245694	-1.779446	-1.408600
6	1.291390	-2.893687	-1.234599
1	1.056384	-3.136322	-2.262338
6	0.503900	-3.203307	-0.099595
1	-0.465088	-3.684609	-0.113900
6	2.374497	-2.042360	0.624318
1	3.080210	-1.521016	1.256831
6	1.132997	-2.632766	1.054485
1	0.766707	-2.683159	2.070744
6	-3.483798	0.278683	-0.121785
1	-3.921269	-0.712581	-0.251402
1	-3.950518	0.797908	0.717394
1	-3.666802	0.861710	-1.031667
8	0.689817	0.416132	-1.925532
6	1.306936	1.452568	-1.636165
8	1.540208	2.399835	-2.499676
6	1.078493	2.196737	-3.852511
1	1.357513	3.103458	-4.385364
1	1.573894	1.325456	-4.284649
1	-0.004330	2.061799	-3.858182
1	1.217596	0.417998	2.832743
35	4.749223	3.790965	1.749473

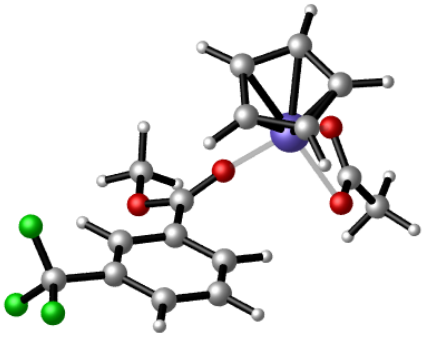
Int2f



E =-1003.824161 Hartrees
G =-1003.598562 Hartrees

8	-1.396654	-0.030746	1.751707
6	-1.723461	0.226266	0.503541
8	-1.012241	-0.082487	-0.455887
6	1.849860	1.680916	-0.506609
6	1.650179	0.632133	0.404686
6	2.305529	2.941492	-0.114286
6	1.927965	0.876182	1.749698
6	2.568489	3.146332	1.231427
6	2.384323	2.126341	2.165413
1	-0.524853	-0.473391	1.777086
1	2.446003	3.729259	-0.846624
1	2.594063	2.301385	3.215732
45	0.926468	-1.054343	-0.436739
6	2.448690	-2.521440	-0.725735
1	3.368671	-2.306003	-1.253516
6	1.272619	-3.161601	-1.297625
1	1.143525	-3.415461	-2.341307
6	0.317922	-3.271798	-0.296701
1	-0.696676	-3.629611	-0.413902
6	2.230825	-2.359784	0.671549
1	2.935632	-1.952904	1.383860
6	0.872689	-2.708312	0.927069
1	0.386937	-2.706104	1.894446
6	-3.033960	0.915447	0.342645
1	-3.224934	1.114469	-0.711168
1	-3.826059	0.282639	0.755126
1	-3.024719	1.851497	0.909201
8	1.170423	0.186598	-2.187489
6	1.535995	1.338582	-1.896926
8	1.655690	2.280853	-2.792015
6	1.340376	1.945713	-4.158847
1	1.475428	2.871587	-4.714629
1	2.025788	1.176204	-4.519435
1	0.307416	1.600477	-4.230650
1	1.791559	0.099260	2.497052
35	3.194511	4.855112	1.818784

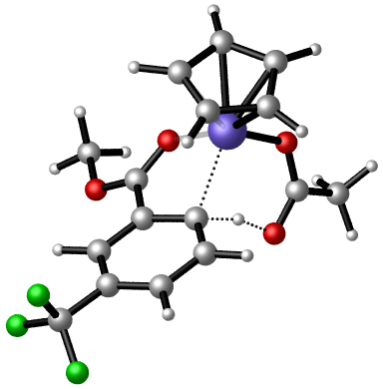
Int1g



E =-1328.199264 Hartrees
G =-1327.963256 Hartrees

8	-1.460060	-0.301877	0.650117
6	-2.219120	-0.530370	-0.346792
8	-1.740233	-1.237765	-1.286865
6	1.856457	1.902681	-0.037067
6	1.271513	1.617130	1.201409
6	3.137711	2.444623	-0.107549
6	1.979273	1.866208	2.369244
6	3.844258	2.669995	1.071432
6	3.271636	2.384447	2.307609
1	0.261765	1.220245	1.245484
1	1.524403	1.660907	3.332330
1	3.824964	2.568977	3.221655
45	0.179408	-1.255656	-0.351859
6	2.210008	-1.628255	0.283705
1	2.925365	-0.840835	0.478534
6	1.976907	-2.262890	-0.987423
1	2.483424	-2.034487	-1.915817
6	0.938675	-3.213408	-0.817252
1	0.492036	-3.809927	-1.602402
6	1.311303	-2.186371	1.224101
1	1.198033	-1.873730	2.254178
6	0.485197	-3.145152	0.542359
1	-0.312263	-3.729161	0.981486
6	-3.593518	0.045586	-0.416395
1	-4.175438	-0.438697	-1.202039
1	-4.093020	-0.063811	0.549791
1	-3.511952	1.116094	-0.635569
8	0.341334	0.645262	-1.424501
6	1.110691	1.600210	-1.279463
8	1.323450	2.453464	-2.248820
6	0.666466	2.204402	-3.508553
1	0.985201	3.015773	-4.160047
1	0.981808	1.239659	-3.910690
1	-0.415946	2.222805	-3.371919
1	3.587262	2.670660	-1.069124
6	5.237840	3.226805	0.965394
9	6.042169	2.403870	0.265441
9	5.248091	4.408839	0.323722
9	5.807934	3.417044	2.163428

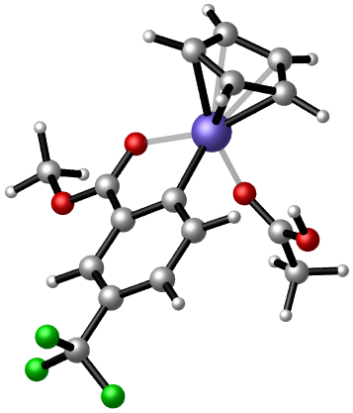
$TS_{1\text{-}2}g$



E =-1328.161041 Hartrees
G =-1327.928989 Hartrees

8	-1.426592	1.105987	0.672403
6	-2.012050	0.172827	0.060753
8	-1.407786	-0.829974	-0.434731
6	1.802492	1.685673	-0.266720
6	1.182138	0.902772	0.726102
6	2.842366	2.561772	0.022172
6	1.645840	1.022503	2.040088
6	3.289818	2.643297	1.337500
6	2.698147	1.879488	2.344738
1	-0.123172	0.822963	0.668801
1	3.303851	3.150973	-0.762450
1	3.055615	1.959923	3.366462
45	0.665507	-1.033698	-0.291078
6	2.463604	-2.148882	-0.777309
1	3.241340	-1.749439	-1.415006
6	1.297228	-2.877468	-1.222166
1	1.059497	-3.131771	-2.246433
6	0.518460	-3.185651	-0.079265
1	-0.446891	-3.674430	-0.084852
6	2.382569	-2.002847	0.624199
1	3.086194	-1.468697	1.248399
6	1.148712	-2.601857	1.066116
1	0.787397	-2.645243	2.084453
6	-3.500515	0.239891	-0.132571
1	-3.945573	-0.747892	0.006564
1	-3.946094	0.960265	0.554639
1	-3.699463	0.557490	-1.162093
8	0.691214	0.425198	-1.928559
6	1.305724	1.463723	-1.638386
8	1.542595	2.407450	-2.504938
6	1.089629	2.197529	-3.859602
1	1.369894	3.102587	-4.394665
1	1.589346	1.325513	-4.285210
1	0.007128	2.060281	-3.871562
1	1.169110	0.456037	2.833967
6	4.465032	3.518322	1.688064
9	4.724374	4.428188	0.738148
9	5.581726	2.784383	1.850565
9	4.263507	4.180487	2.838436

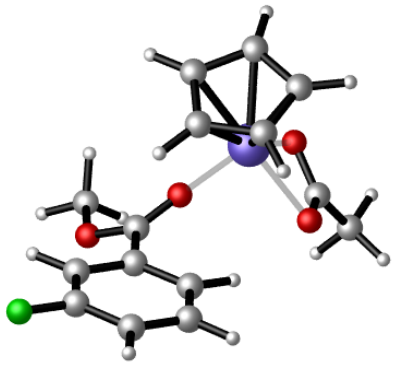
Int2g



E =-1328.197035 Hartrees
G =-1327.957888 Hartrees

8	-1.291747	0.018091	1.759677
6	-1.616830	0.316820	0.520461
8	-0.947397	-0.035801	-0.454206
6	2.036566	1.549131	-0.506996
6	1.766268	0.512921	0.402025
6	2.573237	2.772947	-0.106059
6	2.051756	0.734995	1.750506
6	2.850572	2.964991	1.239162
6	2.590679	1.949042	2.164086
1	-0.455337	-0.489795	1.765412
1	2.766421	3.552953	-0.834526
1	2.808325	2.108880	3.215950
45	0.935042	-1.121274	-0.449643
6	2.357093	-2.678648	-0.759322
1	3.297833	-2.514311	-1.268287
6	1.145280	-3.211246	-1.366127
1	1.011520	-3.419092	-2.419377
6	0.171892	-3.288981	-0.379614
1	-0.864729	-3.565601	-0.521250
6	2.129273	-2.543444	0.640338
1	2.849120	-2.205911	1.373372
6	0.747728	-2.807490	0.868687
1	0.246820	-2.799968	1.828508
6	-2.862789	1.122647	0.391451
1	-3.094019	1.287665	-0.660129
1	-3.689489	0.604761	0.886392
1	-2.718593	2.082669	0.897776
8	1.251207	0.108920	-2.187345
6	1.693958	1.233754	-1.895490
8	1.866522	2.168857	-2.789277
6	1.505541	1.862347	-4.151510
1	1.751542	2.758436	-4.718240
1	2.084092	1.008936	-4.509461
1	0.436525	1.650048	-4.213334
1	1.856684	-0.032676	2.493956
6	3.468550	4.247065	1.720683
9	3.415972	5.217420	0.794893
9	4.765559	4.081684	2.045358
9	2.854466	4.712168	2.823914

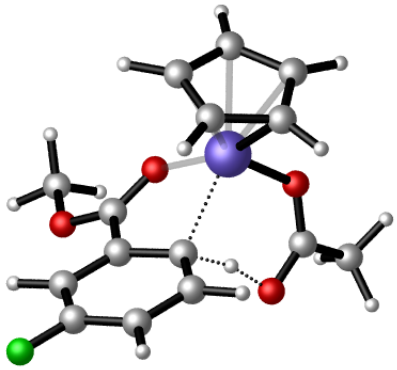
Int1h



E =-1090.456123 Hartrees
G =-1090.228175 Hartrees

8	-1.462892	-0.372652	0.464889
6	-2.188961	-0.558314	-0.563489
8	-1.676696	-1.219675	-1.520261
6	1.877774	1.810684	0.056982
6	1.186518	1.485870	1.227442
6	3.179353	2.315585	0.108322
6	1.807996	1.659517	2.459591
6	3.771692	2.457400	1.351583
6	3.113489	2.138807	2.531061
1	0.166725	1.118971	1.173242
1	3.727496	2.576901	-0.789839
1	1.273235	1.422238	3.373391
1	3.618293	2.273048	3.481766
45	0.214006	-1.269920	-0.535469
6	2.010208	-2.261242	-1.188207
1	2.523862	-2.009744	-2.106615
6	0.969765	-3.215996	-1.048802
1	0.525093	-3.788497	-1.852725
6	0.509626	-3.184223	0.308676
1	-0.291763	-3.778416	0.726513
6	2.240727	-1.667148	0.102634
1	2.954527	-0.884933	0.323232
6	1.334527	-2.246262	1.022148
1	1.217067	-1.963250	2.060150
6	-3.561429	0.017551	-0.662956
1	-4.191558	-0.606926	-1.299678
1	-4.004860	0.122947	0.329160
1	-3.485408	1.011823	-1.117903
8	0.422999	0.683664	-1.500313
6	1.227023	1.590430	-1.254843
8	1.570751	2.459608	-2.171008
6	1.016711	2.291024	-3.491760
1	1.467637	3.081032	-4.089278
1	1.281213	1.308617	-3.887592
1	-0.067705	2.407438	-3.455818
9	5.029874	2.919748	1.415384

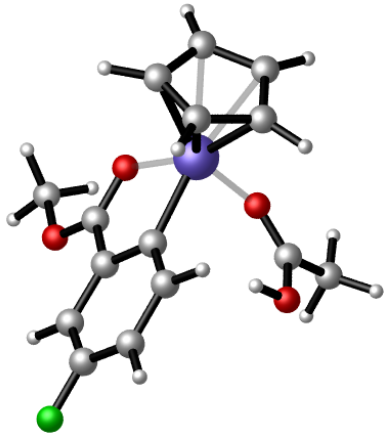
$TS_{1\text{-}2}$h



E =-1090.419871 Hartrees
G =-1090.197179 Hartrees

8	-1.404861	1.143443	0.678088
6	-1.994715	0.201151	0.084035
8	-1.398222	-0.815453	-0.388964
6	1.815405	1.662136	-0.270359
6	1.198875	0.867253	0.720374
6	2.852005	2.540640	0.012927
6	1.679615	0.976040	2.032839
6	3.288948	2.599384	1.330143
6	2.728080	1.834492	2.345226
1	-0.102440	0.852618	0.681486
1	3.324284	3.150395	-0.749254
1	1.211702	0.399215	2.824834
1	3.108165	1.928058	3.356886
45	0.676859	-1.047797	-0.285453
6	2.465596	-2.174969	-0.776202
1	3.251952	-1.777912	-1.404679
6	1.301233	-2.899341	-1.234595
1	1.069835	-3.143119	-2.262851
6	0.511042	-3.207462	-0.103092
1	-0.456473	-3.691632	-0.119306
6	2.377217	-2.042167	0.627000
1	3.080834	-1.519865	1.261065
6	1.135479	-2.633175	1.053468
1	0.767458	-2.686411	2.068944
6	-3.481480	0.287763	-0.117143
1	-3.915834	-0.705119	-0.244509
1	-3.948850	0.806517	0.722125
1	-3.668452	0.869611	-1.026978
8	0.686621	0.413637	-1.928749
6	1.306720	1.448490	-1.640407
8	1.539918	2.395514	-2.504729
6	1.071697	2.193627	-3.855226
1	1.350137	3.099750	-4.389470
1	1.563087	1.321345	-4.290005
1	-0.011447	2.060870	-3.856257
9	4.293722	3.427779	1.630398

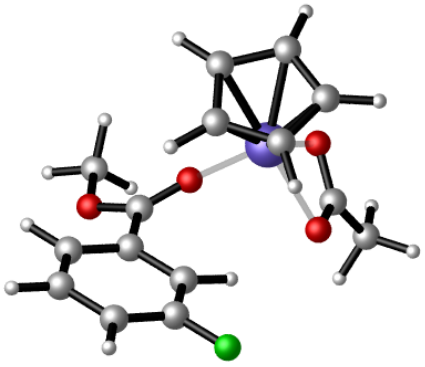
Int2h



E =-1090.451066 Hartrees
G =-1090.224180 Hartrees

8	-1.275719	0.782668	1.534809
6	-1.759867	0.353918	0.390103
8	-1.096262	-0.282717	-0.431222
6	1.847513	1.654020	-0.434828
6	1.669615	0.582209	0.457663
6	2.332019	2.898223	-0.029528
6	2.005962	0.789927	1.798579
6	2.643310	3.054846	1.308804
6	2.489094	2.026897	2.228943
1	-0.320419	0.574355	1.586683
1	2.466616	3.716938	-0.728195
1	1.892827	-0.006382	2.529398
1	2.749477	2.196159	3.268739
45	0.931467	-1.095534	-0.407741
6	2.490200	-2.519643	-0.692132
1	3.419324	-2.279079	-1.192055
6	1.340998	-3.169370	-1.305832
1	1.240194	-3.400703	-2.357942
6	0.364500	-3.321882	-0.330851
1	-0.640345	-3.694238	-0.481565
6	2.234105	-2.396467	0.704045
1	2.913311	-1.991525	1.441592
6	0.877768	-2.774880	0.917570
1	0.357379	-2.775199	1.866198
6	-3.186612	0.717511	0.155921
1	-3.566390	0.200785	-0.724807
1	-3.784939	0.465951	1.035971
1	-3.253336	1.800318	0.004861
8	1.118915	0.201674	-2.134586
6	1.487692	1.346630	-1.823094
8	1.570882	2.316543	-2.692938
6	1.204441	2.023101	-4.056217
1	1.322791	2.964585	-4.589158
1	1.871865	1.262601	-4.465713
1	0.168049	1.683436	-4.099657
9	3.114088	4.239228	1.731791

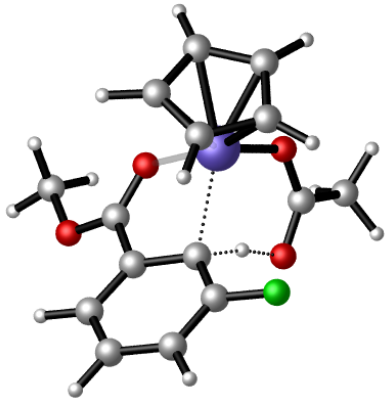
Int1i



E =-1090.456510 Hartrees
G =-1090.229672 Hartrees

8	-1.461665	-0.324017	0.459425
6	-2.196533	-0.534125	-0.559345
8	-1.687658	-1.206874	-1.508535
6	1.898092	1.815566	0.015558
6	1.201008	1.471520	1.176483
6	3.197907	2.323106	0.083487
6	1.840683	1.632723	2.391244
6	3.812946	2.463304	1.324651
6	3.137854	2.116528	2.491941
1	0.182056	1.099756	1.141170
1	3.728354	2.588058	-0.824350
1	3.600328	2.221508	3.467527
45	0.206926	-1.251283	-0.524045
6	2.001442	-2.262016	-1.147970
1	2.523496	-2.024923	-2.065493
6	0.954808	-3.208542	-1.004708
1	0.513939	-3.789774	-1.804484
6	0.482793	-3.155550	0.348780
1	-0.325792	-3.739010	0.767836
6	2.223350	-1.650812	0.136259
1	2.938734	-0.868511	0.351936
6	1.307052	-2.213019	1.056392
1	1.180674	-1.912572	2.088614
6	-3.591409	-0.008515	-0.622796
1	-4.044017	-0.224358	-1.591513
1	-4.184174	-0.471580	0.172661
1	-3.581039	1.071115	-0.445972
8	0.446387	0.677674	-1.536142
6	1.248845	1.587450	-1.295649
8	1.596666	2.448369	-2.217757
6	1.047958	2.268960	-3.539202
1	1.499025	3.055908	-4.140689
1	1.316838	1.284605	-3.927250
1	-0.036912	2.382607	-3.508232
1	4.826439	2.845369	1.386157
9	1.181660	1.298606	3.512869

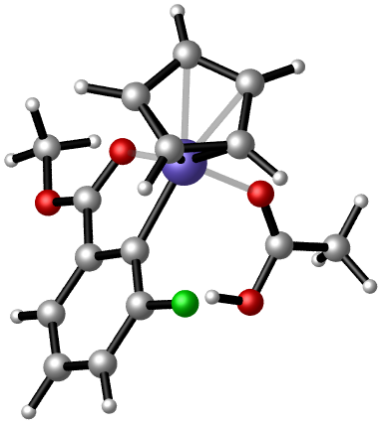
$TS_{1\text{-}2}$i



E =-1090.424301 Hartrees
G =-1090.201309 Hartrees

8	-1.421086	1.153466	0.664042
6	-1.998182	0.201892	0.076246
8	-1.393135	-0.817309	-0.385013
6	1.813311	1.679447	-0.268214
6	1.185382	0.884657	0.717804
6	2.861478	2.540113	0.022493
6	1.693718	0.994215	2.006499
6	3.325226	2.608009	1.339452
6	2.745962	1.836916	2.341451
1	-0.096087	0.867628	0.689172
1	3.326426	3.133839	-0.756821
1	3.096784	1.885125	3.366751
45	0.677748	-1.052435	-0.276532
6	2.465171	-2.179615	-0.766786
1	3.252557	-1.783218	-1.394308
6	1.294988	-2.892923	-1.227388
1	1.060981	-3.130332	-2.256617
6	0.504474	-3.205840	-0.095137
1	-0.465313	-3.685301	-0.113335
6	2.375711	-2.050104	0.636038
1	3.081935	-1.534184	1.272689
6	1.132403	-2.640756	1.061653
1	0.762608	-2.688374	2.076547
6	-3.484947	0.272338	-0.136204
1	-3.909480	-0.725463	-0.258222
1	-3.962433	0.793296	0.696050
1	-3.671618	0.845209	-1.051787
8	0.689412	0.418409	-1.921955
6	1.300094	1.459566	-1.635695
8	1.523511	2.407351	-2.502023
6	1.055480	2.198238	-3.851302
1	1.328078	3.104235	-4.388848
1	1.551171	1.327312	-4.283964
1	-0.026950	2.059470	-3.850976
1	4.149705	3.268611	1.586375
9	1.127178	0.264164	2.977523

