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Oxygen Bridged Bimetallic [Cu-O-Se] Catalyst for Sonogashira Cross-Coupling.

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1. Materials:

Solvents such as acetonitrile (99.8%) 1,4-dioxane (99.8%), DMSO (99.9%), toluene (99.8%), DMF (99.8%), t-BuOH (99.5%) and deuteriated NMR solvents $CDCl_3$ (99.8%) CD_3CN (99.8%) is purchased from Sigma-Aldrich. All other solvents is purchased from Merck of high purity grade. Toluene and acetonitrile was sparged with nitrogen (N_2) for 5 min at room temperature and stored under nitrogen atmosphere. Cs_2CO_3 (*ReagentPlus*®, 99%) and KOH (99%), K_2CO_3 (99%), $KO^{t}Bu$(99%) was purchased from Sigma-Aldrich. All phenyl acetylenes were purchased from Sigma and used directly as received. $CuSeO_3$. $2H_2O$ was purchased from Sigma-Aldrich as well as synthesized in laboratory. Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator using a water bath. ICP standard $Pd(NO_3)_2$ in HNO_3 from Merck was purchased and used for control experiment.

2. Instrumentation:

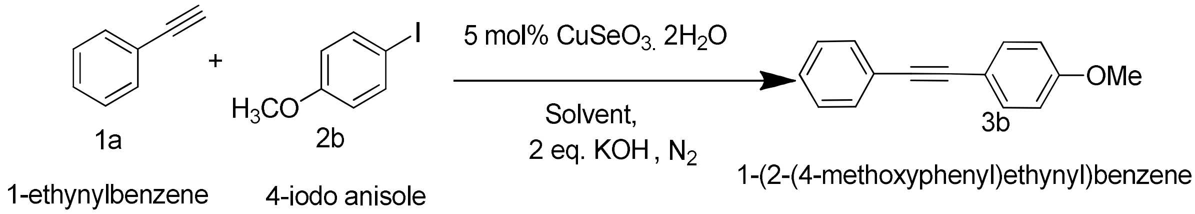
NMR spectra were recorded on Bruker Avance III, 400 MHz (IISER Berhampur) and 500 MHz (University of Hydrabad) spectrometers in appropriate solvents $CDCl_3$ using TMS as internal standard or the solvent signals as secondary standards and the chemical shifts are shown in δ scales. The ^{1}H and ^{13}C NMR spectra were recorded at 400 MHz for ^{1}H and 100 MHz for ^{13}C NMR, respectively. Deuterated solvents were purchased from Sigma-aldrich and used as received. All ^{1}H NMR experiments are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual chloroform (7.26 ppm) in the deuterated solvents. Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = quintet, m = multiplet, dd = doublet of doublets, dt = doublet of triplets…etc, br = broad), coupling constant (Hz) and integration. All ^{13}C NMR spectra are reported in ppm relative to $CDCl_3$ (77.0 ppm). 1,4-di iodobenzene was used as an internal standard for NMR yields from proton analysis. Elemental analysis is performed in 2400 Series II CHNS/O analyzer in CHNS mode. Flash column chromatography was performed by using a 90-120 times weight excess of flash silica gel 60-120 μm from Aldrich. Fractions were analyzed by TLC using TLC silica gel F254 250 μm precoated-plates from Merck and stains (permanganate, 2,4-dnp and CAM) was used for UV-inactive compounds. Melting point is determined in Digital melting point apparatus, Electronics India (EI)-2935 model; Visualized through LCD Screen and is uncorrected by ±5 °C. Internal Standard. XPS is with Al-Kα line at IIT Roorke. HRMS is done at University of Hydrabad and IISER Berhampur in ESI mode. ICP-AES (Inductively Coupled Plasma- Atomic Emission Spectrometry) analysis was carried out at Bhabha Atomic Research Centre (BARC), Trombay, with a Spectro-Arcos SOP unit, Germany. The spectrometer is augmented with a CCD detector array which was used for the analyses. High purity argon plasma was used as the plasma gas, carrier gas and auxiliary gas as well. All the calculations were performed by using Gaussian 09[1]. All the structure were optimized at meta-GGA M06L[2]-level, with Lanl2dz[3] basis set. Effective core potentials were applied for copper, selenium, iodine and potassium atoms. Extra d orbitals were included in the basis set for the selenium and iodine atoms.

3. General Procedure for Sonogashira cross-coupling:

A oven dried 10 mL of two necked round bottom flask (one end with teflon cork and another end connected to N_2 atmosphere) was back filled with nitrogen three times. Then the flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg), halobenzene (0.5 mmol), aryl/alkyl/alkynol/ acetylene (0.6 mmol), KOH (112 mg, 2 eq.) and 1 mL DMF. Then back filled with nitrogen (N_2) for 5 min and placed into an oil bath at temperature 90 °C. The reaction is monitored after every 2 h and up to 48 h with the help of TLC using $KMnO_4$ stain. After the time specified in the schemes, the reaction mixture was cooled, brine solution was added, work up with ethyl acetate and cold water, finally concentrated in rotor. Then the crude mixture was directly subjected to column for flash column chromatography with 230-400 mesh silica Gel using ethylacetate and hexane as efluent to afford corresponding product. All yields are reported after column chromatography. The products were identified and cited with reported literature.

4. Standardization of reaction

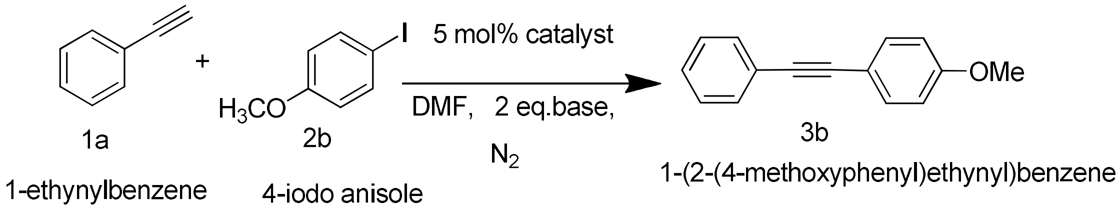
a) Table 1. Standardization of Solvent



Entry	Solvent	(° C)	Yield (%)[a,b]
1	DMSO	90	5
2	CH_3CN	80[d]	0
3	1,4-dioxane	90	0
4	**DMF**	**90**	**80**
5	t-BuOH	80[d]	0
6	Toluene	90	0
7	THF	70	0
8	EtOH	80	0

[a]Phenyl acetylene (1.2 mmol), [b]4-iodo anisole(1 mmol), [c]$CuSeO_3.2H_2O$ catalyst (5 mol%, 11 mg), base 2 equiv. were stirred for 40h, [d]Refluxed using water condenser under respective boiling point.

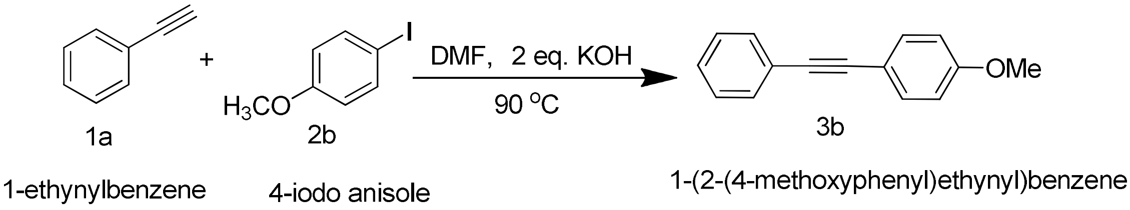
b) Table 2. Standardization of Base



Catalyst	Base	Yield (%)[a,b]
$CuSeO_3 . 2H_2O$	**KOH**	**80**
$CuSeO_3 . 2H_2O$	K_2CO_3	0
$CuSeO_3 . 2H_2O$	KOAc	30
$CuSeO_3 . 2H_2O$	NaOH	0
$CuSeO_3 . 2H_2O$	Na_2CO_3	0
$CuSeO_3 . 2H_2O$	Cs_2CO_3	0
$CuSeO_3 . 2H_2O$	Pyridine	12
$CuSeO_3 . 2H_2O$	Et_3N	0
$CuSeO_3 . 2H_2O$	K_3PO_4	0
$CuSeO_3 . 2H_2O$	t-BuOK	70
$CuSeO_3 . 2H_2O$	-	0[c]

[a]Phenyl acetylene (1.2 mmol), [b]4-iodo anisole(1 mmol), [c]$CuSeO_3 .2H_2O$ catalyst (5 mol%, 11 mg), base 2 equiv. were stirred for 40h, [d]Refluxed using water condenser under respective boiling point.

c) Table 3. Standardization of Catalyst

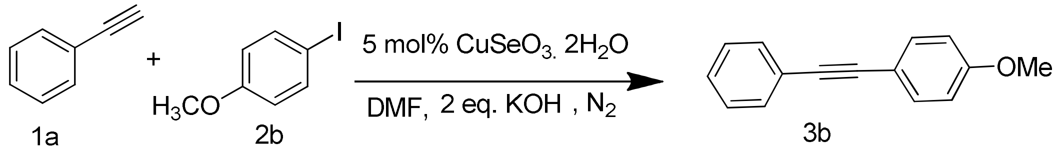


Entry	Catalyst	Base	Yield (%)[a,b]
1	**-**	**KOH**	**0**

2	$CuCl_2$ $2H_2O$	KOH	5
3	SeO_2	KOH	0
4	$CuSeO_3$. $2H_2O$	KOH	90
5	$CuSO_4$. $2H_2O$	KOH	8

[a]Phenyl acetylene (1.2 mmol), [b]4-iodo anisole(1 mmol), [c]$CuSeO_3.2H_2O$ catalyst (5 mol%, 11 mg), base 2 equiv. were stirred for 40 h, [d]Refluxed using water condenser under respective boiling point.

d) Table 4. Standardization at Variant Temperature



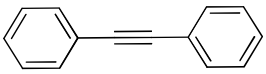
1-ethynylbenzene 4-iodo anisole 1-(2-(4-methoxyphenyl)ethynyl)benzene

Entry	Temperature (°C)	Yield (%)[a,b]	hr
1	30	0	72
2	60	0	54
3	90	90	40
4	120	30	36

[a]Phenyl acetylene (1.2 mmol), [b]4-iodo anisole(1 mmol), [c]$CuSeO_3.2H_2O$ catalyst (5 mol%, 11 mg), base 2 equiv. were stirred for different time, [d]Refluxed using water condenser under respective boiling point.

5. Characterization of Product

1, 2-Diphenylethyne[5]



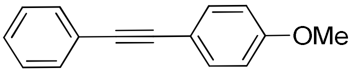
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this iodobenzene (204 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 92% (164 mg) yield.

White solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53–7.55 (m, 4 H), 7.36-34 (m, 4 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 131.61, 128.34, 128.24, 123.28, 89.36.

1-Methoxy-4-(2-phenylethynyl)benzene[3]



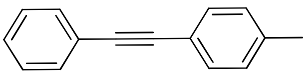
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and2 mL DMF. To this 4-iodoanisole (234 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford in 95% (198 mg) yield.

Yellow solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52 (d, *J* = 8.0 Hz, 2 H), 7.48 (d, *J* = 8.0 Hz, 2 H), 7.34–7.32 (m, 3 H), 6.89 (d, *J* = 8.2 Hz, 2 H), 3.83 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.62, 133.05, 131.04, 128.29, 127.92, 123.60, 113.99, 89.35, 88.05, 55.30.

1-Methyl-4-(2-phenylethynyl)benzene[18]

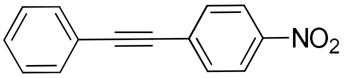


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4- iodo toluene(218 mg, 1 mmol), phenylethyne (122 mg 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (172 mg) yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54 (d, *J* =8.0 Hz, 2 H), 7.45 (d, *J* =8.0 Hz, 2 H), 7.36-7.33 (m, 3 H), 7.17 (d, *J* =8.0 Hz, 2 H), 2.38 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 138.37, 131.54, 131.49, 129.38, 129.10, 128.64, 128.30, 128.06, 126.42, 123.48, 120.19, 21.49.

1-Nitro-4-(2-phenylethynyl)benzene[3]



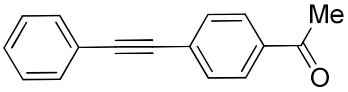
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 1- iodo-4-nitro benzene (248 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 96% (107 mg) yield

Yellow solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 12 Hz, 2 H), 7.68 (d, *J* = 8 Hz, 2 H), 7.58-7.55(m, 2 H), 7.49-7.39 (m, 2 H).

^{13}C NMR (100 MHz, $CDCl_3$): d 147.03, 132.26, 131.84, 129.27, 128.53, 123.64, 122.10, 94.70, 87.54

1-(4-(phenylethynyl)phenyl)ethanone[3]



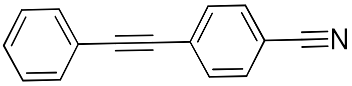
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-iodo acetophenone (226 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 95% (210 mg) yield.

Yellowish solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8 Hz, 2 H), 7.62 (d, *J* = 8 Hz, 2 H), 7.57-7.54(m, 2 H), 7.38-7.36 (m, 3 H), 2.62(s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 197.32, 136.21, 131.74, 131.70, 128.81, 128.44, 128.27, 122.66, 92.71, 88.60, 26.61

4-(phenylethynyl)benzonitrile[13]



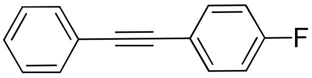
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11mg) and 2 mL DMF. To this 4-bromo benzonitrile (182 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (182 mg) yield.

Colorless liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65-7.61 (m, 4H), 7.56-7.51 (m, 3H), 7.39-7.37 (m, 2H),

^{13}C NMR (100 MHz, $CDCl_3$): δ 133.39, 132.63, 132.06, 132.03, 131.78, 129.11, 128.49, 127.27, 122.21, 118.51, 110.20, 93.77, 87.70.

1-fluoro-4-(phenylethynyl)benzene[8]



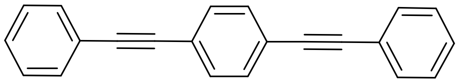
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-Fluoroiodobenzene (222 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 87% (170 mg) yield.

Colorless liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55-7.51 (m, 5H), 7.36 (d, *J* = 8 Hz, 4H),

^{13}C NMR (100 MHz, $CDCl_3$): δ 163.17, 161.36, 138.90, 133.50, 133.42 (J=8 Hz), 132.49, 131.54, 129.19, 128.43, 128.36, 128.31, 121.79, 115.73, 115.51, 89.06, 88.41, 81.54.

1,4-Bis(phenylethynyl)benzene[2]

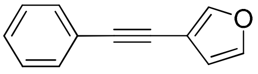


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11mg) and 2 mL DMF. To this 1,4-diiodo benzene (338 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (250 mg) yield**.**

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51-7.54 (m, 8 H), 7.36-7.35 (m, *6* H),

^{13}C NMR (100 MHz, $CDCl_3$): δ 131.62, 131.52, 128.45, 128.38, 123.09, 123.03, 91.21, 89.06.

3-(phenylethynyl)furan[9]



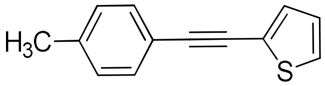
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55-7.53 (m, 3H), 7.38-7.33 (m, 5H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 145.68, 142.90, 132.52, 129.22, 128.46, 128.35, 128.22, 126.48, 121.42, 112.57, 81.57, 73.93.

The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 3-bromobenzofuran (196 mg, 1 mmol), phenylethyne (122 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc an d hexanes as eluent) to afford 70% (118 mg) yield.

brown solid

2-(p-tolylethynyl)thiophene[16]



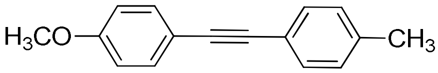
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 2-Iodothiophene (210 mg, 1 mmol), 4-Ethynyltoluene (140 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 75% (138 mg) yield**.**

Light brown solid

^1H NMR (400 MHz, $CDCl_3$): δ 7.45 (d, *J* = 8 Hz, 2H), 7.31 (d, *J* = 8 Hz, 2H), 7.19 (d, *J* = 8 Hz, 2H), 7.03 (d, *J* = 8 Hz, 2H), 2.39 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 138.60, 132.37, 131.63, 131.30, 129.20, 129.13, 127.04, 126.99, 123.543, 119.80, 93.19, 81.90, 21.52.

1-methoxy-4-(p-tolylethynyl)benzene[16]



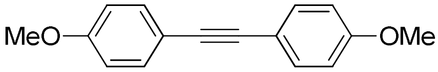
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4- iodo toluene (218 mg, 1 mmol), 4-ethynyl anisole (158 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 82% (182n mg) yield**.**

Light Yellowish solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.45 (d, J=8 HZ, 2H), 7.39 (d, J=8 HZ, 2H), 7.15 (d, J=8 HZ, 2H), 6.88 (d, J=8 HZ, 2H), 3.83(s, 3 H), 2.36(s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.45, 138.24, 132.96, 131.33, 129.34, 129.06, 127.75, 120.43, 115.33, 113.96, 88.72, 88.11, 56.29, 21.47.

1,2-bis(4-methoxyphenyl)ethyne[11]



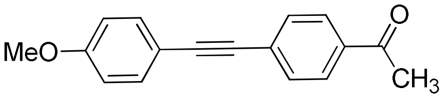
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4- iodo anisole (234 mg, 1 mmol), 4-ethynyl anisole (158 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 85% (202 mg) yield**.**

White solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44-7.41 (m, 4 H), 6.93-6.86 (m, 4 H), 3.82(s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.39, 134.04, 132.87, 127.41, 126.19, 115.74, 114.11, 113.96, 87.94, 55.29

1-(4-((4-methoxyphenyl)ethynyl)phenyl)ethanone[11]



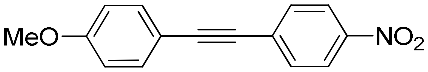
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-iodo acetophenone (246 mg, 1 mmol), 4-ethynyl anisole (158 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (226 mg) yield**.**

Light Yellowish solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8 Hz, 2 H), 7.59 (d, *J* = 8 Hz, 2 H), 7.50 (d, *J* = 8 Hz, 2 H), 6.90 (d, *J* = 8 Hz, 2 H), 3.83(s, 3H), 2.60(s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 197.31, 160.03, 135,85, 133.25, 131.44, 128.58, 128.23, 114.68, 114.09, 92.94, 87.49, 55.29, 26.55.

1-methoxy-4-((4-nitrophenyl)ethynyl)benzene[11]



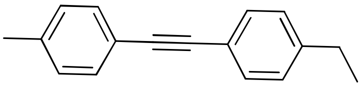
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and2 mL DMF. To this 1-iodo-4-nitro benzene (248 mg, 1 mmol), 4-ethynyl anisole (158 mg, 1.2 mmol), KOH (112mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 93% (236 mg) yield**.**

Yellow solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8 Hz, 2 H), 7.63 (d, *J* = 8 Hz, 2 H), 7.51(t, *J* = 12 Hz, 2H), 6.92 (d, *J* = 12 Hz, 2H), 3.84 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 160.40, 146.66, 133.42, 131.96, 130.67, 123.59, 114.19, 114.10, 95.12, 86.61, 55.13.

1-ethyl-4-(p-tolylethynyl)benzene[15]



The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 1-bromo-4-ethyl benzene(184 mg, 1.2 mmol), 4-ethynyl toluene(140 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water

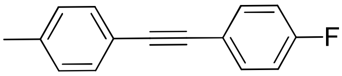
(20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (198 mg) yield**.**

yellow solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46-7.41(m, 4H), 7.19-7.057(m, 4H), 2.67(q, J=4Hz, 2H), 2.37 (s, 3H), 1.25 (t, J=8 Hz, 3H),

^{13}CNMR(100MHz,$CDCl_3$):δ 144.46, 139.47, 138.14, 132.38, 131.51, 131.43, 129.20, 129.06, 127.87, 126. 37, 126.30, 120.62, 120.40, 118.79, 88.85, 81.53, 28.80, 21.59, 15.33.

1-fluoro-4-(phenylethynyl)benzene[16]



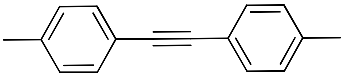
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-Fluoroiodobenzene (222 mg, 1 mmol), 4-ethynyl toluene (140 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 88% (184 mg) yield.

Colorless liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.49 (m, 2H), 7.44 (d, *J* = 8 Hz, 2H), 7.16 (d, *J* = 8 Hz, 2H), 7.04 (t, *J* = 8 Hz, 2H), 2.38(s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 163.61, 161.13, 138.46, 133.41, 133.33, 132.37, 131.42, 129.19, 129.12, 119.97, 115.46, 115.38, 89.19, 87.61, 21.59.

1,2-di-p-tolylethyne[7]



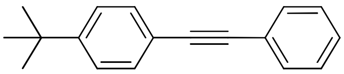
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4- iodo toluene (218 mg, 1 mmol), 4-ethynyl toluene (140 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (186 mg) yield.

Colorless liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (d, *J* = 8 Hz, 4H), 7.16 (t, *J* = 4 Hz, 4H),

^{13}C NMR (100 MHz, $CDCl_3$): δ 139.46, 138.14, 132.36, 131.40, 129.33, 129.19, 129.06, 127.59, 126.28, 120.36, 118.75,88.85, 81.52, 73.43, 21.46.

1-(tert-butyl)-4-(phenylethynyl)benzene[14]



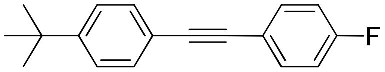
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this iodo benzene(204 mg, 1 mmol)**,** 4-tert-Butyl phenylacetylene (190 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 91% (214 mg) yield.

yellow solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55-7.52(m, 2H), 7.49-7.47(m, 2H), 7.39-7.33(m, 5H), 1.34 (s, 9H).

^{13}CNMR(100MHz,$CDCl_3$):δ 151.97, 140.73, 137.89, 131.56, 131.32, 128.29, 128.04, 125.33, 123.51, 120. 23, 89.52, 88.71, 34.78, 31.17

1-(tert-butyl)-4-((4-fluorophenyl)ethynyl)benzene[4]

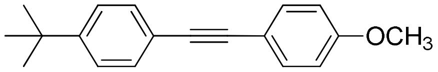


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-fluoroiodobenzene (222 mg, 1 mmol), 4-tert-Butyl phenylacetylene (190 mg, 1,2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 94% (118 mg) yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54-7.47(m, 4H), 7.40(d, *J* = 8 Hz, 2H), 7.05 (d, *J* = 8 Hz, 2H), 1.35 (s, 9H).

^{13}CNMR(100MHz,$CDCl_3$):δ 163.61, 161.13, 151.60, 133.44, 133.36, 132.24, 131.27, 125.45, 125.36, 120. 04, 115.67, 115.45, 189.18, 87.63, 34.77, 31.15

1-(tert-butyl)-4-((4-methoxyphenyl ethynyl)benzene[19]



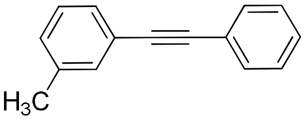
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this iodo anisole (234 mg, 1 mmol), 4-tert-Butyl phenylacetylene (190 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90 °C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 92% (244 mg) yield.

yellow solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48(t, *J* = 4 Hz, 4H), 7.38(d, *J* = 8 Hz, 2H), 6.90(d *J* = 12 Hz, 2H), 3.83(s, 3H), 1.34 (s, 9H).

^{13}CNMR(100MHz,$CDCl_3$):δ 159.47, 151.15, 132.98, 131.15, 127.58, 125.96, 120.54, 115.63, 114.09, 113.9 4, 88.65, 88.16, 55.25, 34.72, 31.16.

1-methyl-3-(phenylethynyl)benzene[12]



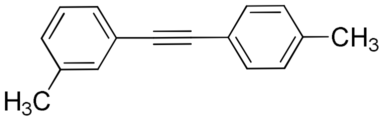
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this iodo benzene(204 mg, 1 mmol), 3-ethynyl toluene (140 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (172 mg) yield.

Colorless liquid

^{1}**H NMR (400 MHz**, CDCl$_3$): δ 7.59-7.57 (m, 2H), 7.41-7.37 (m, 5H), 7.28 (d, *J* = 8 Hz, 1H), 7.20 (d, *J* = 8 Hz, 1H), 2.40 (s, 3 H).

^{13}**C NMR (100 MHz**, CDCl$_3$): δ 137.99, 132.17, 131.58, 129.14, 128.67, 128.31, 128.22, 128.15, 126.45, 123.36, 123.05, 89.54, 89.01, 21.21.

1-methyl-3-(p-tolylethynyl)benzene[15]



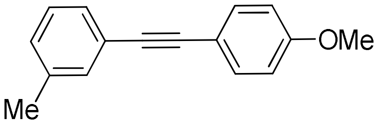
The flask was charged with 5 mol% CuSeO$_3$.2H$_2$O (11 mg) and 2 mL DMF. To this 4- iodo toluene (218 mg, 1 mmol), 3-ethynyl toluene (140 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N$_2$ for three times and stirred at 90°C under N$_2$. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 89% (184 mg) yield.

White solid

^{1}**H NMR (400 MHz**, CDCl$_3$): δ 7.44 (d, *J* = 8 Hz, 2H), 7.35 (t, *J* = 8 Hz, 2H), 7.24 (t, *J* = 8 Hz, 1H), 7.15 (t, *J* = 8 Hz, 2H), 2.38 (s, 3 H), 2.36 (s, 3 H).

^{13}**C NMR (100 MHz**, CDCl$_3$): δ 138.28, 137.95, 132.12, 131.47, 129.08, 128.97, 128.60, 128.20, 126.37, 123.57, 123.24, 120.26, 89.19, 88.87, 21.48, 21.22.

1-((4-methoxyphenyl)ethynyl)-3-methylbenzene[11]



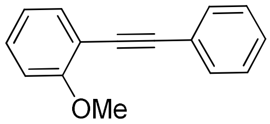
The flask was charged with 5 mol% CuSeO$_3$.2H$_2$O (11 mg) and 2 mL DMF. To this iodoanisole (234mg, 1 mmol), 3-ethynyl toluene (140 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N$_2$ for three times and stirred at 90°C under N$_2$. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 86% (190 mg) yield.

Yellow semi-liquid

^{1}**H NMR (400 MHz**, CDCl$_3$): δ 7.48 (d, *J* = 8 Hz, 2 H), 7.35-7.31 (m, 2 H), 7.23(t, *J* = 8 Hz, 1H), 7.14 (d, *J* = 8 Hz, 1H), 7.89(d, *J* = 8 Hz, 2H), 3.83 (s, 3 H), 2.35(s, 3H).

^{13}**C NMR (100 MHz**, CDCl$_3$): δ 159.55, 137.95, 133.02, 132.03, 128.83, 128.51, 128.19, 127.66, 115.49, 113.97, 89.00, 88.21, 55.29, 21.23.

1-methoxy-2-(phenylethynyl)benzene[3]



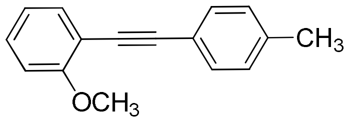
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this iodo benzene (204mg, 1 mmol), 2-ethynyl anisole (158 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 93% (184 mg) yield**.**

Yellow liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 8.0 Hz, 2 H), 7.51 (d, *J* = 8.0 Hz, 1 H), 7.34–7.31 (m, 4 H), 6.96-6.90 (m, 2 H), 3.92 (s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.93, 133.57, 131.65, 129.73, 128.22, 128.08, 123.57, 120.48, 110.73, 93.41, 85.70, 55.85.

1-methoxy-2-(p-tolylethynyl)benzene[10]



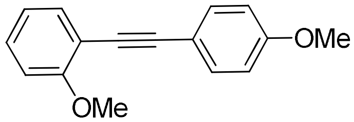
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4- iodo toluene (218 mg, 1 mmol), 2-ethynyl anisole (158 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 90% (200 mg) yield.

Yellow liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.46 (m, 3 H), 7.30 (d, *J* = 8 Hz, 1H), 7.17 (d, *J* = 8 Hz, 1H), 6.96-6.90 (m, 2H), 3.92(s, 3 H), 2.37(s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 159.83, 138.15, 133.50, 131.52, 129.52, 128.97, 120.44, 112.64, 110.67, 93.60, 84.99, 55.80, 21.46.

1-methoxy-2-((4-methoxyphenyl)ethynyl)benzene[6]



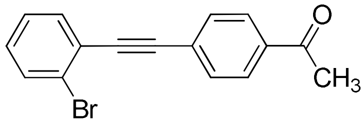
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 1 mL DMF. To this 4- iodoanisole(234 mg, 1 mmol), 2-ethynyl anisole (158 mg, 1.2 mmol),, KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 88% (210 mg) yield**.**

Brownish liquid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.48 (m, 3 H), 7.29 (d, *J* = 8 Hz, 1H), 6.95-6.86 (m, 4 H), 3.91(s, 3 H), 3.82(s, 3 H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 197.31, 160.03, 135.85, 133.25, 131.44, 128.58, 128.23, 114.68, 114.09, 92.94, 87.49, 55.29, 26.55

1-(4-((2-bromophenyl)ethynyl)phenyl)ethanone[17]



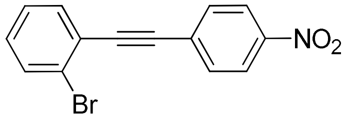
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4- iodo acetophenone (246 mg, 1 mmol), 1-bromo-2-ethynyl benzene (218 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 80% (240 mg) yield.

yellow solid

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8 Hz, 2H), 7.67-7.63 (m, 3H), 7.59(d, *J* = 8 Hz, 1H), 7.32(d, *J* = 8 Hz, 1H), 7.22 (t, *J* = 8 Hz, 1H), 2.62 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 197.83, 136.56, 133.39, 132.57, 131.80, 129.93, 128.28, 127.77, 127.12, 125.80, 92.92, 91.14, 26.63.

1-bromo-2-((4-nitrophenyl)ethynyl)benzene[17]

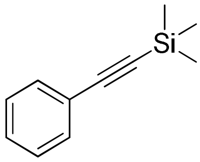


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 1-iodo-4-nitro benzene (248 mg, 1 mmol), 1-bromo-2-ethynyl benzene (218 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 81% (244 mg) yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8 Hz, 2H), 7.72 (d, *J* = 8 Hz, 2H), 7.65(d, *J* = 8 Hz, 1H), 7.58 (d, *J* = 8 Hz, 1H), 7.33(t, *J* = 8 Hz, 1H), 7.24 (d, *J* = 8 Hz, 1H),

^{13}C NMR (100 MHz, $CDCl_3$): δ 147.21, 133.47, 132.64, 132.36, 130.38, 129.77, 127.19, 125.90, 124.31, 123.63, 92.99, 91.69.