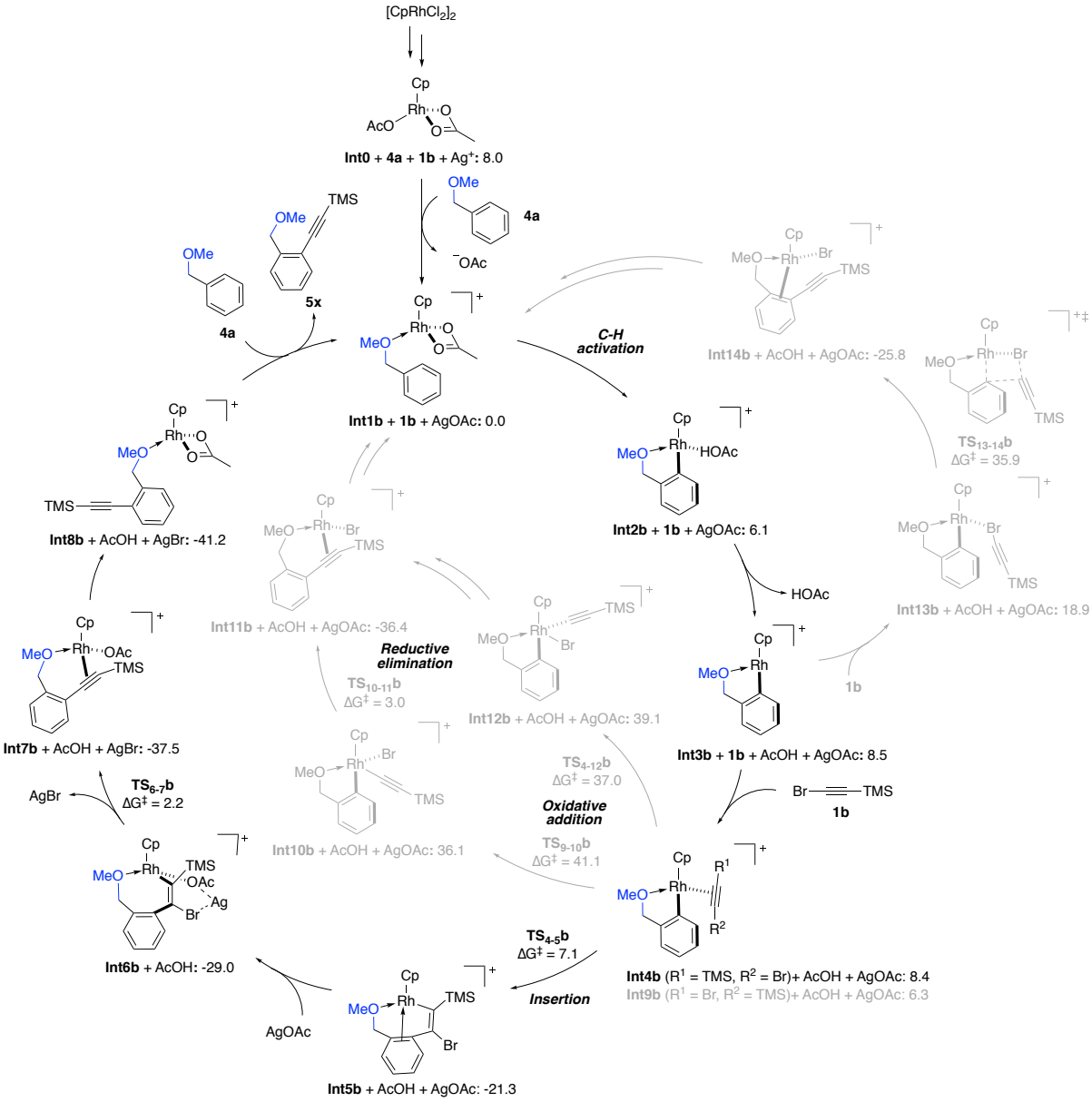
Int2i



E =-1090.454551 Hartrees
G =-1090.225422 Hartrees

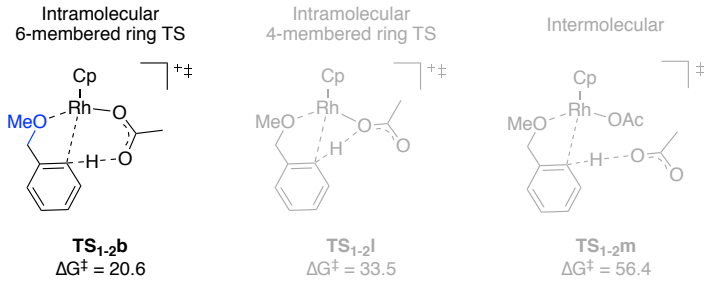
8	-1.260825	1.386645	1.036264
6	-1.820263	0.434640	0.321992
8	-1.185214	-0.460789	-0.237160
6	1.872968	1.643911	-0.384467
6	1.639109	0.569932	0.495722
6	2.394549	2.866766	0.039454
6	1.960358	0.790397	1.827265
6	2.698458	3.033765	1.386463
6	2.480481	1.994534	2.288699
1	-0.288438	1.268013	1.038569
1	2.555745	3.671085	-0.670375
1	2.706605	2.108154	3.344096
45	0.897938	-1.109688	-0.373895
6	2.488942	-2.472012	-0.746276
1	3.397912	-2.188404	-1.260497
6	1.338114	-3.123302	-1.353775
1	1.213827	-3.318020	-2.410818
6	0.392243	-3.337346	-0.357899
1	-0.608097	-3.725333	-0.498075
6	2.264680	-2.402217	0.660192
1	2.949331	-2.006563	1.396509
6	0.925666	-2.826762	0.895391
1	0.428220	-2.863499	1.854935
6	-3.305625	0.535399	0.232312
1	-3.711526	-0.342481	-0.269226
1	-3.731630	0.633221	1.234839
1	-3.567456	1.437760	-0.330371
8	1.022455	0.238561	-2.072165
6	1.487438	1.351680	-1.770959
8	1.646358	2.303596	-2.649190
6	1.261255	2.025714	-4.010610
1	1.504378	2.930864	-4.563990
1	1.828406	1.175423	-4.393415
1	0.190096	1.821275	-4.059754
1	3.103613	3.974799	1.742483
9	1.747389	-0.191665	2.728191

7.3. Mechanism of the Rh-Catalyzed *ortho*-Alkynylation of (Methoxymethyl)benzene



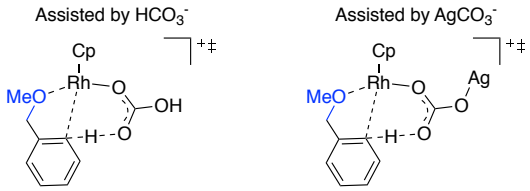
[a] Free energies in kcal/mol.

Scheme S7.3.1 - Rh-catalyzed *ortho*-alkynylation of (methoxymethyl)benzene[a]



[a] Free energies in kcal/mol.

Scheme S7.3.2 - Acetate-assisted C-H activation of (methoxymethyl)benzene

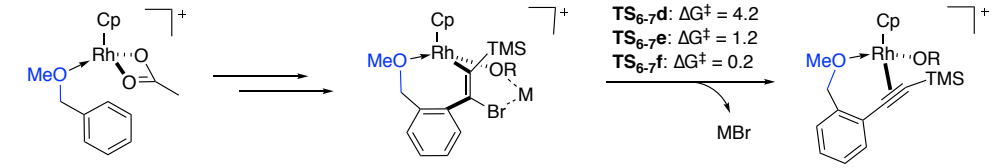


$TS_{1\text{-}2}$n
$\Delta G^{\ddagger}$ = 21.6

$TS_{1\text{-}2}$o
$\Delta G^{\ddagger}$ = 27.3

[a] Free energies in kcal/mol.

Scheme S7.3.3 - Alternative base-assisted C-H activation of (methoxymethyl)benzene



Int1b + **1b** + KOAc**:** 0.0
Int1b + **1b** + $AgHCO_3$**:** 0.0
Int1b + **1b** + Ag_2CO_3**:** 0.0

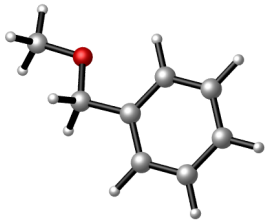
Int6d (M = K, R = Ac) + AcOH**:** -34.5
Int6e (M = Ag, R = CO_2H)+ AcOH**:** -29.1
Int6f (M =Ag, R = CO_2Ag)+ AcOH**:** -35.4

Int7d
Int7e
Int7f

[a] Free energies in kcal/mol.

Scheme S7.3.4 - Alternative base-assisted bromine elimination

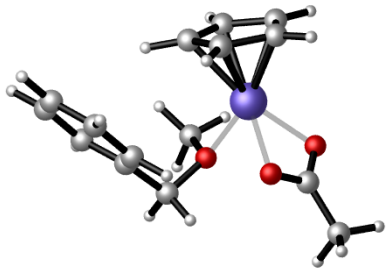
4a



E = -385.953911 Hartrees
G = -385.824823 Hartrees

6	0.839004	-0.657802	-0.213877
6	2.179860	-0.740429	-0.587346
6	3.006657	0.374261	-0.473161
6	2.504817	1.586223	0.008904
6	1.161411	1.663399	0.380316
6	0.334544	0.546196	0.272980
1	0.193252	-1.527236	-0.298530
1	2.584827	-1.675692	-0.963820
1	4.054165	0.301463	-0.757595
1	0.767347	2.600196	0.760718
1	-0.708747	0.619821	0.567648
6	3.405522	2.796072	0.070425
1	4.428596	2.490015	0.344645
1	3.473357	3.255998	-0.930985
8	2.905586	3.729077	0.995466
6	3.671984	4.907264	1.024630
1	3.667988	5.418417	0.049425
1	3.227123	5.568275	1.772850
1	4.717455	4.704289	1.304076

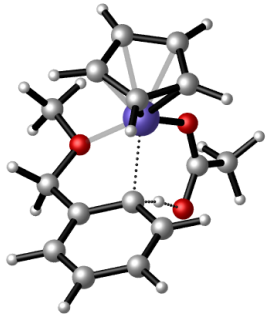
Int1b



E = -917.233578 Hartrees
G = -916.975643 Hartrees

6	1.620820	-3.910266	2.040745
1	2.484198	-3.974718	2.690721
6	1.527075	-3.126819	0.861381
1	2.290448	-2.463324	0.477751
6	0.252069	-3.393619	0.251174
1	-0.109953	-2.970210	-0.676372
6	0.432093	-4.703623	2.147726
1	0.209062	-5.419804	2.926681
6	-0.425714	-4.343847	1.051637
1	-1.383010	-4.794635	0.825780
45	1.413509	-5.221732	0.347265
8	2.879545	-6.721011	0.746703
8	0.942219	-7.265225	-0.066288
6	2.116870	-7.620986	0.274352
6	2.590094	-9.022155	0.081357
1	1.751168	-9.719457	0.128757
1	3.050021	-9.099346	-0.910675
1	3.341787	-9.276936	0.831115
8	2.322324	-5.327643	-1.663248
6	3.208010	-4.243390	-1.956362
1	3.910447	-4.178769	-1.124249
1	3.755415	-4.463650	-2.878284
1	2.663749	-3.299880	-2.064258
6	1.471203	-5.731028	-2.766080
1	2.073902	-5.674268	-3.678080
1	1.229258	-6.774987	-2.564213
6	0.226252	-4.895269	-2.859636
6	-0.949582	-5.335365	-2.245075
6	0.238778	-3.651587	-3.498306
6	-2.090858	-4.536928	-2.249125
1	-0.963964	-6.305499	-1.755082
6	-0.898776	-2.847022	-3.495650
1	1.140399	-3.314485	-4.003490
6	-2.063293	-3.287258	-2.866936
1	-3.000267	-4.889361	-1.771204
1	-0.879823	-1.881293	-3.991821
1	-2.951084	-2.661495	-2.868463

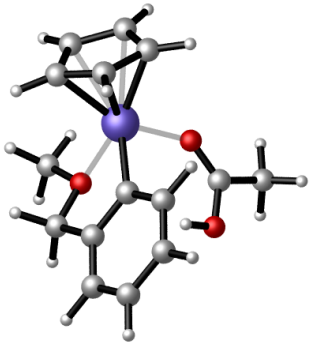
$TS_{1\text{-}2}b$



E = -917.194578 Hartrees
G = -916.942813 Hartrees

8	-1.452374	1.346628	0.475439
6	-2.044652	0.296914	0.107403
8	-1.447776	-0.782218	-0.194436
6	1.847520	1.681959	-0.356980
6	1.134014	0.976240	0.636167
6	2.911330	2.510266	-0.010040
6	1.533986	1.118461	1.979195
6	3.278884	2.639338	1.327309
6	2.593839	1.944580	2.327080
1	-0.164592	1.066221	0.526044
1	3.459124	3.047950	-0.779664
1	0.985045	0.587187	2.752318
1	4.109369	3.287030	1.592811
1	2.887638	2.055164	3.366313
45	0.639396	-0.971084	-0.224112
6	2.441540	-2.078651	-0.721550
1	3.189780	-1.698976	-1.405048
6	1.298656	-2.887968	-1.083149
1	1.042341	-3.211293	-2.083276
6	0.560761	-3.140852	0.090868
1	-0.384531	-3.664457	0.146534
6	2.402796	-1.857668	0.674676
1	3.107184	-1.266953	1.244394
6	1.201132	-2.460902	1.184110
1	0.874263	-2.463783	2.214872
6	-3.544028	0.301211	-0.006432
1	-3.956178	-0.606022	0.442328
1	-3.967401	1.185859	0.470637
1	-3.811986	0.301788	-1.068645
6	1.470345	1.497554	-1.800698
1	2.350899	1.221558	-2.395954
1	1.037108	2.410246	-2.227867
8	0.496417	0.453281	-1.883175
6	0.252282	-0.000186	-3.213123
1	1.154334	-0.457583	-3.635217
1	-0.552656	-0.733077	-3.155798
1	-0.062056	0.845499	-3.833764

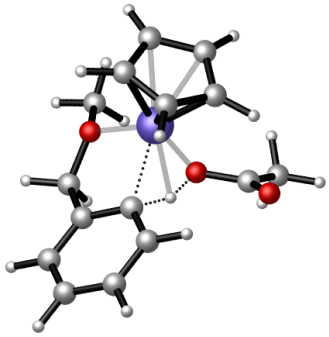
Int2b



E = -917.223158 Hartrees
G = -916.965866 Hartrees

8	-1.282786	1.680502	0.587773
6	-1.890573	0.545697	0.323192
8	-1.297918	-0.495453	0.034325
6	1.915539	1.641119	-0.468977
6	1.556618	0.666856	0.478541
6	2.464651	2.856378	-0.057253
6	1.752080	0.935432	1.837186
6	2.667299	3.105994	1.297312
6	2.305997	2.149469	2.244173
1	-0.309800	1.550229	0.554060
1	2.732398	3.606401	-0.797021
1	1.465667	0.199423	2.583487
1	3.096169	4.051730	1.614368
1	2.453957	2.346720	3.302030
45	0.803750	-1.044038	-0.292764
6	2.465933	-2.321840	-0.675339
1	3.346336	-2.006487	-1.219877
6	1.353655	-3.086045	-1.228012
1	1.221887	-3.327210	-2.274778
6	0.448668	-3.332514	-0.208124
1	-0.519625	-3.804924	-0.306584
6	2.274159	-2.228956	0.734712
1	2.946259	-1.762139	1.441396
6	0.972632	-2.730744	1.012343
1	0.499850	-2.769141	1.984893
6	-3.377534	0.615952	0.429370
1	-3.827456	-0.295975	0.038056
1	-3.646631	0.735148	1.484660
1	-3.751192	1.490153	-0.110036
6	1.695086	1.323454	-1.918107
1	2.604481	0.916817	-2.382001
1	1.367329	2.196103	-2.493632
8	0.664826	0.323989	-1.972098
6	0.463185	-0.207775	-3.282089
1	1.368574	-0.713190	-3.635621
1	-0.363951	-0.914846	-3.215575
1	0.199435	0.606172	-3.965220

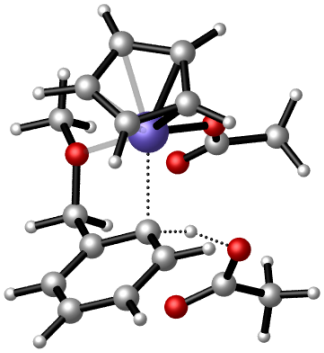
$TS_{1\text{-}2}$l



E = -917.172819 Hartrees
G = -916.922228 Hartrees

6	3.054007	-4.302280	1.833531
1	4.123647	-4.145271	1.848180
6	2.101417	-3.561671	1.033214
1	2.348179	-2.792933	0.313177
6	0.831890	-4.104933	1.264735
1	-0.083942	-3.828526	0.758935
6	2.331712	-5.233755	2.633427
1	2.757466	-5.933172	3.340102
6	0.966076	-5.179222	2.228884
1	0.160549	-5.791460	2.611894
45	2.138528	-5.741201	0.550435
6	1.992346	-8.664315	0.125422
6	3.835736	-8.152954	1.623183
6	2.010382	-9.986573	0.555795
6	3.860925	-9.477848	2.041817
1	4.552082	-7.440160	2.020614
6	2.943229	-10.38643	1.511963
1	1.302381	-10.70431	0.151032
1	4.587054	-9.806244	2.778647
1	2.954765	-11.41983	1.845671
6	1.062434	-8.200164	-0.954538
1	0.131715	-8.775960	-0.981314
1	1.553733	-8.283986	-1.932919
8	0.738124	-6.821847	-0.714064
6	0.222859	-6.158233	-1.872344
1	-0.628744	-6.724121	-2.262529
1	-0.108175	-5.170249	-1.551505
1	1.001929	-6.068694	-2.635953
8	3.454471	-6.046621	-1.241526
8	5.358193	-5.400026	-0.231181
6	4.654907	-5.445028	-1.219663
6	5.025387	-4.856709	-2.554859
1	5.998975	-4.368441	-2.494807
1	5.051376	-5.647204	-3.311598
1	4.264029	-4.133206	-2.863538
6	2.905881	-7.730754	0.660108
1	3.417381	-6.951960	-0.333464

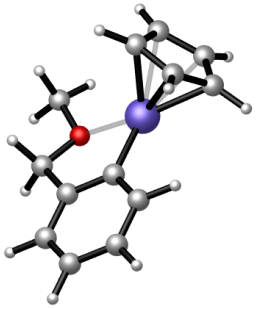
$TS_{1\text{-}2}$m



E = -1145.734608 Hartrees
G = -1145.437298 Hartrees

6	2.773773	-4.296693	2.282037
1	3.824463	-4.150821	2.492337
6	1.897282	-3.346265	1.669956
1	2.197919	-2.394053	1.254051
6	0.611253	-3.930732	1.557846
1	-0.259259	-3.478480	1.102578
6	1.981891	-5.450913	2.637835
1	2.348459	-6.350538	3.111871
6	0.670920	-5.237835	2.168838
1	-0.140480	-5.952234	2.212967
45	2.049924	-5.145000	0.470304
6	2.355260	-7.943770	-0.234802
6	4.157121	-7.357224	1.266043
6	2.255051	-9.188556	0.375611
6	4.068591	-8.605162	1.872433
1	4.914707	-6.651489	1.598501
6	3.115460	-9.519948	1.423263
1	1.508939	-9.903513	0.038841
1	4.738380	-8.871884	2.684927
1	3.037212	-10.49585	1.894268
6	1.419153	-7.514795	-1.322809
1	0.674707	-8.282954	-1.561359
1	1.981725	-7.228481	-2.217125
8	0.729846	-6.360223	-0.810944
6	-0.240422	-5.820457	-1.704938
1	-1.011586	-6.577174	-1.892854
1	-0.689737	-4.961773	-1.202926
1	0.238650	-5.507882	-2.633830
8	2.919630	-4.012468	-1.011205
6	2.983531	-4.189062	-2.293093
8	2.367513	-5.017636	-2.958572
6	3.941409	-3.210553	-2.954033
1	3.827361	-2.204758	-2.538772
1	4.961339	-3.550061	-2.747103
1	3.782415	-3.187065	-4.034721
8	4.957983	-6.015450	-1.610243
8	4.323912	-7.844636	-2.760763
6	4.962559	-6.793266	-2.635712
6	5.827999	-6.303800	-3.795193
1	6.688823	-5.726939	-3.445088
1	6.165278	-7.144992	-4.407474
1	5.215876	-5.649049	-4.427594
6	3.311431	-6.995061	0.197753
1	3.951544	-6.374178	-0.689019

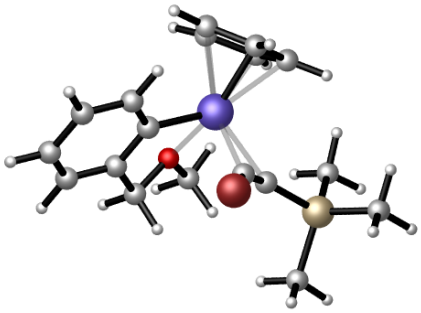
Int3b



E = -688.181088 Hartrees
G = -687.982112 Hartrees

6	2.804012	-4.388089	2.227063
1	3.802149	-4.342830	2.643117
6	2.290016	-3.519124	1.170285
1	2.874025	-2.786140	0.629504
6	0.977804	-3.875074	0.919680
1	0.336196	-3.479236	0.143845
6	1.745848	-5.203989	2.690481
1	1.784525	-5.922151	3.497974
6	0.643680	-4.993958	1.792564
1	-0.318772	-5.486313	1.844408
45	2.246916	-5.796624	0.708832
6	2.275049	-8.636759	0.150980
6	3.392620	-8.149106	2.239868
6	2.620142	-9.982735	0.281156
6	3.739260	-9.493411	2.363913
1	3.705789	-7.444082	3.004903
6	3.348642	-10.40942	1.387665
1	2.319339	-10.69524	-0.482826
1	4.315077	-9.826345	3.222832
1	3.615454	-11.45750	1.486211
6	1.461172	-8.152454	-1.008518
1	0.389430	-8.323717	-0.842341
1	1.748561	-8.623786	-1.954189
8	1.678089	-6.733769	-1.124680
6	0.744710	-6.088944	-1.998345
1	-0.258065	-6.102027	-1.558792
1	1.089558	-5.064027	-2.133968
1	0.739463	-6.608241	-2.961320
6	2.663418	-7.707373	1.130723