Trimethyl(phenylethynyl)silane[20]

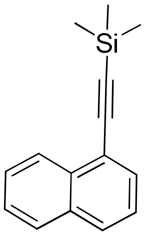


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this iodo benzene(204 mg, 1 mmol), Trimethyl silyl acetylene (186 mg, 2 mmol), KOH(112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 60 °C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 70% as volatile liquid (122 mg) yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.72 (d, J=8 Hz, 2H), 7.33 (t, J=8 Hz, 1H), 7.11 (t, J=8 Hz, 2H), 0.07 (s, 9H)

^{13}C NMR (100 MHz, $CDCl_3$): δ 138.65, 137.43, 132.13, 128.99, 128.55, 127.73, 126.72

Trimethyl(naphthalen-1-ylethynyl)silane



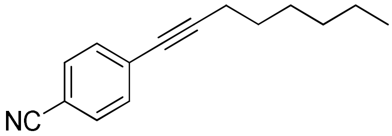
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2mL DMF. To this 1- iodo naphthalene (127 mg, 0.5 mmol), Trimethyl silyl acetylene (186 mg, 2 mmol), KOH (224 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 60 °C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 73% as volatile liquid (162 mg) yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.10 (d, J=8 Hz, 2H), 7.85 (d, J=8 Hz, 1H), 7.78 (d, J=8 Hz, 1H), 7.58 (t, J=8 Hz, 1H), 7.54 (t, J=8 Hz, 1H), 7.19 (t, J=8 Hz, 2H), 0.07 (s,9H)

^{13}C NMR (100 MHz, $CDCl_3$): δ 138.65, 137.43, 132.13, 128.99, 128.55, 127.73, 126.72, 105.14, 100.0

CAS- Sigma-aldrich: 104784-51-2

4-(oct-1-yn-1-yl)benzonitrile[20]

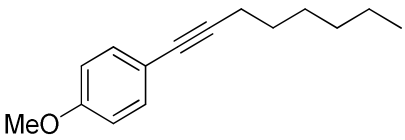


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4- cyano iodobenzene (228 mg, 1 mmol), 1-octyne (132 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 98% as volatile liquid (208 mg) yield.

^{1}**H NMR (400 MHz**, $CDCl_3$): δ = 7.57 (d, J=8Hz, 2H), 7.46 (d, J=, 8 Hz, 2H), 2.42 (t, J=8 Hz, 2H), 1.61 (t, J=6 Hz, 2H), 1.44 (t, J=6 Hz, 2H), 1.32 (t, J=6 Hz, 2H), 0.90 (t, J=8 Hz, 3H).

^{13}**C NMR (100 MHz**, $CDCl_3$): δ 132.07, 131.89, 118.64, 110.74, 95.72, 79.41, 76.78, 31.28, 28.57, 28.39, 22.51, 19.42, 14.02

1-methoxy-4-(oct-1-yn-1-yl)benzene [21]

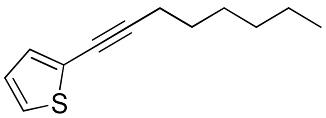


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-methoxy iodobenzene (224 mg, 1 mmol), 1-octyne (132 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 97% as volatile liquid (210 mg) yield.

^{1}**H NMR (400 MHz**, $CDCl_3$): δ = 7.34 (d, J=8Hz, 2H), 6.85 (dd, J=, 8 Hz, 8Hz, 2H), 3.80(3, 3H), 2.38 (t, J=8 Hz, 2H), 1.61 (t, J=6 Hz, 2H), 1.44 (t, J=6 Hz, 2H), 1.31 (t, J=6 Hz, 2H), 0.90 (t, J=8 Hz, 3H).

^{13}**C NMR (100 MHz**, $CDCl_3$): δ =158.94, 132.83, 116.27, 113.77, 113.39, 88.80, 80.20, 55.23, 31.37, 28.84, 28.61, 22.56, 19.40, 14.05.

2-(oct-1-yn-1-yl)thiophene [22]

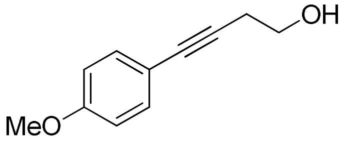


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 2- iodothiopene (210 mg, 1 mmol), 1-octyne (132 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 99% as volatile liquid (190 mg) yield.

^{1}**H NMR (400 MHz**, $CDCl_3$): δ= 7.34 (s, 1H), 7.22 (t, J=4 Hz, 1H), 7.07 (d, J=2 Hz, 1H), 2.38 (t, J=8 Hz, 2H), 1.61 (t, J=8 Hz, 2H), 1.44 (t, J=8 Hz, 2H), 1.31 (t, J=8 Hz, 2H), 0.90 (t, J=8 Hz, 3H).

^{13}**C NMR (100 MHz**, $CDCl_3$): δ =130.0, 127.43, 124.91, 123.02, 89.94, 75.51, 31.35, 28.70, 28.61, 22.54, 19.37, 14.04.

4-(4-methoxyphenyl)but-3-yn-1-ol [23]



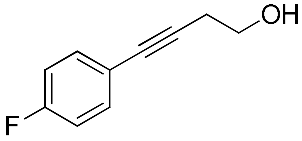
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-methoxyiodobenzene (234 mg, 1 mmol), but-3-yn-1-ol (84 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 95% as volatile liquid (166 mg) yield.

^{1}H NMR (400 MHz, $CDCl_3$): δ= 7.36 (d, J=8 Hz, 2H), 6.83 (d, J=8 Hz, 2H), 3.80 (t, J=6 Hz, 2H), 2.68 (t, J=6 Hz, 2H), 1.86 (s, 1H)

^{13}C NMR (100 MHz, $CDCl_3$): =159.31, 133.02, 115.41, 113.86, 84.63, 82.32, 61.22, 55.25, 23.83

CAS: 52999-15-2

4-(4-fluorophenyl)but-3-yn-1-ol [24]

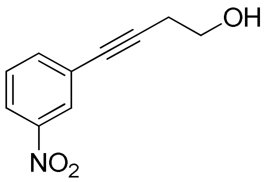


The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-fluoro iodobenzene (220 mg, 1 mmol), but-3-yn-1-ol (84 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 97% as volatile liquid (158 mg) yield

^{1}H NMR (400 MHz, $CDCl_3$): δ= 8.10 (dd, J=4Hz, 4 Hz, 2H), 6.98 (d, J=8 Hz, 2H), 3.81 (t, J=8 Hz, 1H), 2.68 (t, J=6 Hz, 1H), 1.84 (s, 1H)

^{13}C NMR (100 MHz, $CDCl_3$): = 163.05, 161.02, 133.52, 133.43, 119.36, 115.69, 115.37, 85.99, 61.12, 23.73

4-(3-nitrophenyl)but-3-yn-1-ol [25]



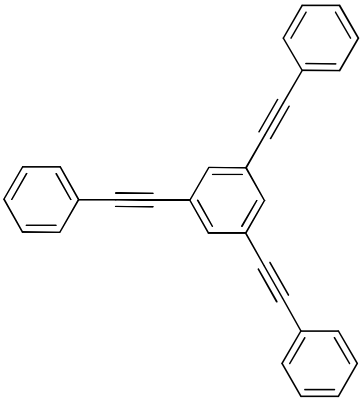
The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this 4-nitro iodobenzene (250 mg, 1 mmol), but-3-yn-1-ol (84 mg, 1.2 mmol), KOH (112 mg, 2 eq.) were added, back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, CH_2Cl_2 and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 96% as volatile liquid (184 mg) yield

^{1}H NMR (400 MHz, $CDCl_3$): δ= 8.24 (s, 1H), 8.14 (d, J=8 Hz, 1H), 7.71 (d, J=8 Hz, 1H), 7.46 (t, J=8 Hz, 1H), 3.85 (t, J=8 Hz, 2H), 2.71 (t, J=6 Hz, 2H), 1.98 (s, 1H)

^{13}C NMR (100 MHz, $CDCl_3$): = 147.99, 137.36, 129.20, 126.48, 125.18, 122.61, 89.65, 80.02, 60.88, 23.66

1,3,5-tris(phenylethynyl)benzene[1]:

The flask was charged with 5 mol% $CuSeO_3.2H_2O$ (11 mg) and 2 mL DMF. To this To this 2,4,6-tribromobenzene (157 mg, 0.5 mmol), phenylethyne (162 mg, 1.5 mmol), KOH (112 mg, 2 eq.) were added back filled with N_2 for three times and stirred at 90°C under N_2. After the time specified in the reaction schemes, the reaction mixture was cooled and worked up with brine solution, ethylacetate and cold water (20 x 5) ml. The organic layer was separated and concentrated in rotor. The product was isolated by flash chromatography (EtOAc and hexanes as eluent) to afford 94% (178 mg) yield.



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 4 Hz, 3 H), 7.57 (t, J = 4 Hz, 6 H), 7.40-7.38(m, 9 H),
^{13}C NMR (100 MHz, $CDCl_3$): δ 134.00, 131.67, 128.57, 128.38, 124.00, 122.77, 90.51, 87.82.

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6: EDX, SEM and Podered XRD of $CuSeO_3$. $2H_2O$

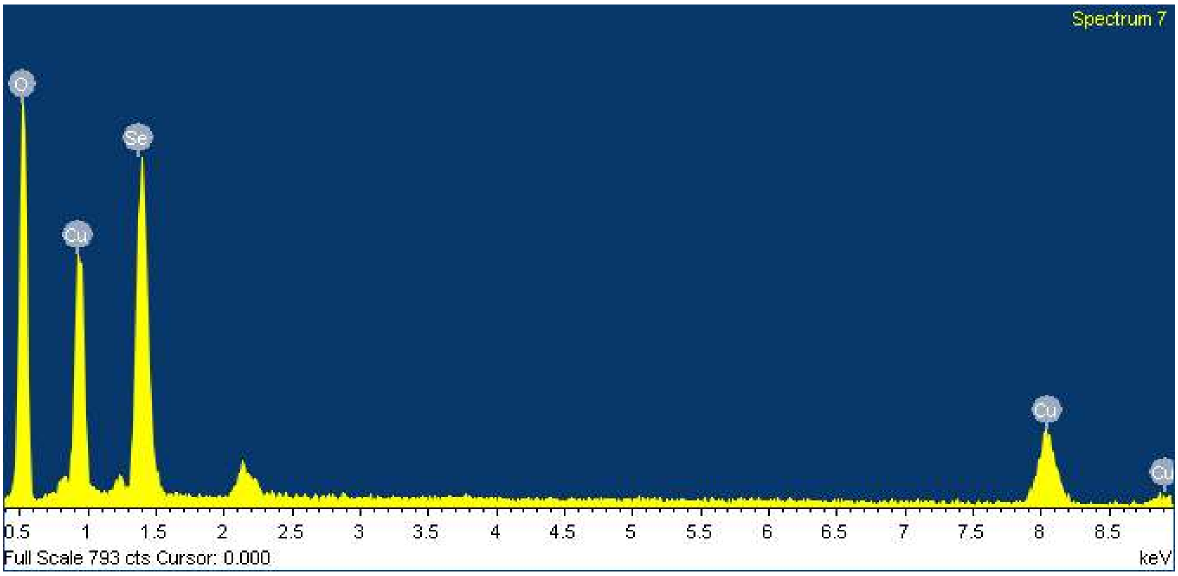

Figure S1: EDXRF spectra of $CuSeO_3$. $2H_2O$ (EDX Sigma)

Table 5: EDXRF spectra of $CuSeO_3$. $2H_2O$ (EDX Sigma)

Element	App	Intensity	Weight%	Weight%	Atomic%
	Conc.	Corrn.		Sigma	
O K	34.83	1.2604	37.44	0.60	72.66
Cu L	12.66	0.5983	28.68	0.59	14.02
Se L	13.69	0.5471	33.88	0.58	13.32
Totals			100.00		

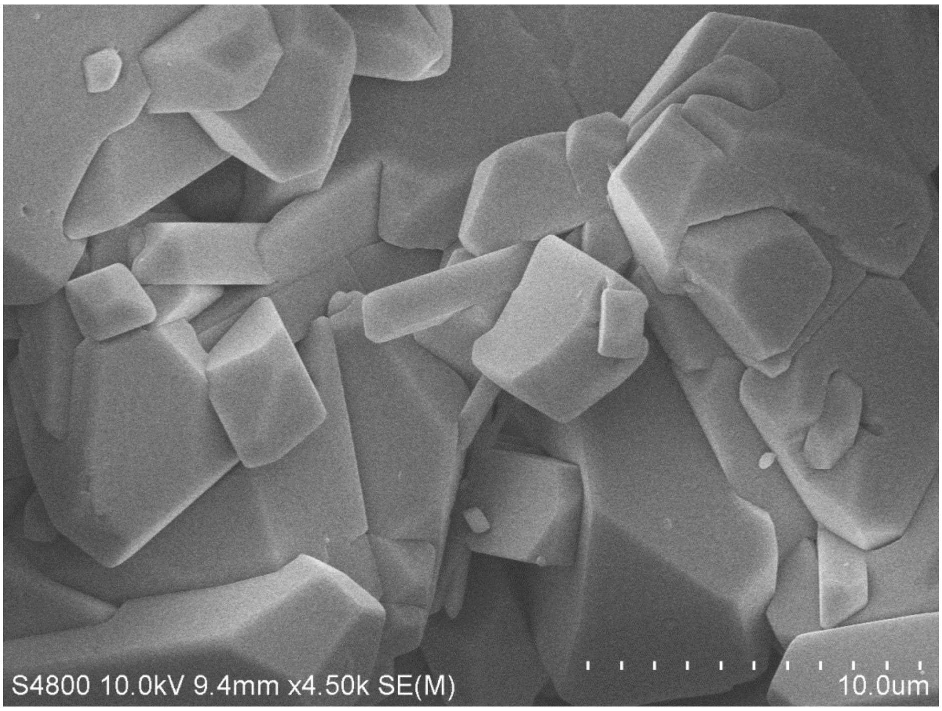

Figure S2: Catalytic Surface of $CuSeO_3 \cdot 2H_2O$ in FE-SEM (Sigma)

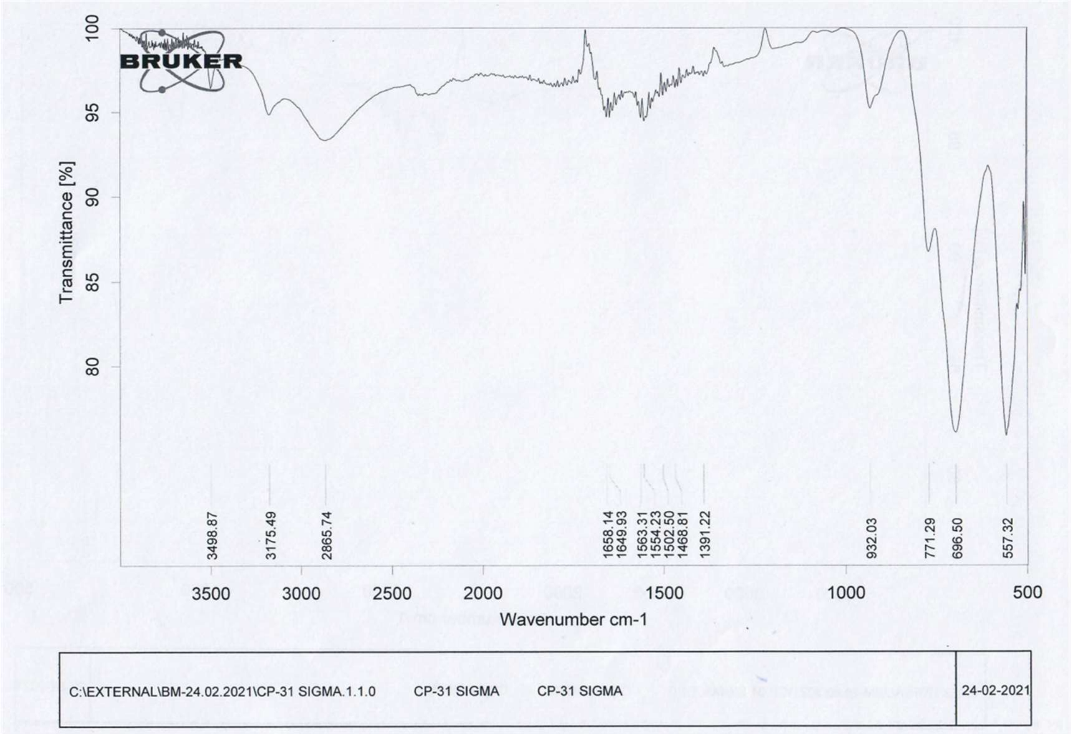

Figure S3: IR of $CuSeO_3 \cdot 2H_2O$ catalyst

IR characterization: 3327 cm^{-1} (O-H vibration), 1555 cm^{-1} (Se-O streching), 1429 cm^{-1} (Se=O streching), 671 cm^{-1} (Cu-O streching), 584 cm^{-1} (Cu-O-Se streching frequency).

Reference: a) R.J.M. Konings, A.S. Booij , A. Kovacs, Chemical Physics Letters **1998**, 292, 447–45; b) N. Dukstiene, L. Tatariskinaite, M. Andrulevicius, Materials Science-Poland, **2010**, 28, 93-103.

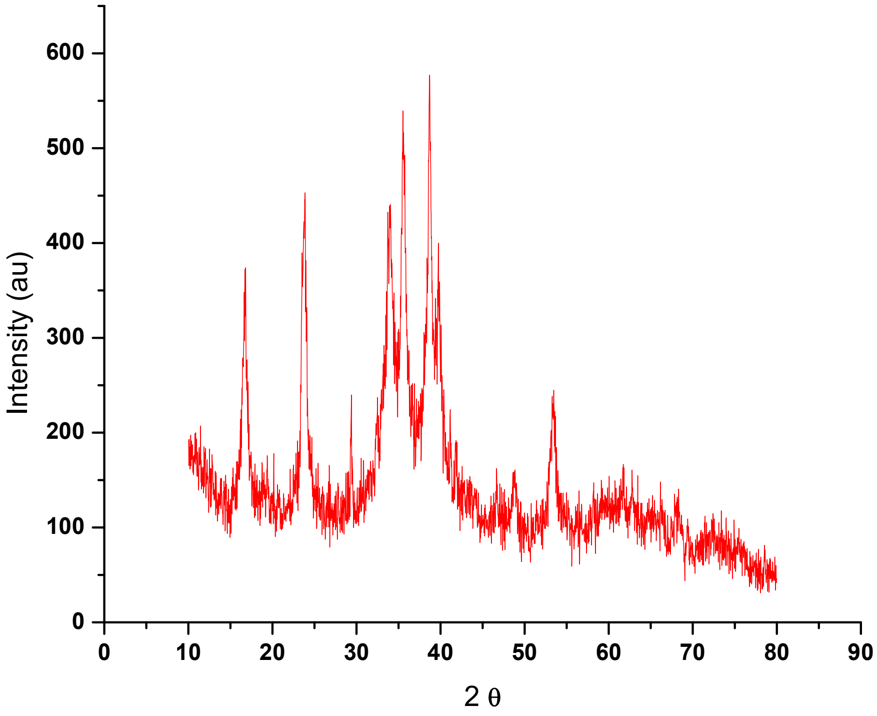

Figure S4: Powder XRD of $CuSeO_2.2H_2O$ catalyst (Sigma)

The X-ray diffraction analysis has been used to study the crystal structure of materilas. The powder XRD patterns at room temperature were recorded by using Rigaku model TTRX-III equipped with rotating anode-based Cu-Kα radiation (λ= 1.5418 A°). X-ray diffractometer was operating at 100mA and 50kV. XRD machine was operated with the following conditions: (i) 2θ-θ scanning mode, (ii) fixed monochromater (iii) continuous scanning, and (iv) measurement angle between 10-80° with 0.02° step.

7. ICP- AES study

ICP-AES (Inductively Coupled Plasma- Atomic Emission Spectrometry) analysis was carried out at Bhabha Atomic Research Centre (BARC), Trombay, with a Spectro-Arcos SOP unit, Germany. The spectrometer is augmented with a CCD detector array which was used for the analyses. High purity argon plasma was used as the plasma gas, carrier gas and auxiliary gas as well. To establish the calibration curves for the analyses, ICP standard solution purchased from MERCK was used. All measurements were done in triplicate. High pure Ar gas (total flow rate of 12 liters per minute) was also used for flushing of the detector before all the measurements to minimize the background. The detector set consists of thermally stabilized linear arrays of CCD detectors (3648 pixels/array). The detection limits are mentioned in the individual figures itself for each spectral line for easy ref. There are five analytical lines of 'Pd' available in the instrumental library on which measurements were done. All the samples were dissolved in 1M nitric acid (prepared from AR grade, Merck).

Figure S5: ICP-AES (Inductively Coupled Plasma- Atomic Emission Spectrometry) analysis was carried out at Bhabha Atomic Research Centre (BARC), Trombay, with a Spectro-Arcos SOP unit, Germany.

Procedure:

All experiments were repeated thrice for consistency of result. All analytes were dissolved in minimum quantity of 1M HNO_3 (prepared from AR grade, Merck) under IR lamp. ICP standard of $Pd(NO_3)_2$ solution purchased from Merck was used as control. The analytes were fed directly into the ICP after digestion with 1M HNO_3. Calibration curves were established for the ICP standard of $Pd(NO_3)_2$ solution after which the actual samples were run. There are 5 analytical lines (229.651, 324.270, 340.458, 344.140, 360.955 for palladium). The spectrometer can detection up to 0.2 ppm (200 ppb). All the four analytes showed no palladium impurity up to 0.2 ppm (200 ppb).

References:

(20) For ICP-OES Analysis See: Morrison, C.; Sun, H.; Yao, Y.; Loomis, R. A.; Buhro, W. E.; Methods for the ICP-OES Analysis of Semiconductor Materials. *Chem. Mater.* **2020**, 32, 1760–1768;

Instrumentation Details for ICP-OES/AES

Table 6. Instrumentation Details. ICP-AES spectrometer Spectro-Arcos SOP, Germany. Version 2.0.0.22336 software.

Gas Flow	
Plasma	15 L/min
Auxiliary	0.2 L/min
Nebulizer	0.70 L/min
RF Power	1300 Watts
Pump Flow Rate	1.5 mL/min

Spectrometer	
Resolution	High (0.0035 nm)
Read Time (sec)	Min 5; Max 20
Delay Time	60
Replicates	3
Calibration	Hg Realignment at 253 nm

Plasma	
Conditions	Same for all elements
Plasma View	Axial
Source Equilibration Delay	15 sec

Peristaltic Pump	
Sample Flow Rate	1.50 mL/min
Flush Time	60 sec

8. Mechanism Study by Computational DFT Study

All the calculations were performed by using Gaussian 09[1]. We optimized all the structure at meta-GGA M06L[2]-level, with Lanl2dz[3] basis set. Effective core potentials were applied for copper, selenium, iodine and potassium atoms. Extra d orbitals were included in the basis set for the selenium and iodine atoms. All the optimized structures were confirmed as the energetically minimized structures by the analytical frequency calculations with no imaginary value. Single-point electronic energies were generated for all optimized structures at M06-2X[4] level with SDD[5] for heavy atoms (Cu, Se, I and K) and 6-311+G(2d,p) basis set was used small atoms. The solvent effect of the reaction was considered by calculating the single-point energies through the SMD[6] model at M062X/SDD (Cu, Se, I and K)/6-311+G(2d,p) level. Dimethylformamide was used as a solvent. All the energy calculations were performed at a temperature of 363.15 K. The final free energies were calculated as

$$G= E_{M062X/SDD/6\text{-}311G(2d,p)} + G_{corr} + \Delta G_{sol}\ (G_{sol}\text{-}G_g)$$

The free energy correction (G_{corr}) was taken at M06L/Lanl2dz level. The ΔG_{sol} is the difference in the free energies between the solvent phase to the gas phase at M062X/SDD/6-311+G(2d, p).

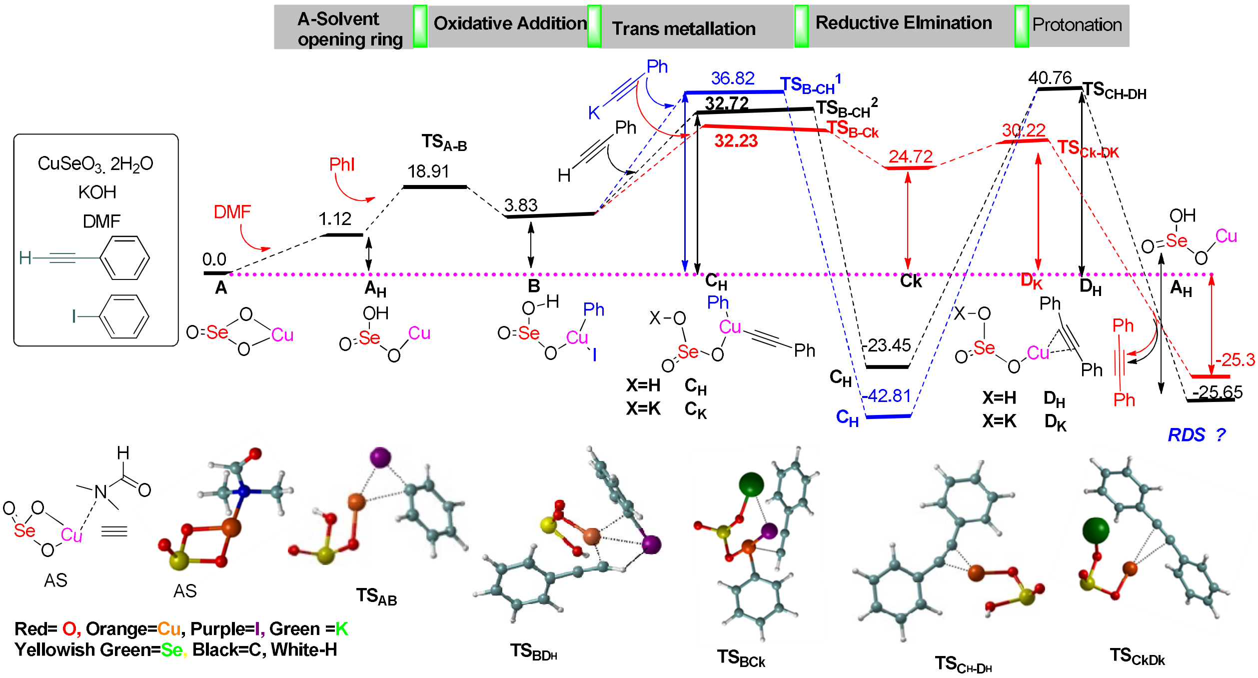

Figure S6: Free energy profile for $CuSeO_3.2H_2O$ mediated Sonogashira cross-coupling reaction using DFT Study

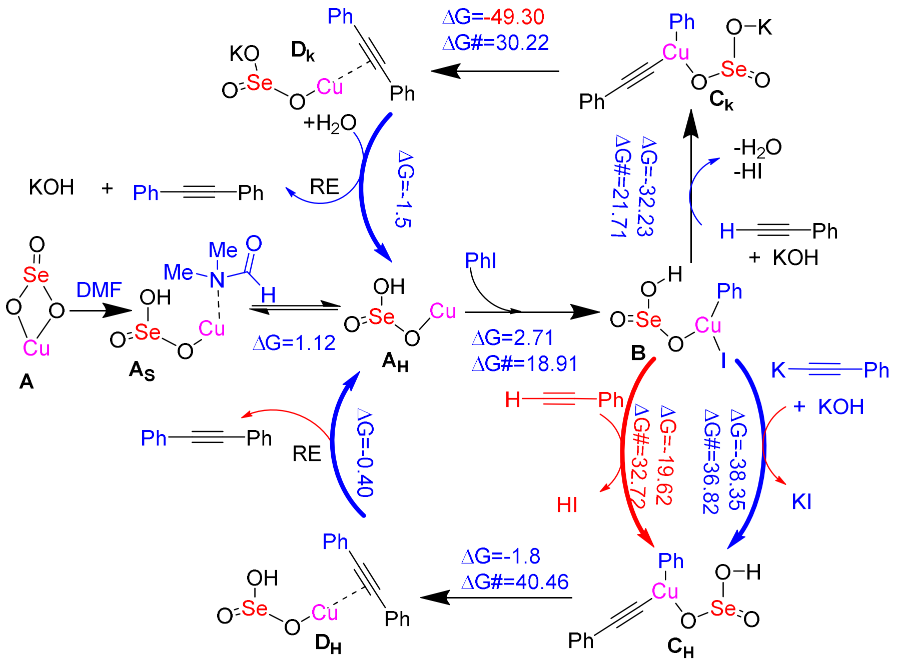

Figure S7: Plausible mechanism for $CuSeO_3.2H_2O$ mediated Sonogashira cross-coupling reaction using DFT

DMF is believed to open the [Se-O-Cu] bridge of $CuSeO_3$. $2H_2O$ **A** at an initial stage forming precursor complex **B** by forming solvated complex **AH** with ($\Delta \mathbf{G_{A-AH}}$=1.12 Kcal/Mol) (Figure 3).[23-28] The precursor complex **AH** undergoes oxidative addition of iodobenzene to generate successor complex **B** with (ΔG_{A-AH}=2.71Kcal/mol) through transition state TS_{AH-B} ($\Delta G^{\neq}$=18.91 Kcal/mol). The complex **B** could then undergo transmetallation with phenyl acetylene by two possible pathways. In the first pathway potassium plays the counter ion role. Complex B is transformed to $\mathbf{C_k}$ (K=potassium) with a free energy of 21.71 kcal/mol through transition state $TS_{BCk}^{\neq}$= 32.23; Whereas subsequent reductive elimination of $\mathbf{C_k}$ results in formation of stable intermediate $\mathbf{D_k}$ ($\Delta G^{\neq}$=-25.3 Kcal/mol) and diaryl acetylene product leaving $\mathbf{A_H}$ metal complex through transition. state $TS_{CkD}^{\neq}$ =30.22 Kcal/mol. Alternatively; complex B is transformed to $\mathbf{C_H}$ (H=hydrogen) via two ways; with free energy -23.72 Kcal/mol with transmetallation of phenylacetylene through transition state $TS_{BCH}^{\neq 1}$=36.82 Kcal/ mol or with free energy -42.81 Kcal/mol with transmetallation of the potassium salt of phenyl acetylene through transition state $TS_{BCH}^{\neq 2}$= 32.72 Kcal/mol to give the final complex C_H. whereas subsequent reductive elimination of $\mathbf{C_H}$ results in formation of the stable intermediate A_H ($\Delta G^{\neq}$=-25.65 Kcal/mol) and diarylacetylene product leaving $\mathbf{A_H}$ metal complex through transition state $TS_{CH-DH}^{\neq}$=40.46 Kcal/mol. As per the reduction potential data, both oxidative addition, transmetallation and reductive elimination was supposed to occurs at the copper centre assisted by the selenium metal.[17-18] The mechanism of A-A_S-A_H-B to C_k-D_K (activation barriers 21 and 30 kcal/mol) is more plausible in comparison to C_H-D_H (36 and 40 kcal/mol) activation barriers 36 and 40 kcal/mol. The activation energy barrier value is agreeing with experimental findings that correspond to relatively longer reaction time at 90 °C.