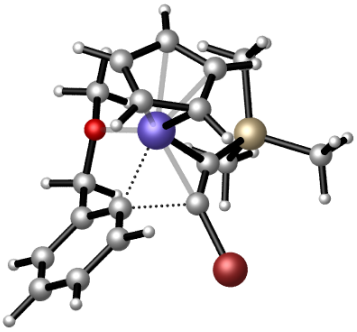
Int4b



E = -1186.717087 Hartrees
G = -1186.405831 Hartrees

6	2.247958	-3.468927	1.386003
1	3.242022	-3.094335	1.181107
6	1.018761	-2.977668	0.792465
1	0.960009	-2.244418	-0.000818
6	-0.046366	-3.688322	1.351277
1	-1.088971	-3.603912	1.075706
6	1.889887	-4.398243	2.412863
1	2.570632	-4.920276	3.069737
6	0.494731	-4.606391	2.331702
1	-0.079873	-5.300084	2.931512
45	1.420738	-5.182892	0.392164
6	2.648897	-6.794167	0.710352
6	2.157035	-8.010343	0.226775
6	3.862777	-6.765022	1.394145
6	2.866763	-9.190657	0.451836
6	4.571243	-7.946655	1.611342
1	4.278430	-5.827855	1.751578
6	4.074415	-9.160304	1.142301
1	2.471675	-10.13246	0.079136
1	5.514670	-7.913492	2.149056
1	4.622631	-10.08125	1.316495
6	0.879344	-7.999676	-0.552273
1	0.294472	-8.914683	-0.409617
1	1.059224	-7.859840	-1.627693
8	0.120217	-6.884947	-0.066151
6	-1.152435	-6.755857	-0.692128
1	-1.715942	-7.682985	-0.543570
1	-1.668978	-5.930946	-0.202448
1	-1.042904	-6.563689	-1.764061
6	1.511809	-4.798911	-1.793006
6	2.650640	-5.150788	-1.410844
35	4.430952	-5.413797	-1.748523
14	0.320014	-4.000485	-3.011340
6	-1.243859	-3.420512	-2.163586
1	-1.025265	-2.738543	-1.334855
1	-1.850640	-2.866533	-2.891453
1	-1.856621	-4.244439	-1.786930
6	1.289407	-2.542661	-3.684632
1	2.238780	-2.867626	-4.125614
1	0.713860	-2.029987	-4.465371
1	1.513038	-1.813526	-2.897336
6	-0.007072	-5.275522	-4.345369
1	-0.516034	-6.165650	-3.959154
1	-0.639176	-4.843320	-5.131027
1	0.931243	-5.598503	-4.811183

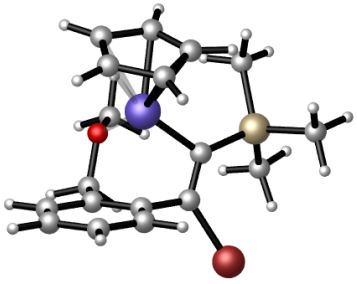
$TS_{4\text{-}5}b$



E = -1186.707528 Hartrees
G = -1186.394512 Hartrees

6	2.095478	-3.436370	1.548199
1	3.082222	-3.036266	1.353989
6	0.868892	-2.972867	0.944646
1	0.795486	-2.227525	0.164529
6	-0.176242	-3.753586	1.460165
1	-1.218629	-3.697984	1.176488
6	1.758943	-4.402543	2.560849
1	2.459645	-4.927094	3.195627
6	0.381852	-4.647064	2.463796
1	-0.178363	-5.379452	3.030475
45	1.300632	-5.109227	0.472541
6	2.718336	-6.660303	0.362351
6	2.166152	-7.887479	-0.031108
6	3.928311	-6.627341	1.061593
6	2.841488	-9.071982	0.267146
6	4.588070	-7.813063	1.358507
1	4.361283	-5.677974	1.361187
6	4.052527	-9.035718	0.948759
1	2.408910	-10.02278	-0.031899
1	5.525265	-7.783983	1.906150
1	4.574998	-9.960808	1.171994
6	0.837279	-7.878855	-0.711816
1	0.333930	-8.848583	-0.647463
1	0.920808	-7.588861	-1.769601
8	0.050811	-6.894846	-0.023753
6	-1.269384	-6.769684	-0.546217
1	-1.791647	-7.725539	-0.431485
1	-1.775273	-6.001646	0.038630
1	-1.247281	-6.490037	-1.604325
6	1.512824	-4.899760	-1.605701
6	2.652033	-5.322320	-1.223254
35	4.423404	-5.229641	-1.803248
14	0.463776	-4.102409	-2.939338
6	-1.077990	-3.363712	-2.171484
1	-0.835222	-2.520984	-1.514346
1	-1.738262	-2.985172	-2.962091
1	-1.644009	-4.099832	-1.591243
6	1.530530	-2.765267	-3.711830
1	2.425237	-3.188941	-4.182031
1	0.968078	-2.228511	-4.486140
1	1.856513	-2.032882	-2.964154
6	0.063959	-5.446458	-4.186470
1	-0.629284	-6.195951	-3.788767
1	-0.401621	-5.005818	-5.077026
1	0.976072	-5.962782	-4.508259

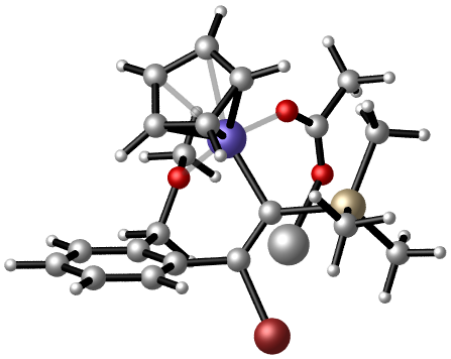
Int5b



E = -1186.767805 Hartrees
G = -1186.453093 Hartrees

6	2.175229	-3.861431	1.605309
1	3.225589	-3.638274	1.470962
6	1.096893	-3.246975	0.914868
1	1.176674	-2.494806	0.142477
6	-0.097001	-3.897648	1.352171
1	-1.099201	-3.692674	0.999538
6	1.624309	-4.758840	2.612992
1	2.208619	-5.371798	3.286598
6	0.245423	-4.777823	2.462981
1	-0.453540	-5.404420	3.000946
45	1.167066	-5.353285	0.455319
6	2.975892	-6.793851	-0.555083
6	2.165848	-7.812814	0.005273
6	4.233576	-6.523237	0.021322
6	2.634391	-8.530946	1.114132
6	4.677404	-7.246521	1.114527
1	4.855173	-5.745078	-0.411602
6	3.877453	-8.256518	1.661028
1	2.011113	-9.314789	1.534043
1	5.649630	-7.031373	1.546264
1	4.230609	-8.825671	2.515061
6	0.808631	-8.115204	-0.572010
1	0.440774	-9.093516	-0.248928
1	0.819747	-8.079047	-1.666810
8	-0.079349	-7.102818	-0.068208
6	-1.301177	-7.000129	-0.796762
1	-1.824252	-7.961366	-0.760016
1	-1.900188	-6.234375	-0.303576
1	-1.108872	-6.721415	-1.838806
6	1.475451	-5.163651	-1.562658
6	2.485834	-6.007256	-1.726518
35	3.431419	-6.337864	-3.395599
14	0.569454	-4.036735	-2.774921
6	-0.991591	-3.353676	-1.976312
1	-0.780417	-2.598524	-1.211501
1	-1.606576	-2.869728	-2.745789
1	-1.597715	-4.145087	-1.520948
6	1.725107	-2.623737	-3.227933
1	2.636828	-2.993693	-3.710931
1	1.234342	-1.929802	-3.921646
1	2.022608	-2.053267	-2.339440
6	0.063579	-5.022740	-4.296432
1	-0.502893	-5.921614	-4.023813
1	-0.579467	-4.406476	-4.937753
1	0.926511	-5.338210	-4.891243

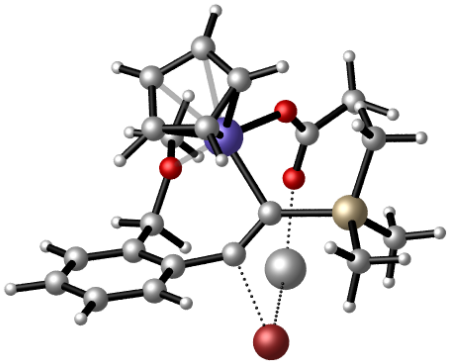
Int6b



E = -1561.006941 Hartrees
G = -1560.648051 Hartrees

6	-2.762750	-0.100206	0.617511
6	-4.547079	-2.019514	1.621564
6	-1.833822	0.856438	-0.058782
6	-0.664355	0.577703	-0.678898
6	-2.489396	-0.743091	1.835109
1	-3.173548	-2.191238	3.262897
6	-3.390760	-1.696473	2.320158
6	-3.933045	-0.429982	-0.079400
6	-4.815317	-1.382898	0.411426
1	-5.234040	-2.761249	2.016698
1	-5.711512	-1.626268	-0.150951
1	-4.147683	0.061103	-1.023839
6	0.303437	-2.330819	-2.136836
6	-1.088785	-2.168631	-1.848015
6	0.850608	-3.280001	-1.180896
1	-1.792336	-1.562224	-2.402511
1	1.884653	-3.595355	-1.139037
6	-1.344668	-2.854012	-0.632787
1	-2.293559	-2.901477	-0.115682
6	-0.145168	-3.589450	-0.263342
1	-0.035075	-4.197356	0.624989
1	0.828650	-1.933566	-2.993053
14	0.050476	1.578149	-2.166709
35	-2.773429	2.606893	-0.315216
6	1.592256	0.793044	-2.907263
1	1.336443	0.051340	-3.671497
1	2.240674	0.316828	-2.168010
1	2.167457	1.581934	-3.409233
6	-1.285771	1.516607	-3.489509
1	-2.205653	2.037752	-3.208684
1	-1.539660	0.473697	-3.717273
1	-0.907302	1.972302	-4.413354
6	0.532333	3.341644	-1.698921
1	0.773766	3.884777	-2.622723
1	1.440385	3.352282	-1.080631
1	-0.251896	3.904786	-1.184391
8	2.141868	-0.597847	-0.024843
6	2.858653	0.309759	0.495010
8	2.460813	1.325477	1.121633
47	0.303407	1.809363	1.105044
6	4.352112	0.155563	0.299244
1	4.630093	-0.897055	0.216167
1	4.627711	0.657364	-0.636145
1	4.900337	0.631616	1.114865
6	-1.238265	-0.491832	2.617201
1	-1.333786	-0.912330	3.623546
1	-1.030599	0.583285	2.736859
8	-0.130015	-1.133262	1.970847
6	1.014362	-1.248878	2.817631
1	1.763280	-1.821552	2.272264
1	1.416743	-0.261140	3.068343
1	0.735357	-1.782069	3.732848
45	0.117987	-1.309790	-0.289049

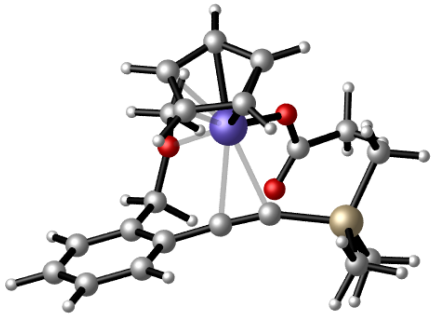
$TS_{6\text{-}7}b$



E = -1561.00179 Hartrees
G = -1560.644501 Hartrees

6	-2.711836	-0.202693	0.547902
6	-4.653965	-1.852446	1.683219
6	-1.680198	0.576018	-0.139552
6	-0.604046	0.425188	-0.841884
6	-2.485075	-0.773619	1.810382
1	-3.287305	-2.057822	3.330445
6	-3.463640	-1.603232	2.359326
6	-3.908322	-0.456077	-0.132418
6	-4.876479	-1.275221	0.433886
1	-5.405002	-2.497147	2.128820
1	-5.801982	-1.465740	-0.100327
1	-4.070435	-0.007913	-1.108100
6	0.472340	-2.637932	-2.096633
6	-0.937369	-2.483928	-1.889130
6	0.993586	-3.454699	-1.021678
1	-1.619580	-1.939622	-2.528111
1	2.030749	-3.733644	-0.891690
6	-1.250246	-3.071435	-0.637057
1	-2.222986	-3.083921	-0.163299
6	-0.052059	-3.711017	-0.129766
1	0.030460	-4.218711	0.822331
1	1.034508	-2.298365	-2.954128
14	0.170675	1.490064	-2.221652
35	-2.408501	2.762873	0.134402
6	1.425600	0.490132	-3.193836
1	0.938540	-0.267533	-3.817301
1	2.155437	-0.000686	-2.543247
1	1.967323	1.164311	-3.869477
6	-1.250223	1.928267	-3.371654
1	-1.980834	2.587809	-2.892406
1	-1.775193	1.025038	-3.706044
1	-0.864300	2.437983	-4.263635
6	1.025798	3.048535	-1.601775
1	1.483246	3.540585	-2.470692
1	1.831386	2.841437	-0.888140
1	0.331473	3.770185	-1.156562
8	2.060107	-0.548268	-0.144412
6	2.490901	0.467636	0.492760
8	1.845449	1.187042	1.287209
47	-0.010853	2.446257	1.375543
6	3.939141	0.818055	0.219950
1	4.515781	-0.064717	-0.064313
1	3.966176	1.528179	-0.615922
1	4.387870	1.302075	1.090154
6	-1.197668	-0.556355	2.545113
1	-1.287470	-0.926652	3.571769
1	-0.934291	0.510331	2.602528
8	-0.137679	-1.267653	1.902360
6	0.995242	-1.436489	2.753711
1	1.768992	-1.934687	2.170009
1	1.364577	-0.466435	3.098644
1	0.715537	-2.063569	3.608059
45	0.171230	-1.477233	-0.343310

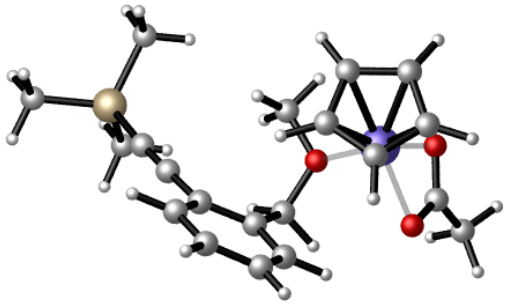
Int7b



E = -1401.989703 Hartrees
G = -1401.626971 Hartrees

6	-2.668559	-0.503996	0.464936
6	-4.734774	-1.403489	2.089535
6	-1.601348	-0.064072	-0.383520
6	-0.740679	0.381873	-1.145191
6	-2.407142	-0.792418	1.817150
1	-3.265453	-1.471783	3.661208
6	-3.453904	-1.246122	2.615598
6	-3.951715	-0.674118	-0.069491
6	-4.983906	-1.117408	0.748679
1	-5.539461	-1.753017	2.728856
1	-5.980801	-1.241734	0.338058
1	-4.128833	-0.453038	-1.117209
6	1.073079	-2.851197	-1.980282
6	-0.283035	-2.556530	-2.295353
6	1.087345	-3.599033	-0.758260
1	-0.622012	-1.959769	-3.131633
1	1.963898	-3.969179	-0.244223
6	-1.123476	-3.153072	-1.292596
1	-2.201640	-3.088310	-1.240911
6	-0.276500	-3.803060	-0.363074
1	-0.598907	-4.285736	0.550760
1	1.939725	-2.499981	-2.524262
14	0.121688	1.477885	-2.404561
6	1.558104	0.543610	-3.159462
1	1.203130	-0.315593	-3.740846
1	2.245752	0.177307	-2.391332
1	2.114174	1.199812	-3.840373
6	-1.191142	1.833620	-3.696835
1	-2.072649	2.310449	-3.253064
1	-1.516939	0.916848	-4.202216
1	-0.792563	2.513202	-4.460607
6	0.647869	3.038680	-1.514109
1	1.264628	3.665596	-2.169903
1	1.217789	2.814520	-0.607222
1	-0.230905	3.623760	-1.217489
8	1.999822	-0.660440	-0.146349
6	2.159366	0.460422	0.494103
8	1.307819	1.034116	1.167624
6	3.542125	1.054230	0.299822
1	4.311374	0.278167	0.277811
1	3.563935	1.576092	-0.665064
1	3.757866	1.777051	1.089427
6	-1.026639	-0.614836	2.375028
1	-1.041037	-0.780188	3.456256
1	-0.609761	0.372646	2.159434
8	-0.134291	-1.595500	1.795943
6	1.017613	-1.819805	2.617429
1	1.664750	-2.518315	2.087565
1	1.544870	-0.880356	2.800150
1	0.691801	-2.263013	3.564286
45	0.223340	-1.674276	-0.397002

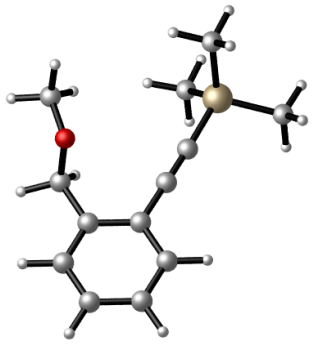
Int8b



E = -1401.992141 Hartrees
G = -1401.632981 Hartrees

6	1.526955	-3.804770	2.052885
1	2.350942	-3.857870	2.753213
6	1.500896	-3.039306	0.858042
1	2.283227	-2.378781	0.509170
6	0.262892	-3.320009	0.179998
1	-0.047435	-2.913202	-0.773474
6	0.335370	-4.599739	2.103749
1	0.070097	-5.305769	2.878757
6	-0.457647	-4.260949	0.954066
1	-1.399151	-4.717247	0.678164
45	1.418630	-5.137678	0.367802
8	2.878998	-6.617781	0.846394
8	0.986544	-7.186615	-0.049501
6	2.152289	-7.526501	0.335786
6	2.658744	-8.916368	0.148217
1	1.832827	-9.630429	0.162580
1	3.151671	-8.975375	-0.829133
1	3.391041	-9.162822	0.919590
8	2.408441	-5.269708	-1.600384
6	3.374777	-4.237561	-1.829609
1	4.020773	-4.217889	-0.950338
1	3.967958	-4.490866	-2.713133
1	2.894818	-3.265366	-1.968223
6	1.629557	-5.674442	-2.752668
1	2.274440	-5.587124	-3.631390
1	1.405198	-6.727561	-2.579617
6	0.352793	-4.891120	-2.903193
6	-0.803983	-5.366288	-2.283132
6	0.292961	-3.674136	-3.613887
6	-1.994059	-4.646094	-2.328080
1	-0.761788	-6.313028	-1.751619
6	-0.907004	-2.948165	-3.649354
6	-2.040401	-3.428172	-3.003314
1	-2.882044	-5.035753	-1.839825
1	-0.942393	-2.010686	-4.195114
1	-2.963546	-2.858153	-3.040746
6	1.438419	-3.176268	-4.315881
6	2.428553	-2.775216	-4.899230
14	4.010407	-2.240653	-5.695536
6	5.117594	-1.570816	-4.332216
1	6.076867	-1.237096	-4.747251
1	4.655851	-0.714110	-3.827361
1	5.329765	-2.335914	-3.575652
6	4.778014	-3.758007	-6.493373
1	4.116948	-4.184260	-7.256975
1	5.727723	-3.499465	-6.977871
1	4.982656	-4.538386	-5.750713
6	3.636131	-0.919408	-6.973627
1	3.190082	-0.029984	-6.513486
1	4.558263	-0.608140	-7.479845
1	2.942166	-1.288414	-7.737722

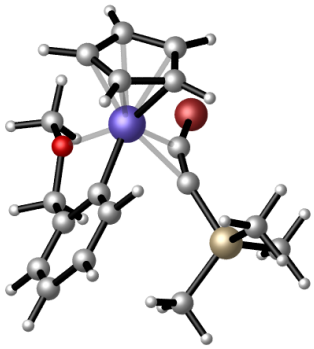
5x



E = -870.712250 Hartrees
G = -870.482376 Hartrees

6	0.959414	-0.725074	-0.165994
6	2.349888	-0.714572	-0.127141
6	3.047411	0.500479	-0.121511
6	2.338733	1.719898	-0.153483
6	0.947394	1.686948	-0.189970
6	0.256484	0.476222	-0.198304
1	0.427826	-1.671781	-0.171184
1	2.905183	-1.647254	-0.104015
1	0.397632	2.624379	-0.210951
1	-0.829139	0.472927	-0.228032
6	3.086507	3.027277	-0.136345
1	3.869818	3.018270	-0.910984
1	2.403681	3.859195	-0.367390
8	3.669564	3.201775	1.137459
6	4.637677	4.220342	1.140798
1	4.210099	5.193672	0.853566
1	5.031501	4.293942	2.158002
1	5.466881	3.990288	0.453101
6	4.480998	0.501605	-0.096686
6	5.698526	0.520516	-0.090442
14	7.543009	0.601966	-0.071823
6	8.077009	1.865164	-1.356327
1	7.632061	2.847689	-1.159326
1	9.167768	1.984338	-1.349112
1	7.780190	1.558376	-2.366207
6	8.086284	1.133002	1.646227
1	7.762006	0.412650	2.406150
1	9.179524	1.209102	1.699259
1	7.666890	2.111255	1.909313
6	8.217877	-1.100388	-0.490297
1	7.885881	-1.428898	-1.482188
1	9.315118	-1.090708	-0.490219
1	7.889986	-1.849301	0.240079

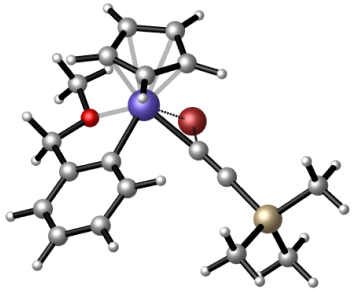
Int9b



E = -1186.718858 Hartrees
G = -1186.409151 Hartrees

6	2.245635	-3.457464	1.459812
1	3.255123	-3.095428	1.317994
6	1.066988	-2.966470	0.771734
1	1.070805	-2.234716	-0.025457
6	-0.041798	-3.668635	1.254626
1	-1.061407	-3.579315	0.904326
6	1.808336	-4.374443	2.467268
1	2.437245	-4.897667	3.173228
6	0.422404	-4.577021	2.284940
1	-0.198694	-5.261086	2.848415
45	1.461938	-5.168825	0.418248
6	2.658578	-6.791831	0.804518
6	2.180698	-8.005941	0.299488
6	3.811317	-6.782466	1.588443
6	2.852259	-9.195685	0.582679
6	4.483118	-7.974206	1.864705
1	4.202682	-5.853007	1.989995
6	4.005506	-9.182136	1.361711
1	2.467796	-10.13382	0.190270
1	5.380184	-7.953596	2.477131
1	4.524583	-10.11072	1.578828
6	0.952509	-7.987535	-0.555806
1	0.349113	-8.894058	-0.438769
1	1.198029	-7.862130	-1.619924
8	0.179249	-6.858675	-0.128556
6	-1.072285	-6.741969	-0.801545
1	-1.694704	-7.605560	-0.544880
1	-1.546608	-5.827642	-0.445845
1	-0.931290	-6.702132	-1.886768
6	1.636796	-4.796502	-1.684497
6	2.796973	-5.178108	-1.416015
35	0.384474	-4.123138	-2.842129
14	4.607805	-5.474447	-1.821760
6	5.655786	-4.512132	-0.605052
1	6.712218	-4.586341	-0.892305
1	5.387036	-3.449457	-0.608776
1	5.563728	-4.893073	0.416327
6	4.751595	-4.750492	-3.548742
1	5.772563	-4.877587	-3.930281
1	4.068896	-5.248468	-4.247111
1	4.521301	-3.678841	-3.554539
6	4.976772	-7.307556	-1.839839
1	5.977923	-7.467731	-2.260246
1	4.957352	-7.746621	-0.838354
1	4.263370	-7.850081	-2.470518

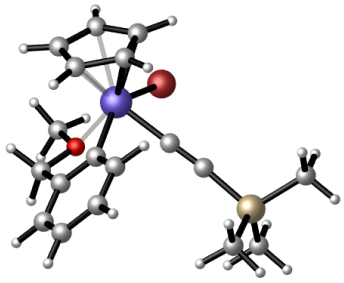
$TS_{9\text{-}10}b$



E = -1186.651651 Hartrees
G = -1186.343551 Hartrees

45	0.271096	0.935013	-0.350668
6	-0.343695	2.809666	-0.961434
6	-0.359931	3.947316	-0.163623
6	-0.693281	2.886411	-2.309959
6	-0.741876	5.170680	-0.708902
1	-0.093045	3.885131	0.885050
6	-1.094797	4.115133	-2.843106
6	-1.117164	5.254643	-2.048379
1	-0.753438	6.054692	-0.077711
1	-1.383899	4.170601	-3.889452
1	-1.428540	6.204370	-2.472028
6	-0.581996	1.675977	-3.177093
1	0.358102	1.679639	-3.745966
1	-1.416640	1.583130	-3.879984
8	-0.590536	0.536617	-2.306710
6	-0.288470	-0.687512	-2.983257
1	0.719677	-0.647398	-3.409510
1	-1.027654	-0.843868	-3.774292
1	-0.363590	-1.490838	-2.250548
6	1.780086	0.837684	1.223740
1	1.521858	0.978401	2.264558
6	2.129159	1.872527	0.306184
6	1.958218	-0.441620	0.564372
1	2.154139	2.931831	0.517086
6	2.332687	1.253144	-0.957606
1	1.791786	-1.409569	1.017454
6	2.269706	-0.187787	-0.768055
1	2.573970	1.761214	-1.882457
1	2.389588	-0.926659	-1.549607
35	-1.612504	-0.639762	0.380782
6	-1.065984	1.357852	1.187935
6	-1.511458	1.995512	2.135274
14	-2.180798	3.030418	3.507471
6	-4.004737	2.632407	3.717318
1	-4.432207	3.216170	4.542138
1	-4.569754	2.871787	2.808753
1	-4.159905	1.570387	3.940323
6	-1.954813	4.839078	3.047312
1	-2.393943	5.484592	3.818513
1	-0.894948	5.104081	2.955765
1	-2.449152	5.070603	2.096820
6	-1.217582	2.608775	5.065745
1	-1.336896	1.551728	5.331160
1	-0.146596	2.807920	4.940312
1	-1.573579	3.208799	5.912320

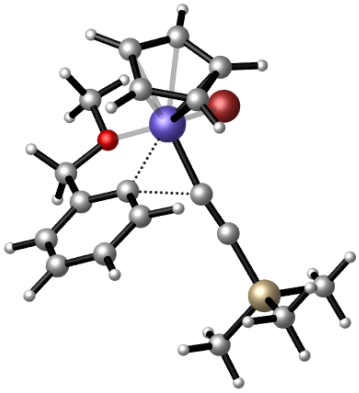
Int10b



E = -1186.670104 Hartrees
G = -1186.361553 Hartrees

45	0.547722	0.863806	-0.142987
6	0.035992	2.831168	-0.787600
6	0.343624	4.012123	-0.126208
6	-0.672539	2.818934	-1.979967
6	-0.071631	5.218377	-0.681494
1	0.868454	4.008750	0.821031
6	-1.094277	4.040953	-2.516281
6	-0.792321	5.234062	-1.875302
1	0.157599	6.145515	-0.165338
1	-1.661805	4.041035	-3.442773
1	-1.126141	6.175369	-2.299727
6	-0.946014	1.533142	-2.677925
1	-0.164050	1.303024	-3.414563
1	-1.914858	1.539508	-3.186274
8	-0.964596	0.494541	-1.684167
6	-1.075082	-0.797241	-2.305421
1	-0.148981	-1.044007	-2.835601
1	-1.914363	-0.769190	-3.005967
1	-1.273079	-1.523298	-1.522225
6	2.379338	0.289140	0.860340
1	2.368383	-0.118782	1.861888
6	2.442536	1.664771	0.524336
6	2.391755	-0.474103	-0.380579
1	2.480307	2.488233	1.223924
6	2.460441	1.755264	-0.913569
1	2.346144	-1.551526	-0.456407
6	2.453380	0.429191	-1.449135
1	2.537353	2.665512	-1.490611
1	2.430880	0.177923	-2.501133
35	-0.358552	-1.260220	0.984674
6	-0.629410	1.666850	1.225576
6	-1.322118	2.179195	2.090239
14	-2.378155	3.103711	3.281418
6	-4.128942	2.427242	3.189831
1	-4.779696	2.944041	3.906289
1	-4.557896	2.561308	2.189676
1	-4.153384	1.356619	3.424827
6	-2.339038	4.914490	2.770665
1	-2.982057	5.519285	3.422717
1	-1.323823	5.324740	2.832170
1	-2.692085	5.041469	1.740413
6	-1.681571	2.889335	5.013875
1	-1.676206	1.834455	5.312881
1	-0.654008	3.265769	5.083137
1	-2.288968	3.441233	5.742185

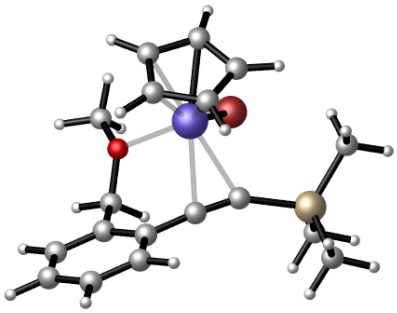
$TS_{10\text{-}11}b$



E = -1186.668836 Hartrees
G = -1186.356866 Hartrees

45	0.257314	0.873088	-0.268613
6	0.258114	2.995346	-0.637996
6	0.847421	3.964265	0.171619
6	-0.187530	3.290154	-1.920146
6	0.982194	5.258620	-0.310328
1	1.161683	3.731695	1.180974
6	-0.052308	4.606506	-2.381627
6	0.523684	5.585101	-1.587902
1	1.433531	6.015070	0.323985
1	-0.400427	4.844816	-3.383241
1	0.619788	6.599248	-1.961795
6	-0.727302	2.245848	-2.838177
1	-0.043958	2.104163	-3.685147
1	-1.717062	2.504848	-3.228403
8	-0.842809	1.007571	-2.124403
6	-0.878956	-0.116233	-3.016637
1	0.082870	-0.218882	-3.529989
1	-1.681898	0.043311	-3.742088
1	-1.095940	-0.999540	-2.420089
6	2.012735	1.055022	0.989338
1	2.042211	1.758463	1.810112
6	2.454833	1.285714	-0.360723
6	1.529984	-0.276651	1.060682
1	2.886807	2.200221	-0.742158
6	2.273417	0.080682	-1.101922
1	1.133059	-0.761282	1.942083
6	1.677353	-0.871948	-0.255482
1	2.474427	-0.043411	-2.157945
1	1.386527	-1.876841	-0.528225
35	-1.483951	-0.938196	0.306802
6	-1.013468	2.011110	0.761698
6	-1.799502	2.570149	1.512776
14	-2.903652	3.571303	2.595426
6	-1.800017	4.645719	3.674195
1	-1.157645	5.290131	3.061958
1	-2.404292	5.292078	4.322863
1	-1.154181	4.035743	4.317058
6	-3.958709	2.433505	3.652745
1	-4.592431	1.787743	3.033628
1	-3.339796	1.790096	4.289203
1	-4.614776	3.021599	4.306605
6	-3.980628	4.640630	1.487887
1	-4.631580	5.285195	2.091711
1	-3.369143	5.285658	0.845821
1	-4.620061	4.027952	0.841610

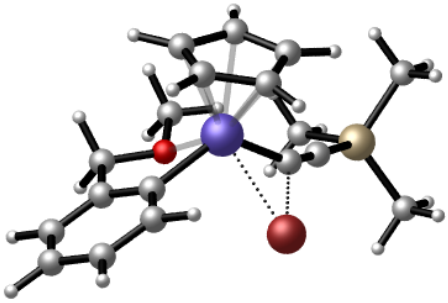
Int11b



E = -1186.786991 Hartrees
G = -1186.477124 Hartrees

45	0.055828	1.199614	0.304724
6	-0.295558	4.119714	-1.068017
6	0.363244	5.338594	-0.864637
6	-0.406793	3.567671	-2.357645
6	0.901758	6.015598	-1.952338
1	0.440680	5.747010	0.137850
6	0.150234	4.255639	-3.431208
6	0.794518	5.475366	-3.232794
1	1.405093	6.964997	-1.800632
1	0.073760	3.835907	-4.430135
1	1.219110	6.002648	-4.081291
6	-1.073461	2.237844	-2.542751
1	-1.175928	2.014637	-3.608123
1	-2.065246	2.198586	-2.077187
8	-0.246191	1.219238	-1.943110
6	-0.412777	-0.052415	-2.581543
1	-0.084841	0.033077	-3.622683
1	-1.455270	-0.379153	-2.536649
1	0.217456	-0.768332	-2.054824
6	1.615636	1.975042	1.600327
1	1.525737	2.950800	2.059595
6	2.194399	1.702437	0.335643
6	1.058997	0.757379	2.118851
1	2.650795	2.423387	-0.329093
6	2.034207	0.296182	0.079422
1	0.552761	0.637119	3.066069
6	1.363525	-0.289983	1.180839
1	2.333475	-0.218244	-0.824754
1	1.077935	-1.328833	1.272725
35	-1.958088	-0.331581	0.465598
6	-0.865075	3.415959	0.040111
6	-1.422444	2.892160	1.010578
14	-2.616588	2.847159	2.464880
6	-2.021658	1.658023	3.780622
1	-1.056963	1.973298	4.194705
1	-2.745826	1.642496	4.604844
1	-1.928801	0.638342	3.394063
6	-4.310950	2.422038	1.793436
1	-4.618836	3.141229	1.025708
1	-4.324485	1.420674	1.352416
1	-5.053523	2.453064	2.600621
6	-2.577269	4.611177	3.108265
1	-3.272299	4.720318	3.950317
1	-1.578032	4.892183	3.461065
1	-2.877916	5.324918	2.332682

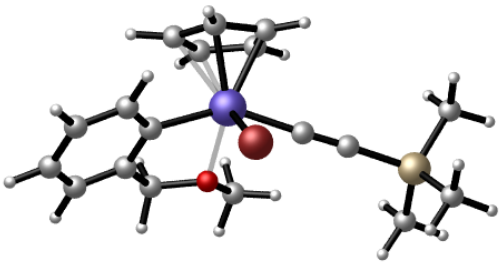
$TS_{4\text{-}12}b$



E = -1186.654088 Hartrees
G = -1186.346826 Hartrees

45	0.362372	1.017535	-0.280109
6	0.516654	2.979661	-0.878558
6	0.985104	4.005601	-0.067127
6	0.100938	3.224492	-2.184627
6	1.038821	5.303343	-0.573503
1	1.307831	3.810773	0.950770
6	0.147711	4.531128	-2.676858
6	0.620203	5.565332	-1.876554
1	1.405234	6.107853	0.057120
1	-0.189612	4.730862	-3.690373
1	0.656696	6.577090	-2.268164
6	-0.358967	2.081931	-3.027606
1	0.464086	1.672891	-3.630040
1	-1.178955	2.359804	-3.697507
8	-0.826331	1.061254	-2.131921
6	-1.117846	-0.162674	-2.815066
1	-0.223520	-0.531271	-3.330104
1	-1.919938	0.020563	-3.536362
1	-1.452356	-0.875689	-2.065098
6	-1.324279	0.067969	0.419982
6	-2.110668	-0.871456	0.412993
14	-3.289565	-2.288790	0.334668
6	-2.379833	-3.825771	0.917805
1	-3.050852	-4.693803	0.915727
1	-1.995696	-3.702897	1.937353
1	-1.531953	-4.057181	0.261879
6	-3.838349	-2.475808	-1.454234
1	-3.005346	-2.761388	-2.107564
1	-4.266394	-1.543062	-1.840088
1	-4.606902	-3.254734	-1.534919
6	-4.761004	-1.912147	1.438261
1	-4.453944	-1.764495	2.480150
1	-5.484804	-2.736356	1.413556
1	-5.277304	-1.003148	1.107634
35	-1.189052	1.996329	1.522781
6	2.007484	0.537295	1.088072
1	2.047750	0.918102	2.100358
6	2.578063	1.162157	-0.059682
6	1.482914	-0.754953	0.693644
1	3.088691	2.113860	-0.082390
6	2.236120	0.360100	-1.180278
1	0.998805	-1.461300	1.353560
6	1.600784	-0.854198	-0.693943
1	2.474792	0.575043	-2.213995
1	1.225529	-1.656798	-1.314792

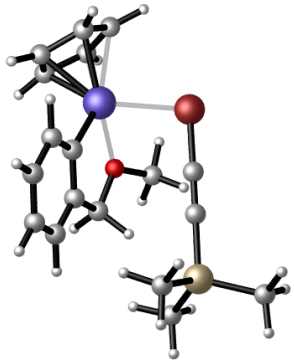
Int12b



E = -1186.666716 Hartrees
G = -1186.356805 Hartrees

45	0.187320	1.027671	-0.314950
6	0.578937	3.062742	-0.831875
6	1.049015	4.039085	0.034555
6	0.269201	3.344533	-2.154189
6	1.212962	5.337106	-0.441426
1	1.281028	3.815353	1.069101
6	0.419903	4.658603	-2.612056
6	0.896892	5.647966	-1.763270
1	1.581348	6.105491	0.231429
1	0.159742	4.892282	-3.640773
1	1.015904	6.662986	-2.128843
6	-0.196650	2.255752	-3.056134
1	0.645496	1.774690	-3.573163
1	-0.909364	2.615577	-3.804539
8	-0.858717	1.275503	-2.237587
6	-1.209043	0.117558	-3.014283
1	-0.304297	-0.426153	-3.308586
1	-1.753690	0.453681	-3.900992
1	-1.849551	-0.507553	-2.398632
6	-1.242804	-0.339082	-0.000443
6	-2.054598	-1.239045	0.145552
14	-3.306911	-2.586596	0.299766
6	-2.420877	-4.133255	0.895640
1	-3.133688	-4.957984	1.021090
1	-1.928658	-3.969024	1.861551
1	-1.658560	-4.457756	0.177312
6	-4.053211	-2.874785	-1.401198
1	-3.293326	-3.194208	-2.124112
1	-4.531245	-1.967198	-1.788103
1	-4.818470	-3.659816	-1.354637
6	-4.626005	-2.057045	1.525614
1	-4.200074	-1.888378	2.521722
1	-5.398985	-2.830408	1.616327
1	-5.114547	-1.129263	1.205705
35	-1.356221	2.222833	1.298542
6	1.945432	1.011911	0.955109
1	2.040103	1.683177	1.797939
6	2.439626	1.238659	-0.372262
6	1.321014	-0.274339	0.980957
1	3.007289	2.094134	-0.706882
6	2.095392	0.103495	-1.164420
1	0.859533	-0.738745	1.841728
6	1.420225	-0.835070	-0.341162
1	2.287050	-0.006801	-2.223991
1	1.021595	-1.788433	-0.658284

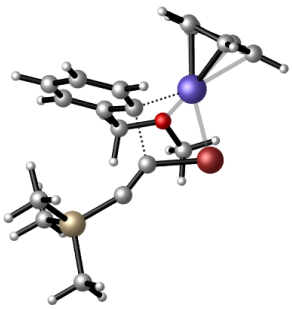
Int13b



E = -1186.697942 Hartrees
G = -1186.389073 Hartrees

6	-1.492050	-4.739663	1.240328
1	-2.140133	-5.372952	0.647936
6	-1.216124	-4.905696	2.667816
1	-1.566477	-5.725724	3.281703
6	-0.370660	-3.883659	3.063860
1	0.082215	-3.760234	4.038566
6	-0.896739	-3.527381	0.811853
1	-0.953579	-3.094607	-0.177128
6	-0.084582	-3.059404	1.893550
1	0.534038	-2.171219	1.885818
45	0.647603	-4.945538	1.287510
6	1.527266	-4.796309	-0.514312
6	2.924571	-4.680462	-0.514110
6	0.841425	-4.803617	-1.731648
6	3.614343	-4.550382	-1.722038
6	1.535926	-4.696254	-2.934773
1	-0.240260	-4.905147	-1.747837
6	2.923263	-4.557128	-2.929384
1	4.697225	-4.449177	-1.715582
1	0.993110	-4.713201	-3.875548
1	3.465921	-4.457747	-3.864804
6	3.675716	-4.747611	0.781911
1	4.257247	-3.839282	0.980442
1	4.357665	-5.605250	0.790913
8	2.723086	-4.914974	1.842444
6	3.256634	-5.530712	3.013522
1	4.119643	-4.956924	3.366101
1	2.473428	-5.519696	3.771910
1	3.559496	-6.561873	2.796184
6	2.398179	-8.005011	0.292553
6	3.444120	-8.188442	-0.295992
14	5.028450	-8.473272	-1.235321
35	0.834674	-7.726878	1.150406
6	4.654838	-8.190795	-3.049372
1	4.252140	-7.185938	-3.219603
1	5.569911	-8.296881	-3.644990
1	3.923520	-8.916567	-3.423348
6	6.296058	-7.251843	-0.588551
1	5.995494	-6.215917	-0.780172
1	6.458803	-7.372296	0.488617
1	7.258221	-7.415841	-1.090139
6	5.557449	-10.24023	-0.900430
1	5.735440	-10.41076	0.167633
1	4.799797	-10.95657	-1.237938
1	6.489816	-10.46228	-1.434339

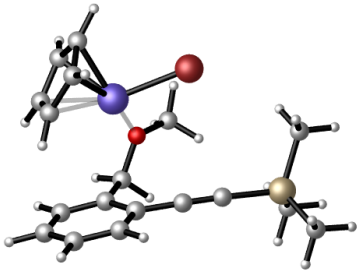
$TS_{13\text{-}14}b$



E = -1186.638864 Hartrees
G = -1186.331866 Hartrees

6	0.298126	-3.672236	2.731479
1	0.959527	-2.864672	3.016122
6	-0.932035	-3.533138	1.968392
1	-1.292359	-2.617700	1.517762
6	-1.501433	-4.798742	1.833660
1	-2.382564	-5.048123	1.257258
6	0.399906	-5.030377	3.155781
1	1.193996	-5.454192	3.755264
6	-0.646477	-5.752585	2.520067
1	-0.823127	-6.817407	2.596141
45	0.592725	-4.879571	0.995956
6	2.484462	-5.746466	0.858731
6	2.319615	-7.100339	0.425553
6	3.429831	-5.478608	1.888038
6	3.157168	-8.090762	0.900624
6	4.276948	-6.472261	2.341984
1	3.518110	-4.466061	2.272310
6	4.152955	-7.768965	1.831422
1	3.052617	-9.113989	0.550724
1	5.031766	-6.253507	3.090307
1	4.822359	-8.548531	2.182480
6	1.336237	-7.356068	-0.669735
1	0.888827	-8.353744	-0.611094
1	1.839951	-7.252759	-1.640752
8	0.297152	-6.372172	-0.576973
6	-0.363426	-6.105319	-1.814582
1	-0.790770	-7.034038	-2.205689
1	-1.160894	-5.392644	-1.603501
1	0.338980	-5.682862	-2.541290
6	3.134108	-4.802464	-0.626608
6	4.091689	-5.065473	-1.377740
14	5.522022	-6.000380	-2.046036
35	1.789924	-3.342023	-0.647366
6	6.838718	-6.167675	-0.711105
1	6.463949	-6.740756	0.144612
1	7.721050	-6.685496	-1.108569
1	7.166128	-5.188133	-0.342358
6	4.904162	-7.699976	-2.572355
1	4.482120	-8.248076	-1.721872
1	4.134306	-7.628731	-3.350001
1	5.730450	-8.297086	-2.978599
6	6.253200	-5.106298	-3.531417
1	5.512774	-4.982035	-4.330689
1	6.619786	-4.110132	-3.255601
1	7.099567	-5.670791	-3.942918