References

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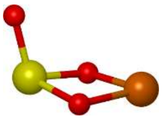
9: Cartesian Co-ordinates used for DFT Study:

a



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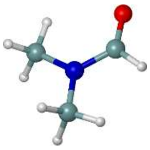
DMF



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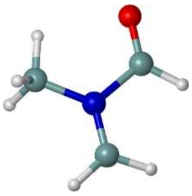
DMF-H



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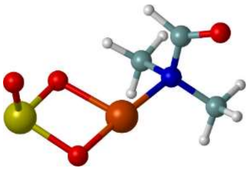

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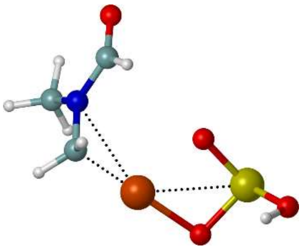

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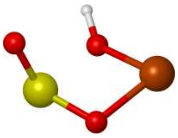

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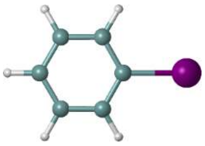

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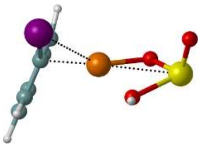

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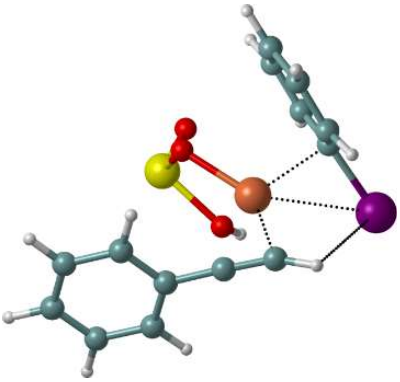

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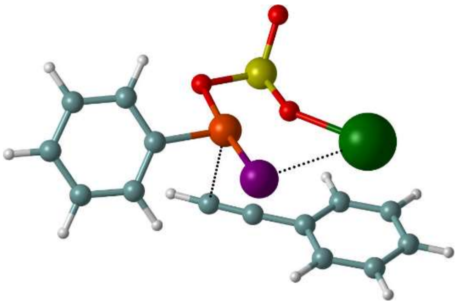

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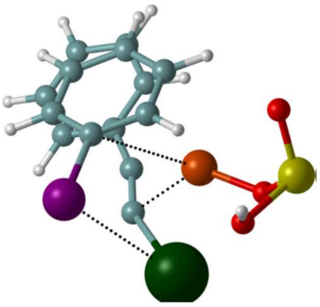

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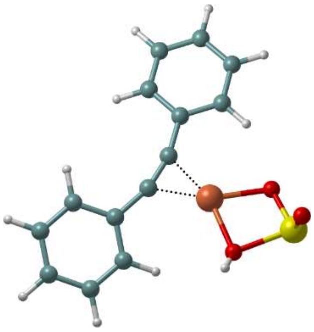

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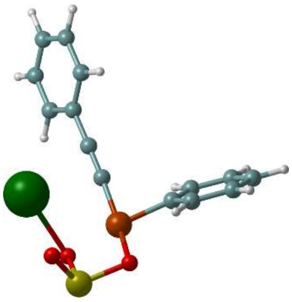

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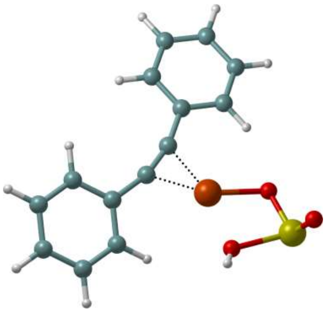
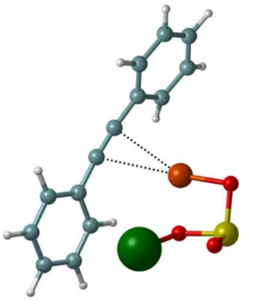
C	0.72085200	2.14059400	-0.11604300
C	1.49762100	2.58984900	0.95511300
C	-0.04947600	2.99608600	-0.90821800
C	0.78310600	4.86049000	0.42255000
C	1.52566600	3.97264900	1.21564900
C	0.00490100	4.37660600	-0.63917700
C	-0.86822300	0.11215000	-0.47893500
C	-2.08681000	-0.06914700	-0.32198300
C	-3.48882700	-0.29138200	-0.14090300
C	-4.13094200	0.13705900	1.04727300
C	-4.26181300	-0.94103300	-1.13376100
C	-5.50025700	-0.08051100	1.23306100
C	-5.63146500	-1.15312100	-0.94103300
C	-6.25640300	-0.72708400	0.24216700
H	2.11044200	1.90069900	1.52598800
H	2.13883400	4.34499300	2.02944800
H	0.80932800	5.92391000	0.63306300
H	-0.57195700	5.05973500	-1.25338800
H	-0.67355300	2.61456200	-1.70642500
H	-3.54707600	0.64905900	1.80407900
H	-5.97892300	0.25831600	2.14499000
H	-7.31788700	-0.89134700	0.38731700
H	-6.21183600	-1.64664700	-1.71235200
H	-3.77831700	-1.26186400	-2.04968700
Se	3.07744000	-1.54668500	-0.20770200
K	-0.00698400	-2.62500600	0.85382500



O	-2.31952300	0.31685500	-0.34291800
O	-0.84796800	2.33932000	-0.15042800
O	-3.23259300	2.24781300	1.44305800
Cu	-0.33569900	0.37646700	-0.11564300
C	0.15235700	-2.62049200	-0.01105500
C	-1.24805400	-2.78268800	-0.11807900
C	0.98207100	-3.76350700	0.09759500
C	-0.97766800	-5.19692300	-0.01693900
C	-1.80263700	-4.06603400	-0.12182500
C	0.41396000	-5.04083300	0.09396200
C	0.74549100	-1.31285300	-0.01235600
C	1.55015400	-0.33490100	-0.02321500
C	2.73072200	0.48058700	-0.00496000
C	3.95844500	-0.06673700	0.44051800
C	2.69076100	1.82748000	-0.43236400
C	5.11316100	0.72177700	0.45277400
C	3.85116500	2.60686600	-0.41811000
C	5.06532400	2.05860300	0.02550000
H	-1.88303700	-1.90355400	-0.19357100
H	-2.87651500	-4.18309700	-0.20413500
H	-1.41260800	-6.18981200	-0.01983200
H	1.05281200	-5.91266600	0.17526700
H	2.05636300	-3.63884700	0.17968100
H	3.99209500	-1.09816600	0.77302500
H	6.04904100	0.29671800	0.79628700
H	5.96327400	2.66478800	0.03770400
H	3.81180100	3.63689300	-0.75236200
H	1.74779200	2.24026100	-0.78141800
Se	-2.83445900	1.93484800	-0.12830600
H	-0.54494300	3.09111800	0.39901300



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Cu	-2.05460600	0.40605100	0.57407700
C	-0.16077700	2.35687000	-0.01863200
C	-1.03966000	2.09726000	1.09670400
C	-0.66548200	3.00588500	-1.16012200
C	-2.89493800	3.10216000	-0.18773000
C	-2.42281100	2.46057900	0.98738800
C	-2.02124600	3.38052900	-1.24034600
C	1.17764200	1.88374000	0.03253500
C	2.29784200	1.37632700	0.08561600
C	3.54710700	0.69792800	0.17550700
C	4.61183900	0.98302300	-0.71492300
C	3.72714200	-0.30939000	1.15990300
C	5.81796200	0.28167400	-0.61937200
C	4.93761100	-1.00477500	1.24482600
C	5.98653800	-0.71393200	0.35711200
H	-0.60713900	1.80494000	2.04768400
H	-3.06439500	2.40611100	1.86040200
H	-3.94031400	3.37619700	-0.25787200
H	-2.38781500	3.87395500	-2.13164000
H	0.00318600	3.20676500	-1.98959400
H	4.48274000	1.75753500	-1.46216200
H	6.62784900	0.51252000	-1.30143500
H	6.92399000	-1.25243700	0.42814200
H	5.06505300	-1.76744800	2.00374300
H	2.91835100	-0.52181800	1.85172100
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K	0.91392600	-1.27696700	-1.09440300

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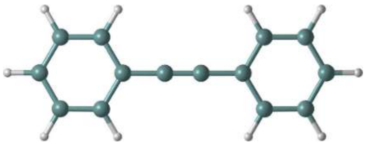

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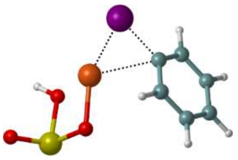
C	-2.03844200	-0.00382300	-0.00042700
C	-2.76393300	-1.21981600	0.00105800
C	-2.75600100	1.21688000	-0.00130300
C	-4.16216300	-1.21065900	0.00164000
C	-4.15422200	1.21703600	-0.00076600
C	-4.86379100	0.00550600	0.00072400
H	-2.21985500	-2.15734400	0.00180400
H	-4.70557300	-2.14869800	0.00282600
H	-5.94770200	0.00908800	0.00115900
H	-4.69133900	2.15870800	-0.00148500
H	-2.20562600	2.15071400	-0.00244900
C	2.03840200	-0.00385600	-0.00073600
C	2.75597200	1.21690400	0.00078200
C	2.76397300	-1.21972900	-0.00158600
C	4.15417200	1.21703100	0.00167300
H	2.20566100	2.15079600	0.00136200
C	4.16221100	-1.21062600	-0.00070200
H	2.21993300	-2.15729900	-0.00289100
C	4.86383200	0.00550900	0.00100600
H	4.69125700	2.15873000	0.00296500
H	4.70545600	-2.14875900	-0.00130300
H	5.94773900	0.00914300	0.00181700

TS1



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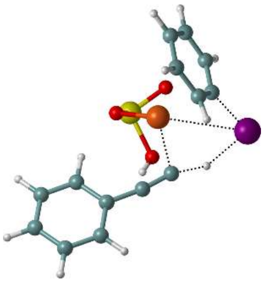
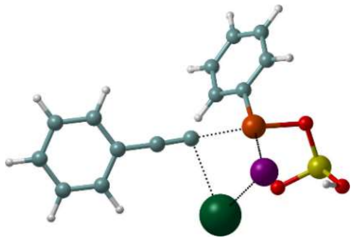
O	-3.99438900	-0.81465600	-0.61985500
O	-1.67317200	0.72773300	-0.75153700
Cu	-0.40207500	-0.52067900	0.22714900
C	1.96223800	0.63004600	-0.07680700
C	1.39694700	1.36870800	-1.12962700
C	2.58151500	1.24878100	1.02039300
C	2.06233800	3.40884700	0.02240900
C	1.44758900	2.76858100	-1.06340200
C	2.62637000	2.65094900	1.05881600
I	1.90881000	-1.51660300	-0.16879400
H	0.90178100	0.87954600	-1.95909400
H	0.99071800	3.34603000	-1.85708900
H	2.09509000	4.49069000	0.06464800
H	3.09999700	3.14145600	1.90077800
H	3.01114300	0.66387700	1.82422300
Se	-3.17360500	0.46915900	0.02577700
H	-2.47929500	-1.12456100	2.00199200

TS2



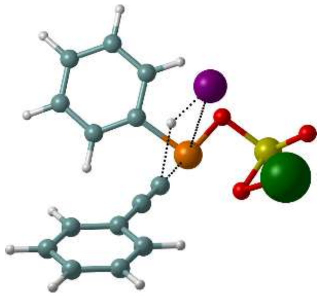
O	-0.85769500	1.75715200	0.40151200
O	-0.37495300	1.25472600	-2.20308800
O	1.56266200	2.39815200	-0.72010000
Cu	0.03206800	0.05695500	0.72476100
C	2.12183300	-0.59392600	0.81278100
C	2.78810300	0.61653900	1.11346600
C	1.32819600	-1.26307000	1.79670100
C	1.82429700	0.56371200	3.35263200
C	2.64258500	1.17755400	2.38955400
C	1.16191900	-0.63723800	3.05996100
C	-0.83009900	-1.48565100	-0.51420900
C	-2.06263700	-1.38126800	-0.38542000
C	-3.44070000	-1.09661400	-0.13828600
C	-4.43658500	-2.08355500	-0.31580700
C	-3.80945900	0.20298100	0.29068500
C	-5.77869000	-1.77529800	-0.07040600
C	-5.15471400	0.49460200	0.53773000
C	-6.14174400	-0.48850300	0.35791300
H	3.36195200	1.12607400	0.35437200
H	3.14321500	2.11089200	2.61066700
H	1.69968000	1.01911200	4.32675100
H	0.54567600	-1.12363700	3.80588700
H	0.94232900	-2.26013800	1.62141300
H	-4.14988300	-3.07552800	-0.64536900
H	-6.53893100	-2.53462900	-0.21124000
H	-7.18251900	-0.25446100	0.54993800
H	-5.43341700	1.48825800	0.86883900
H	-3.03368100	0.95335100	0.42753400
Se	-0.07546600	2.58655000	-0.91786300
H	0.46728300	-1.76001000	-1.02207300
I	2.54796300	-1.56144000	-1.02080000
H	-1.14183200	0.69081400	-1.94543900

TS3



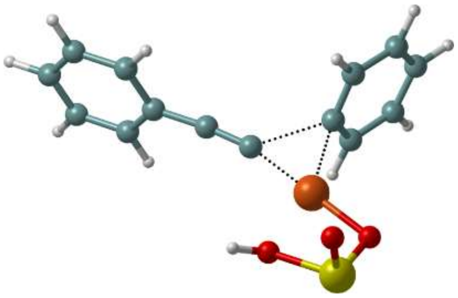
O	-1.73405400	-0.35080900	1.79187900
O	-3.87309800	-1.51950400	0.44095200
O	-2.66425700	0.83037100	-0.35401900
Cu	-0.76276800	0.60530000	-0.39551700
C	-0.50444700	2.54973600	-0.30193500
C	0.42355200	3.14936100	0.54470900
C	-1.33868500	3.24860100	-1.17180400
C	-0.28709400	5.29843600	-0.37172400
C	0.51981600	4.55600400	0.50203600
C	-1.20809700	4.65162700	-1.20703000
C	1.51470000	0.23419100	-0.15507600
C	2.73927300	0.05572500	-0.03055700
C	4.15702200	-0.11132400	0.07388300
C	4.72626200	-1.03167800	0.98570700
C	5.02542000	0.64883400	-0.74608300
C	6.11366000	-1.18736200	1.07661300
C	6.41185600	0.48788200	-0.65269700
C	6.96359700	-0.42778100	0.25779100
H	1.07327700	2.56766000	1.18492300
H	1.24144300	5.05138600	1.14276700
H	-0.19967700	6.37853500	-0.39984700
H	-1.84582400	5.22173800	-1.87354100
H	-2.08743800	2.74786100	-1.77364300
H	4.07255100	-1.62735800	1.61811000
H	6.53137300	-1.89934800	1.77948400
H	8.03842800	-0.54905800	0.32653700
H	7.06277400	1.07558300	-1.28994100
H	4.59733500	1.35283300	-1.44944400
Se	-3.23006900	0.03227200	1.09814800
I	-0.88557900	-2.43281900	-1.26337000
H	-3.21842700	-1.97624700	-0.16205900
K	0.43382800	-1.70890000	1.79656600

TS4



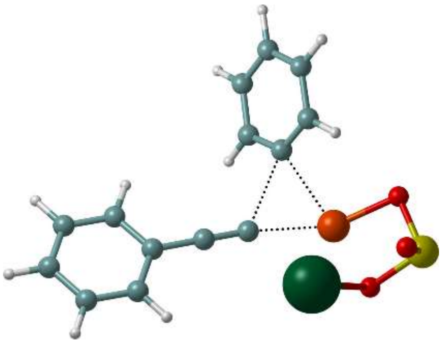
O	0.87634200	1.99746500	-0.83853700
O	0.89555900	0.86607000	1.44461100
O	-0.61190000	3.10483100	1.26411000
Cu	0.10390700	0.16589300	-0.43057100
C	-2.04775900	-0.01633000	-0.79886300
C	-2.49693100	1.24028300	-0.32613400
C	-1.42216600	-0.13472800	-2.08212700
C	-1.67739400	2.27341400	-2.37442500
C	-2.27410300	2.37972700	-1.10577000
C	-1.25750600	1.03099900	-2.85982700
C	0.41175500	-1.89898900	-0.07831900
C	1.64976000	-1.82608400	-0.22364800
C	3.05429700	-1.59948900	-0.35687600
C	3.97450500	-2.66230600	-0.20272500
C	3.52839600	-0.29614900	-0.64509100
C	5.34658300	-2.42587800	-0.33392500
C	4.90337100	-0.07554500	-0.77576600
C	5.81451500	-1.13308500	-0.62080400
H	-2.95379400	1.34034500	0.65019600
H	-2.52142900	3.34572800	-0.68936900
H	-1.51046900	3.16428800	-2.96552400
H	-0.77441600	0.95040100	-3.82563900
H	-1.17295700	-1.10893800	-2.48715000
H	3.60565500	-3.65923700	0.01303200
H	6.04869900	-3.24347800	-0.21561400
H	6.87880900	-0.95278800	-0.72303700
H	5.26235400	0.92304200	-0.99563200
H	2.81307500	0.51846100	-0.75563000
Se	0.92580500	2.53958000	0.84541600
H	-0.93526900	-2.33870400	0.01429100
I	-2.95012500	-1.78508600	0.06451300
K	-0.37885700	-0.65095600	2.84461200

TS5



O	3.05937200	0.00710800	-0.34404400
O	1.60235000	-1.97777700	-0.49887300
O	3.67007600	-2.03018200	1.45690800
Cu	1.10490600	0.03923100	-0.23523700
C	-0.12951300	2.10586300	0.01303200
C	0.00105600	2.61921100	1.29840300
C	-0.17602600	2.84588800	-1.16312100
C	0.12326200	4.81641100	0.24412900
C	0.14083800	4.01660300	1.39793600
C	-0.03423600	4.24015000	-1.02632100
C	-0.98793300	0.07369600	-0.11930300
C	-2.19459000	-0.24041500	-0.05508100
C	-3.51569000	-0.76035200	0.00001000
C	-4.07938300	-1.16235900	1.23770800
C	-4.29295900	-0.88584600	-1.17961600
C	-5.37816400	-1.67417300	1.28906800
C	-5.59141900	-1.39779600	-1.11784700
C	-6.13860700	-1.79502600	0.11373400
H	0.00458500	1.98395700	2.17286500
H	0.26269000	4.46726300	2.37564500
H	0.22866200	5.89057200	0.33562700
H	-0.04905000	4.86279500	-1.91292900
H	-0.30839600	2.37974800	-2.12937400
H	-3.48598600	-1.06984300	2.13977100
H	-5.79847300	-1.98117800	2.23960200
H	-7.14535100	-2.19406100	0.15705000
H	-6.17720000	-1.48984800	-2.02499600
H	-3.86377400	-0.58077000	-2.12677800
Se	3.52860400	-1.63049000	-0.14129000
H	1.18328500	-2.77400300	-0.10906600

TS6



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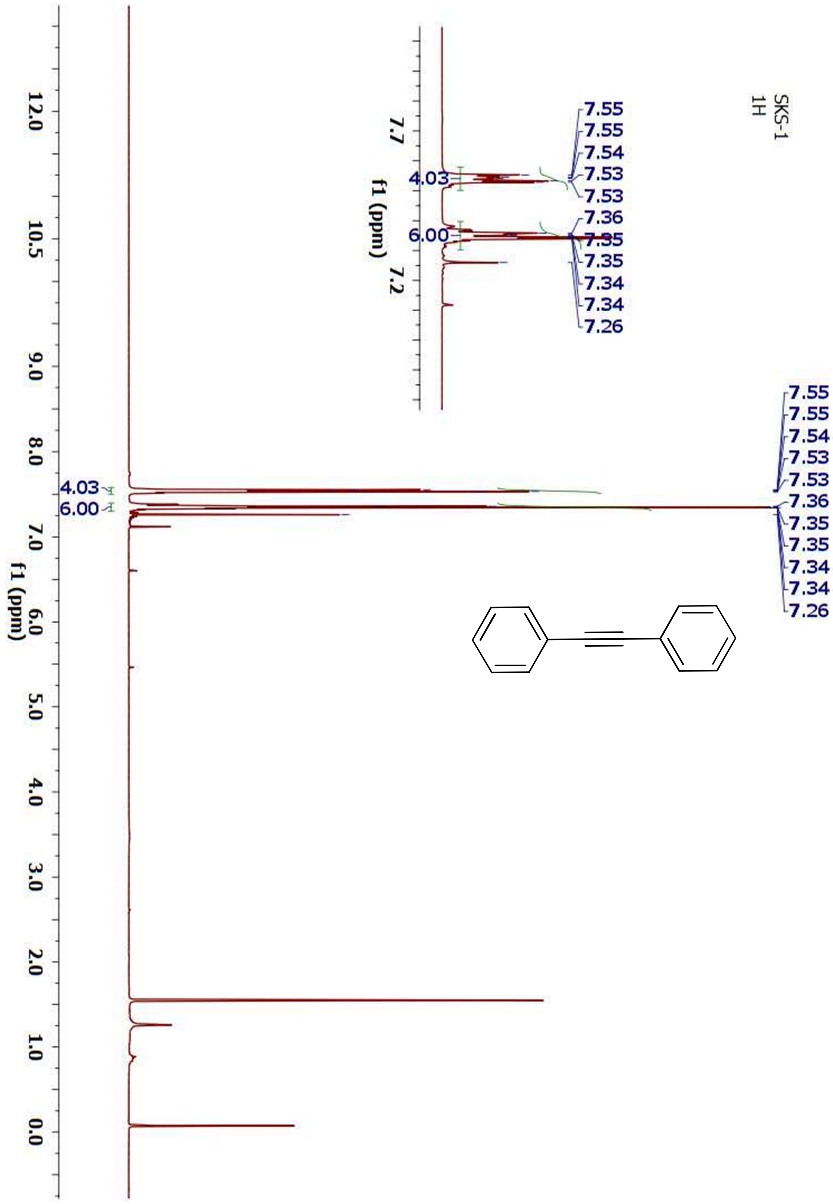
O	2.21383400	-1.51261200	-1.10180400
O	3.06408600	-1.58348600	1.44679900
Cu	1.27881600	0.23730900	-0.95276600
C	-0.09499600	2.11470500	-0.12275200
C	0.59538700	2.44660700	1.03599900
C	-0.96632900	2.93748500	-0.82335300
C	-0.43380700	4.65257800	0.83097700
C	0.41876800	3.76516000	1.50566200
C	-1.11779300	4.24872000	-0.32696300
C	-1.02662600	-0.08212900	-0.56225600
C	-2.21041700	-0.41598800	-0.34655800
C	-3.58193500	-0.77780400	-0.16360500
C	-4.58888700	0.21683400	-0.22533000
C	-3.97120500	-2.11685100	0.07935700
C	-5.93387000	-0.12172700	-0.04634400
C	-5.31815200	-2.44919000	0.25720000
C	-6.30607200	-1.45372300	0.19633200
H	1.29214200	1.76653700	1.51306700
H	0.96383900	4.08632000	2.38609700
H	-0.56593200	5.65990300	1.20807300
H	-1.77442900	4.93805500	-0.84644400
H	-1.49802200	2.59821300	-1.70205300
H	-4.29920800	1.24523100	-0.41063300
H	-6.69227100	0.65125400	-0.09696300
H	-7.34964200	-1.71237000	0.33302900
H	-5.59892700	-3.48054800	0.43873700
H	-3.21140800	-2.89226700	0.11206200
Se	3.57566300	-0.98665300	-0.05111800
K	0.58129100	-2.35698400	0.89789500

10: Proton(400 MHz) and Carbon NMR(100 MHz)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7.34
7.34
7.26
4.03
6.00
7.7
7.2
f1 (ppm)
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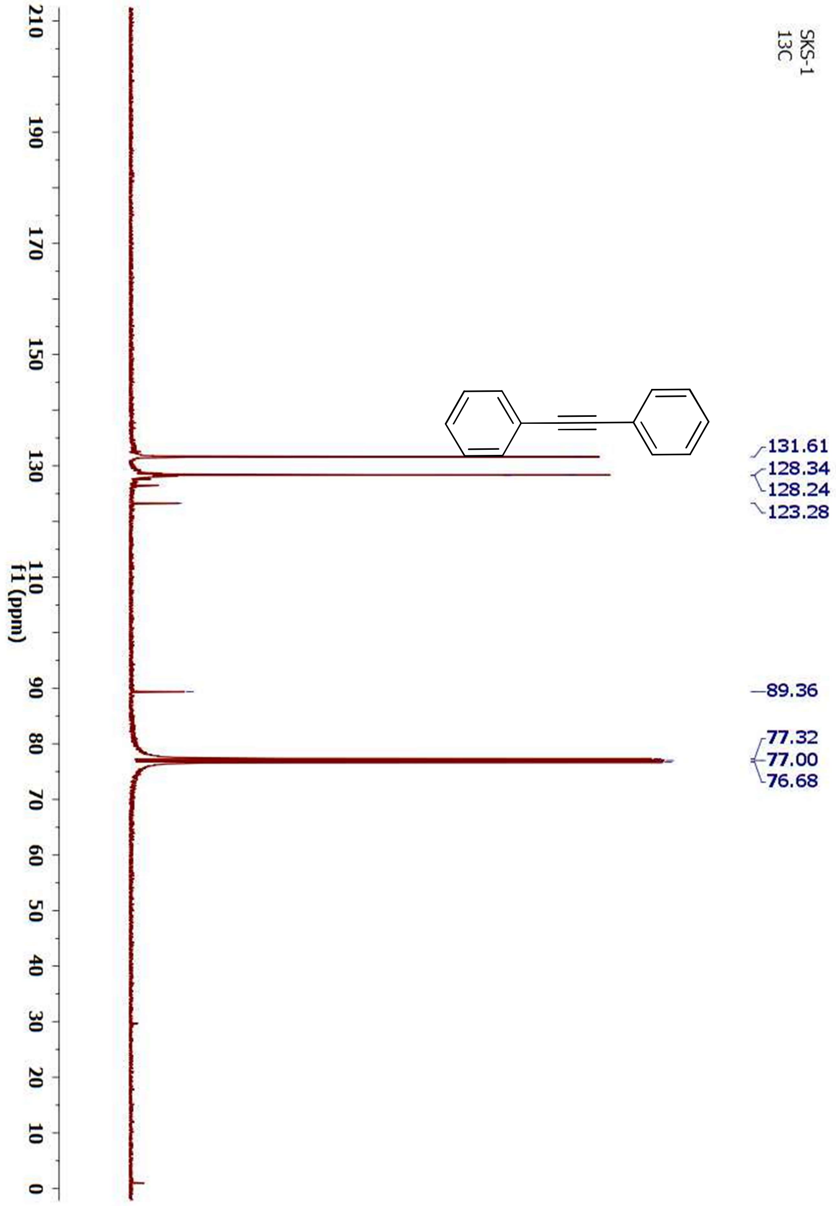
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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77.32
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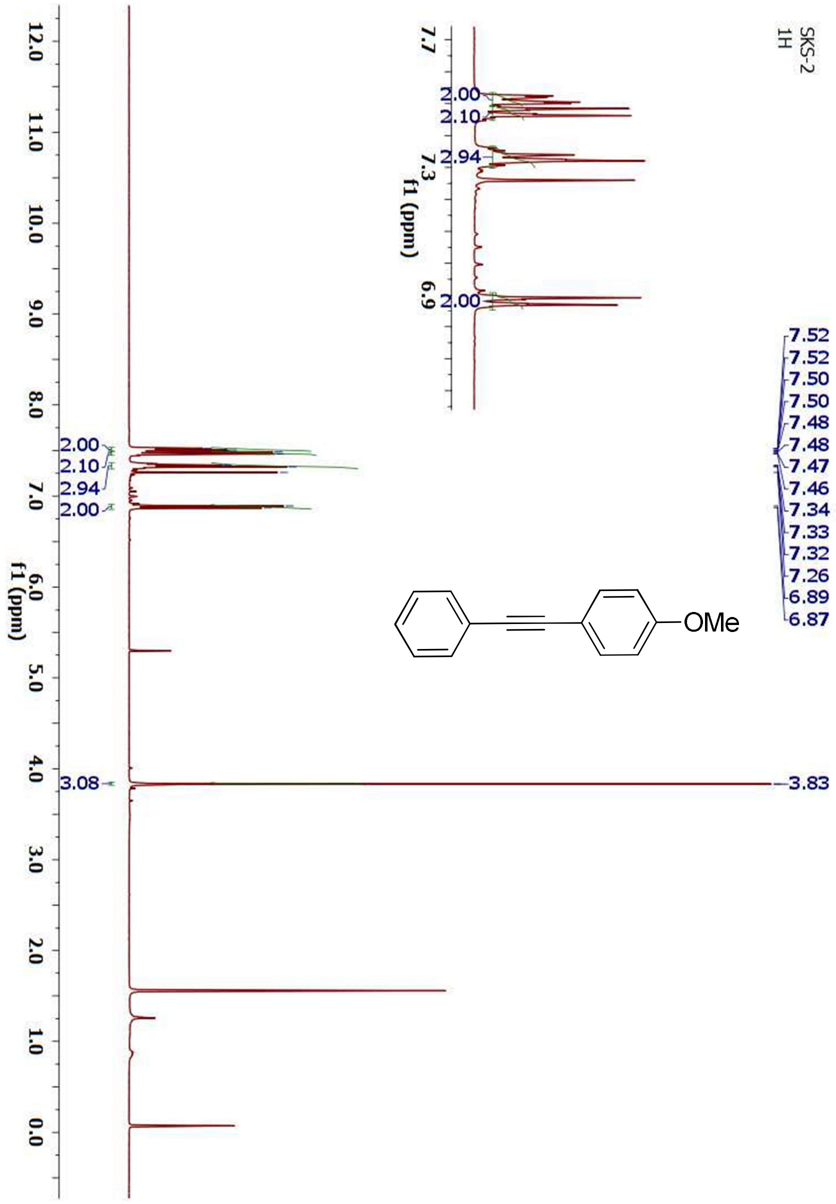
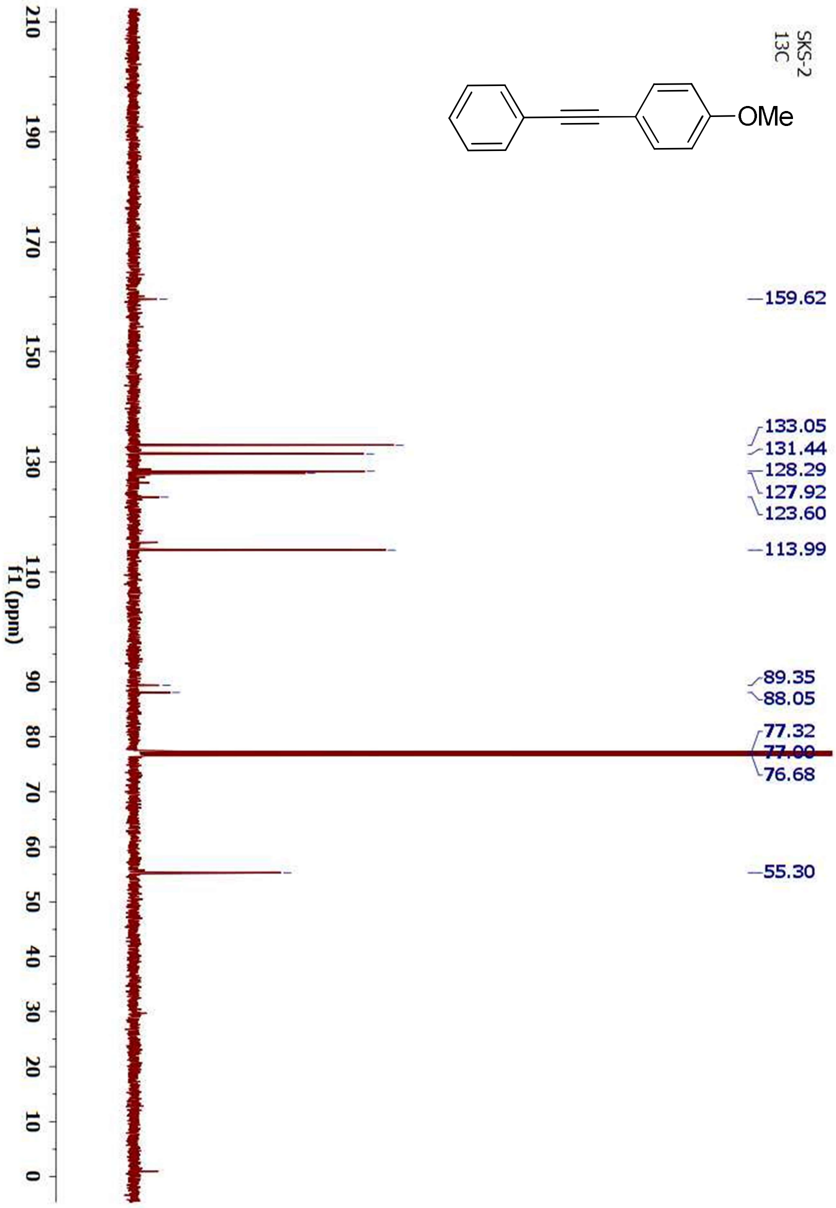
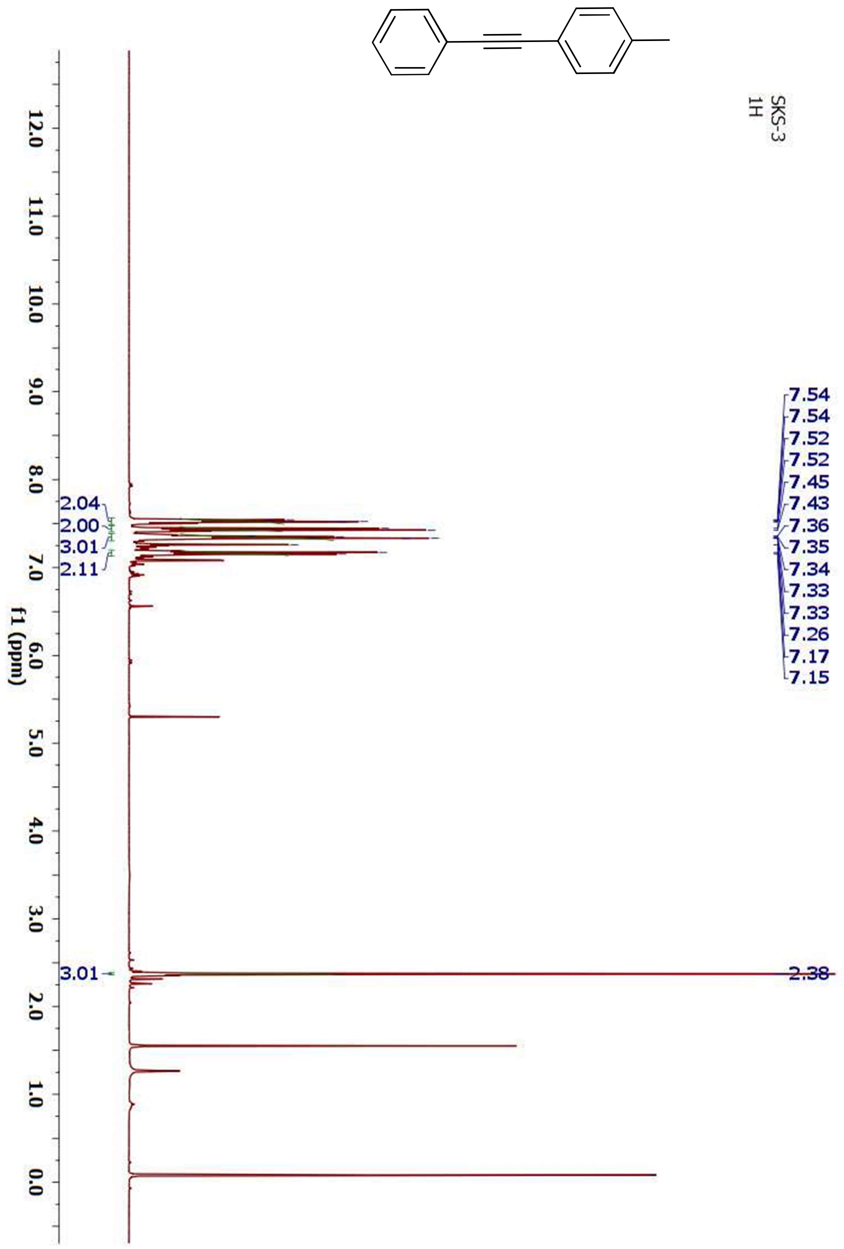
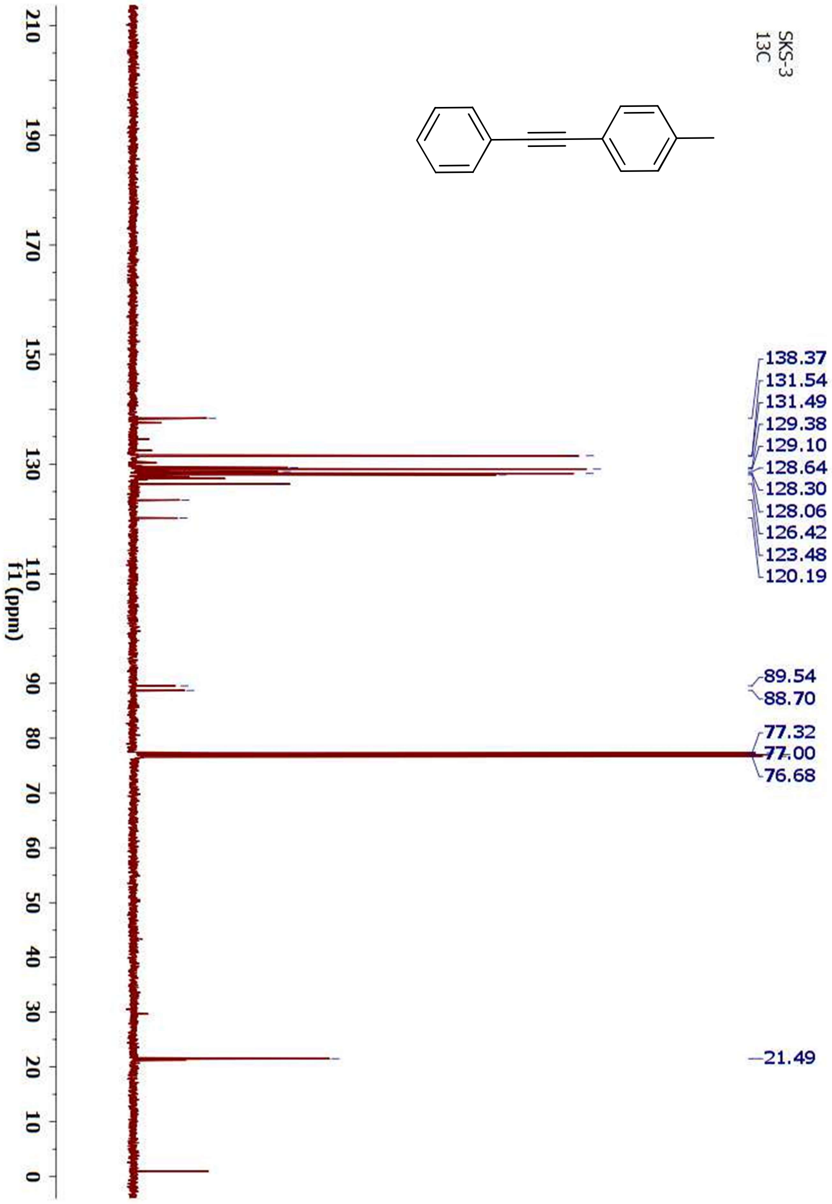
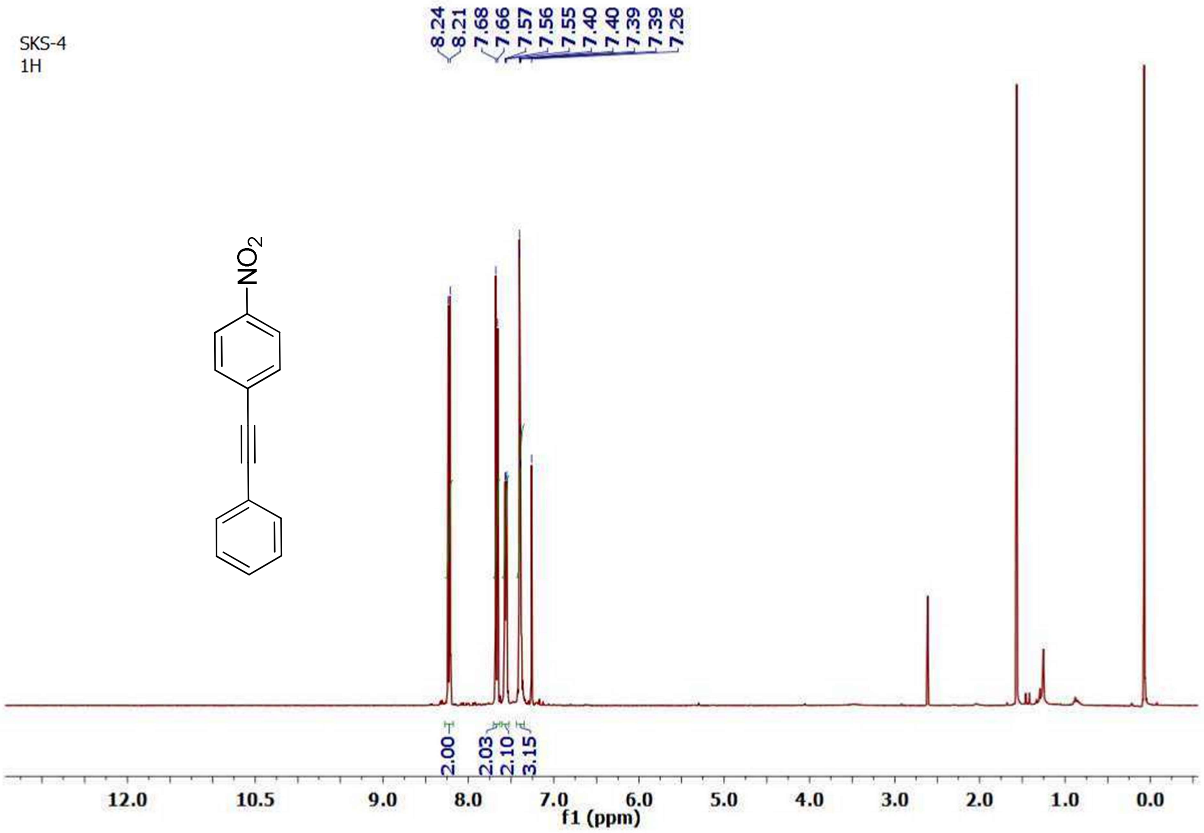
76.68
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

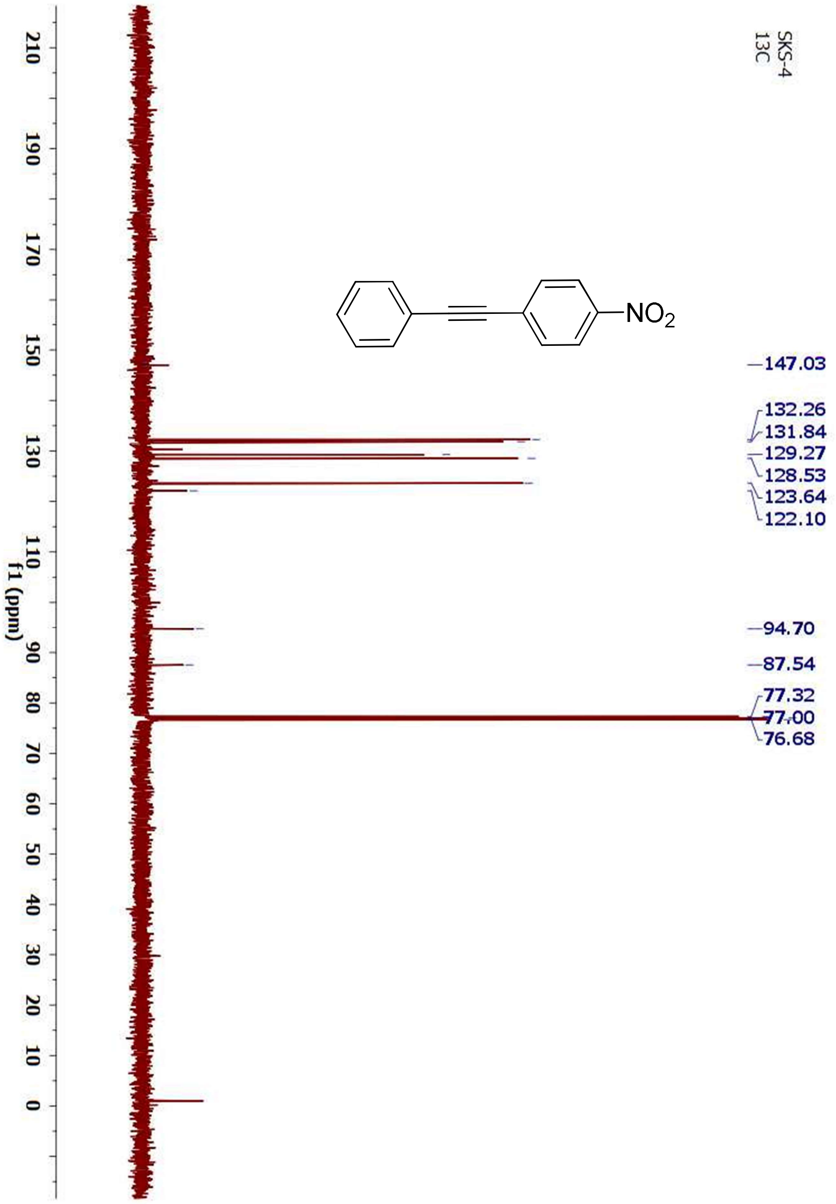

SKS-2
1H
7.52
7.52
7.50
7.50
7.48
7.48
7.47
7.46
7.34
7.33
7.32
7.26
6.89
6.87
3.83
OMe
2.00
2.10
2.94
2.00
3.08
7.7
7.3
6.9
f1 (ppm)
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

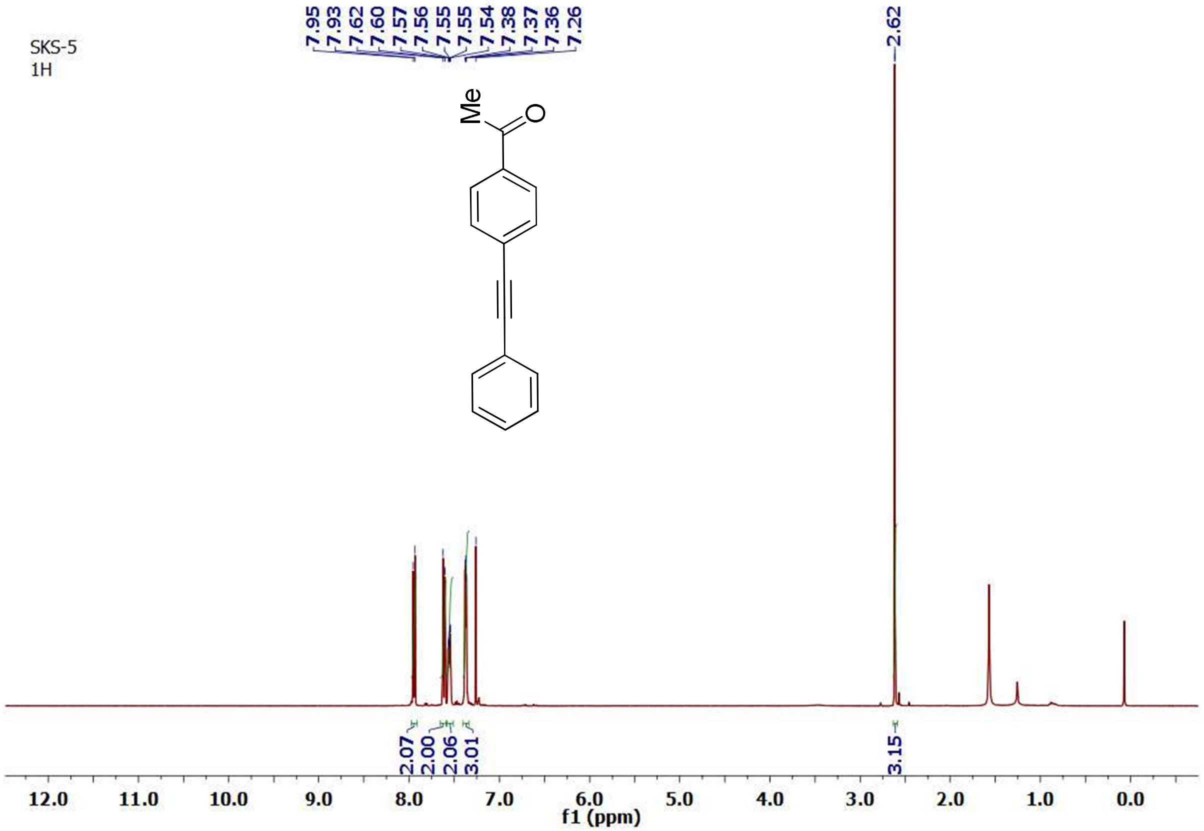
SKS-2
13C
OMe
159.62
133.05
131.44
128.29
127.92
123.60
113.99
89.35
88.05
77.32
77.00
76.68
55.30
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

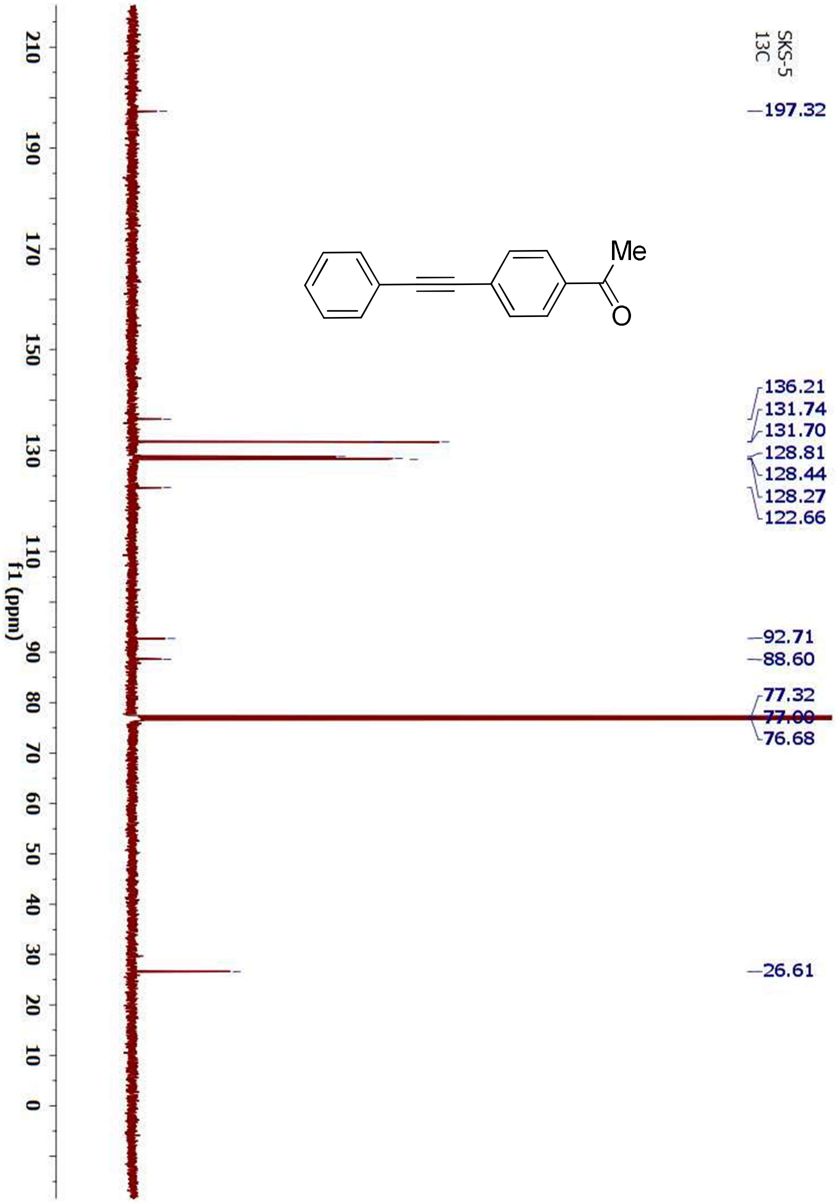

SKS-3
1H
7.54
7.54
7.52
7.52
7.45
7.43
7.36
7.35
7.34
7.33
7.33
7.26
7.17
7.15
2.38
2.04
2.00
3.01
2.11
3.01
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

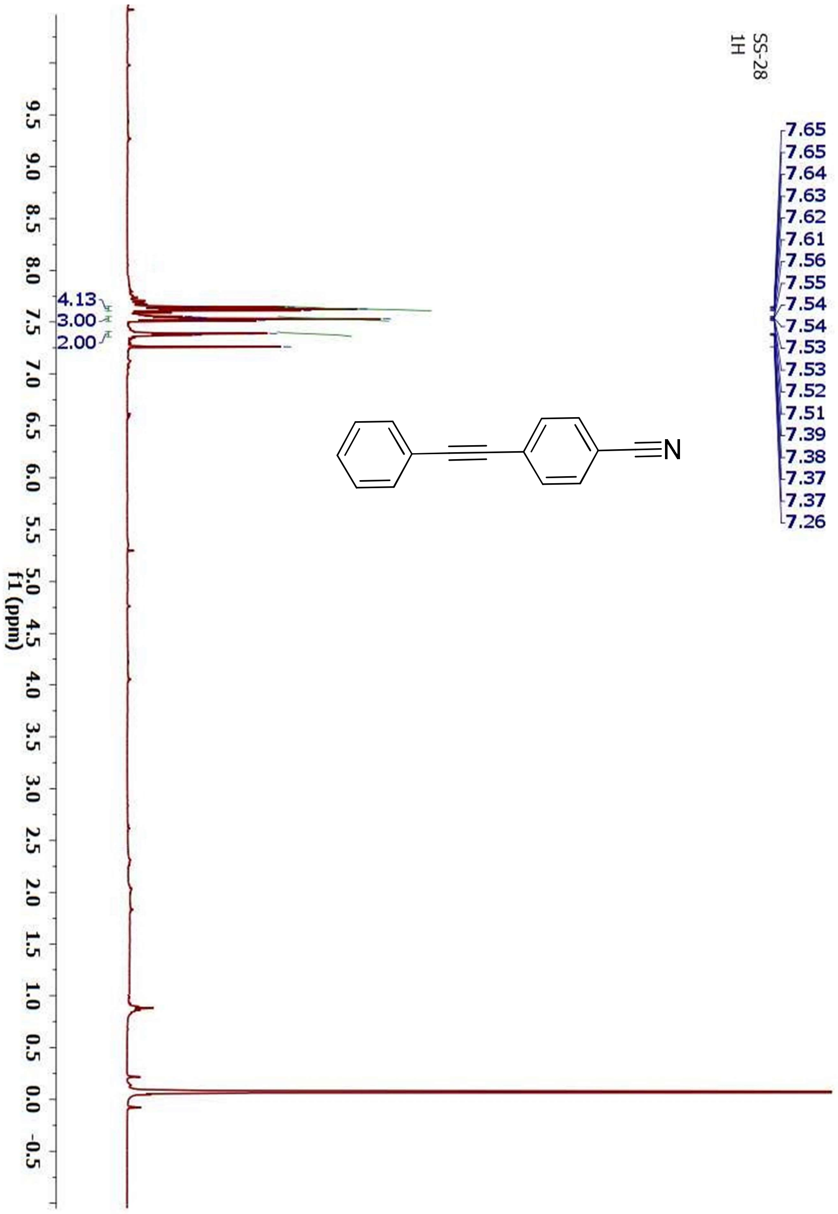

SKS-3
13C
138.37
131.54
131.49
129.38
129.10
128.64
128.30
128.06
126.42
123.48
120.19
89.54
88.70
77.32
77.00
76.68
21.49
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

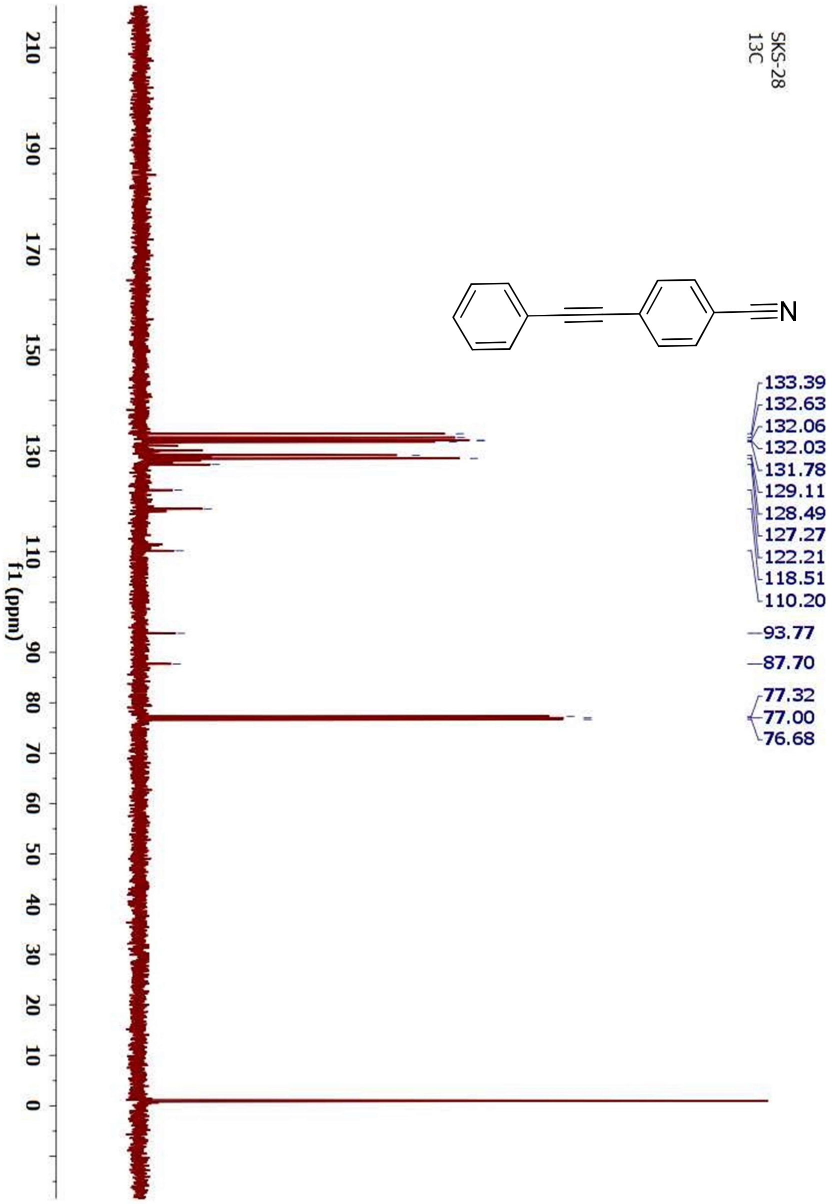

SKS-4
1H
NO2
8.24
8.21
7.68
7.66
7.57
7.56
7.55
7.40
7.40
7.39
7.39
7.26
2.00
2.03
2.10
3.15
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

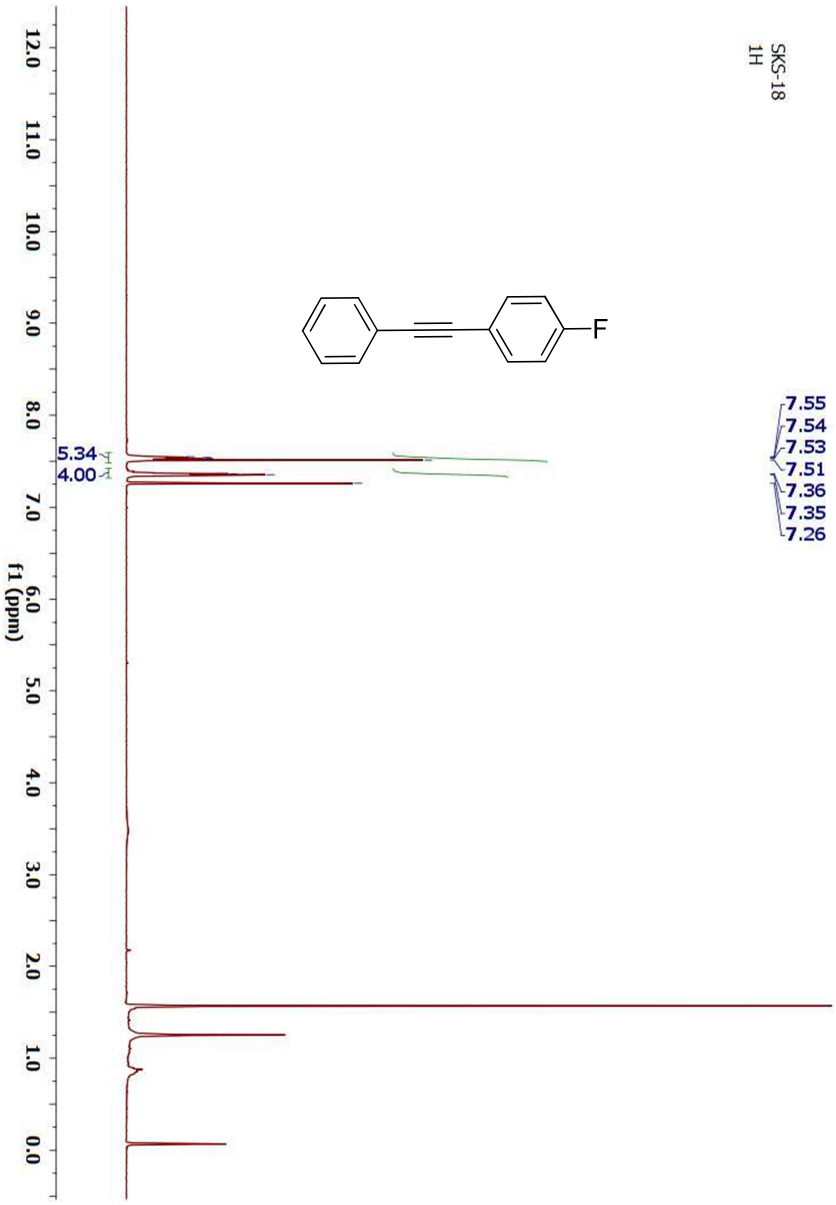

SKS-4
13C
NO2
147.03
132.26
131.84
129.27
128.53
123.64
122.10
94.70
87.54
77.32
77.00
76.68
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