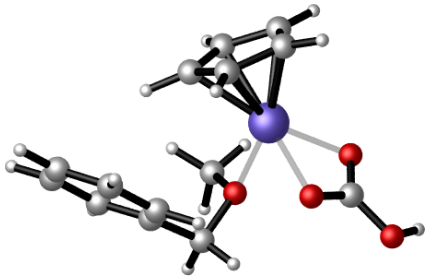
Int14b



E = -1186.769571 Hartrees
G = -1186.460327 Hartrees

6	0.493188	-3.420406	2.344137
1	1.207959	-2.684605	2.687317
6	-0.514374	-3.222081	1.363001
1	-0.701730	-2.312805	0.807728
6	-1.189738	-4.480028	1.173585
1	-1.966507	-4.674038	0.445013
6	0.395379	-4.784887	2.805229
1	1.065096	-5.254467	3.514516
6	-0.646699	-5.426775	2.100687
1	-0.932021	-6.466182	2.187321
45	0.857164	-4.685373	0.681264
6	3.418923	-6.831645	1.346901
6	2.178043	-7.505418	1.292334
6	4.017018	-6.586728	2.590980
6	1.597054	-7.961342	2.473557
6	3.414016	-7.036618	3.760975
1	4.968568	-6.066254	2.628634
6	2.212186	-7.739902	3.703812
1	0.652651	-8.496398	2.427100
1	3.894235	-6.852908	4.717028
1	1.750471	-8.108972	4.614206
6	1.505035	-7.725987	-0.030637
1	0.607488	-8.343560	0.077262
1	2.187787	-8.210109	-0.737934
8	1.127207	-6.456410	-0.596447
6	1.009323	-6.488328	-2.019545
1	0.346305	-7.309458	-2.311908
1	0.581226	-5.538905	-2.336334
1	1.998683	-6.619381	-2.470258
6	4.091700	-6.467998	0.135417
6	4.651285	-6.211643	-0.914571
14	5.523919	-5.901873	-2.517420
35	1.976064	-3.245504	-0.985697
6	7.363584	-5.780463	-2.159372
1	7.743526	-6.702184	-1.703368
1	7.921849	-5.611203	-3.088625
1	7.585966	-4.950486	-1.478496
6	5.162099	-7.366718	-3.637211
1	5.526900	-8.303685	-3.200173
1	4.086692	-7.476430	-3.821691
1	5.655202	-7.235622	-4.608737
6	4.885765	-4.313387	-3.285134
1	3.807281	-4.363276	-3.469867
1	5.074889	-3.449785	-2.638150
1	5.387468	-4.135139	-4.245012

Int1n



E = -953.139058 Hartrees
G = -952.903794 Hartrees

6	1.618148	-3.949278	2.047932
1	2.476518	-4.022529	2.703656
6	1.540261	-3.163255	0.867801
1	2.310997	-2.504334	0.491195
6	0.268079	-3.420642	0.247918
1	-0.083145	-2.994457	-0.682643
6	0.423522	-4.733027	2.144867
1	0.192242	-5.453052	2.917930
6	-0.422973	-4.368185	1.042434
1	-1.380959	-4.813023	0.807668
45	1.412869	-5.247085	0.345283
8	2.910646	-6.754975	0.717688
8	0.939302	-7.304132	-0.076441
6	2.115056	-7.630614	0.262210
8	2.300717	-5.357500	-1.672045
6	3.200140	-4.284154	-1.964540
1	3.911135	-4.237026	-1.138462
1	3.735860	-4.504619	-2.893102
1	2.669165	-3.331766	-2.059394
6	1.440466	-5.748056	-2.772876
1	2.042687	-5.700811	-3.685724
1	1.183298	-6.788174	-2.570320
6	0.209040	-4.892574	-2.863601
6	-0.976614	-5.320301	-2.259637
6	0.243803	-3.642896	-3.490079
6	-2.105342	-4.503931	-2.260291
1	-1.010441	-6.295594	-1.781068
6	-0.881155	-2.820945	-3.484764
1	1.153050	-3.314454	-3.987280
6	-2.055322	-3.248856	-2.865377
1	-3.022189	-4.847210	-1.790066
1	-0.844897	-1.851059	-3.971730
1	-2.932991	-2.608998	-2.864665
8	2.482480	-8.890703	0.122417
1	3.407657	-8.981964	0.413453

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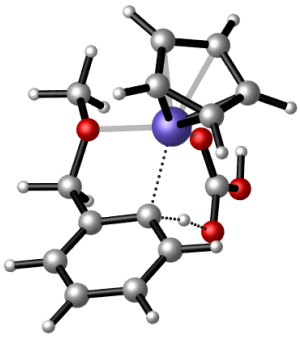
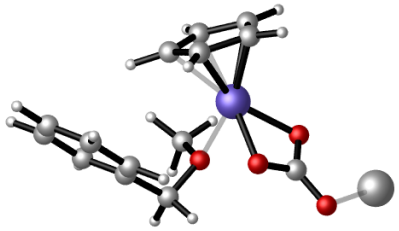


E = -953.101193 Hartrees
G = -952.869429 Hartrees

8	-1.250561	1.254474	0.938203
6	-1.851927	0.463577	0.165515
8	-1.316492	-0.463946	-0.506763
6	1.780868	1.753478	-0.449118
6	1.328792	0.933817	0.614288
6	2.813013	2.662261	-0.259238
6	1.956836	1.068048	1.867072
6	3.408859	2.778914	0.997813
6	2.982630	1.986437	2.062209
1	0.023488	0.977597	0.785940
1	3.157163	3.279883	-1.084022
1	1.602289	0.475298	2.705688
1	4.211307	3.495882	1.144193
1	3.447155	2.090003	3.037863
45	0.742907	-0.990068	-0.227150
6	2.502884	-2.193892	-0.069232
1	3.496943	-1.840518	-0.306951
6	1.598868	-2.865743	-0.971732
1	1.776683	-3.034407	-2.026152
6	0.411962	-3.164481	-0.276945
1	-0.478452	-3.612642	-0.696818
6	1.871704	-2.141755	1.208214
1	2.287534	-1.698257	2.101921
6	0.555508	-2.672291	1.072375
1	-0.190601	-2.731821	1.853651
6	1.105541	1.591065	-1.776658
1	1.650511	2.079546	-2.590364
1	0.083504	1.993871	-1.743856
8	1.043428	0.180845	-2.047624
6	0.234851	-0.137468	-3.183991
1	0.621196	0.394937	-4.058655
1	0.317950	-1.213497	-3.339660
1	-0.808385	0.136747	-3.001518
8	-3.166272	0.635406	0.055084
1	-3.510985	-0.042950	-0.551271

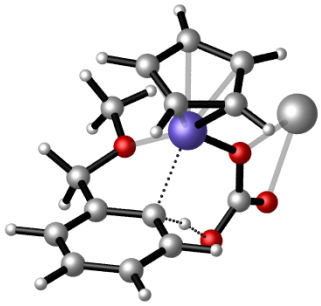
Int1o



E = -1098.337084 Hartrees
G = -1098.117886 Hartrees

6	1.654961	-3.938462	2.054482
1	2.518947	-3.993907	2.703983
6	1.547753	-3.159937	0.881896
1	2.301617	-2.489961	0.490999
6	0.264209	-3.434265	0.278676
1	-0.105236	-3.010709	-0.646118
6	0.469781	-4.746347	2.164392
1	0.252435	-5.457468	2.949832
6	-0.408043	-4.377112	1.085282
1	-1.370205	-4.823771	0.872623
45	1.426967	-5.276178	0.362782
8	2.850706	-6.763411	0.716157
8	0.883476	-7.224571	-0.104803
6	2.049519	-7.684992	0.234203
8	2.330861	-5.352139	-1.688223
6	3.188796	-4.247415	-1.970928
1	3.917146	-4.201013	-1.159726
1	3.709876	-4.420985	-2.918544
1	2.630366	-3.306928	-2.024542
6	1.468737	-5.744307	-2.781303
1	2.063392	-5.695742	-3.699910
1	1.215484	-6.784337	-2.574908
6	0.230424	-4.895998	-2.871320
6	-0.952376	-5.330400	-2.265964
6	0.253671	-3.649692	-3.504557
6	-2.088534	-4.525049	-2.273754
1	-0.973916	-6.300845	-1.777525
6	-0.878752	-2.837515	-3.505389
1	1.160044	-3.315533	-4.003450
6	-2.049963	-3.272939	-2.886164
1	-3.002758	-4.874311	-1.802588
1	-0.850603	-1.869983	-3.997799
1	-2.934133	-2.641955	-2.891061
8	2.394608	-8.878910	0.120214
47	4.546573	-8.795211	0.864087

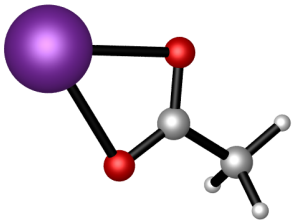
$TS_{1\text{-}2}o$



E = -1098.288339 Hartrees
G = -1098.074333 Hartrees

8	-1.514793	1.395847	0.404199
6	-2.110247	0.348374	0.000551
8	-1.424547	-0.783275	-0.160086
6	1.823904	1.680008	-0.344561
6	1.069663	1.043515	0.665899
6	2.967123	2.407195	-0.024728
6	1.510381	1.152960	1.998897
6	3.373031	2.506897	1.304464
6	2.648392	1.880430	2.321327
1	-0.195281	1.100238	0.531551
1	3.546535	2.889143	-0.808103
1	0.934466	0.671783	2.785201
1	4.266597	3.074220	1.548862
1	2.974745	1.965815	3.353367
45	0.617777	-0.955105	-0.185126
6	2.433018	-2.053596	-0.703852
1	3.163722	-1.678906	-1.408492
6	1.276325	-2.855014	-1.031730
1	0.998847	-3.192210	-2.021775
6	0.565679	-3.102453	0.166090
1	-0.376716	-3.627770	0.249223
6	2.417359	-1.808526	0.686295
1	3.128925	-1.205096	1.233620
6	1.229749	-2.413961	1.233715
1	0.926617	-2.401157	2.271630
6	1.393597	1.531178	-1.778673
1	2.251363	1.290188	-2.420351
1	0.923045	2.446819	-2.158025
8	0.437800	0.472316	-1.842741
6	0.097075	0.065699	-3.162345
1	0.965638	-0.372128	-3.668561
1	-0.698386	-0.674762	-3.070072
1	-0.268881	0.928804	-3.728274
8	-3.345240	0.293613	-0.254178
47	-3.426041	-1.909321	-0.944847

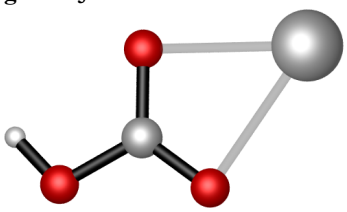
KOAc



E = -256.633763 Hartrees
G = -256.615211 Hartrees

6	0.096694	-0.861685	-0.680851
1	0.662950	-1.714709	-1.071366
1	-0.164371	-0.191538	-1.504136
1	-0.823956	-1.263279	-0.240899
6	0.911935	-0.141882	0.399909
8	1.322451	-0.848588	1.361248
8	1.110526	1.094891	0.261879
19	2.480065	1.212570	2.503125

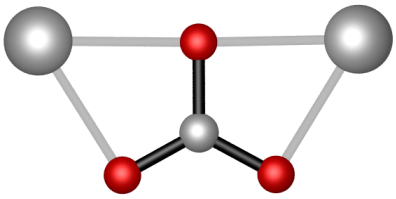
$AgHCO_3$



E = -410.109700 Hartrees
G = -410.112227 Hartrees

6	0.858198	-0.271812	0.393913
8	1.315405	-0.881007	1.389875
8	0.985075	0.959587	0.146830
47	2.282675	1.196824	2.130783
8	0.163208	-1.021587	-0.498560
1	-0.113649	-0.420974	-1.207777

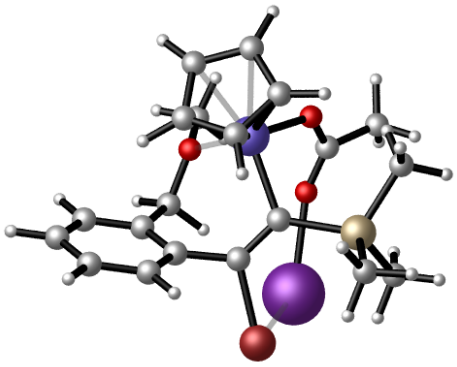
Ag_2CO_3



E = -555.284018 Hartrees
G = -555.302740 Hartrees

6	0.830665	-0.322676	0.359354
8	1.340382	-0.841462	1.412164
8	0.996306	0.969707	0.147511
47	2.257063	1.164772	2.113532
8	0.168310	-1.003800	-0.497633
47	-0.224982	0.829977	-1.851324

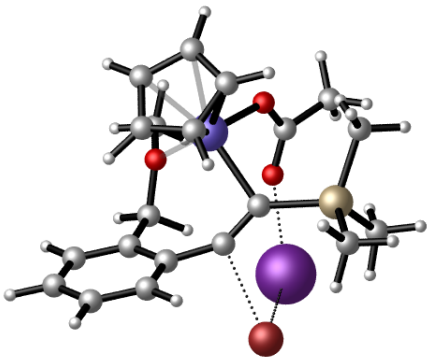
Int6d



E = -1443.448507 Hartrees
G = -1443.089301 Hartrees

6	-2.725016	-0.145285	0.587616
6	-4.495252	-1.917485	1.843958
6	-1.784321	0.726396	-0.164006
6	-0.622298	0.443832	-0.740859
6	-2.394759	-0.702436	1.830752
1	-3.019018	-2.025380	3.402495
6	-3.285278	-1.589036	2.443236
6	-3.950142	-0.473168	-0.006255
6	-4.826992	-1.355118	0.611367
1	-5.176783	-2.605998	2.333912
1	-5.768179	-1.603948	0.130653
1	-4.208131	-0.037385	-0.967195
6	0.223586	-2.459788	-2.206304
6	-1.160331	-2.294904	-1.869825
6	0.793123	-3.419926	-1.277649
1	-1.875651	-1.674381	-2.392130
1	1.824197	-3.748213	-1.273467
6	-1.385776	-2.992492	-0.659907
1	-2.316566	-3.026814	-0.109022
6	-0.177114	-3.730317	-0.329464
1	-0.043107	-4.349495	0.547769
1	0.719104	-2.061804	-3.079865
14	0.216306	1.473738	-2.112510
35	-2.613129	2.568881	-0.328954
6	1.681887	0.602363	-2.916455
1	1.345797	-0.063355	-3.719912
1	2.285861	0.019441	-2.217821
1	2.325388	1.360399	-3.381929
6	-1.049597	1.715875	-3.488334
1	-1.889048	2.356779	-3.203288
1	-1.456341	0.749707	-3.812633
1	-0.556912	2.171968	-4.356958
6	0.862189	3.154663	-1.533021
1	1.313668	3.650816	-2.401572
1	1.659285	3.046273	-0.787583
1	0.079987	3.831527	-1.170353
8	2.048444	-0.681376	-0.062840
6	2.385944	0.409447	0.516220
8	1.624854	1.165571	1.145576
6	3.847597	0.776903	0.351245
1	4.483122	-0.112171	0.355694
1	3.970123	1.268781	-0.622115
1	4.165297	1.471004	1.132425
6	-1.063866	-0.449433	2.470771
1	-1.119802	-0.627367	3.549927
1	-0.703444	0.568878	2.301866
8	-0.111410	-1.352431	1.908092
6	1.036562	-1.535247	2.734615
1	1.723223	-2.185537	2.193755
1	1.518195	-0.575857	2.943771
1	0.729882	-2.016186	3.670376
45	0.110864	-1.453132	-0.337862
19	0.121290	3.095883	1.598194

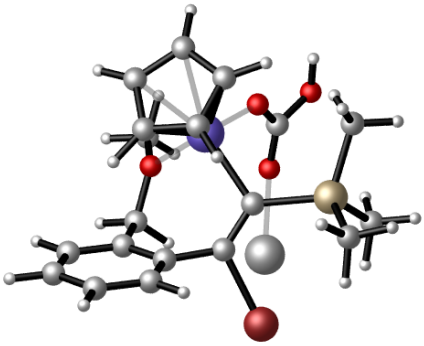
$TS_{6\text{-}7}$d



E = -1443.439781 Hartrees
G = -1443.082653 Hartrees

6	-2.696832	-0.189783	0.568708
6	-4.618444	-1.710360	1.897032
6	-1.661054	0.491252	-0.183948
6	-0.579900	0.430764	-0.852644
6	-2.410926	-0.711504	1.841470
1	-3.161260	-1.892848	3.468434
6	-3.381604	-1.476901	2.489179
6	-3.940590	-0.429405	-0.028316
6	-4.897439	-1.183712	0.635300
1	-5.364593	-2.302281	2.417907
1	-5.860803	-1.362683	0.168386
1	-4.147338	-0.010141	-1.007180
6	0.382350	-2.570820	-2.203384
6	-1.019731	-2.460009	-1.912150
6	0.970479	-3.427099	-1.200718
1	-1.742087	-1.885429	-2.476256
1	2.018391	-3.687604	-1.132263
6	-1.263342	-3.131322	-0.690868
1	-2.210486	-3.182816	-0.170622
6	-0.027995	-3.757191	-0.270201
1	0.112516	-4.317435	0.644871
1	0.888501	-2.170434	-3.069654
14	0.223984	1.496168	-2.199967
35	-2.673162	2.852702	-0.111987
6	1.649700	0.595028	-3.027886
1	1.285543	-0.111582	-3.782090
1	2.276801	0.051591	-2.315754
1	2.276296	1.328855	-3.550934
6	-1.120359	1.800358	-3.473072
1	-1.957402	2.357427	-3.040052
1	-1.506352	0.852569	-3.868162
1	-0.719394	2.374149	-4.318110
6	0.891162	3.121383	-1.522542
1	1.373908	3.655557	-2.350851
1	1.659550	2.963863	-0.756709
1	0.091277	3.771711	-1.152008
8	2.059024	-0.692809	-0.079874
6	2.339285	0.407393	0.522022
8	1.547274	1.093840	1.186630
6	3.770266	0.867085	0.329531
1	4.460885	0.020425	0.309710
1	3.840208	1.376562	-0.639899
1	4.059692	1.570294	1.113327
6	-1.061878	-0.522684	2.466731
1	-1.114980	-0.725710	3.541130
1	-0.670605	0.486925	2.319550
8	-0.130203	-1.437675	1.877898
6	1.013484	-1.657687	2.705203
1	1.695053	-2.302587	2.151433
1	1.505890	-0.710036	2.939898
1	0.695848	-2.157772	3.626802
45	0.171161	-1.539172	-0.363624
19	0.023344	3.063246	1.598769

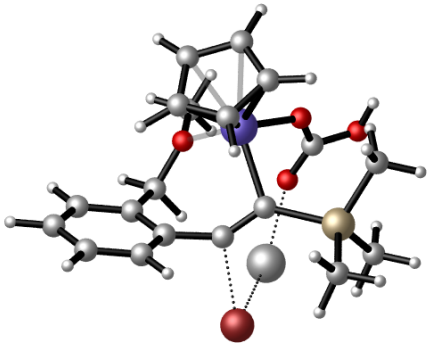
Int6e



E = -1596.913305 Hartrees
G = -1596.577696 Hartrees

6	-2.693431	-0.148369	0.602978
6	-4.575273	-1.900336	1.702966
6	-1.700253	0.709508	-0.089044
6	-0.590869	0.410658	-0.752328
6	-2.429352	-0.773816	1.829949
1	-3.167795	-2.141987	3.309614
6	-3.377322	-1.650668	2.363183
6	-3.903221	-0.396464	-0.054829
6	-4.838174	-1.268537	0.488382
1	-5.300384	-2.584553	2.132472
1	-5.769499	-1.456580	-0.036884
1	-4.102116	0.090336	-1.005567
6	0.294502	-2.598785	-2.175454
6	-1.093876	-2.358794	-1.925195
6	0.778326	-3.531971	-1.173066
1	-1.754265	-1.742006	-2.519243
1	1.792963	-3.900254	-1.098638
6	-1.409571	-2.985794	-0.691943
1	-2.369837	-2.967909	-0.193801
6	-0.251101	-3.755176	-0.265970
1	-0.187399	-4.327886	0.649972
1	0.857826	-2.256814	-3.031357
14	0.224922	1.445681	-2.146055
35	-2.363742	2.658266	-0.014400
6	1.498578	0.453617	-3.107955
1	1.022834	-0.262258	-3.786512
1	2.199012	-0.082025	-2.461587
1	2.073383	1.150552	-3.731750
6	-1.147139	1.879762	-3.360042
1	-1.858319	2.614485	-2.970822
1	-1.710087	0.981731	-3.644103
1	-0.703567	2.293727	-4.274715
6	1.107415	3.000526	-1.544037
1	1.482061	3.528182	-2.431516
1	1.979873	2.767012	-0.921664
1	0.465414	3.711564	-1.009896
8	2.083429	-0.699383	-0.153206
6	2.595322	0.281884	0.465603
8	2.069765	1.087658	1.255332
47	0.188041	2.311947	1.347411
6	-1.127563	-0.580187	2.545164
1	-1.209499	-0.932247	3.578865
1	-0.829419	0.479342	2.583085
8	-0.107082	-1.336413	1.891471
6	1.043022	-1.540001	2.711865
1	1.747422	-2.138835	2.134962
1	1.501846	-0.583737	2.978716
1	0.749921	-2.086867	3.615086
45	0.109558	-1.498713	-0.366468
8	3.916097	0.460922	0.251607
1	4.210490	-0.231518	-0.362326

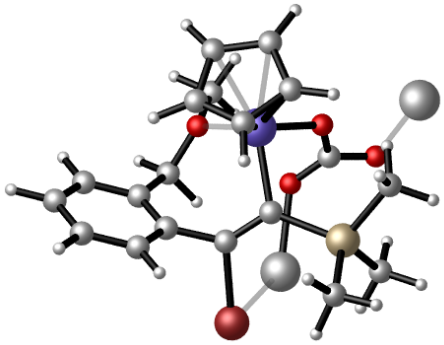
$TS_{6\text{-}7}e$



E = -1596.911467 Hartrees
G = -1596.575811 Hartrees

6	-2.673030	-0.189626	0.576656
6	-4.650977	-1.756905	1.764144
6	-1.629325	0.552027	-0.130753
6	-0.566002	0.375992	-0.844337
6	-2.435141	-0.771770	1.832108
1	-3.249645	-2.022383	3.373260
6	-3.432957	-1.559699	2.407264
6	-3.896600	-0.392413	-0.071689
6	-4.882597	-1.170296	0.520764
1	-5.417255	-2.367548	2.231235
1	-5.829393	-1.320790	0.011763
1	-4.067037	0.064676	-1.041794
6	0.405744	-2.678247	-2.174837
6	-0.995063	-2.486149	-1.948203
6	0.913990	-3.536801	-1.125641
1	-1.667040	-1.905112	-2.565323
1	1.943387	-3.851045	-1.015147
6	-1.311873	-3.094903	-0.705650
1	-2.278767	-3.086025	-0.219841
6	-0.128286	-3.782946	-0.227641
1	-0.051928	-4.316418	0.710673
1	0.968523	-2.332528	-3.029307
14	0.244393	1.433893	-2.210665
35	-2.296924	2.764796	0.157759
6	1.434003	0.400421	-3.230746
1	0.900038	-0.290802	-3.891926
1	2.131366	-0.167696	-2.608377
1	2.019901	1.072043	-3.871381
6	-1.160327	1.978244	-3.333355
1	-1.846167	2.671647	-2.837104
1	-1.740233	1.113097	-3.677481
1	-0.751942	2.479163	-4.220291
6	1.200555	2.920916	-1.563586
1	1.594575	3.455589	-2.438415
1	2.062132	2.643246	-0.945514
1	0.580289	3.636717	-1.011401
8	2.060672	-0.642021	-0.154340
6	2.441270	0.367298	0.518210
8	1.824895	1.016939	1.380016
47	0.080906	2.443342	1.396449
6	-1.116454	-0.617395	2.528126
1	-1.198240	-0.975023	3.559841
1	-0.786239	0.430247	2.566482
8	-0.122629	-1.398684	1.859896
6	1.008559	-1.673604	2.686820
1	1.706981	-2.262769	2.092634
1	1.486831	-0.743585	3.004660
1	0.685596	-2.255171	3.557668
45	0.151824	-1.557400	-0.388756
8	3.708679	0.760729	0.272881
1	4.074024	0.172410	-0.408294

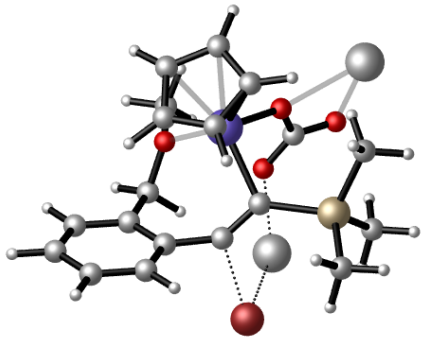
Int6f



E = -1742.098632 Hartrees
G = 1741.778248 Hartrees

6	-2.654318	-0.148720	0.594247
6	-4.585965	-1.782076	1.787345
6	-1.646020	0.665176	-0.124626
6	-0.559574	0.350208	-0.803604
6	-2.398477	-0.731877	1.842726
1	-3.165183	-2.012298	3.384862
6	-3.370114	-1.551349	2.421978
6	-3.879919	-0.380848	-0.040674
6	-4.840518	-1.192826	0.549442
1	-5.331387	-2.418112	2.254842
1	-5.785503	-1.366370	0.043707
1	-4.072345	0.075663	-1.007754
6	0.390393	-2.671611	-2.147496
6	-1.009378	-2.465496	-1.912574
6	0.888905	-3.567661	-1.122537
1	-1.678847	-1.876660	-2.524693
1	1.910860	-3.910829	-1.030109
6	-1.323723	-3.081632	-0.677029
1	-2.287168	-3.071281	-0.184586
6	-0.146539	-3.801053	-0.221103
1	-0.076141	-4.352487	0.707294
1	0.944702	-2.343199	-3.013779
14	0.246867	1.368624	-2.200901
35	-2.221695	2.649970	0.010651
6	1.386160	0.311718	-3.265736
1	0.817015	-0.325974	-3.951553
1	2.043706	-0.327172	-2.667272
1	2.010036	0.973999	-3.879677
6	-1.133724	1.931760	-3.355482
1	-1.748300	2.733429	-2.935158
1	-1.798501	1.097427	-3.611339
1	-0.693318	2.302281	-4.290409
6	1.252422	2.861504	-1.640175
1	1.677611	3.329950	-2.538347
1	2.091564	2.585539	-0.989923
1	0.645142	3.633498	-1.150932
8	2.031039	-0.608679	-0.094309
6	2.292484	0.496007	0.583542
8	1.468531	0.937607	1.444060
47	0.279204	2.795582	1.367519
6	-1.067277	-0.570186	2.511758
1	-1.148048	-0.818673	3.576020
1	-0.664350	0.442691	2.417231
8	-0.149930	-1.481825	1.902589
6	0.989078	-1.750620	2.716864
1	1.645047	-2.407201	2.144528
1	1.512934	-0.823572	2.960314
1	0.663489	-2.261594	3.630849
45	0.158532	-1.542428	-0.357169
8	3.412917	1.054994	0.343736
47	4.171332	-0.316137	-1.298216

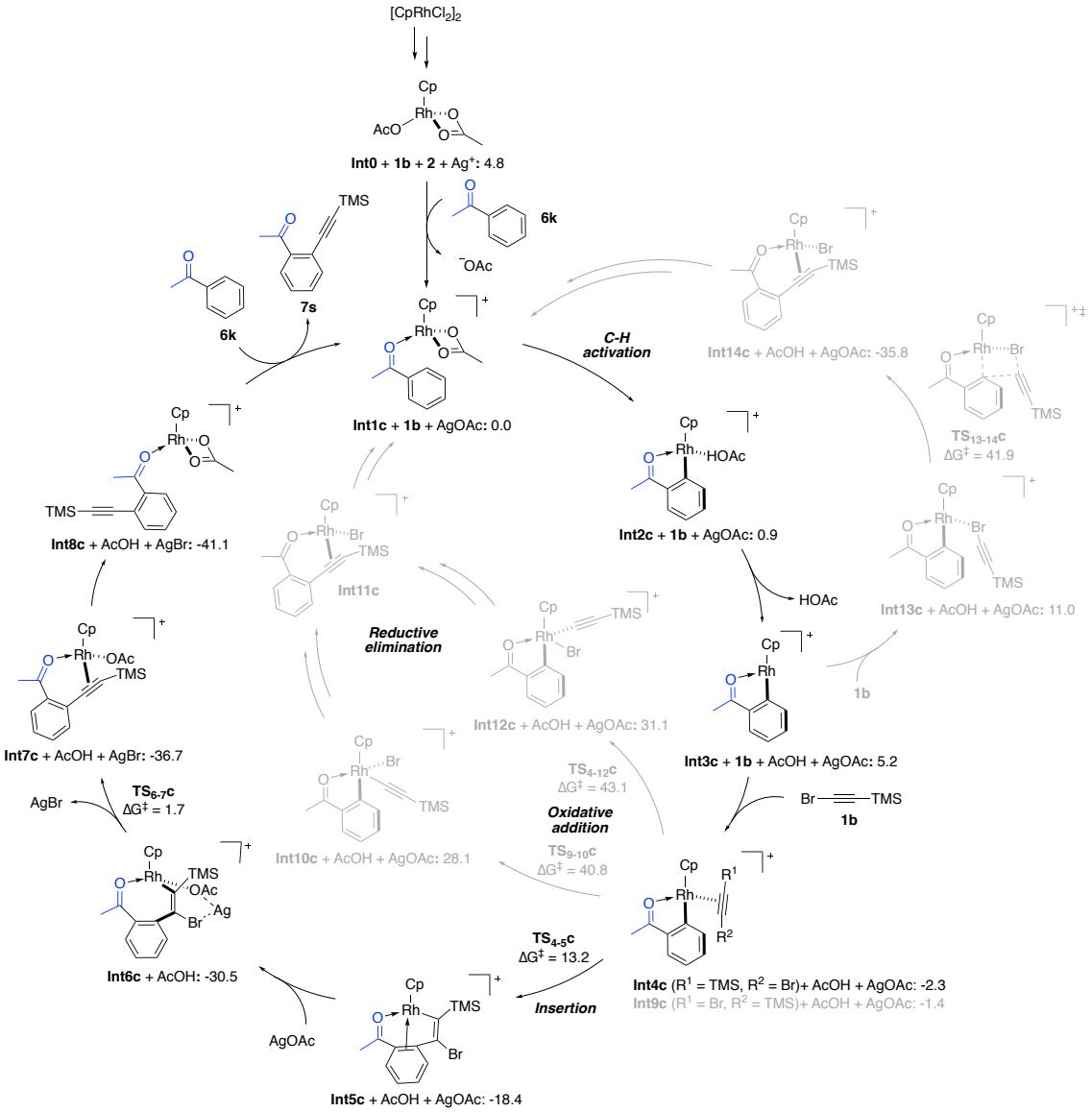
$TS_{6\text{-}7}$f



E = -1742.097573 Hartrees
G = -1741.777940 Hartrees

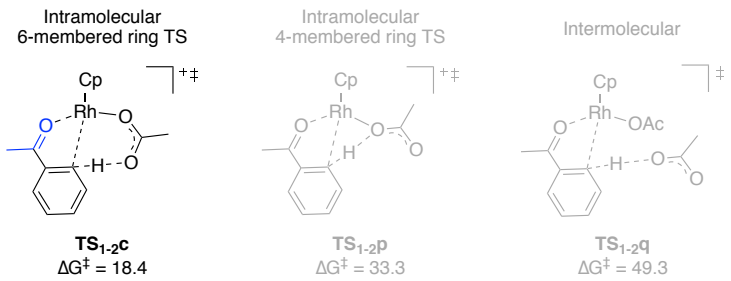
6	-2.659144	-0.214285	0.581290
6	-4.627661	-1.798175	1.766825
6	-1.621219	0.545829	-0.119518
6	-0.555650	0.364492	-0.831838
6	-2.418122	-0.798906	1.834004
1	-3.220982	-2.059536	3.372737
6	-3.410114	-1.594815	2.408603
6	-3.883360	-0.421765	-0.065147
6	-4.863822	-1.208558	0.525345
1	-5.389695	-2.415493	2.232428
1	-5.810298	-1.363555	0.016794
1	-4.058710	0.037914	-1.033333
6	0.484315	-2.645289	-2.192174
6	-0.925226	-2.486203	-1.974199
6	0.998532	-3.514038	-1.156803
1	-1.601839	-1.907394	-2.588429
1	2.031783	-3.813284	-1.040715
6	-1.244282	-3.130374	-0.754177
1	-2.215715	-3.154255	-0.278684
6	-0.049431	-3.795621	-0.274164
1	0.027271	-4.346395	0.654037
1	1.041892	-2.280533	-3.041915
14	0.227359	1.444610	-2.187540
35	-2.269212	2.727819	0.191947
6	1.341777	0.407869	-3.292909
1	0.759616	-0.237770	-3.959710
1	2.023614	-0.222790	-2.712081
1	1.942825	1.075523	-3.923218
6	-1.181752	2.054518	-3.273715
1	-0.772664	2.523440	-4.177911
1	-1.814841	2.789548	-2.767678
1	-1.819489	1.220196	-3.591032
6	1.250401	2.890323	-1.551951
1	2.089735	2.570883	-0.922322
1	0.656951	3.642567	-1.017267
1	1.677169	3.397764	-2.428158
8	2.043244	-0.607603	-0.104542
6	2.319905	0.473280	0.612495
8	1.512588	0.886575	1.499658
47	0.157423	2.631720	1.408707
6	-1.087345	-0.656495	2.508869
1	-1.170383	-0.943193	3.562926
1	-0.694902	0.364015	2.457165
8	-0.156868	-1.536981	1.872919
6	0.974130	-1.827984	2.693260
1	1.636873	-2.468970	2.111118
1	1.494729	-0.907494	2.966199
1	0.638210	-2.363177	3.589201
45	0.194675	-1.558393	-0.386899
8	3.440615	1.028273	0.371689
47	4.120844	-0.289205	-1.367513

7.4. Mechanism of the Rh-Catalyzed *ortho*-Alkynylation of Acetophenone



[a] Free energies in kcal/mol.

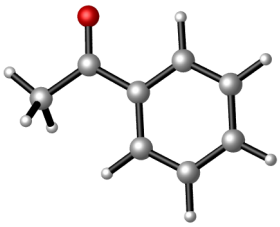
Scheme S7.4.1 - Rh-catalyzed *ortho*-alkynylation of acetophenone



[a] Free energies in kcal/mol.

Scheme S7.4.2 - Acetate-assisted C-H activation of acetophenone

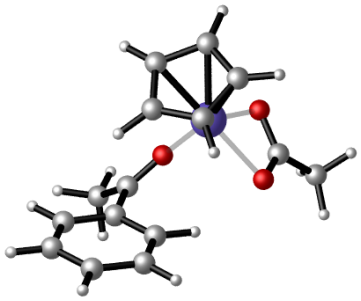
6k



E = -384.773156 Hartrees
G = -384.666479 Hartrees

6	0.852308	-0.643246	-0.195352
6	2.184525	-0.746468	-0.590387
6	3.024077	0.361604	-0.510794
6	2.535511	1.582719	-0.032663
6	1.195762	1.676332	0.362230
6	0.358056	0.570813	0.282651
1	0.198366	-1.508245	-0.259170
1	2.571219	-1.690147	-0.963439
1	4.059245	0.264829	-0.822819
1	0.825011	2.627522	0.730819
1	-0.680334	0.653919	0.589600
6	3.394787	2.807374	0.066395
8	2.930211	3.854119	0.487177
6	4.838869	2.716742	-0.364009
1	5.371777	1.960800	0.223678
1	4.911535	2.425669	-1.417926
1	5.317267	3.687831	-0.223547

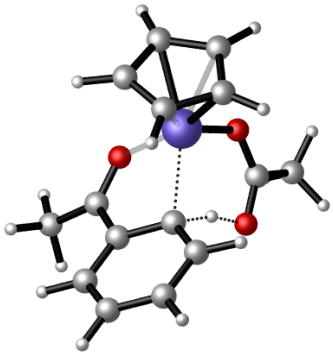
Int1c



E = -916.045039 Hartrees
G = -915.812138 Hartrees

8	-1.445809	-0.254124	0.406032
6	-2.136008	-0.473309	-0.639855
8	-1.586475	-1.150733	-1.564564
6	1.928879	1.820835	0.034315
6	1.233622	1.505439	1.208921
6	3.262896	2.238824	0.101915
6	1.874100	1.596182	2.438630
6	3.906473	2.297738	1.334330
6	3.213648	1.979341	2.501099
1	0.188631	1.214755	1.157086
1	3.810121	2.485307	-0.802779
1	1.328059	1.368518	3.348953
1	4.948416	2.597762	1.383968
1	3.715839	2.038735	3.461892
45	0.265643	-1.193050	-0.504447
6	2.051427	-2.248207	-1.071270
1	2.592911	-2.042083	-1.984900
6	0.983371	-3.173085	-0.924198
1	0.545037	-3.762997	-1.719040
6	0.492643	-3.084388	0.418451
1	-0.333108	-3.643787	0.836598
6	2.265139	-1.615740	0.202909
1	2.991066	-0.842242	0.414548
6	1.320699	-2.138779	1.117459
1	1.184376	-1.814013	2.140802
6	-3.531811	0.036206	-0.782437
1	-3.636232	0.558247	-1.737788
1	-4.223293	-0.813113	-0.788529
1	-3.785734	0.704799	0.041418
8	0.520998	0.711366	-1.529502
6	1.242217	1.684340	-1.271975
6	1.388105	2.763256	-2.294713
1	0.988354	3.697539	-1.883636
1	2.446406	2.940921	-2.514150
1	0.857939	2.497836	-3.210334

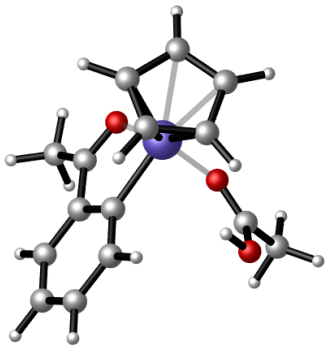
$TS_{1\text{-}2}$c



E = -916.010921 Hartrees
G = -915.782859 Hartrees

8	-1.374835	1.184772	0.601770
6	-1.967335	0.245594	0.004975
8	-1.377013	-0.788177	-0.437721
6	1.867270	1.668559	-0.265673
6	1.226896	0.884418	0.724141
6	2.899462	2.545989	0.059804
6	1.665893	1.001176	2.046600
6	3.327664	2.628644	1.383824
6	2.714221	1.861121	2.372836
1	-0.078691	0.864823	0.648605
1	3.383952	3.144968	-0.705162
1	1.169138	0.433949	2.828452
1	4.139685	3.299603	1.645183
1	3.048387	1.942126	3.402714
45	0.694098	-1.020137	-0.270283
6	2.454199	-2.191347	-0.776545
1	3.216317	-1.825843	-1.452350
6	1.264529	-2.914946	-1.158678
1	0.993424	-3.207636	-2.164046
6	0.519796	-3.169562	0.020333
1	-0.452550	-3.642570	0.063597
6	2.420287	-1.991755	0.621801
1	3.154053	-1.450712	1.203642
6	1.194777	-2.559572	1.123759
1	0.866597	-2.565350	2.153973
6	-3.446121	0.357477	-0.237607
1	-3.596401	0.930744	-1.159549
1	-3.895432	-0.628684	-0.364975
1	-3.926301	0.895527	0.581999
8	0.755789	0.419120	-1.891145
6	1.380252	1.465950	-1.641202
6	1.598303	2.475509	-2.714282
1	1.212879	3.449020	-2.393278
1	2.673460	2.593819	-2.893325
1	1.108697	2.160478	-3.636579

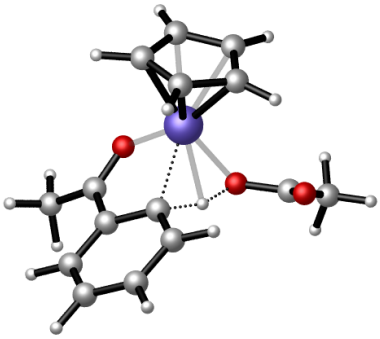
Int2c



E = -916.045118 Hartrees
G = -915.810661 Hartrees

8	-1.424185	0.017520	1.680005
6	-1.709295	0.253827	0.416996
8	-0.977965	-0.088655	-0.515206
6	1.899338	1.676587	-0.520678
6	1.657085	0.646772	0.412137
6	2.335448	2.943117	-0.109976
6	1.867084	0.911467	1.764158
6	2.538000	3.189006	1.240647
6	2.304950	2.173677	2.170495
1	-0.557738	-0.433694	1.737382
1	2.511795	3.726651	-0.841402
1	1.693755	0.142746	2.513111
1	2.878319	4.164455	1.572898
1	2.467344	2.366532	3.227324
45	0.970792	-1.053727	-0.415556
6	2.529085	-2.502100	-0.594185
1	3.473326	-2.280770	-1.074329
6	1.400044	-3.178307	-1.215914
1	1.333353	-3.454609	-2.259723
6	0.396255	-3.294353	-0.265139
1	-0.601517	-3.680342	-0.428368
6	2.231162	-2.322999	0.787728
1	2.887818	-1.889155	1.529500
6	0.872529	-2.702009	0.977114
1	0.334840	-2.695278	1.916661
6	-2.983939	0.994247	0.201656
1	-2.813329	2.048424	0.448608
1	-3.290742	0.914678	-0.841011
1	-3.763465	0.612969	0.865106
8	1.290281	0.143691	-2.150002
6	1.657166	1.312755	-1.912570
6	1.820138	2.272577	-3.042130
1	1.090422	3.084066	-2.938213
1	2.818042	2.722149	-3.016193
1	1.665953	1.763982	-3.994923

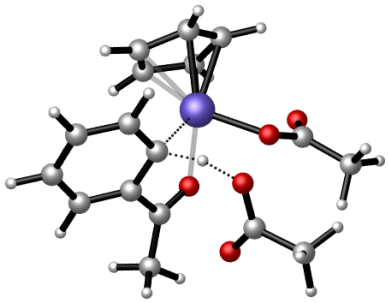
$TS_{1\text{-}2}p$



E = -915.988275 Hartrees
G = -915.759053 Hartrees

6	2.930605	-4.314444	1.841826
1	3.990050	-4.154167	1.983619
6	2.077944	-3.584434	0.934623
1	2.404613	-2.819599	0.242367
6	0.786346	-4.130429	1.013989
1	-0.063844	-3.850920	0.405757
6	2.121487	-5.257737	2.541807
1	2.468299	-5.966656	3.281604
6	0.810749	-5.202267	1.985203
1	-0.030878	-5.819085	2.271158
45	2.165554	-5.735725	0.436145
6	2.048920	-8.662182	0.091036
6	3.979239	-8.167867	1.468586
6	2.098705	-9.999310	0.471565
6	4.021583	-9.508052	1.860974
1	4.728432	-7.468168	1.825477
6	3.087292	-10.41411	1.366347
1	1.375390	-10.71590	0.095250
1	4.788406	-9.846326	2.550737
1	3.128119	-11.45425	1.673421
8	3.614599	-5.940145	-1.227398
8	5.409250	-5.294298	-0.028917
6	4.803613	-5.335229	-1.081084
6	5.294680	-4.730718	-2.369545
1	6.263892	-4.253237	-2.218714
1	5.377195	-5.508370	-3.135224
1	4.568757	-3.994215	-2.729181
6	2.994985	-7.730988	0.582650
1	3.503116	-6.899585	-0.350689
8	0.916834	-6.875393	-0.899854
6	1.023498	-8.112189	-0.816523
6	0.134332	-8.986409	-1.630008
1	0.738732	-9.657276	-2.250020
1	-0.473221	-9.612553	-0.966187
1	-0.517640	-8.379270	-2.259277