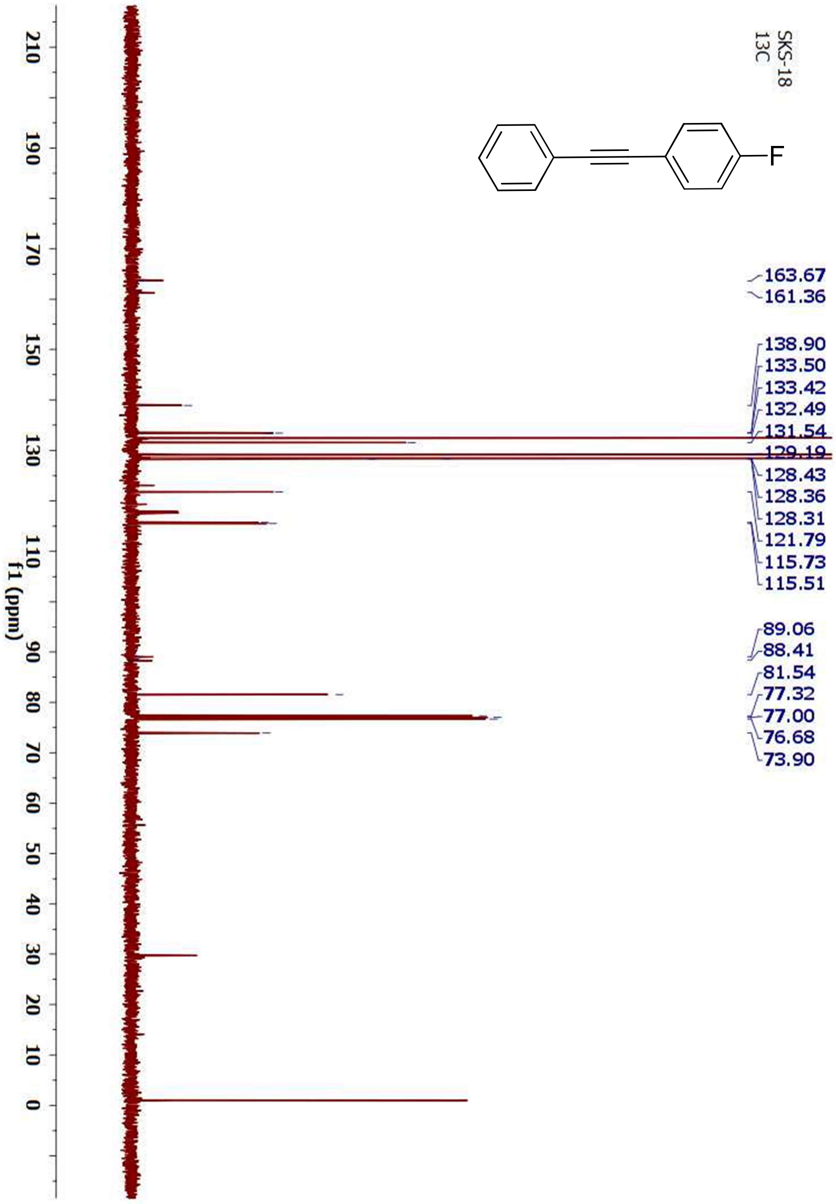

SKS-5
1H
7.95
7.93
7.62
7.60
7.57
7.56
7.55
7.55
7.54
7.38
7.37
7.36
7.26
2.62
Me
O
2.07
2.00
2.06
3.01
3.15
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

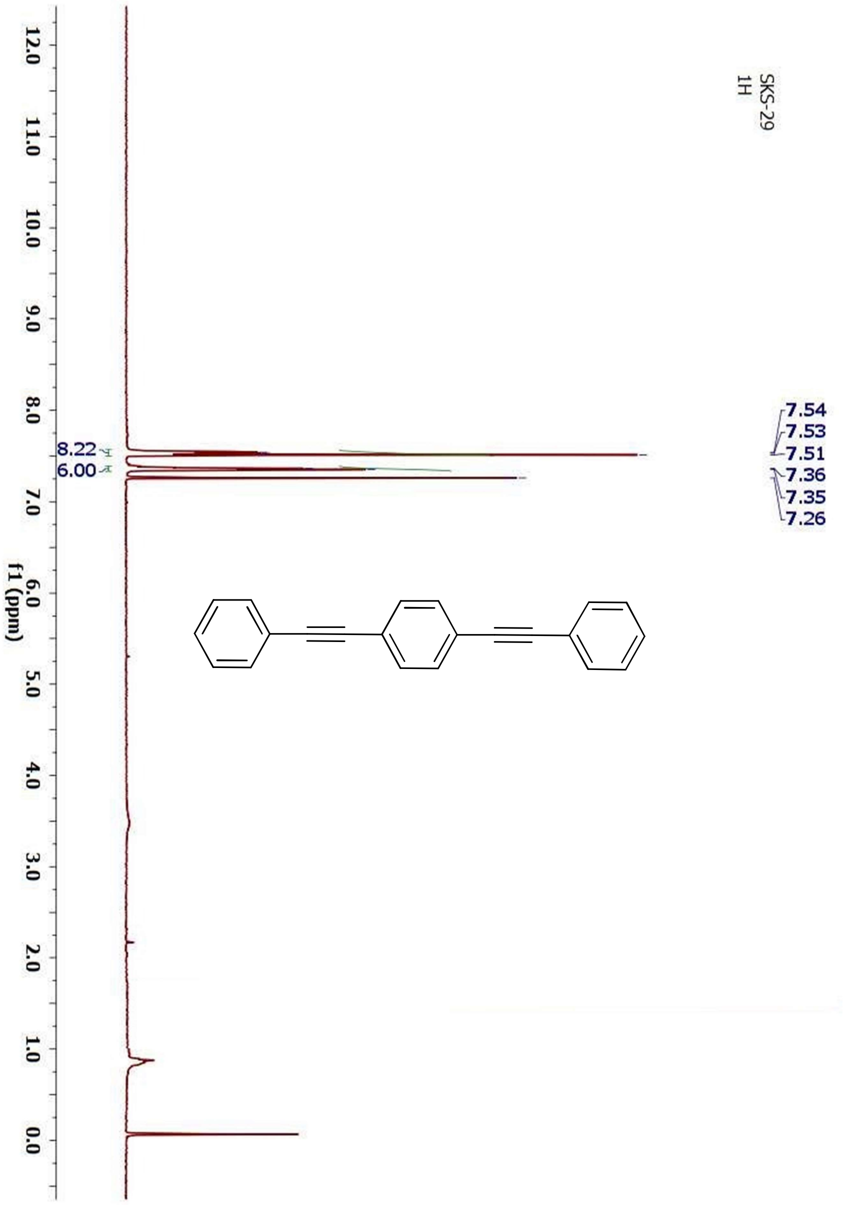

SKS-5
13C
197.32
Me
O
136.21
131.74
131.70
128.81
128.44
128.27
122.66
92.71
88.60
77.32
77.00
76.68
26.61
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

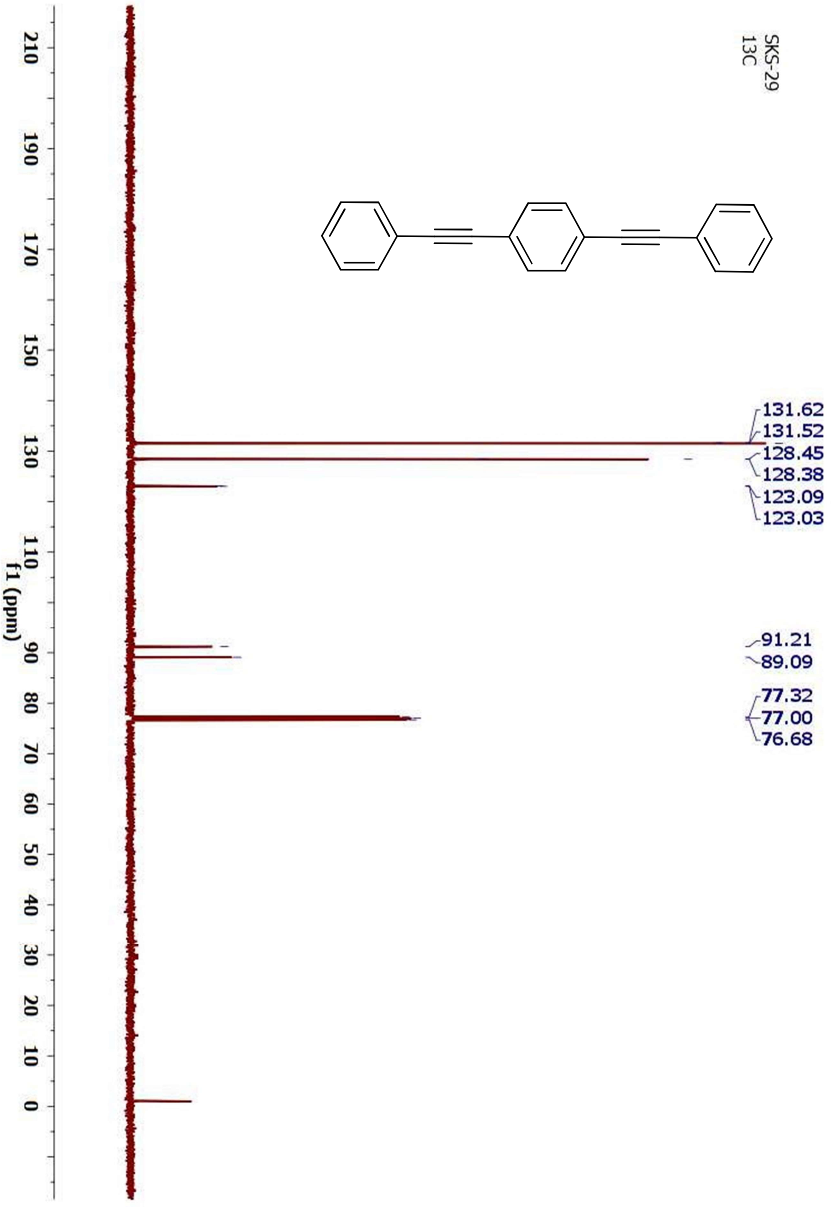

SS-28
1H
7.65
7.65
7.64
7.63
7.62
7.61
7.56
7.55
7.54
7.54
7.53
7.53
7.52
7.51
7.39
7.38
7.37
7.37
7.26
N
4.13
3.00
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

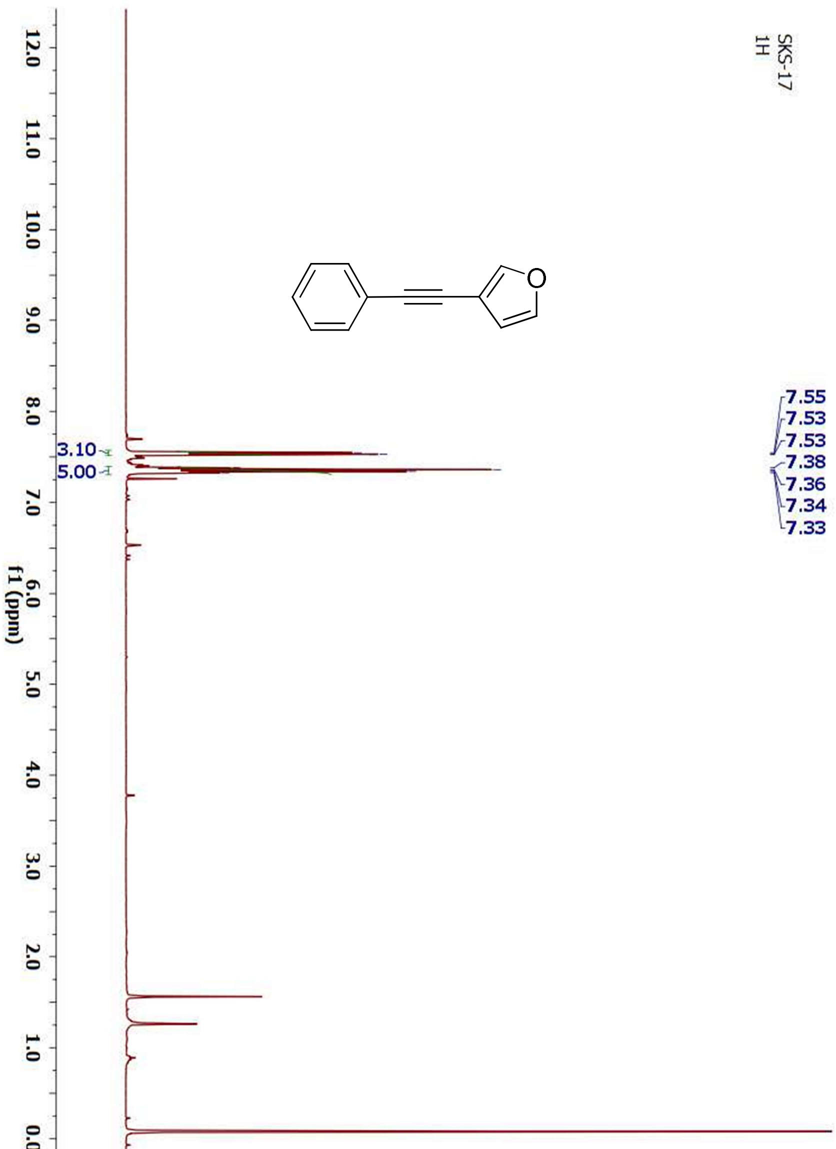

SKS-28
13C
N
133.39
132.63
132.06
132.03
131.78
129.11
128.49
127.27
122.21
118.51
110.20
93.77
87.70
77.32
77.00
76.68
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

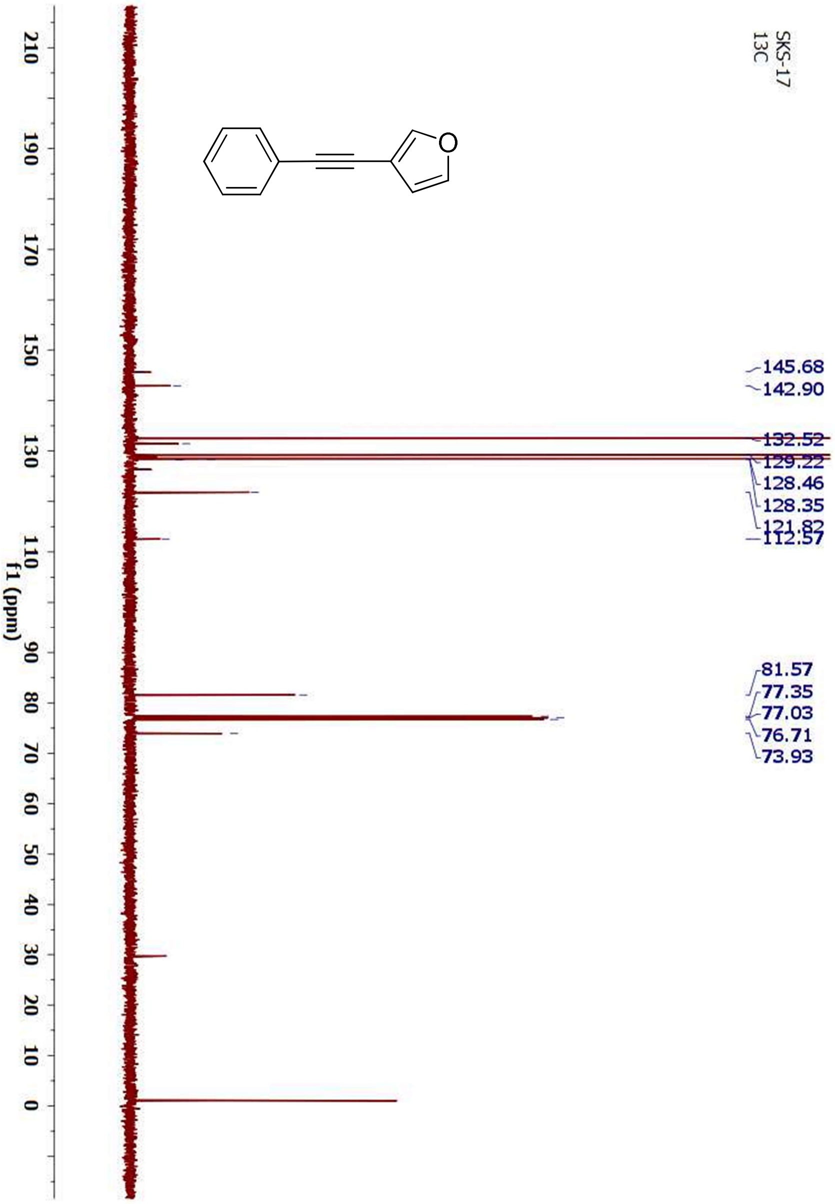

SKS-18
1H
F
7.55
7.54
7.53
7.51
7.36
7.35
7.26
5.34
4.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

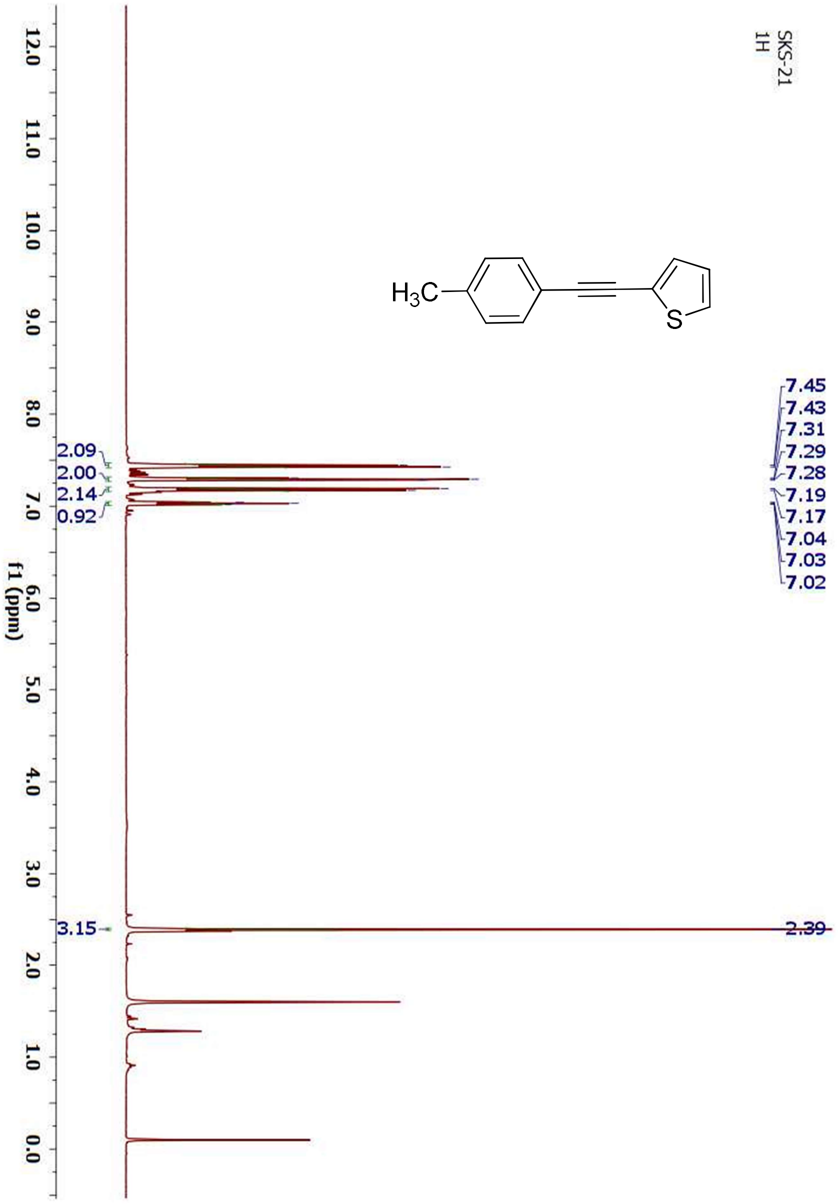

SKS-18
13C
F
163.67
161.36
138.90
133.50
133.42
132.49
131.54
129.19
128.43
128.36
128.31
121.79
115.73
115.51
89.06
88.41
81.54
77.32
77.00
76.68
73.90
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

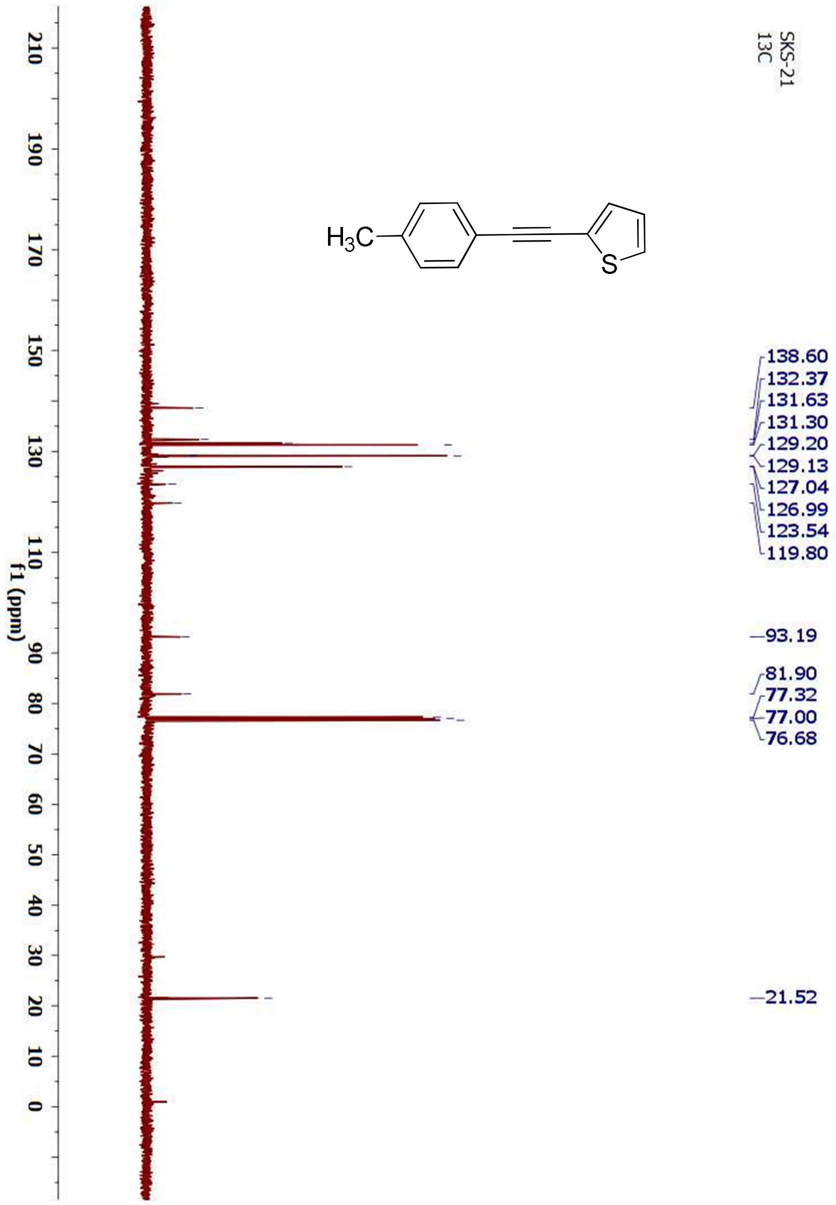

SKS-29
1H
7.54
7.53
7.51
7.36
7.35
7.26
8.22
6.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
f1 (ppm)
5.0
4.0
3.0
2.0
1.0
0.0

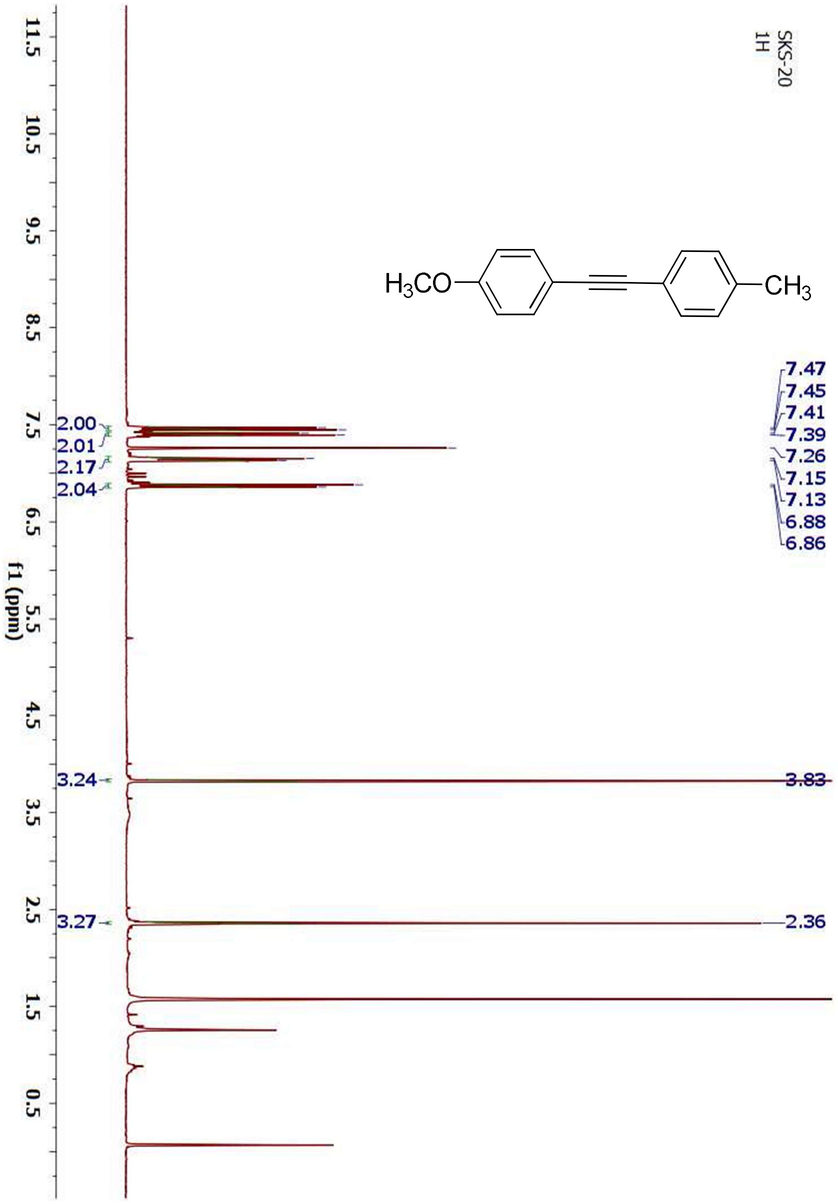

SKS-29
13C
131.62
131.52
128.45
128.38
123.09
123.03
91.21
89.09
77.32
77.00
76.68
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

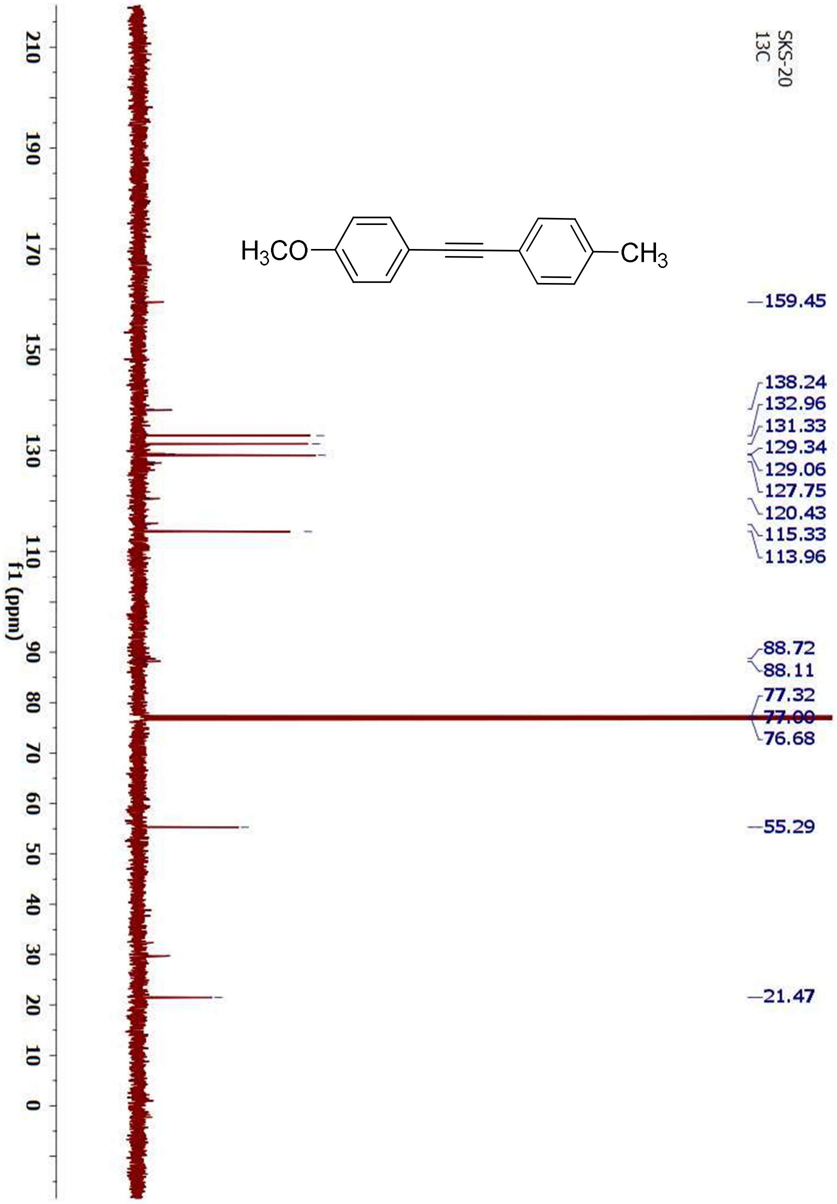

SKS-17
1H
7.55
7.53
7.53
7.38
7.36
7.34
7.33
3.10
5.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)
O

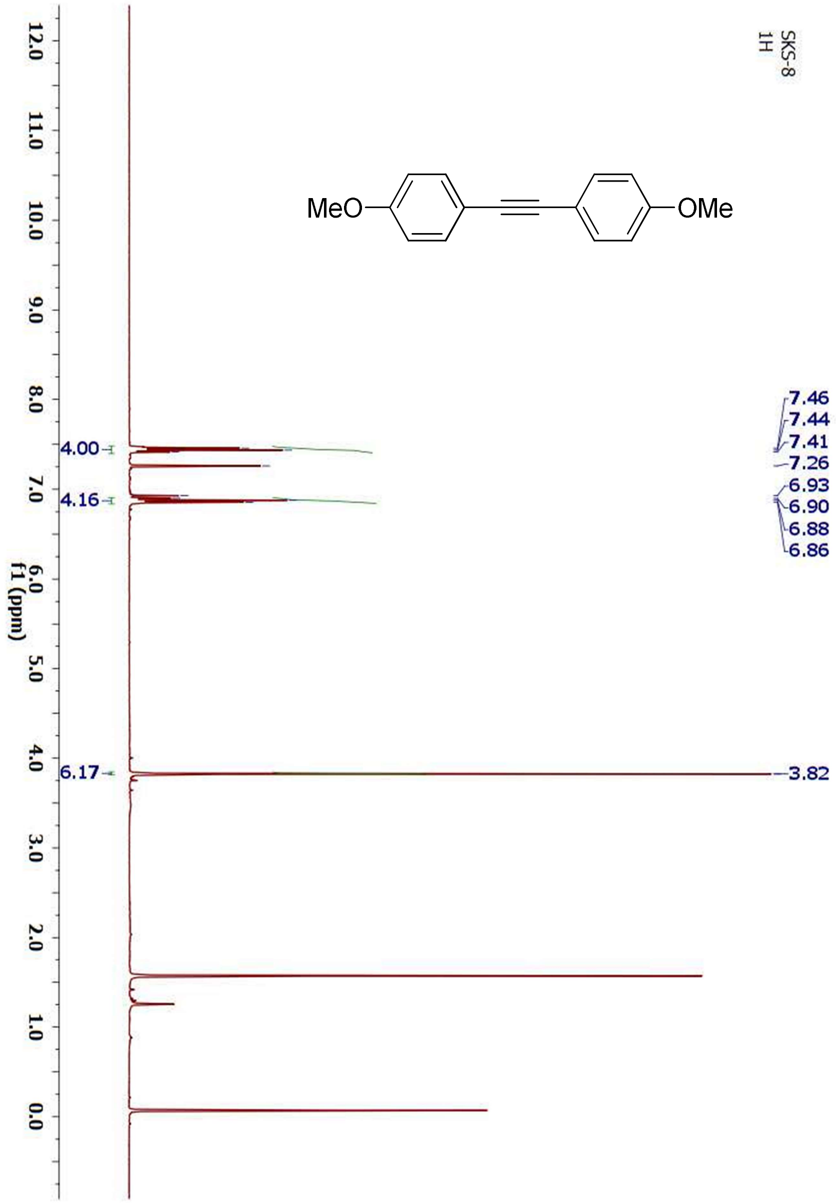

SKS-17
13C
O
145.68
142.90
132.52
129.22
128.46
128.35
121.82
112.57
81.57
77.35
77.03
76.71
73.93
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