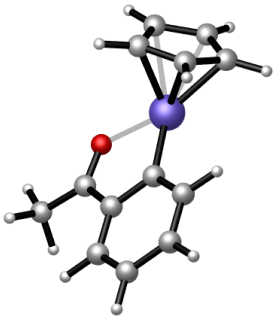
$TS_{1\text{-}2}q$



E = -1144.556545 Hartrees
G = -1144.285138 Hartrees

6	2.810343	-4.317656	2.260787
1	3.818800	-4.164721	2.619957
6	2.036377	-3.395057	1.497763
1	2.381257	-2.449334	1.104034
6	0.784939	-4.005029	1.201523
1	0.004122	-3.580746	0.587070
6	1.982519	-5.475038	2.516357
1	2.285723	-6.361013	3.057421
6	0.749202	-5.285766	1.866712
1	-0.060408	-6.002166	1.819546
45	2.355081	-5.205417	0.369042
6	2.559711	-8.050200	-0.250923
6	4.267440	-7.624190	1.392008
6	2.348184	-9.321992	0.273698
6	4.043376	-8.884083	1.943564
1	5.044998	-6.986499	1.804499
6	3.088542	-9.731774	1.383110
1	1.599934	-9.983324	-0.154052
1	4.621649	-9.214656	2.801526
1	2.920503	-10.71652	1.808610
8	3.357702	-4.306183	-1.160468
6	2.781862	-3.353510	-1.827595
8	1.715694	-2.809800	-1.546414
6	3.579238	-2.965092	-3.061569
1	3.152608	-2.076125	-3.531354
1	4.625816	-2.780628	-2.801324
1	3.558512	-3.797041	-3.774357
8	5.279776	-6.344557	-1.462370
8	3.771471	-7.160801	-2.917133
6	4.855060	-6.619457	-2.636428
6	5.812331	-6.232988	-3.761527
1	5.987735	-5.151484	-3.741022
1	6.782795	-6.720489	-3.615677
1	5.408144	-6.514538	-4.737128
6	3.528326	-7.174021	0.288928
1	4.207892	-6.526704	-0.526833
8	1.424144	-6.279184	-1.251549
6	1.711271	-7.484522	-1.323107
6	1.097055	-8.340758	-2.377408
1	0.707413	-7.717507	-3.183535
1	1.830187	-9.049858	-2.766164
1	0.268451	-8.906807	-1.932835

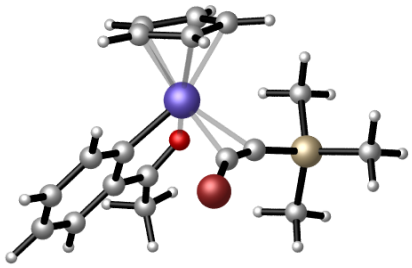
Int3c



E = -687.000304 Hartrees
G = -686.823898 Hartrees

6	2.852516	-4.297149	2.156129
1	3.868943	-4.172249	2.506391
6	2.207630	-3.484942	1.128323
1	2.699054	-2.719503	0.542181
6	0.909720	-3.935680	0.969133
1	0.191475	-3.594388	0.235877
6	1.889691	-5.176731	2.699025
1	2.033339	-5.878219	3.509266
6	0.716295	-5.063831	1.874659
1	-0.205438	-5.616632	2.002762
45	2.278920	-5.770653	0.682243
6	2.178571	-8.621040	0.215877
6	3.453838	-8.145801	2.206499
6	2.420306	-9.991912	0.362013
6	3.693904	-9.515091	2.350005
1	3.867840	-7.453407	2.933766
6	3.178708	-10.43674	1.437509
1	2.024054	-10.70216	-0.358262
1	4.287972	-9.867030	3.188865
1	3.370082	-11.49696	1.567478
6	2.689870	-7.681277	1.138442
8	1.296664	-6.799126	-0.916849
6	1.424124	-8.042144	-0.891842
6	0.823643	-8.858410	-1.984023
1	1.614019	-9.405197	-2.510793
1	0.136630	-9.600540	-1.563153
1	0.290704	-8.215574	-2.685933

Int4c



E = -1185.546161 Hartrees
G = -1185.259339 Hartrees

6	2.125062	-3.294799	1.555962
1	3.060975	-2.770308	1.414579
6	0.847907	-2.910665	0.989519
1	0.690226	-2.104197	0.286211
6	-0.104553	-3.830443	1.427477
1	-1.141980	-3.871911	1.122970
6	1.907867	-4.391979	2.440225
1	2.659914	-4.885350	3.040153
6	0.552808	-4.794128	2.291181
1	0.070166	-5.615014	2.804624
45	1.549166	-5.017887	0.365854
6	2.649253	-6.702370	0.567891
6	2.073940	-7.833520	-0.047348
6	3.858083	-6.852308	1.242144
6	2.701461	-9.087155	0.004460
6	4.473035	-8.102537	1.298609
1	4.334669	-6.003401	1.722255
6	3.902984	-9.219367	0.681046
1	2.246594	-9.946750	-0.479006
1	5.414562	-8.207484	1.830379
1	4.398383	-10.18319	0.733065
6	1.925160	-4.402398	-1.759095
6	3.034122	-4.613526	-1.230377
35	4.861023	-4.643847	-1.239948
14	0.557077	-4.019326	-2.989597
6	-1.035309	-3.676017	-2.069600
1	-0.937466	-2.824504	-1.388113
1	-1.830120	-3.441274	-2.788639
1	-1.349097	-4.552188	-1.492741
6	1.163296	-2.508633	-3.920175
1	2.118979	-2.699880	-4.421380
1	0.433128	-2.217760	-4.685391
1	1.298879	-1.656504	-3.244055
6	0.411491	-5.526217	-4.092766
1	0.114390	-6.408271	-3.514510
1	-0.346109	-5.360753	-4.868830
1	1.361826	-5.748152	-4.591600
8	0.329006	-6.437798	-0.637293
6	0.804824	-7.593553	-0.707061
6	0.054029	-8.644981	-1.449415
1	-0.160994	-9.488270	-0.784089
1	-0.879473	-8.238376	-1.840815
1	0.668062	-9.024446	-2.273466

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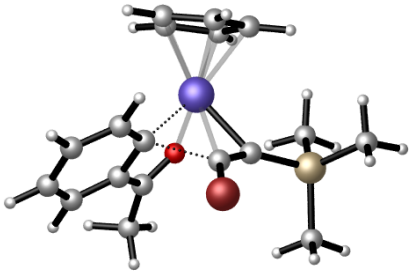
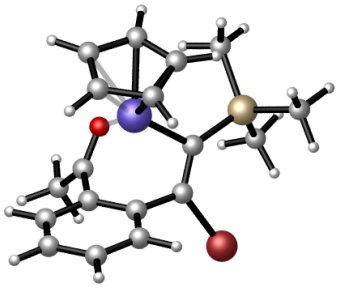


E = -1185.525351 Hartrees
G = -1185.238304 Hartrees

6	2.114477	-3.315591	1.525556
1	3.091145	-2.870229	1.387862
6	0.901925	-2.895854	0.876794
1	0.823083	-2.124238	0.122992
6	-0.125585	-3.754801	1.305806
1	-1.153037	-3.747871	0.967538
6	1.786567	-4.352990	2.466460
1	2.487077	-4.868242	3.109498
6	0.425496	-4.658247	2.303388
1	-0.125238	-5.432150	2.821684
45	1.410841	-5.018832	0.354277
6	2.761510	-6.623295	0.241632
6	2.107743	-7.844361	-0.037104
6	4.009382	-6.651732	0.872214
6	2.727210	-9.066716	0.252383
6	4.590933	-7.868586	1.203794
1	4.531439	-5.724385	1.086481
6	3.964839	-9.076389	0.877013
1	2.225237	-10.00032	0.018278
1	5.551715	-7.880059	1.709332
1	4.445146	-10.01909	1.117195
6	1.687203	-4.829102	-1.710216
6	2.762381	-5.423164	-1.369761
35	4.472556	-5.612041	-2.106568
14	0.565387	-4.018697	-2.972467
6	-1.139535	-3.829235	-2.220943
1	-1.134431	-3.092015	-1.410297
1	-1.852505	-3.483613	-2.979852
1	-1.505780	-4.781019	-1.820442
6	1.325309	-2.351459	-3.373346
1	2.328141	-2.462679	-3.801506
1	0.705338	-1.811690	-4.099795
1	1.406755	-1.727510	-2.475458
6	0.549046	-5.174523	-4.449142
1	0.181633	-6.167594	-4.164607
1	-0.109669	-4.785322	-5.235348
1	1.551783	-5.292700	-4.875982
8	0.179262	-6.629182	-0.432409
6	0.746651	-7.732970	-0.548282
6	0.029760	-8.871837	-1.190312
1	-0.088706	-9.687966	-0.468395
1	-0.952619	-8.549063	-1.538091
1	0.617786	-9.257672	-2.029759

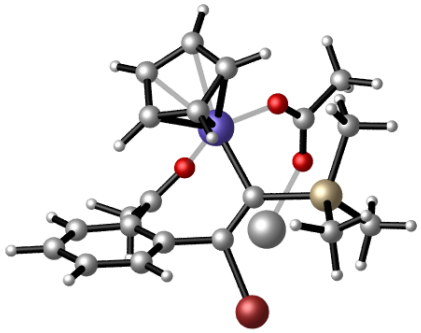
Int5c



E = -1185.572444 Hartrees
G = -1185.284928 Hartrees

6	2.049855	-3.813768	1.566560
1	3.097154	-3.554551	1.482694
6	0.979213	-3.212101	0.855600
1	1.058625	-2.436862	0.105891
6	-0.208933	-3.915415	1.228513
1	-1.202337	-3.738034	0.837996
6	1.486283	-4.757684	2.526665
1	2.064957	-5.372374	3.203931
6	0.115103	-4.810727	2.330600
1	-0.585460	-5.466353	2.830164
45	1.131789	-5.299685	0.333448
6	2.983863	-6.767898	-0.626673
6	2.146601	-7.781776	-0.092104
6	4.256453	-6.585410	-0.054890
6	2.600133	-8.588929	0.960600
6	4.680589	-7.369728	1.004807
1	4.912275	-5.825113	-0.468126
6	3.853838	-8.376994	1.510745
1	1.954107	-9.367429	1.354303
1	5.663359	-7.207921	1.435472
1	4.192793	-8.998271	2.333228
6	1.564794	-5.061852	-1.654030
6	2.549269	-5.938358	-1.793306
35	3.545134	-6.276294	-3.430332
14	0.669282	-3.924710	-2.865372
6	-1.022821	-3.512201	-2.154806
1	-0.964676	-2.782075	-1.340263
1	-1.655913	-3.076311	-2.937871
1	-1.530811	-4.408259	-1.779336
6	1.700018	-2.363780	-3.054467
1	2.685325	-2.586489	-3.480450
1	1.200920	-1.648463	-3.719886
1	1.854855	-1.868816	-2.087986
6	0.419235	-4.783920	-4.519932
1	-0.024571	-5.778504	-4.391624
1	-0.266155	-4.189524	-5.137703
1	1.354132	-4.901779	-5.075846
8	-0.013570	-6.990206	-0.495940
6	0.743045	-7.962759	-0.575810
6	0.283261	-9.269663	-1.110423
1	0.467255	-10.06166	-0.375504
1	-0.777324	-9.229860	-1.362823
1	0.877109	-9.516137	-1.998817

Int6c



E = -1559.818870 Hartrees
G = -1559.486969 Hartrees

6	-2.767515	-0.101252	0.529584
6	-4.619379	-1.867406	1.705347
6	-1.843759	0.827170	-0.195564
6	-0.680853	0.550785	-0.815326
6	-2.487093	-0.719079	1.764188
1	-3.210066	-2.038589	3.309618
6	-3.427939	-1.572942	2.353796
6	-3.986579	-0.389106	-0.091616
6	-4.893789	-1.275796	0.474943
1	-5.328889	-2.551790	2.158355
1	-5.821539	-1.495812	-0.043618
1	-4.223317	0.083071	-1.040030
6	0.555442	-2.521836	-1.938183
6	-0.853310	-2.318111	-1.841864
6	0.972252	-3.335610	-0.810911
1	-1.475289	-1.787450	-2.550285
1	1.987947	-3.648019	-0.608481
6	-1.267729	-2.841295	-0.585971
1	-2.276136	-2.838859	-0.194638
6	-0.131231	-3.519798	0.014254
1	-0.136067	-4.009134	0.979576
1	1.191707	-2.228458	-2.760355
14	0.081453	1.546965	-2.277232
35	-2.756772	2.589147	-0.466752
6	1.409307	0.549505	-3.151327
1	0.971508	-0.258793	-3.747250
1	2.148874	0.128580	-2.464726
1	1.927469	1.218414	-3.850975
6	-1.273502	1.856251	-3.552099
1	-1.862213	2.754869	-3.348296
1	-1.966701	1.008638	-3.619440
1	-0.805671	1.978847	-4.537529
6	0.860572	3.164291	-1.702267
1	1.201038	3.717226	-2.587844
1	1.740530	2.985968	-1.072130
1	0.165962	3.819158	-1.162417
8	2.123991	-0.379166	-0.119414
6	2.760159	0.574549	0.422770
8	2.290360	1.516164	1.109811
47	0.112313	1.967583	1.139308
6	4.252015	0.590474	0.155115
1	4.644817	-0.421741	0.037137
1	4.422015	1.133006	-0.782898
1	4.783463	1.113375	0.953101
45	0.161245	-1.251590	-0.263920
8	-0.119387	-0.618983	1.809109
6	-1.184190	-0.546791	2.441590
6	-1.134336	-0.279349	3.909290
1	-1.832754	0.520758	4.172924
1	-1.447454	-1.176780	4.456486
1	-0.116339	-0.022589	4.207268

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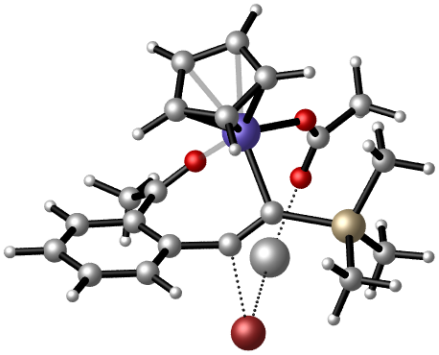
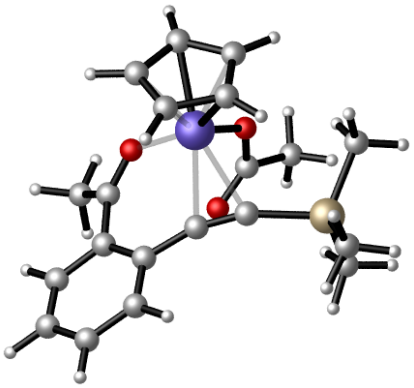


E = -1559.813585 Hartrees
G = -1559.484248 Hartrees

6	-2.735313	-0.175810	0.464737
6	-4.730180	-1.641898	1.770450
6	-1.728986	0.594654	-0.273662
6	-0.670319	0.455688	-1.001082
6	-2.484619	-0.737335	1.732365
1	-3.311051	-1.890573	3.356980
6	-3.496051	-1.452087	2.381838
6	-3.985466	-0.358135	-0.130163
6	-4.972987	-1.094887	0.512761
1	-5.500908	-2.213033	2.277295
1	-5.935280	-1.236296	0.031470
1	-4.180361	0.089587	-1.099507
6	0.595695	-2.653090	-2.025115
6	-0.820537	-2.562753	-1.846035
6	1.146462	-3.339550	-0.877353
1	-1.525060	-2.118806	-2.536610
1	2.196492	-3.540391	-0.711367
6	-1.118529	-3.057383	-0.547354
1	-2.097537	-3.093776	-0.088662
6	0.106409	-3.577136	0.027256
1	0.204433	-4.004549	1.016577
1	1.151359	-2.351941	-2.901260
14	0.110424	1.504854	-2.385067
35	-2.455115	2.777405	0.041844
6	1.339195	0.473013	-3.354344
1	0.847714	-0.345085	-3.892488
1	2.116507	0.056641	-2.706351
1	1.823029	1.112425	-4.103967
6	-1.313232	1.969433	-3.521022
1	-2.033282	2.631071	-3.028432
1	-1.849494	1.074845	-3.860607
1	-0.929996	2.485743	-4.410256
6	0.985818	3.039721	-1.742301
1	1.456932	3.540767	-2.598619
1	1.780494	2.805596	-1.025408
1	0.298052	3.760600	-1.285826
8	2.034989	-0.310696	-0.226058
6	2.541044	0.603658	0.499526
8	1.946354	1.405836	1.255894
47	-0.060643	2.344935	1.258972
6	4.045992	0.741237	0.372294
1	4.520898	-0.237717	0.271830
1	4.263255	1.314126	-0.537284
1	4.460839	1.277601	1.227796
45	0.192221	-1.360453	-0.376398
8	-0.108916	-0.746345	1.704735
6	-1.147179	-0.625107	2.363614
6	-1.043286	-0.342857	3.828026
1	-1.670487	0.515094	4.091631
1	-1.412020	-1.202160	4.400350
1	-0.001931	-0.156008	4.094569

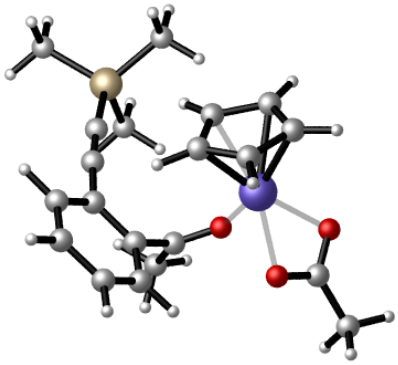
Int7c



E = -1400.800083 Hartrees
G = -1400.462265 Hartrees

6	-2.471882	-0.313668	0.537949
6	-4.537059	-0.367191	2.422604
6	-1.458695	-0.178477	-0.468476
6	-0.786147	0.190228	-1.438845
6	-2.193663	-0.685217	1.871081
1	-3.044254	-0.959308	3.832712
6	-3.238838	-0.687380	2.801515
6	-3.779735	0.021344	0.168879
6	-4.807357	-0.015038	1.103778
1	-5.333201	-0.390661	3.159199
1	-5.817609	0.241254	0.801417
1	-3.978529	0.316345	-0.856108
6	1.391359	-2.824761	-2.007504
6	0.077854	-2.599553	-2.508435
6	1.279699	-3.581132	-0.802222
1	-0.176632	-2.035485	-3.395827
1	2.094413	-3.903018	-0.167926
6	-0.858731	-3.268503	-1.642768
1	-1.934324	-3.276148	-1.752090
6	-0.114948	-3.877610	-0.607294
1	-0.531735	-4.401357	0.243650
1	2.302573	-2.413454	-2.420414
14	0.024605	1.269343	-2.747983
6	1.686157	0.550743	-3.218532
1	1.580409	-0.377177	-3.791035
1	2.278254	0.340025	-2.322223
1	2.236685	1.265677	-3.842361
6	-1.164685	1.300095	-4.196916
1	-2.157036	1.651816	-3.891755
1	-1.278386	0.305385	-4.644032
1	-0.794298	1.977829	-4.976147
6	0.190982	2.944437	-1.923766
1	0.780009	3.625542	-2.550024
1	0.687929	2.856268	-0.951084
1	-0.791835	3.400610	-1.757246
8	1.753955	-0.411398	-0.104530
6	1.650407	0.642441	0.660107
8	0.663746	0.990061	1.301306
6	2.926779	1.465997	0.660122
1	3.800747	0.829641	0.826511
1	3.046852	1.943262	-0.319546
1	2.877804	2.239039	1.429619
45	0.227127	-1.718700	-0.534868
8	-0.043236	-1.698529	1.581515
6	-0.856715	-1.135756	2.322752
6	-0.482982	-1.001574	3.767231
1	-0.997844	-1.771600	4.354148
1	0.592934	-1.145495	3.871672
1	-0.775285	-0.023956	4.158428

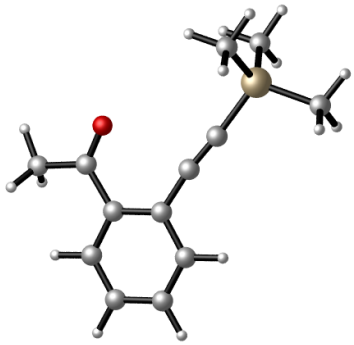
Int8c



E = -1400.801560 Hartrees
G = -1400.469227 Hartrees

6	2.554770	-3.204772	0.556614
1	3.626106	-3.082703	0.644159
6	1.777091	-2.952276	-0.601045
1	2.157170	-2.628057	-1.562552
6	0.418236	-3.312078	-0.321637
1	-0.416632	-3.246125	-1.005283
6	1.675733	-3.718598	1.575878
1	1.966668	-4.033834	2.569154
6	0.359141	-3.756665	1.035235
1	-0.518232	-4.146532	1.535011
45	1.648546	-5.056483	-0.079340
8	2.826593	-6.723519	0.624608
8	0.704242	-6.944460	0.226243
6	1.816117	-7.484676	0.537796
6	1.922623	-8.960046	0.738083
1	1.010749	-9.348259	1.197367
1	2.041423	-9.434560	-0.242954
1	2.792293	-9.202953	1.351422
6	0.207833	-5.247832	-3.078959
6	-0.878506	-5.887933	-2.486842
6	0.054966	-3.982797	-3.674962
6	-2.130293	-5.278738	-2.504886
1	-0.739509	-6.850112	-2.004294
6	-1.209671	-3.382307	-3.685654
6	-2.295112	-4.032676	-3.108016
1	-2.977303	-5.777891	-2.045424
1	-1.328429	-2.402734	-4.136975
1	-3.271847	-3.559921	-3.120894
6	1.216170	-3.310828	-4.174217
6	2.268368	-2.812822	-4.529505
14	3.931822	-2.172377	-5.037342
6	4.782341	-1.539210	-3.487747
1	5.777631	-1.147381	-3.731847
1	4.212056	-0.728857	-3.018842
1	4.912235	-2.338661	-2.748323
6	4.855729	-3.631197	-5.772310
1	4.332538	-4.030947	-6.648733
1	5.862355	-3.332482	-6.090353
1	4.962011	-4.441913	-5.041728
6	3.689858	-0.802192	-6.294794
1	3.131047	0.038894	-5.868339
1	4.661156	-0.420681	-6.633478
1	3.145448	-1.160310	-7.176195
8	2.205736	-5.935551	-1.991738
6	1.555408	-5.893892	-3.038785
6	2.087603	-6.530169	-4.276288
1	3.101046	-6.902510	-4.119171
1	1.420023	-7.356324	-4.551613
1	2.065741	-5.812261	-5.103277