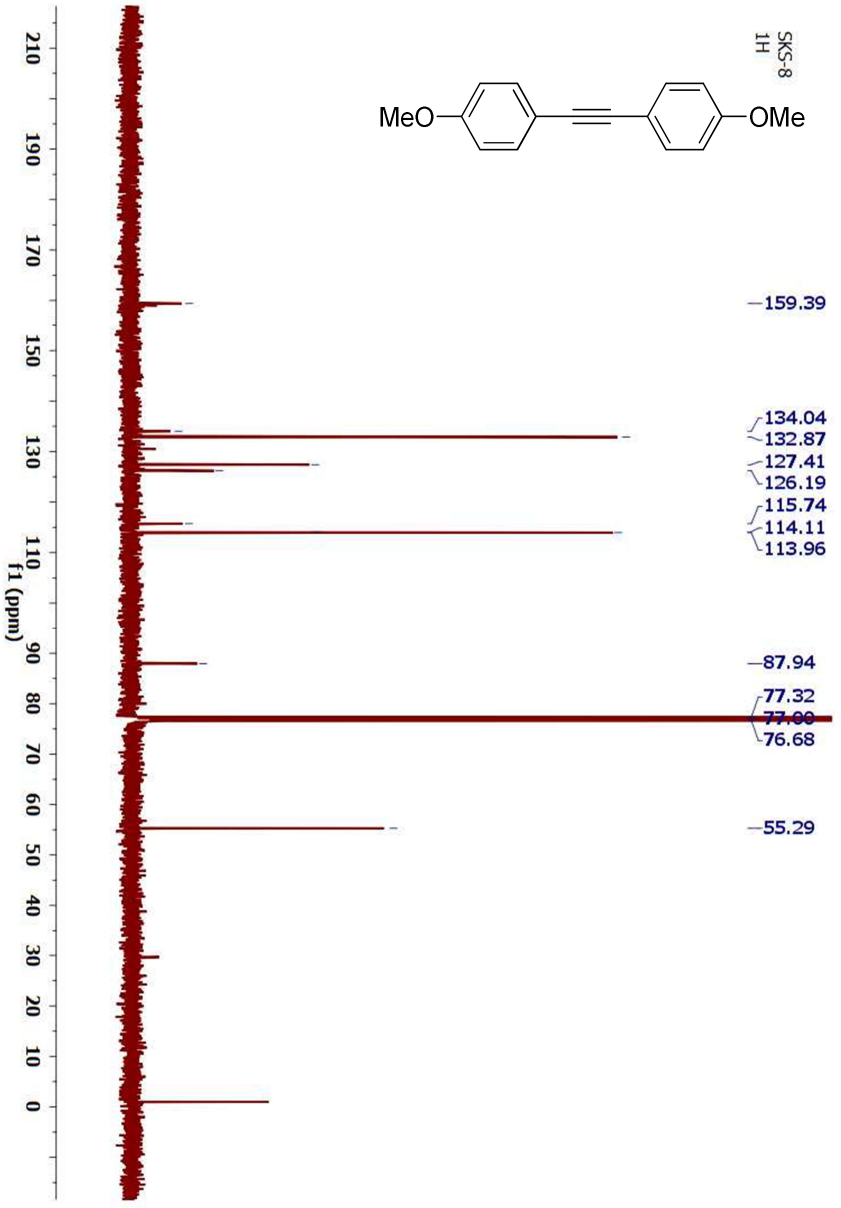

SKS-21
1H
H3C
S
7.45
7.43
7.31
7.29
7.28
7.19
7.17
7.04
7.03
7.02
2.39
2.09
2.00
2.14
0.92
3.15
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

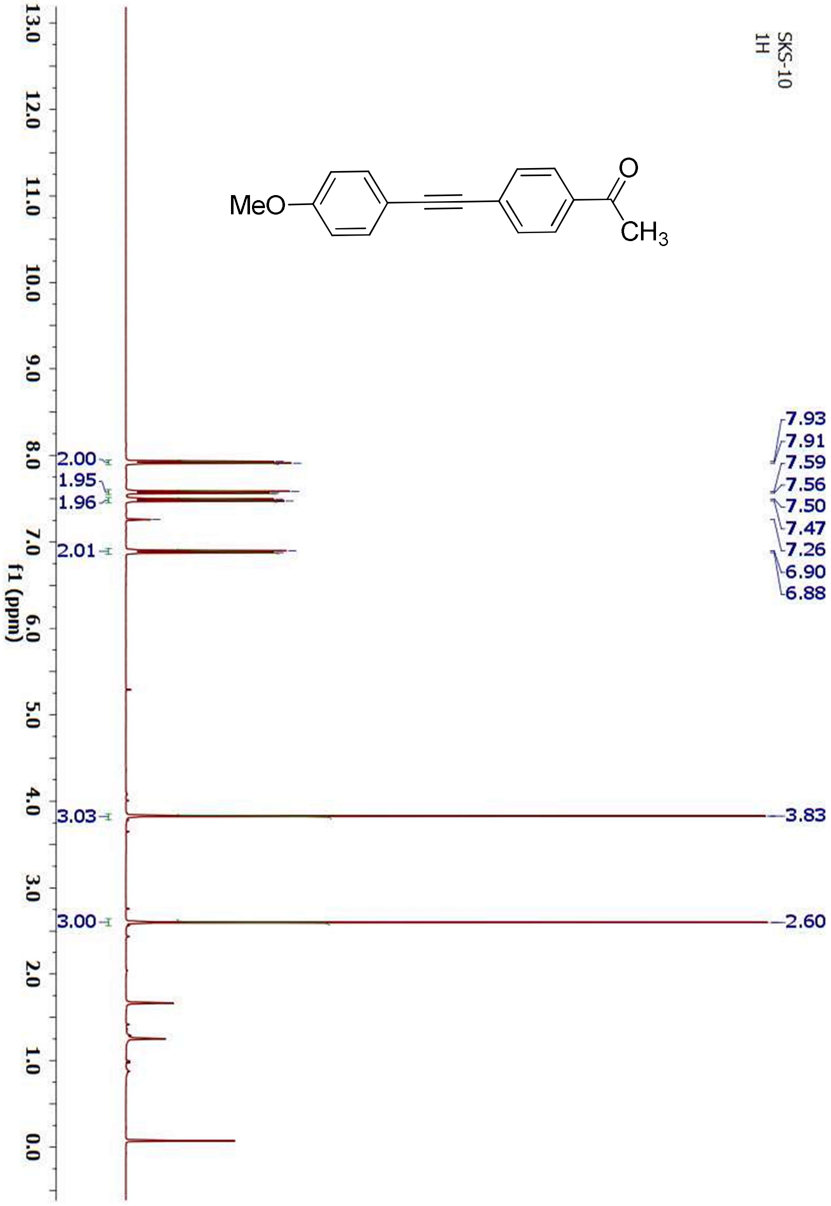

SKS-21
13C
H3C
S
138.60
132.37
131.63
131.30
129.20
129.13
127.04
126.99
123.54
119.80
93.19
81.90
77.32
77.00
76.68
21.52
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

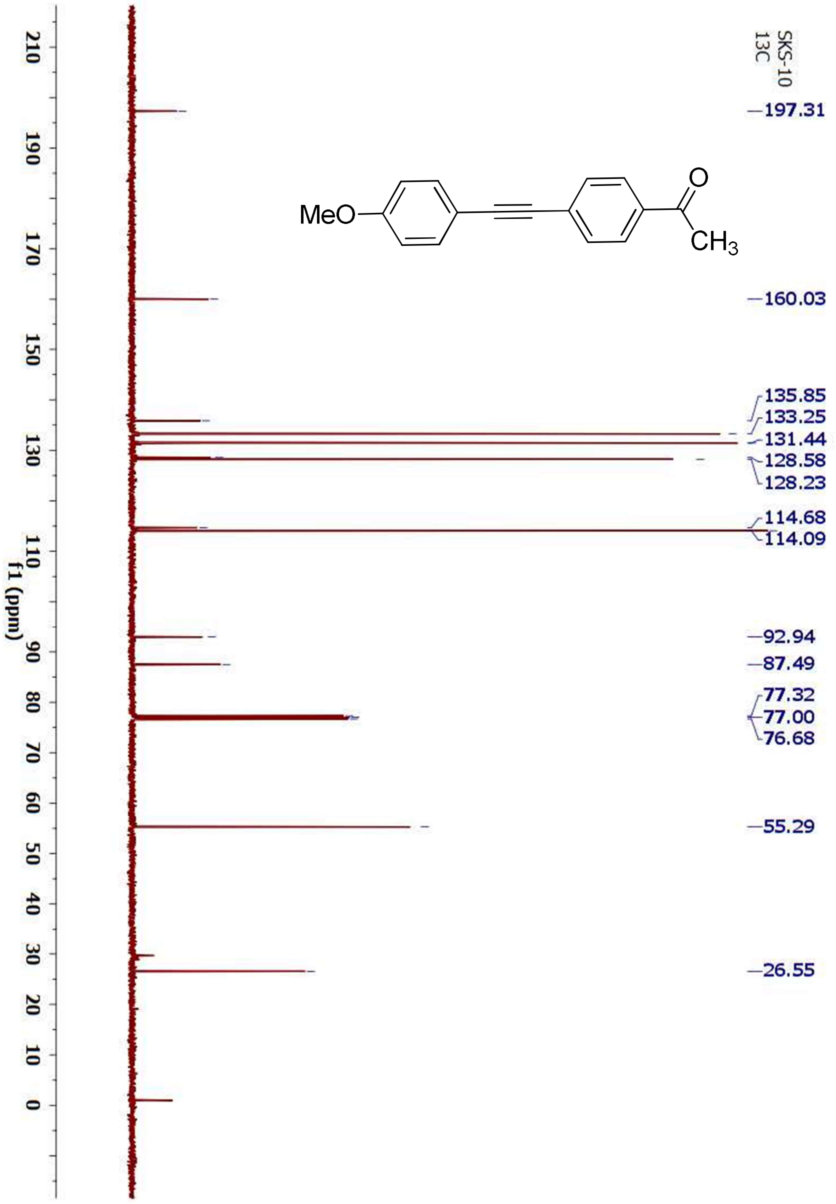

SKS-20
1H
H3CO
CH3
7.47
7.45
7.41
7.39
7.26
7.15
7.13
6.88
6.86
3.83
2.36
2.00
2.01
2.17
2.04
3.24
3.27
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

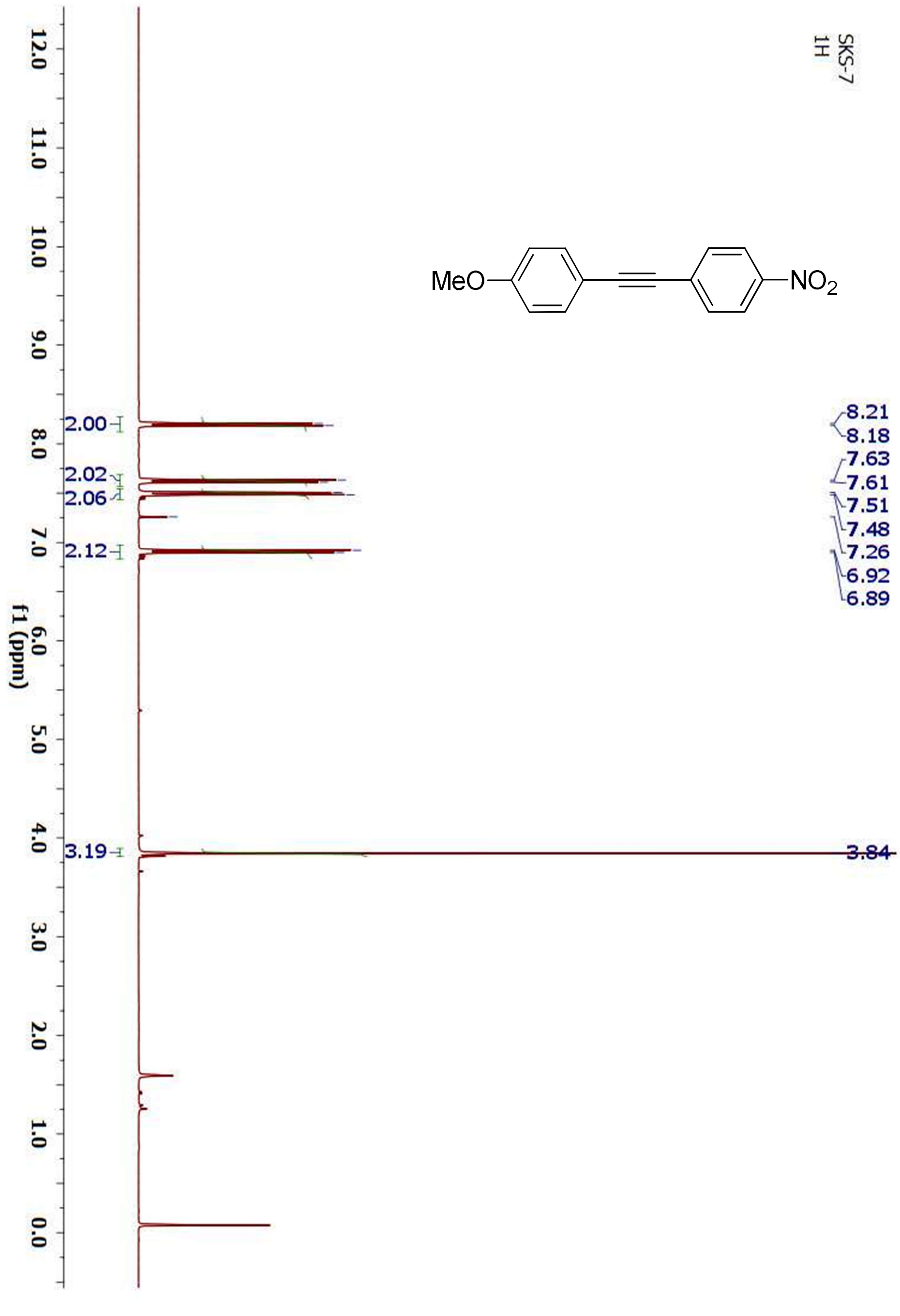

SKS-20
13C
H$_3$CO
CH$_3$
159.45
138.24
132.96
131.33
129.34
129.06
127.75
120.43
115.33
113.96
88.72
88.11
77.32
77.00
76.68
55.29
21.47
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

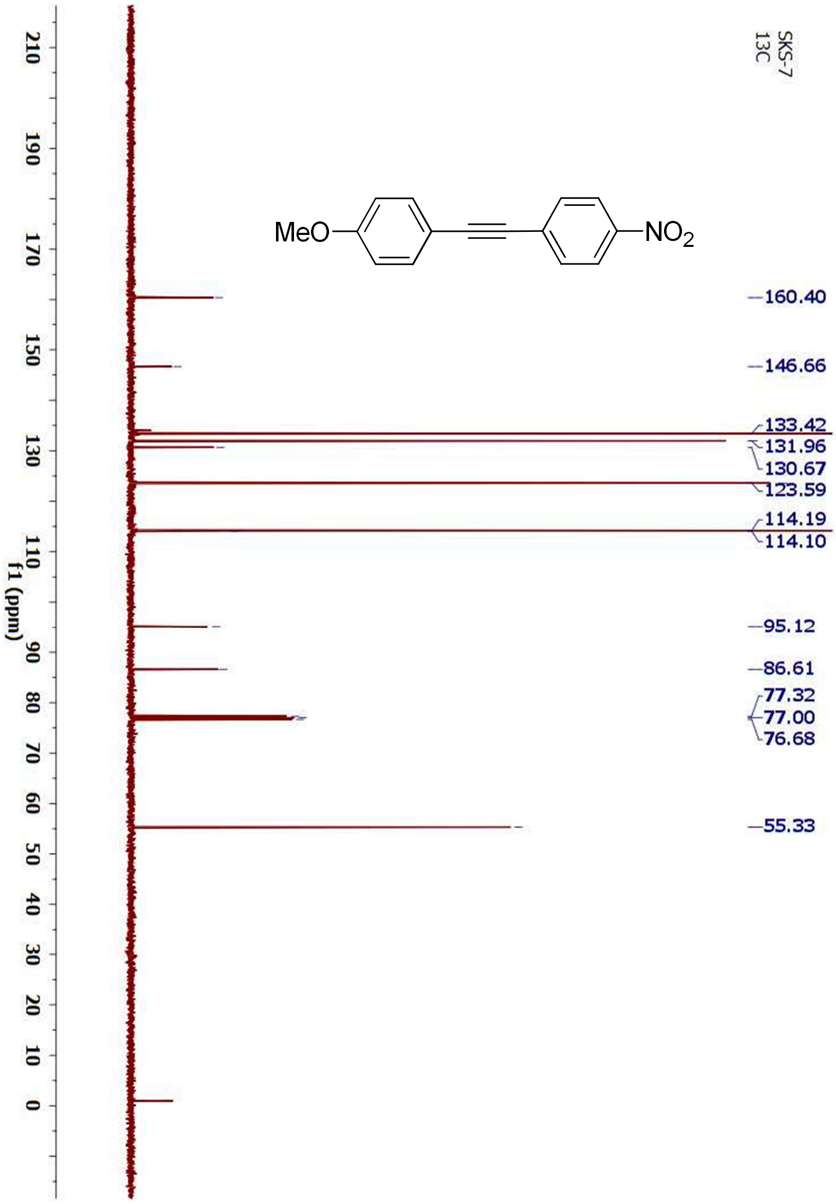

SKS-8
1H
MeO
OMe
7.46
7.44
7.41
7.26
6.93
6.90
6.88
6.86
3.82
4.00
4.16
6.17
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

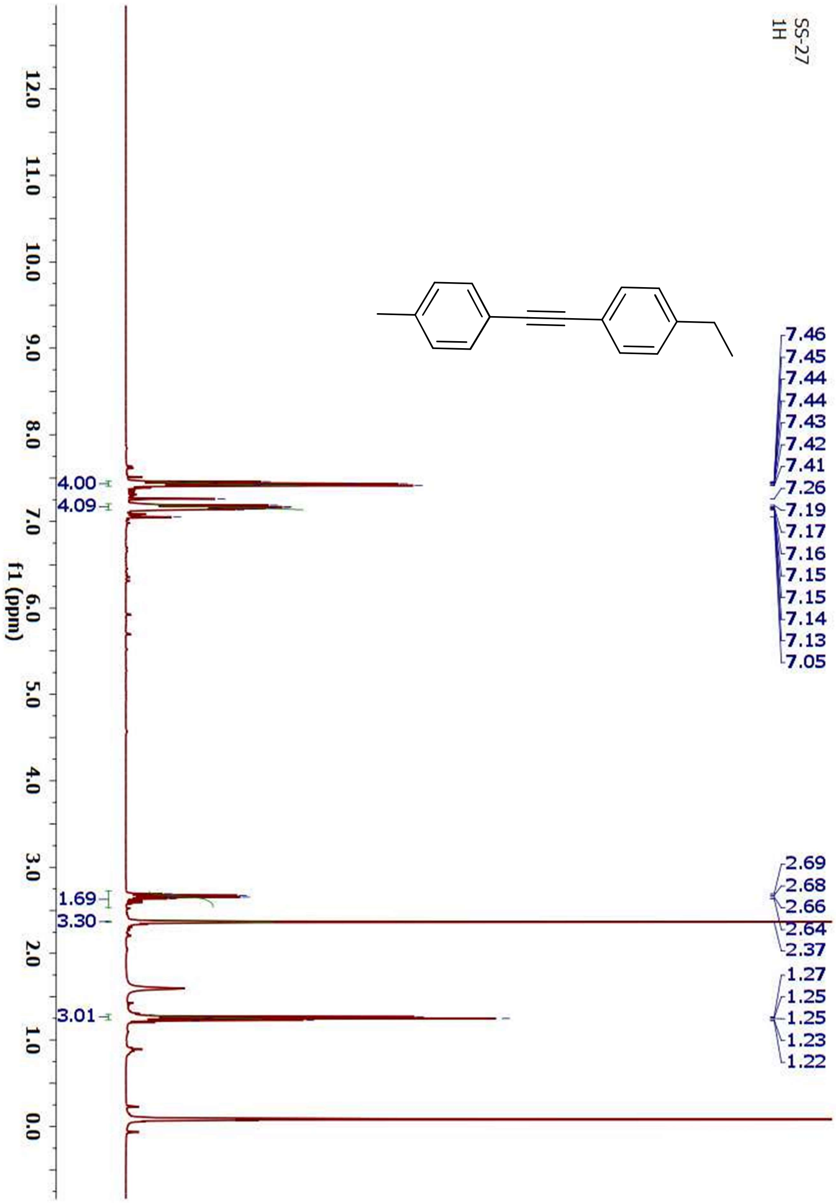

SKS-8
1H
MeO
OMe
159.39
134.04
132.87
127.41
126.19
115.74
114.11
113.96
87.94
77.32
77.00
76.68
55.29
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

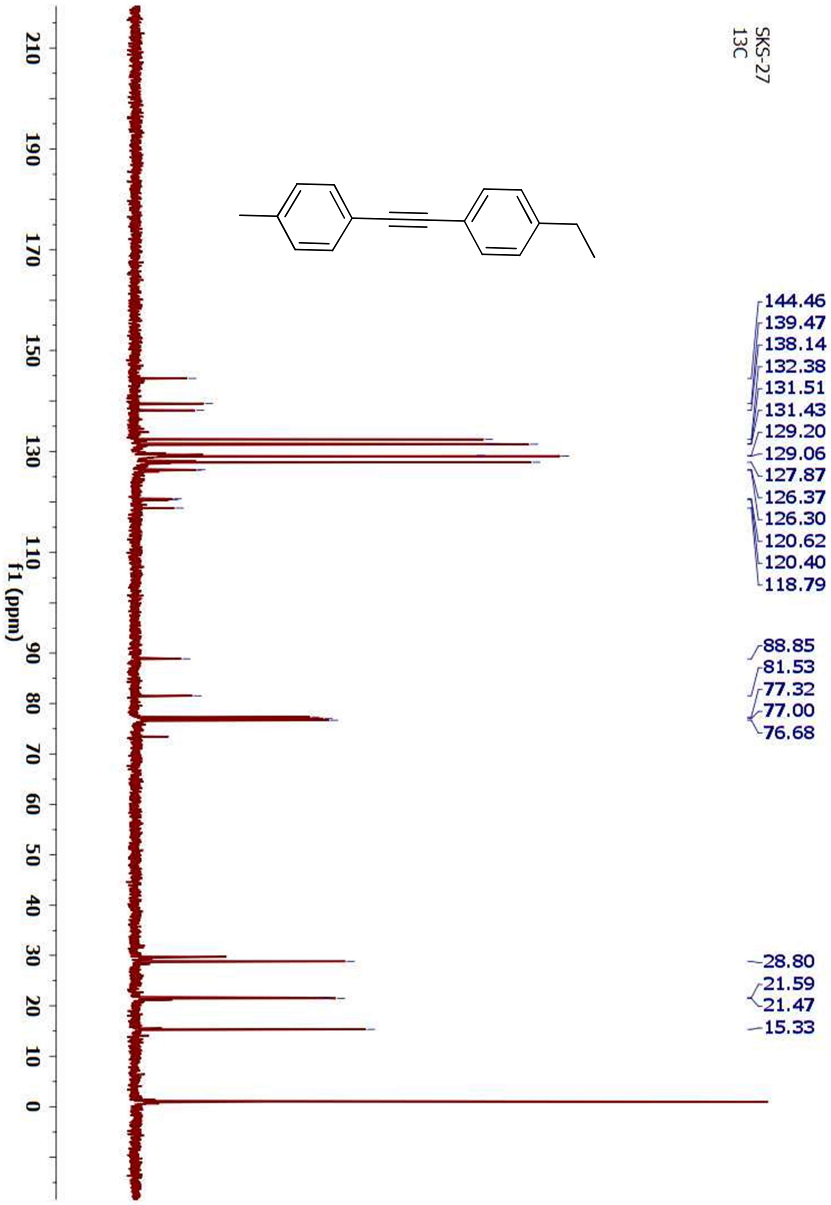

SKS-10
1H
MeO
O
CH3
7.93
7.91
7.59
7.56
7.50
7.47
7.26
6.90
6.88
3.83
2.60
2.00
1.95
1.96
2.01
3.03
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

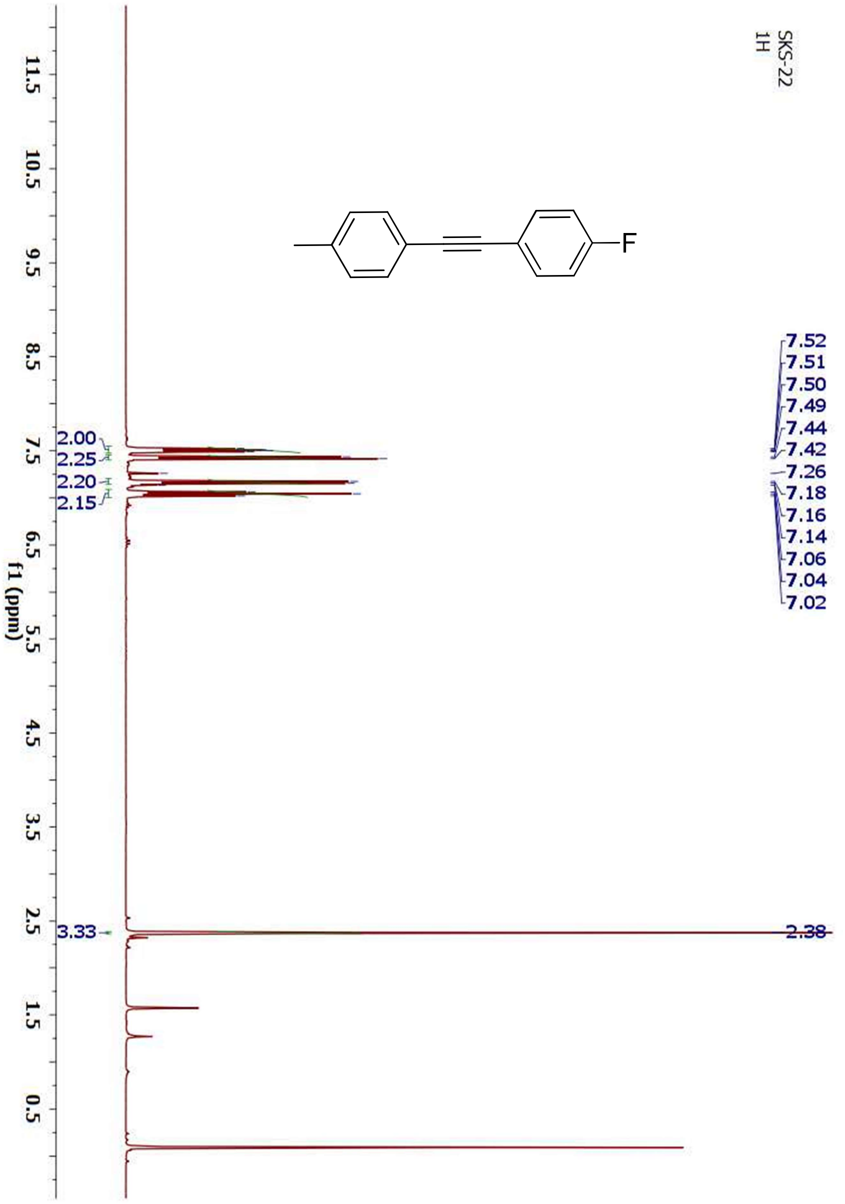

SKS-10
13C
197.31
MeO
O
CH3
160.03
135.85
133.25
131.44
128.58
128.23
114.68
114.09
92.94
87.49
77.32
77.00
76.68
55.29
26.55
210
190
170
150
130
110
f1 (ppm)
90
80
70
60
50
40
30
20
10
0

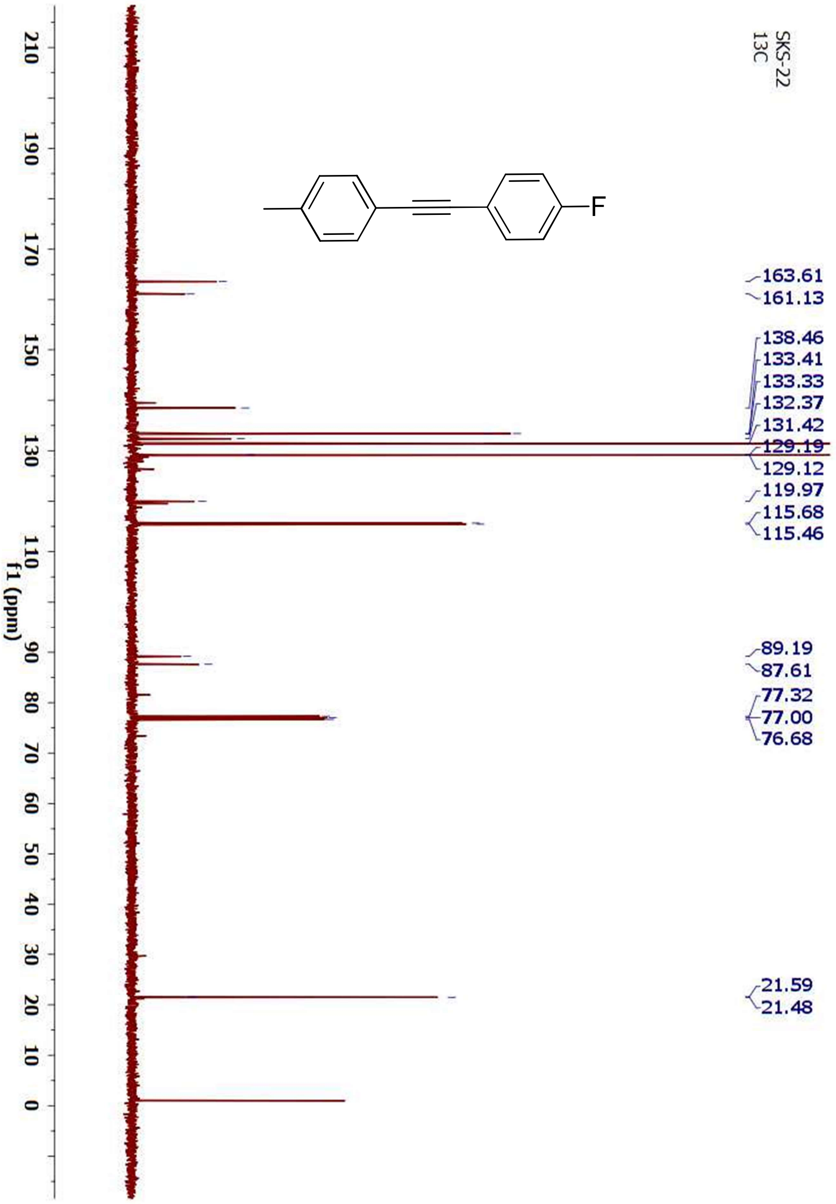

SKS-7
1H
MeO
NO2
8.21
8.18
7.63
7.61
7.51
7.48
7.26
6.92
6.89
3.84
2.00
2.02
2.06
2.12
3.19
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

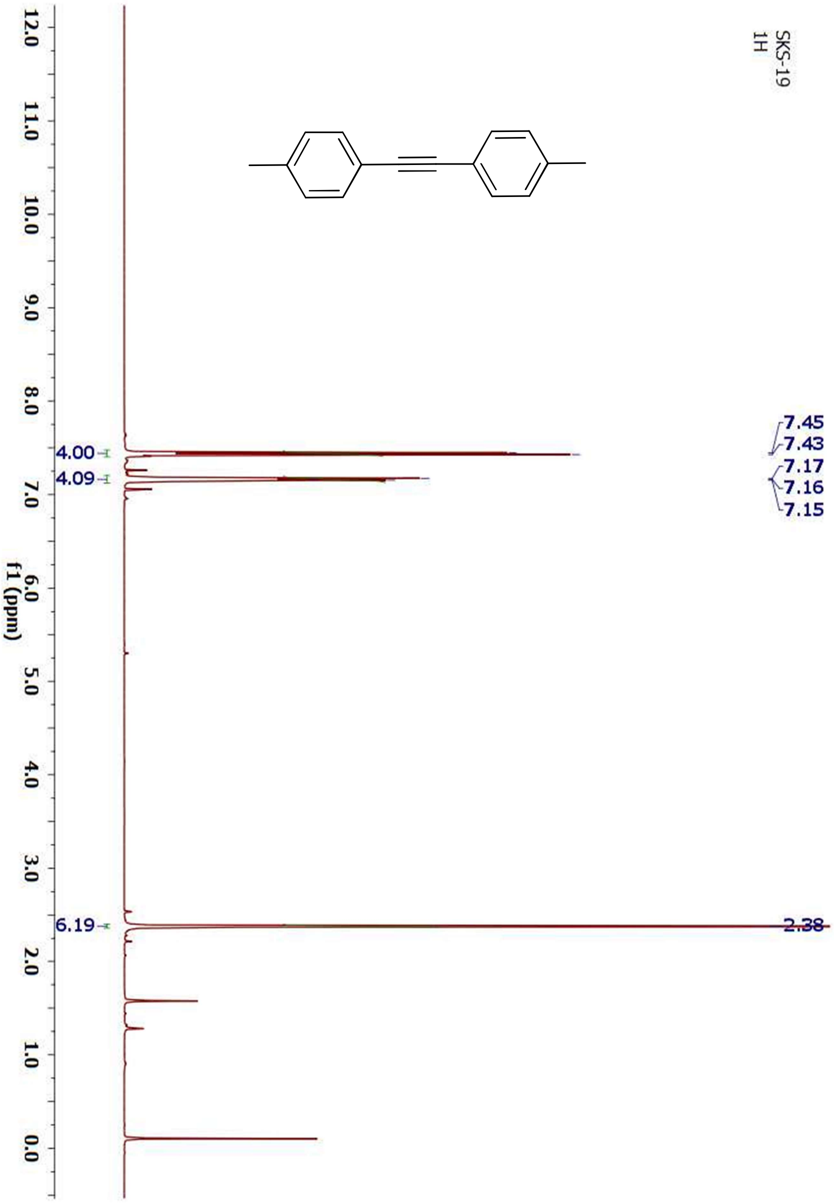

SKS-7
13C
MeO
NO2
160.40
146.66
133.42
131.96
130.67
123.59
114.19
114.10
95.12
86.61
77.32
77.00
76.68
55.33
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

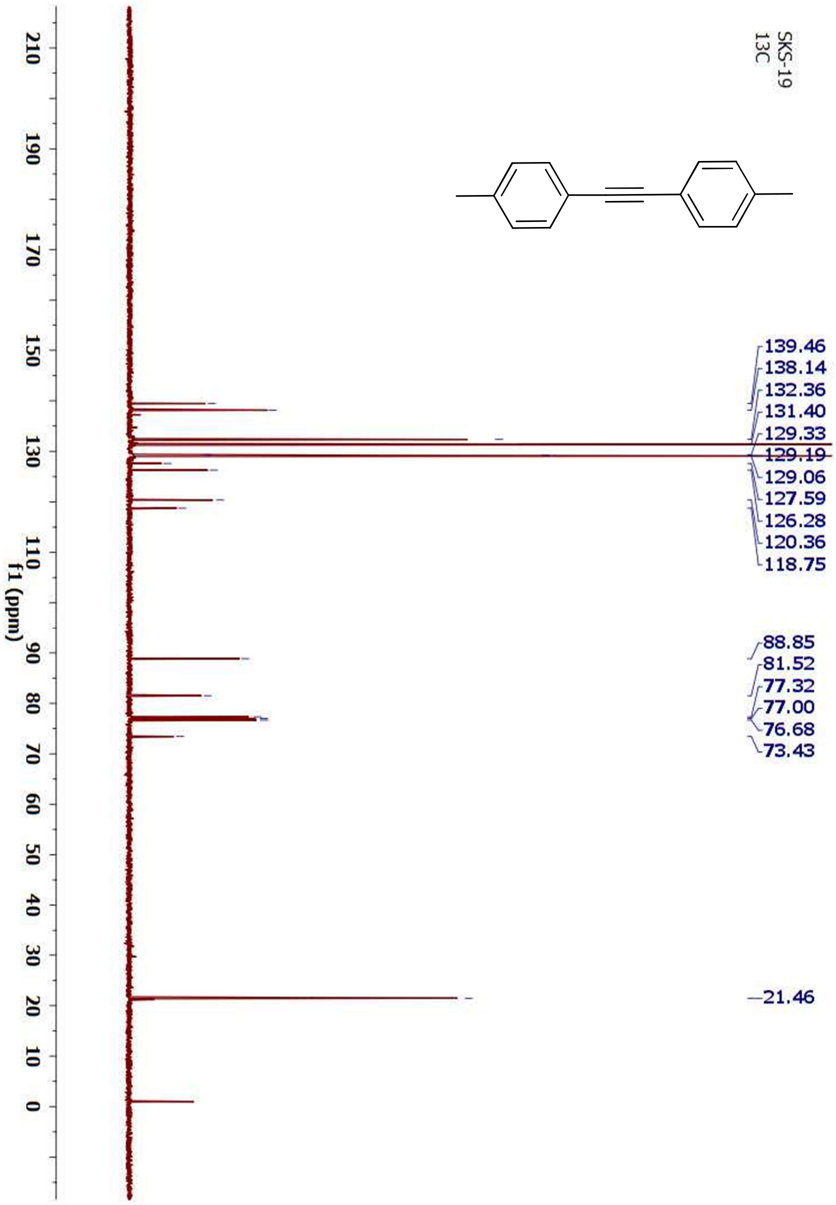

SS-27
1H
7.46
7.45
7.44
7.44
7.43
7.42
7.41
7.26
7.19
7.17
7.16
7.15
7.15
7.14
7.13
7.05
2.69
2.68
2.66
2.64
2.37
1.27
1.25
1.25
1.23
1.22
4.00
4.09
1.69
3.30
3.01
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

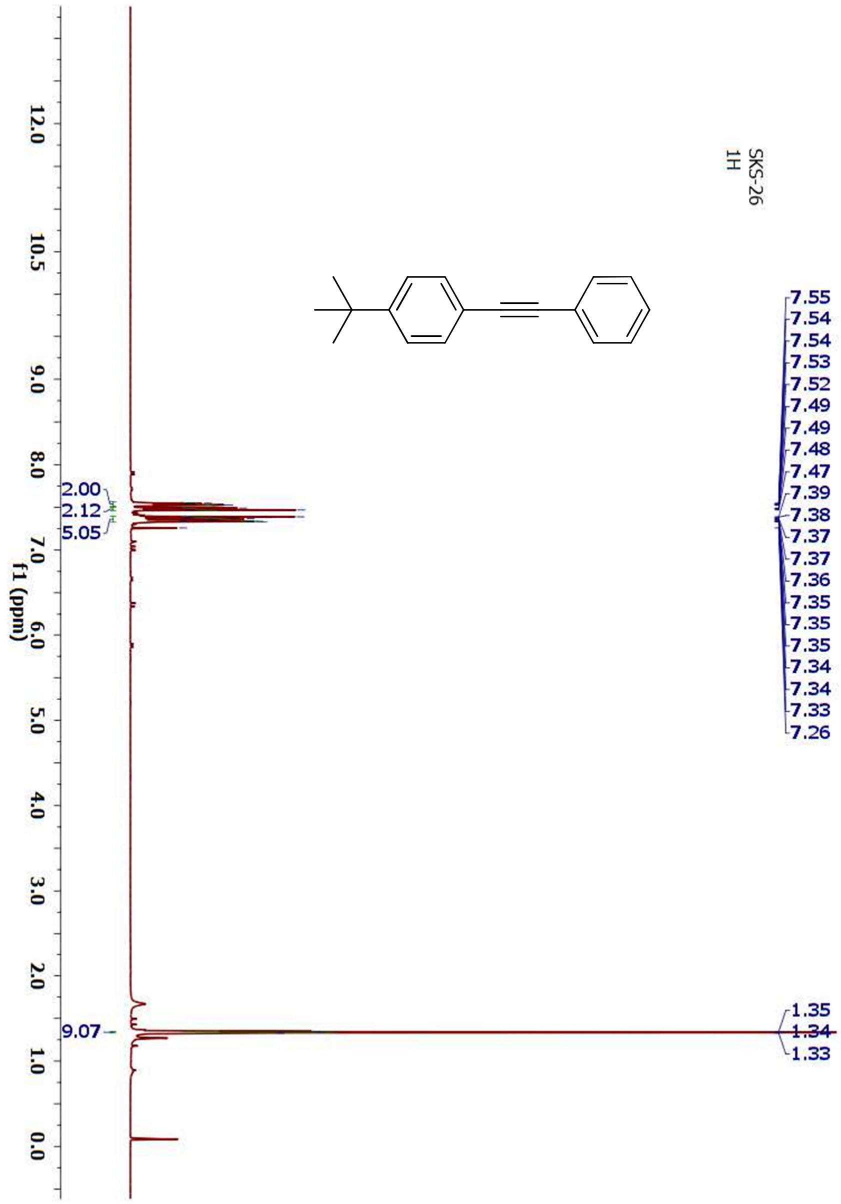

SKS-27
13C
144.46
139.47
138.14
132.38
131.51
131.43
129.20
129.06
127.87
126.37
126.30
120.62
120.40
118.79
88.85
81.53
77.32
77.00
76.68
28.80
21.59
21.47
15.33
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

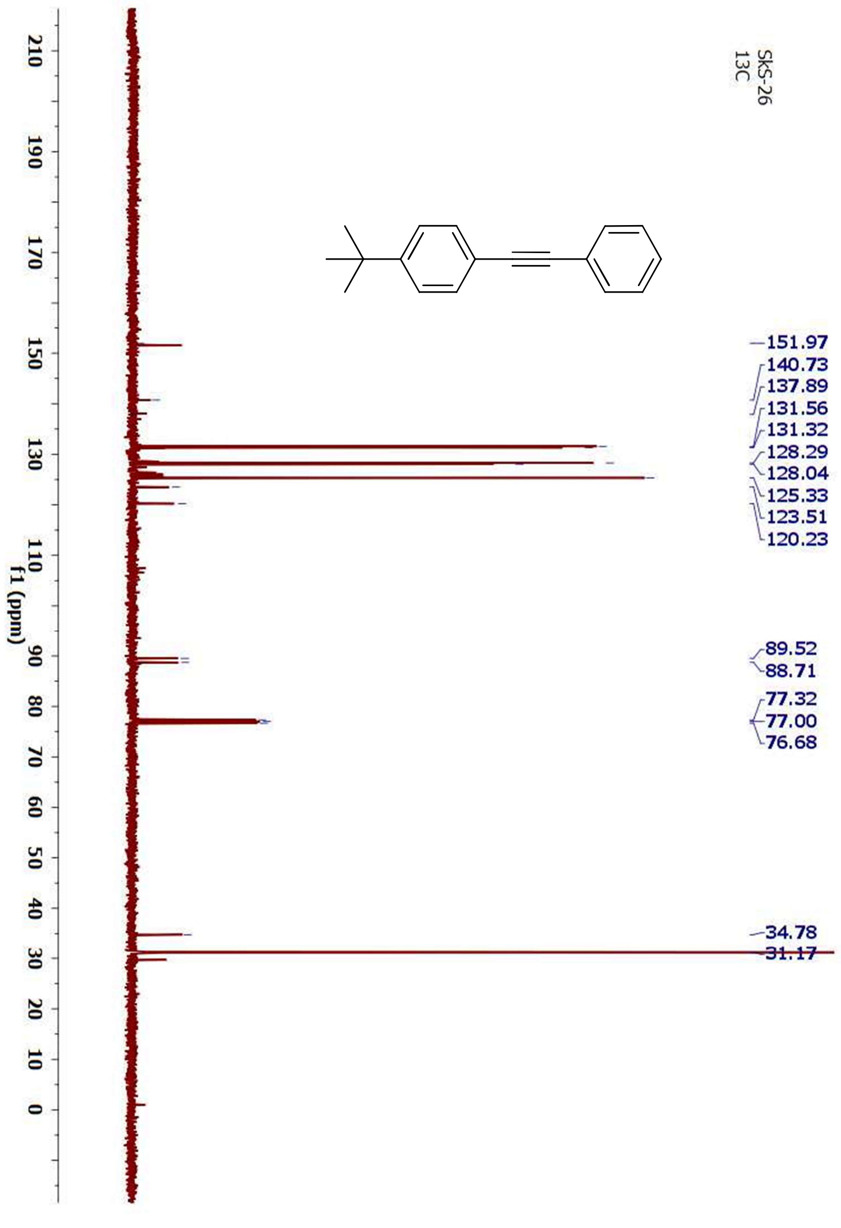

SKS-22
1H
F
7.52
7.51
7.50
7.49
7.44
7.42
7.26
7.18
7.16
7.14
7.06
7.04
7.02
2.38
2.00
2.25
2.20
2.15
3.33
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

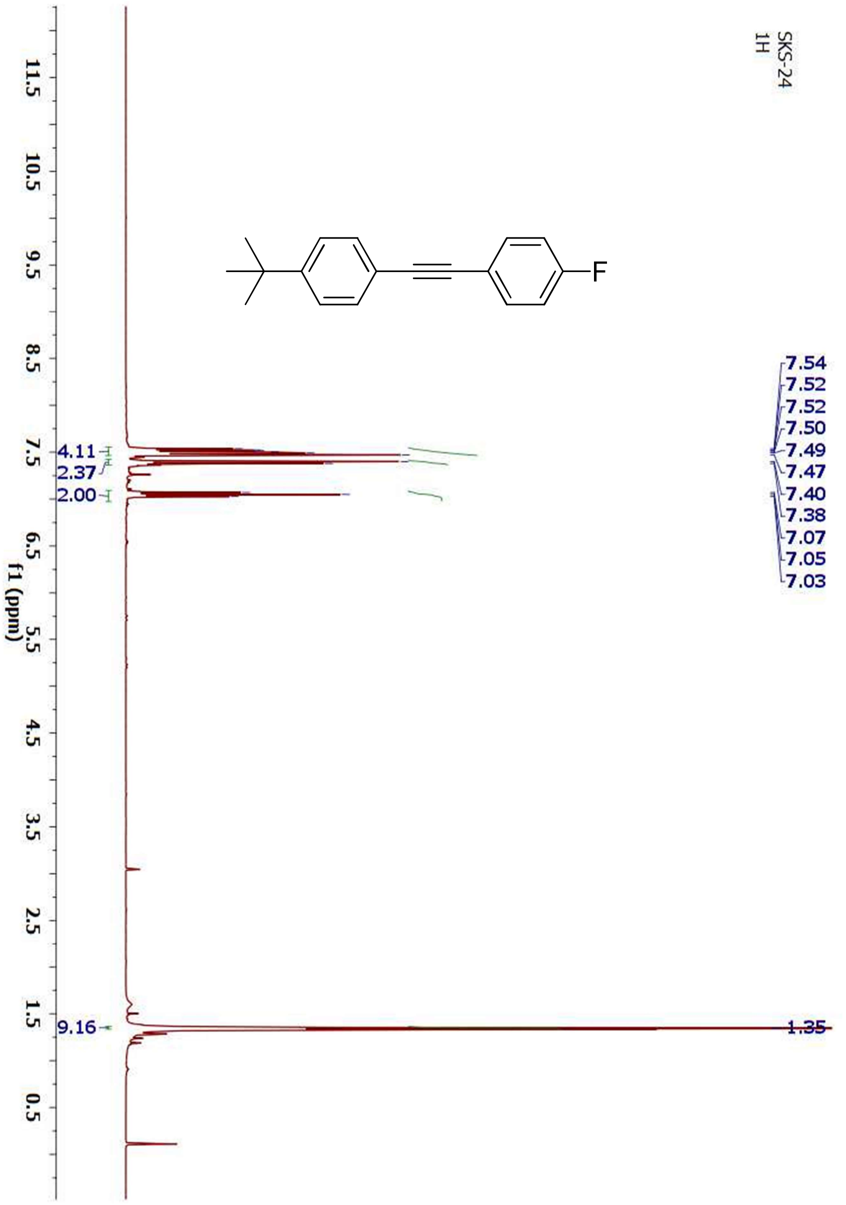

SKS-22
13C
F
163.61
161.13
138.46
133.41
133.33
132.37
131.42
129.19
129.12
119.97
115.68
115.46
89.19
87.61
77.32
77.00
76.68
21.59
21.48
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

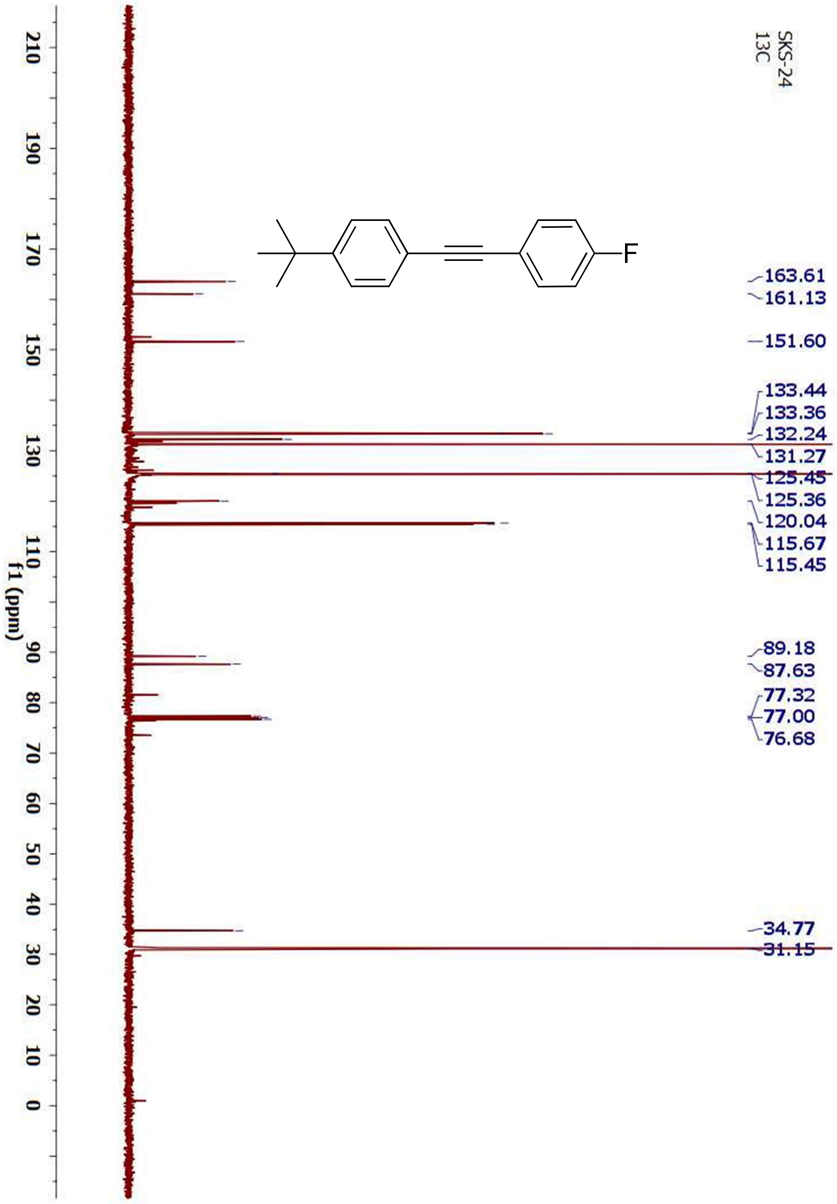
SKS-19
1H
7.45
7.43
7.17
7.16
7.15
2.38
4.00
4.09
6.19
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

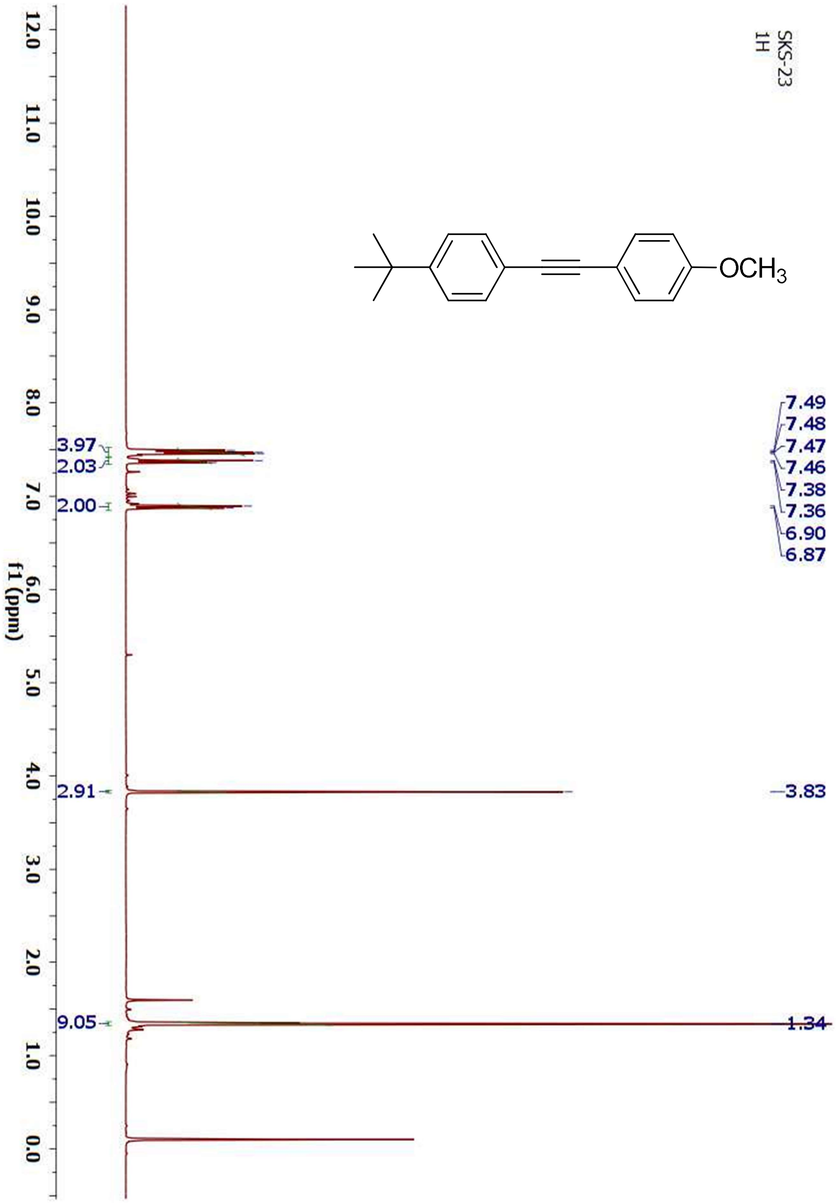

SKS-19
13C
139.46
138.14
132.36
131.40
129.33
129.19
129.06
127.59
126.28
120.36
118.75
88.85
81.52
77.32
77.00
76.68
73.43
21.46
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

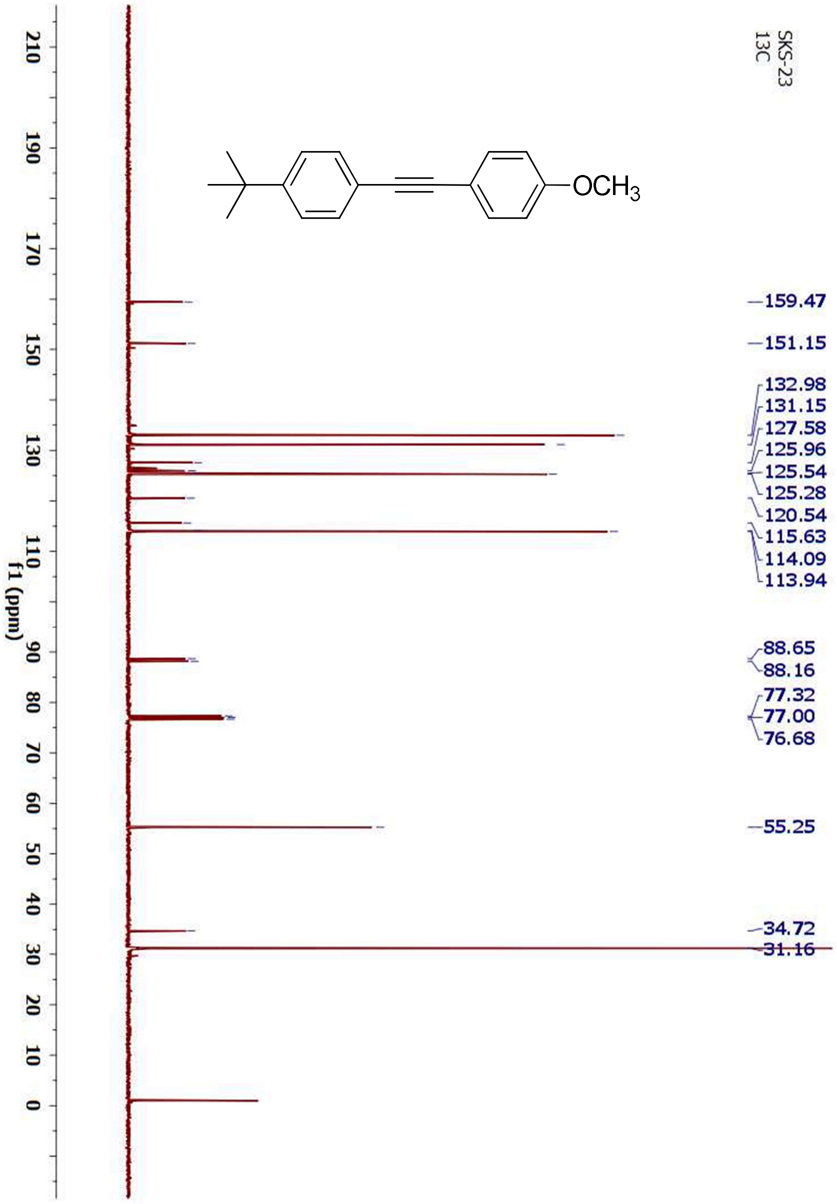

SKS-26
1H
7.55
7.54
7.54
7.53
7.52
7.49
7.49
7.48
7.47
7.39
7.38
7.37
7.37
7.36
7.35
7.35
7.35
7.34
7.34
7.33
7.26
1.35
1.34
1.33
2.00
2.12
5.05
9.07
12.0
10.5
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

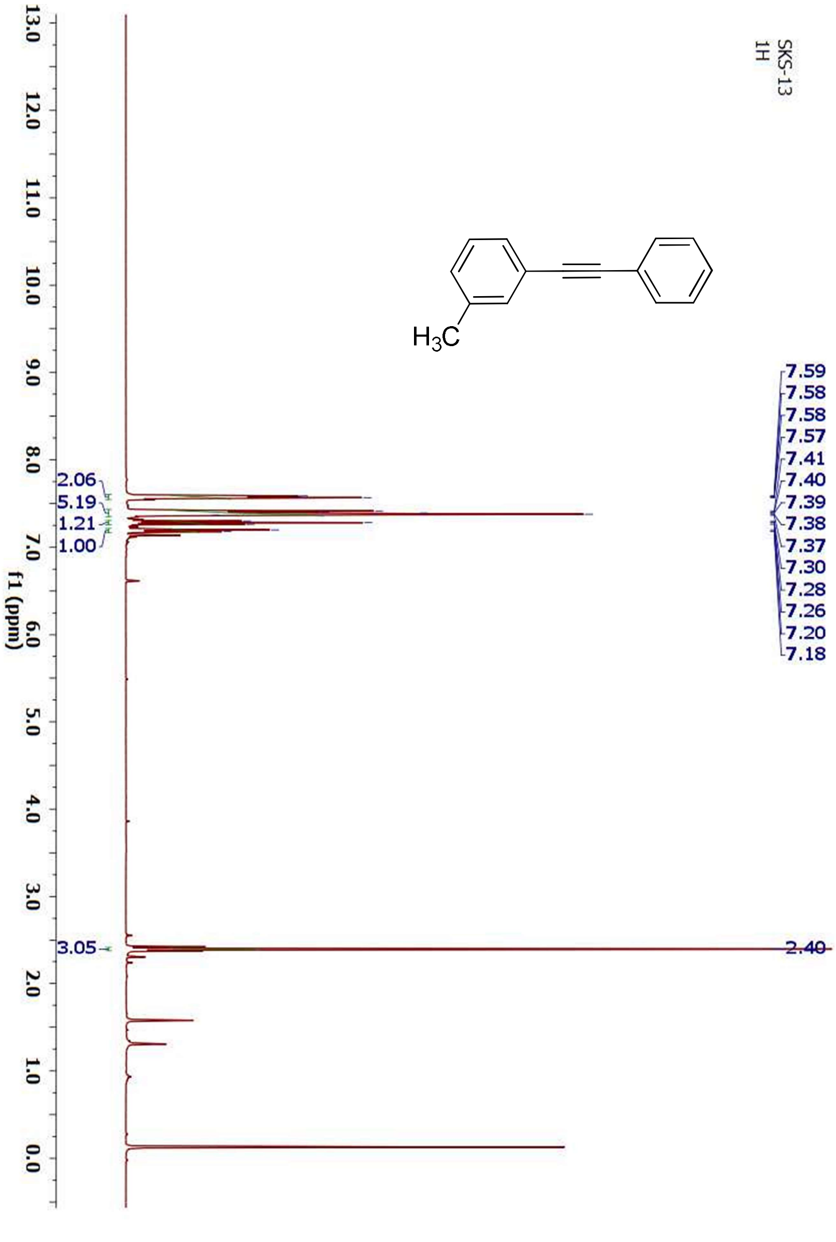

SKS-26
13C
151.97
140.73
137.89
131.56
131.32
128.29
128.04
125.33
123.51
120.23
89.52
88.71
77.32
77.00
76.68
34.78
31.17
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