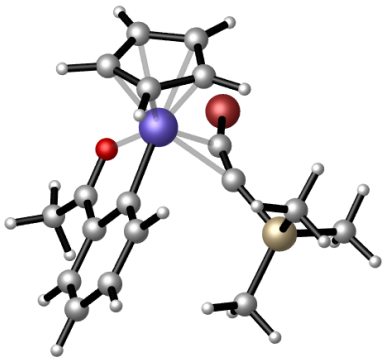
7s



E = -869.524316 Hartrees
G = -869.318095 Hartrees

6	1.134758	-0.668874	-0.303289
6	2.516228	-0.540099	-0.242183
6	3.121879	0.720922	-0.126766
6	2.307409	1.877236	-0.073811
6	0.918516	1.720948	-0.143761
6	0.330743	0.466386	-0.255288
1	0.688698	-1.654626	-0.391975
1	3.148790	-1.421100	-0.285282
1	0.277028	2.594425	-0.106723
1	-0.749816	0.376948	-0.305146
6	4.555571	0.736860	-0.093220
6	5.765473	0.598895	-0.094328
14	7.609055	0.520170	-0.102441
6	8.228065	1.571664	-1.531751
1	7.890049	2.610205	-1.437180
1	9.325044	1.575047	-1.558919
1	7.869661	1.186606	-2.493778
6	8.237263	1.190418	1.536417
1	7.861821	0.601359	2.381290
1	9.333735	1.158607	1.566526
1	7.927427	2.231180	1.686659
6	8.134307	-1.269857	-0.328210
1	7.745512	-1.686696	-1.264919
1	9.228604	-1.346818	-0.357560
1	7.777135	-1.899838	0.494981
6	2.901172	3.248889	0.065959
6	1.979930	4.445437	-0.022183
1	1.419448	4.445701	-0.963390
1	1.253076	4.439306	0.797881
1	2.581060	5.354244	0.042333
8	4.094883	3.404171	0.250574

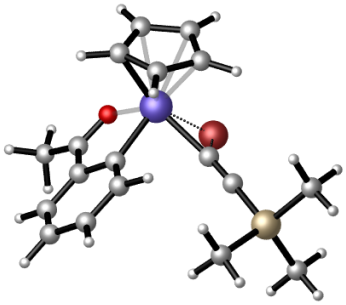
Int9c



E = -1185.543915 Hartrees
G = -1185.257799 Hartrees

45	0.480120	1.252720	0.075390
6	0.057079	3.156744	-0.483165
6	0.411663	4.340274	0.161279
6	-0.634219	3.244536	-1.709296
6	0.078016	5.571749	-0.402587
1	0.945381	4.323645	1.105025
6	-0.989516	4.484276	-2.260890
6	-0.630698	5.650369	-1.604176
1	0.369467	6.484582	0.109379
1	-1.530362	4.529295	-3.201704
1	-0.889313	6.616621	-2.024376
6	1.772276	0.992732	1.810806
1	1.481982	1.293040	2.808859
6	2.462305	1.799298	0.861782
6	1.637382	-0.338297	1.256291
1	2.744056	2.834481	0.991459
6	2.608123	1.032604	-0.326665
1	1.171132	-1.179843	1.750725
6	2.133070	-0.310236	-0.049547
1	3.073109	1.362232	-1.246152
1	2.111192	-1.125116	-0.761667
35	-2.032359	-1.256608	0.126174
6	-1.431056	0.380688	0.663345
6	-1.479819	1.479621	1.248758
14	-2.137943	2.761909	2.450455
6	-3.442759	1.811590	3.407529
1	-3.912603	2.460604	4.157029
1	-4.231106	1.438838	2.743377
1	-3.006636	0.953095	3.931216
6	-2.913531	4.168306	1.489965
1	-3.461349	4.823431	2.179032
1	-2.173637	4.775998	0.961558
1	-3.631381	3.786545	0.754584
6	-0.735744	3.278813	3.579039
1	-0.358555	2.415689	4.139859
1	0.100300	3.731932	3.038161
1	-1.097056	4.013823	4.309054
8	-0.420894	0.945168	-1.817800
6	-0.879122	1.972834	-2.364929
6	-1.619693	1.840906	-3.651094
1	-1.082738	2.374981	-4.443105
1	-1.720503	0.788952	-3.921480
1	-2.610421	2.298485	-3.558882

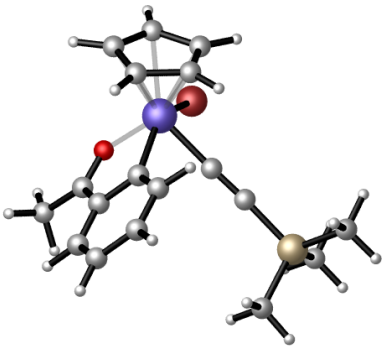
$TS_{9\text{-}10}c$



E = -1185.476722 Hartrees
G = -1185.192919 Hartrees

45	0.431354	1.024710	-0.378744
6	-0.235169	2.862387	-0.968644
6	-0.267028	4.023012	-0.209958
6	-0.641349	2.905612	-2.315690
6	-0.698721	5.213196	-0.793981
1	0.012601	4.009016	0.837246
6	-1.088101	4.104604	-2.892014
6	-1.112416	5.259422	-2.128080
1	-0.719948	6.117621	-0.192536
1	-1.407097	4.122428	-3.929813
1	-1.453826	6.193508	-2.561197
6	1.748709	0.671496	1.360551
1	1.353498	0.609749	2.365524
6	2.136653	1.872318	0.694719
6	2.043882	-0.450998	0.502430
1	2.078728	2.872243	1.100402
6	2.521338	1.510620	-0.627534
1	1.863146	-1.490769	0.737842
6	2.494973	0.058822	-0.715246
1	2.856932	2.185446	-1.403908
1	2.724050	-0.513977	-1.604925
35	-1.559415	-0.535185	0.056173
6	-1.029488	1.355861	1.072950
6	-1.506380	1.967372	2.021884
14	-2.171469	2.980826	3.411230
6	-3.991623	2.576815	3.639913
1	-4.409946	3.152909	4.474749
1	-4.569020	2.821936	2.740657
1	-4.141399	1.512745	3.856725
6	-1.955972	4.796002	2.970358
1	-2.394605	5.429564	3.751690
1	-0.898102	5.068414	2.876667
1	-2.456640	5.037812	2.025646
6	-1.187141	2.544176	4.952150
1	-1.298171	1.483147	5.205099
1	-0.118699	2.749476	4.815131
1	-1.534363	3.131120	5.811444
8	-0.095330	0.668025	-2.392461
6	-0.549982	1.648724	-3.026466
6	-0.960245	1.466569	-4.444156
1	-0.380704	2.140189	-5.085014
1	-0.801787	0.433115	-4.754638
1	-2.017290	1.730727	-4.557459

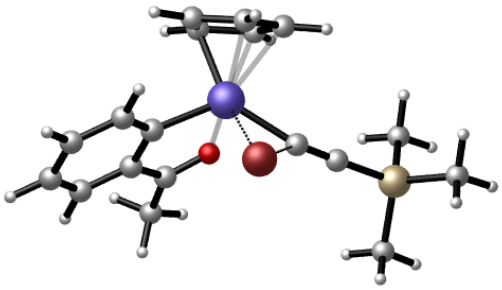
Int10c



E = -1185.495930 Hartrees
G = -1185.210840 Hartrees

45	0.560540	0.858729	-0.207639
6	0.266063	2.867307	-0.732515
6	0.776707	3.994820	-0.109505
6	-0.530464	2.993045	-1.881811
6	0.503207	5.248366	-0.653411
1	1.365387	3.926407	0.796913
6	-0.806867	4.262997	-2.410135
6	-0.285144	5.388956	-1.797882
1	0.910345	6.129288	-0.166702
1	-1.427936	4.353179	-3.295798
1	-0.489638	6.374468	-2.201628
6	2.136590	-0.035720	1.021409
1	1.910067	-0.515857	1.963772
6	2.416870	1.336686	0.832020
6	2.244352	-0.694692	-0.272264
1	2.435434	2.091343	1.606312
6	2.661135	1.536939	-0.576188
1	2.082032	-1.747445	-0.456101
6	2.578640	0.271681	-1.233193
1	2.921340	2.473499	-1.049480
1	2.686324	0.104597	-2.296588
35	-0.776261	-1.228237	0.452782
6	-0.681083	1.698377	1.083296
6	-1.406493	2.216329	1.917341
14	-2.503576	3.092857	3.110445
6	-3.933087	1.966956	3.575990
1	-4.605822	2.470656	4.281390
1	-4.521011	1.683266	2.695068
1	-3.574883	1.046807	4.052487
6	-3.125191	4.649275	2.258114
1	-3.762798	5.236724	2.930595
1	-2.290147	5.287673	1.944856
1	-3.713325	4.405525	1.365242
6	-1.491375	3.535399	4.631904
1	-1.090619	2.638997	5.119663
1	-0.647832	4.188052	4.376879
1	-2.113365	4.064517	5.364686
8	-0.684596	0.695123	-1.875153
6	-1.029352	1.757343	-2.441413
6	-1.915261	1.685288	-3.632370
1	-1.435450	2.180606	-4.483168
1	-2.132621	0.645400	-3.878714
1	-2.848799	2.219277	-3.421589

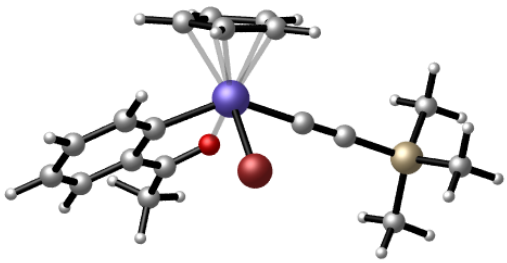
$TS_{4\text{-}12}c$



E = -1185.474784 Hartrees
G = -1185.190562 Hartrees

45	0.591534	0.883616	-1.130060
6	0.837000	2.830215	-0.574544
6	2.025361	3.416082	-0.165047
6	-0.344421	3.590004	-0.617764
6	2.030038	4.767606	0.183952
1	2.944537	2.841892	-0.106355
6	-0.330148	4.944992	-0.258786
6	0.862210	5.531875	0.136045
1	2.961323	5.228220	0.500109
1	-1.248188	5.524337	-0.282780
1	0.887538	6.580377	0.413136
6	-0.412309	-0.536190	-0.013322
6	-1.264587	-1.408798	0.091671
14	-2.580438	-2.700107	0.127666
6	-3.024719	-3.129666	-1.647413
1	-3.804639	-3.901024	-1.671982
1	-2.155602	-3.515024	-2.193705
1	-3.402643	-2.252291	-2.185422
6	-4.067319	-1.989322	1.027848
1	-4.439233	-1.086089	0.530373
1	-3.822009	-1.729661	2.064248
1	-4.883714	-2.721834	1.049450
6	-1.906255	-4.210162	1.018054
1	-1.007739	-4.598171	0.524300
1	-2.655937	-5.011097	1.026863
1	-1.648895	-3.980115	2.058510
35	1.031865	0.444283	1.367610
6	2.474729	-0.068440	-1.840004
1	3.282781	-0.337987	-1.172296
6	2.321601	1.181475	-2.500869
6	1.420257	-0.953473	-2.285079
1	2.973561	2.038261	-2.408137
6	1.094381	1.129012	-3.220942
1	1.276742	-1.972483	-1.954103
6	0.571407	-0.223291	-3.120952
1	0.666163	1.929552	-3.810306
1	-0.357885	-0.569266	-3.553545
8	-1.388740	1.643241	-1.285675
6	-1.529889	2.858033	-1.022551
6	-2.879090	3.473555	-1.139129
1	-3.166332	3.917653	-0.179962
1	-2.850690	4.280236	-1.880323
1	-3.613403	2.723949	-1.435755

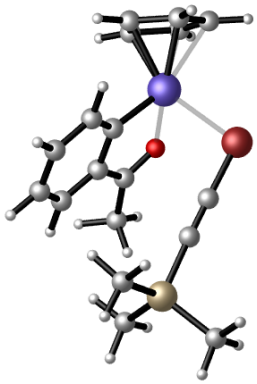
Int12c



E = -1185.490031 Hartrees
G = -1185.206039 Hartrees

45	0.479854	0.873420	-1.077914
6	0.935406	2.855615	-0.531993
6	2.170050	3.375312	-0.175976
6	-0.200190	3.679909	-0.539192
6	2.265158	4.725371	0.158454
1	3.062598	2.761268	-0.146351
6	-0.091618	5.035952	-0.191365
6	1.143303	5.557447	0.151524
1	3.235125	5.130473	0.430614
1	-0.976446	5.665007	-0.187460
1	1.239893	6.604163	0.418570
6	-0.736099	-0.653448	-0.612600
6	-1.529270	-1.557628	-0.409200
14	-2.748766	-2.899862	-0.065961
6	-3.228446	-3.684069	-1.705471
1	-3.979462	-4.469727	-1.554635
1	-2.362438	-4.142043	-2.198356
1	-3.653949	-2.942834	-2.392722
6	-4.250566	-2.131972	0.761656
1	-4.715108	-1.376096	0.117505
1	-3.980505	-1.649213	1.708120
1	-5.004993	-2.898610	0.978228
6	-1.938697	-4.164156	1.062804
1	-1.048287	-4.605115	0.599540
1	-2.636792	-4.979669	1.289830
1	-1.634223	-3.708522	2.012308
35	0.920604	0.649622	1.406780
6	2.521420	0.506604	-1.782759
1	3.381838	0.642876	-1.141782
6	1.957387	1.484485	-2.668993
6	1.759046	-0.691311	-1.903826
1	2.326463	2.485985	-2.836518
6	0.837037	0.890251	-3.319751
1	1.931496	-1.614333	-1.367181
6	0.715002	-0.450952	-2.866197
1	0.170247	1.386581	-4.012937
1	-0.039517	-1.159296	-3.176838
8	-1.406037	1.808147	-1.138395
6	-1.447260	3.032364	-0.879013
6	-2.757620	3.732402	-0.934982
1	-2.976976	4.178006	0.041315
1	-2.709687	4.545823	-1.667483
1	-3.547573	3.032148	-1.207968

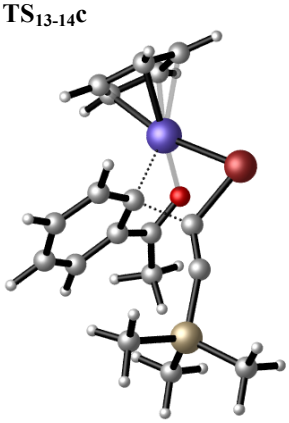
Int13c



E = -1185.521235 Hartrees
G = -1185.238039 Hartrees

6	0.155308	-3.526460	2.724341
1	0.837548	-2.728833	2.988538
6	-0.986097	-3.403796	1.822390
1	-1.246361	-2.516269	1.260189
6	-1.622779	-4.635220	1.758465
1	-2.459728	-4.896945	1.124885
6	0.134923	-4.824251	3.289104
1	0.828505	-5.218877	4.018750
6	-0.886034	-5.563128	2.606704
1	-1.145702	-6.598899	2.782715
45	0.558969	-4.988714	1.176432
6	2.202671	-6.113423	1.453816
6	2.285921	-7.226757	0.592546
6	3.224967	-5.901143	2.374504
6	3.358982	-8.123899	0.665994
6	4.298570	-6.791641	2.438090
1	3.200262	-5.046637	3.044159
6	4.364434	-7.905760	1.597234
1	3.403904	-8.981592	0.001044
1	5.090799	-6.619301	3.161239
1	5.198874	-8.595781	1.669329
6	3.254456	-4.444995	-1.209824
6	4.201404	-5.104385	-1.587520
14	5.708000	-6.032817	-2.174677
35	1.846288	-3.450584	-0.666145
6	6.935635	-6.031722	-0.759561
1	6.519682	-6.523286	0.127201
1	7.849666	-6.566142	-1.046317
1	7.216461	-5.009442	-0.480985
6	5.180467	-7.769118	-2.643683
1	4.806589	-8.328075	-1.779668
1	4.402630	-7.756301	-3.415614
1	6.039774	-8.318093	-3.048642
6	6.359567	-5.103456	-3.667016
1	5.621679	-5.088039	-4.477215
1	6.612105	-4.066528	-3.417656
1	7.266356	-5.589622	-4.047204
8	0.332362	-6.430111	-0.364401
6	1.224429	-7.307269	-0.400587
6	1.181818	-8.343793	-1.468740
1	2.032001	-8.196002	-2.145229
1	1.277943	-9.343823	-1.033986
1	0.250815	-8.267518	-2.032002

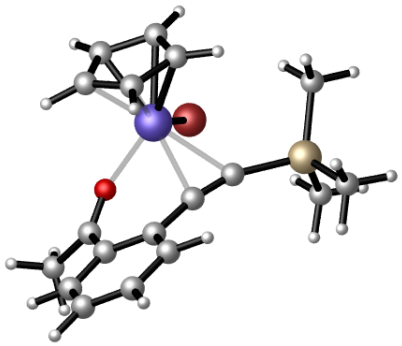
$TS_{13\text{-}14}$c



E = -1185.455058 Hartrees
G = -1185.171285 Hartrees

6	0.291095	-3.641540	2.666455
1	0.926233	-2.806813	2.931598
6	-0.925042	-3.566282	1.881267
1	-1.307841	-2.676928	1.397733
6	-1.456579	-4.856332	1.774399
1	-2.322755	-5.145768	1.194208
6	0.437914	-4.984862	3.117467
1	1.241755	-5.366907	3.732323
6	-0.584225	-5.760722	2.497759
1	-0.728344	-6.827621	2.605899
45	0.622733	-4.890728	0.951832
6	2.554960	-5.728772	0.795910
6	2.337294	-7.090438	0.382411
6	3.499872	-5.502305	1.836647
6	3.190863	-8.101998	0.791455
6	4.310422	-6.530798	2.279321
1	3.630267	-4.495732	2.223318
6	4.192845	-7.812053	1.722802
1	3.072441	-9.116661	0.423900
1	5.057163	-6.345778	3.044943
1	4.861754	-8.601683	2.049566
6	3.114344	-4.804071	-0.626501
6	4.096874	-5.074756	-1.347682
14	5.561238	-5.971985	-2.002341
35	1.749332	-3.367783	-0.769271
6	6.838322	-6.160990	-0.632500
1	6.496914	-6.866914	0.132789
1	7.782413	-6.539013	-1.045393
1	7.048620	-5.204133	-0.140387
6	4.978802	-7.657232	-2.607227
1	4.588393	-8.261901	-1.780666
1	4.196071	-7.564611	-3.369307
1	5.815606	-8.206489	-3.057242
6	6.307858	-5.005844	-3.431980
1	5.582131	-4.862701	-4.241260
1	6.652848	-4.015952	-3.110063
1	7.171093	-5.542452	-3.845574
8	0.384377	-6.349441	-0.623082
6	1.231858	-7.264894	-0.557762
6	1.119529	-8.453337	-1.446661
1	2.006282	-8.507744	-2.089435
1	1.092456	-9.370610	-0.847404
1	0.218679	-8.386873	-2.058067

Int14c



E = -1185.599940 Hartrees
G = -1185.312744 Hartrees

6	2.042946	-3.333556	0.361853
1	3.004956	-2.859585	0.222983
6	0.936472	-3.254975	-0.531450
1	0.924024	-2.732762	-1.478015
6	-0.117322	-4.068192	-0.002917
1	-1.084847	-4.234320	-0.456226
6	1.653410	-4.139758	1.487995
1	2.276672	-4.396071	2.334172
6	0.328006	-4.582099	1.261127
1	-0.227714	-5.261391	1.894973
45	1.601009	-5.298676	-0.382608
6	3.265565	-7.359062	1.383121
6	2.176425	-8.252637	1.469463
6	4.216101	-7.316107	2.406489
6	2.081699	-9.098968	2.577192
6	4.089197	-8.149396	3.513437
1	5.054239	-6.632142	2.322994
6	3.023086	-9.039358	3.599775
1	1.260623	-9.803092	2.654001
1	4.831653	-8.106730	4.303698
1	2.925613	-9.694565	4.458849
6	3.469595	-6.507501	0.244477
6	3.892266	-5.825516	-0.695033
14	5.061404	-5.064915	-1.955973
35	1.371211	-5.584100	-2.894515
6	6.705994	-5.032682	-1.049836
1	7.026179	-6.044156	-0.773433
1	7.482932	-4.599724	-1.692287
1	6.653131	-4.431107	-0.134888
6	5.134060	-6.199509	-3.441382
1	5.425378	-7.215106	-3.149190
1	4.164758	-6.253559	-3.946451
1	5.877342	-5.828501	-4.158336
6	4.493185	-3.334006	-2.383405
1	3.472515	-3.337191	-2.779599
1	4.534809	-2.665332	-1.516089
1	5.153466	-2.914722	-3.153152
8	0.877280	-7.352066	-0.323955
6	1.139852	-8.311134	0.411201
6	0.346455	-9.567202	0.223554
1	0.987886	-10.45164	0.260165
1	-0.390430	-9.650039	1.032197
1	-0.185416	-9.519292	-0.727579

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