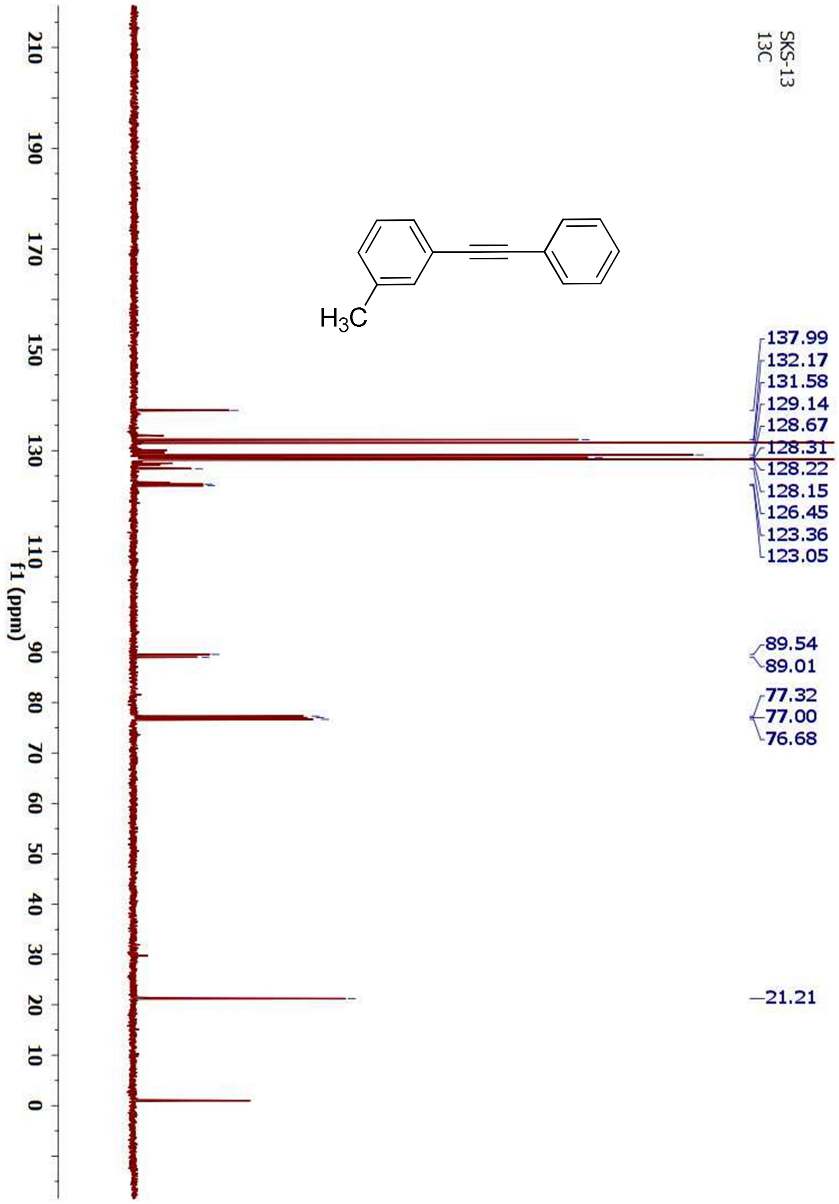

SKS-24
1H
F
7.54
7.52
7.52
7.50
7.49
7.47
7.40
7.38
7.07
7.05
7.03
1.35
4.11
2.37
2.00
9.16
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

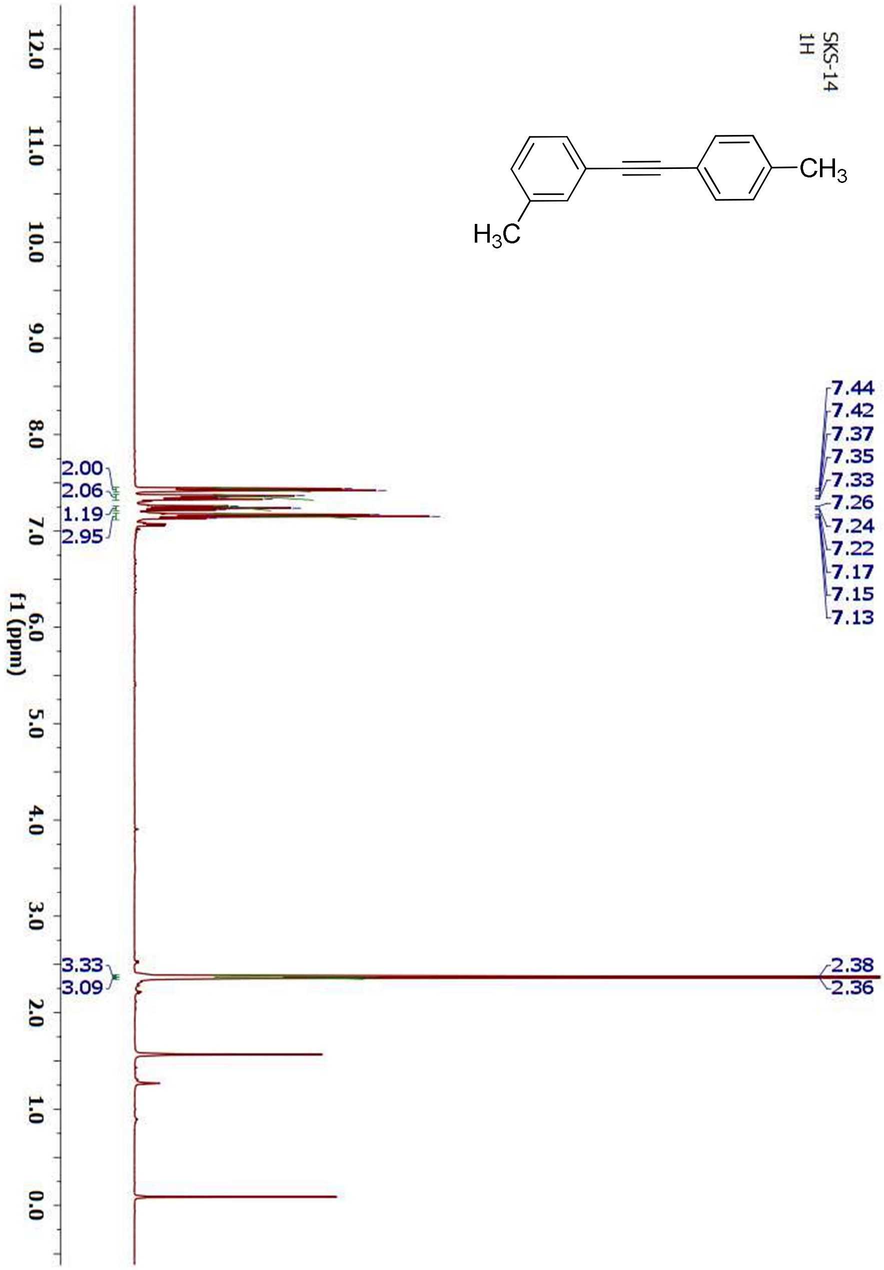

SKS-24
13C
F
163.61
161.13
151.60
133.44
133.36
132.24
131.27
125.45
125.36
120.04
115.67
115.45
89.18
87.63
77.32
77.00
76.68
34.77
31.15
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

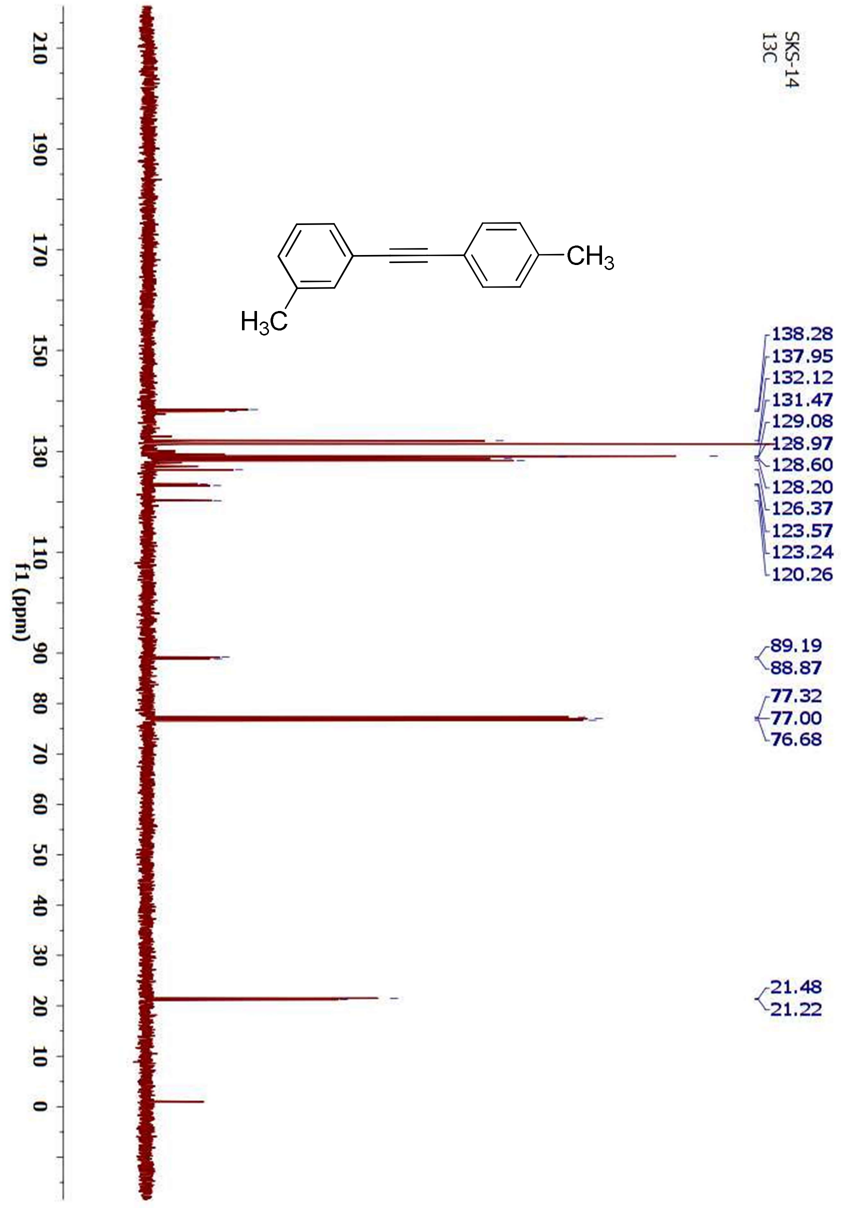

SKS-23
1H
OCH3
7.49
7.48
7.47
7.46
7.38
7.36
6.90
6.87
3.83
1.34
3.97
2.03
2.00
2.91
9.05
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

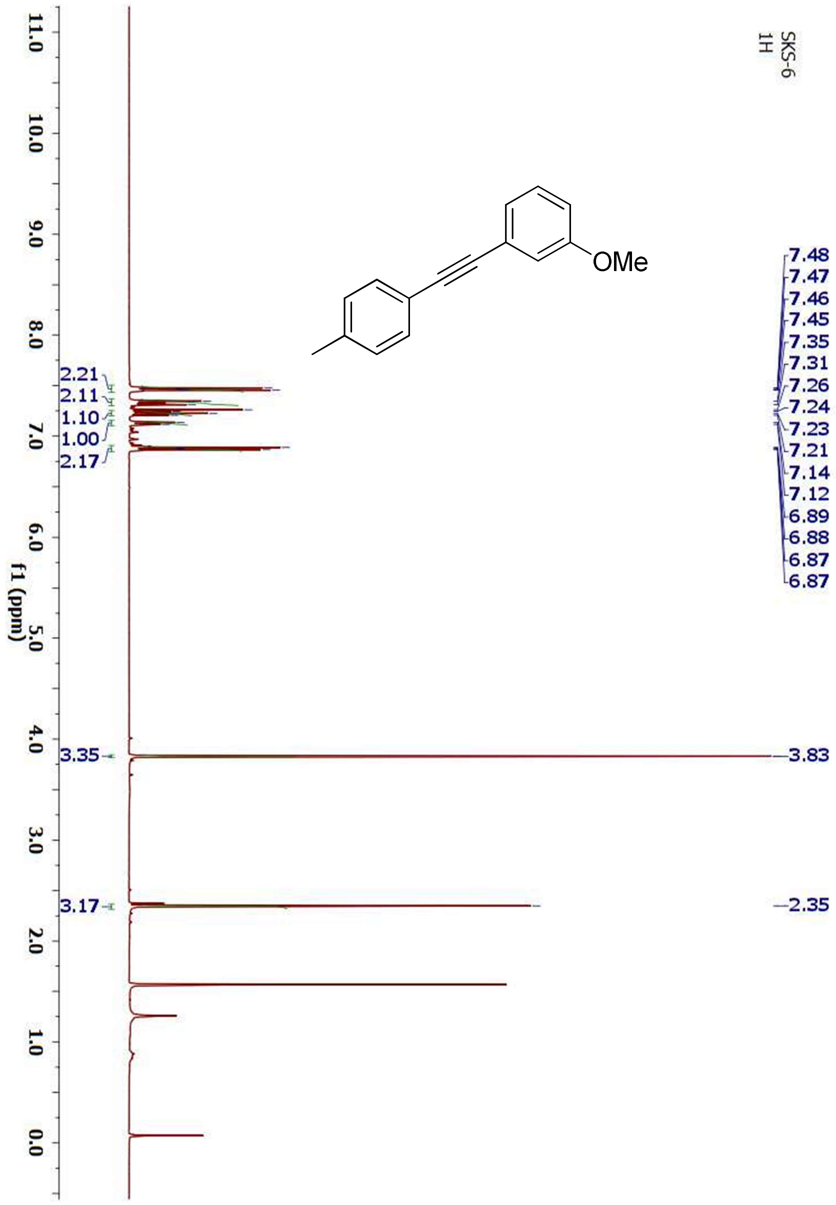

SKS-23
13C
OCH3
159.47
151.15
132.98
131.15
127.58
125.96
125.54
125.28
120.54
115.63
114.09
113.94
88.65
88.16
77.32
77.00
76.68
55.25
34.72
31.16
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

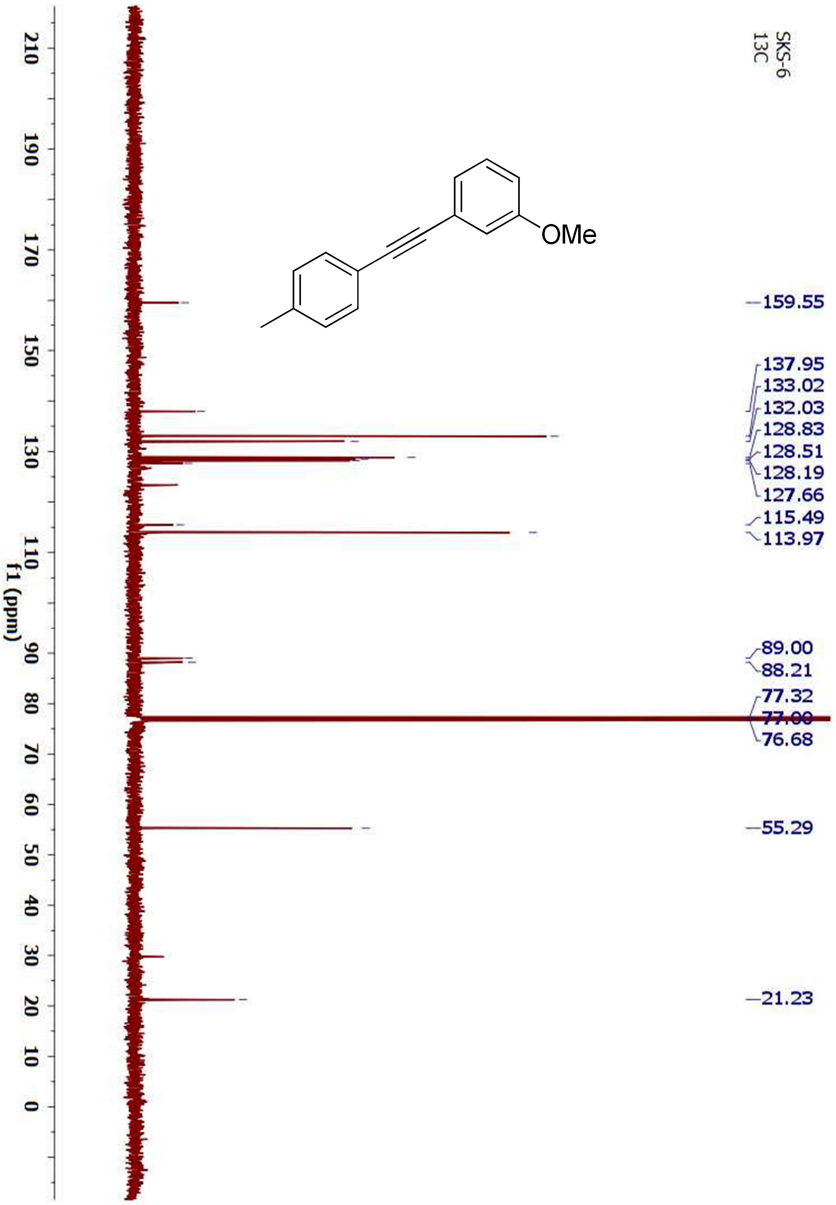

SKS-13
1H
H3C
7.59
7.58
7.58
7.57
7.41
7.40
7.39
7.38
7.37
7.30
7.28
7.26
7.20
7.18
2.40
2.06
5.19
1.21
1.00
3.05
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

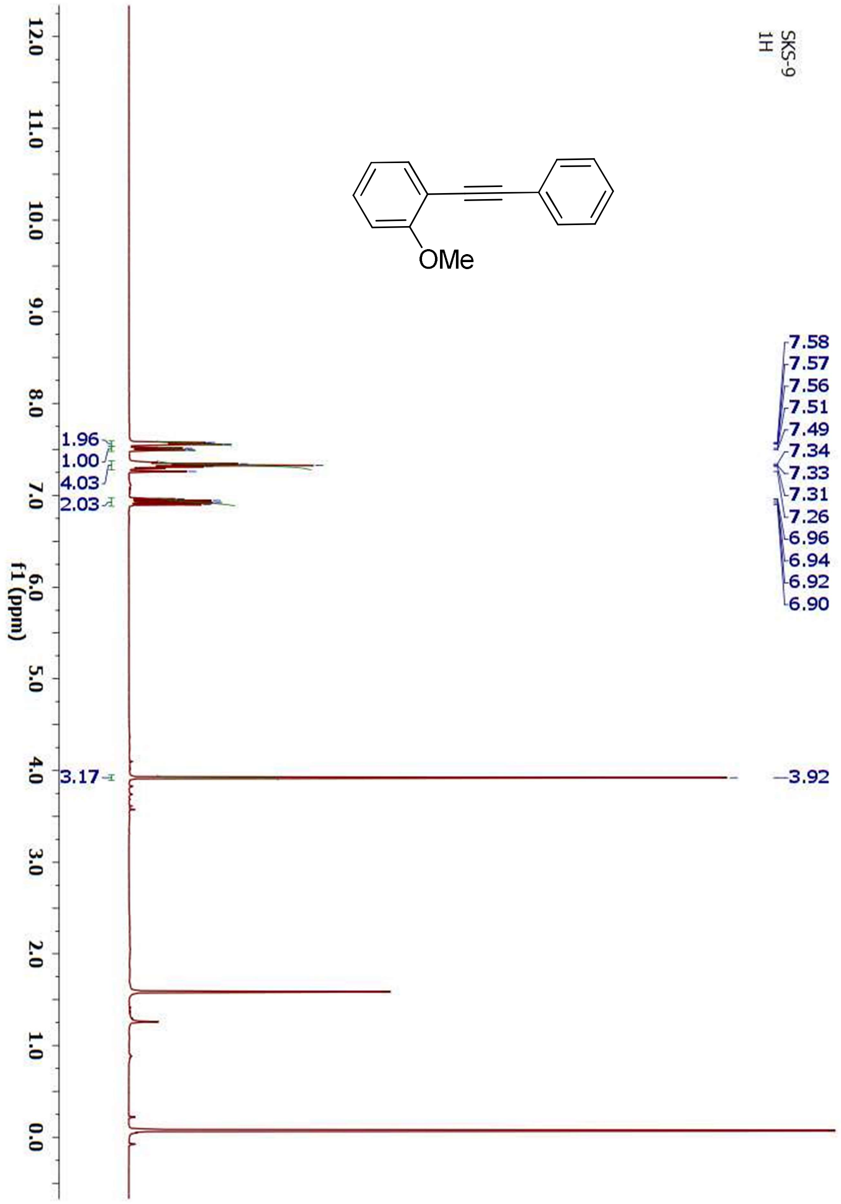

SKS-13
13C
H$_3$C
137.99
132.17
131.58
129.14
128.67
128.31
128.22
128.15
126.45
123.36
123.05
89.54
89.01
77.32
77.00
76.68
21.21
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

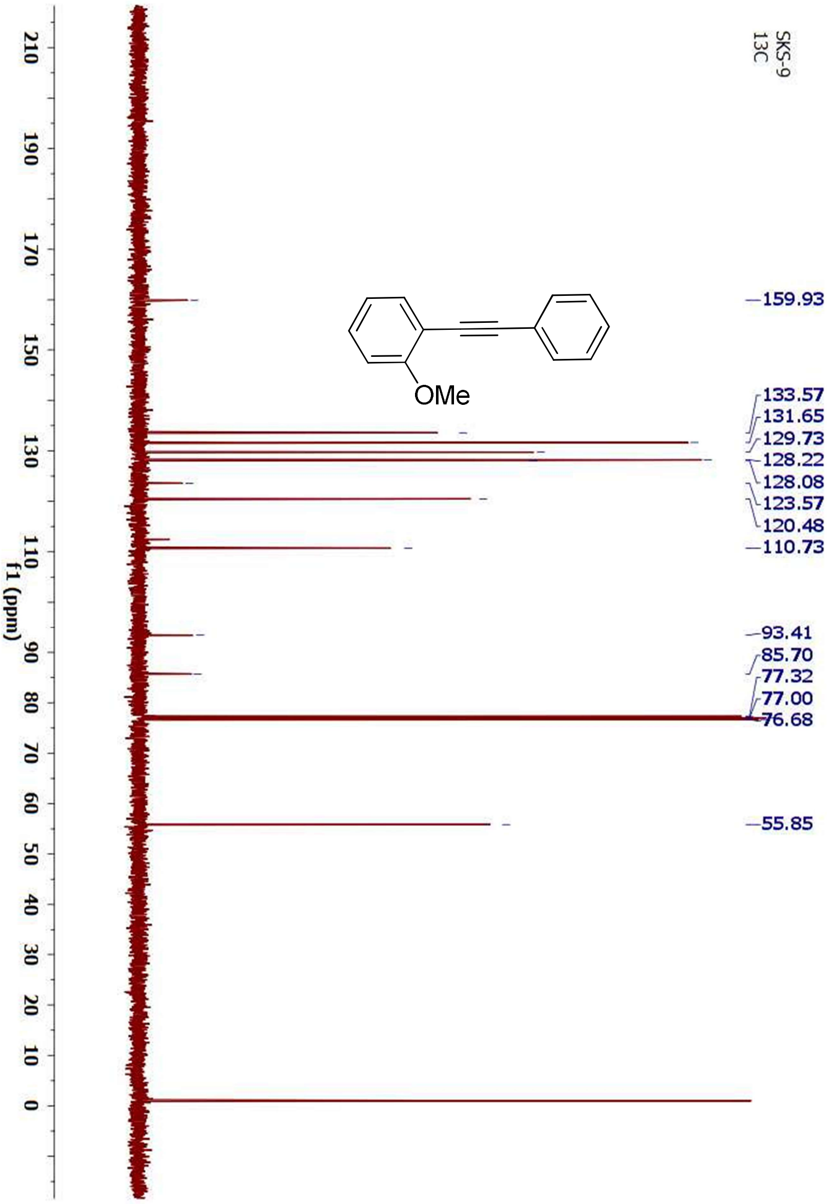

SKS-14
1H
CH3
H3C
7.44
7.42
7.37
7.35
7.33
7.26
7.24
7.22
7.17
7.15
7.13
2.38
2.36
2.00
2.06
1.19
2.95
3.33
3.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

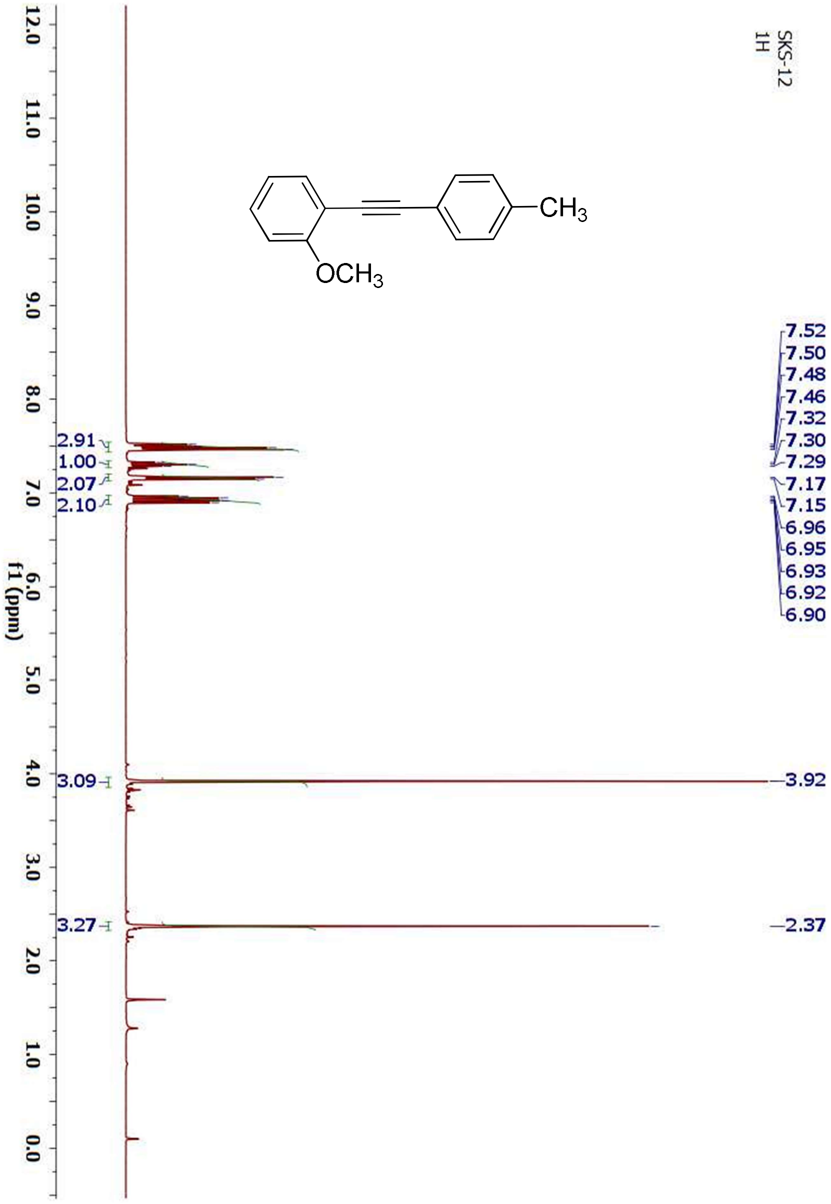

SKS-14
13C
CH3
H3C
138.28
137.95
132.12
131.47
129.08
128.97
128.60
128.20
126.37
123.57
123.24
120.26
89.19
88.87
77.32
77.00
76.68
21.48
21.22
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

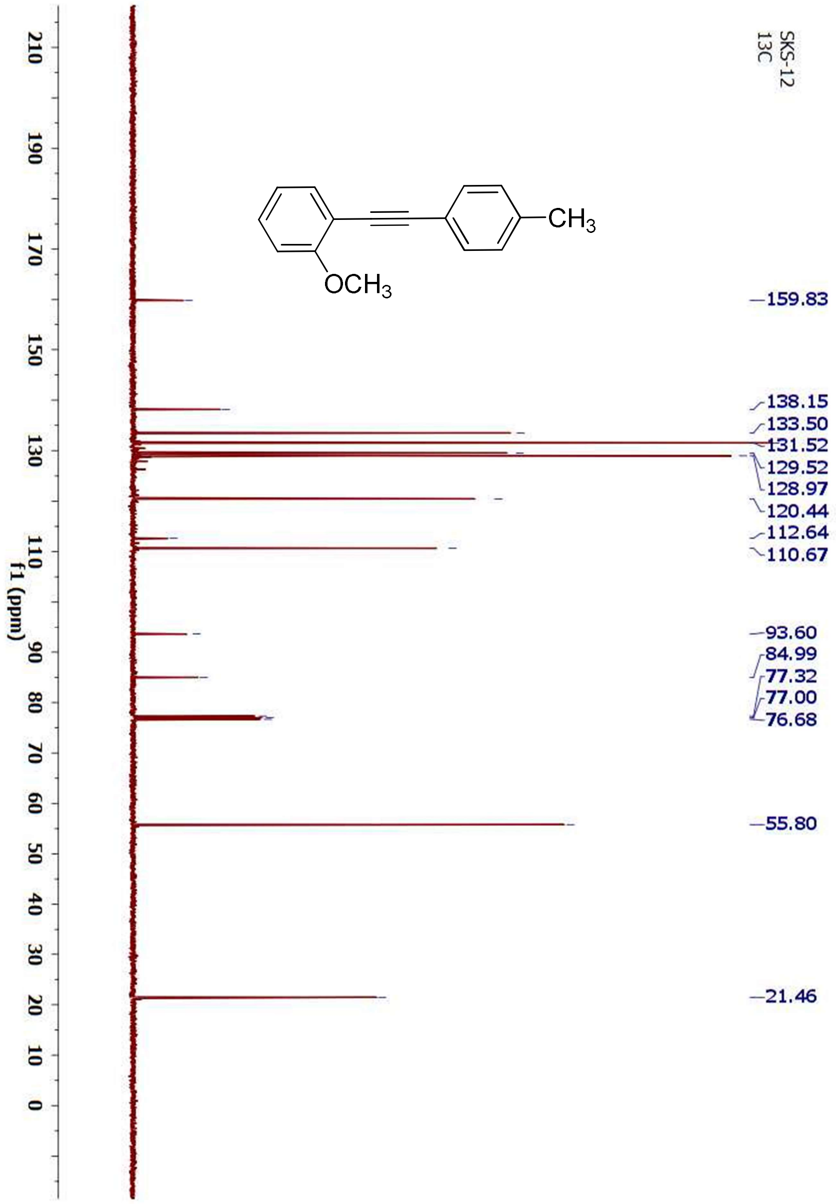

SKS-6
1H
OMe
7.48
7.47
7.46
7.45
7.35
7.31
7.26
7.24
7.23
7.21
7.14
7.12
6.89
6.88
6.87
6.87
3.83
2.35
2.21
2.11
1.10
1.00
2.17
3.35
3.17
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

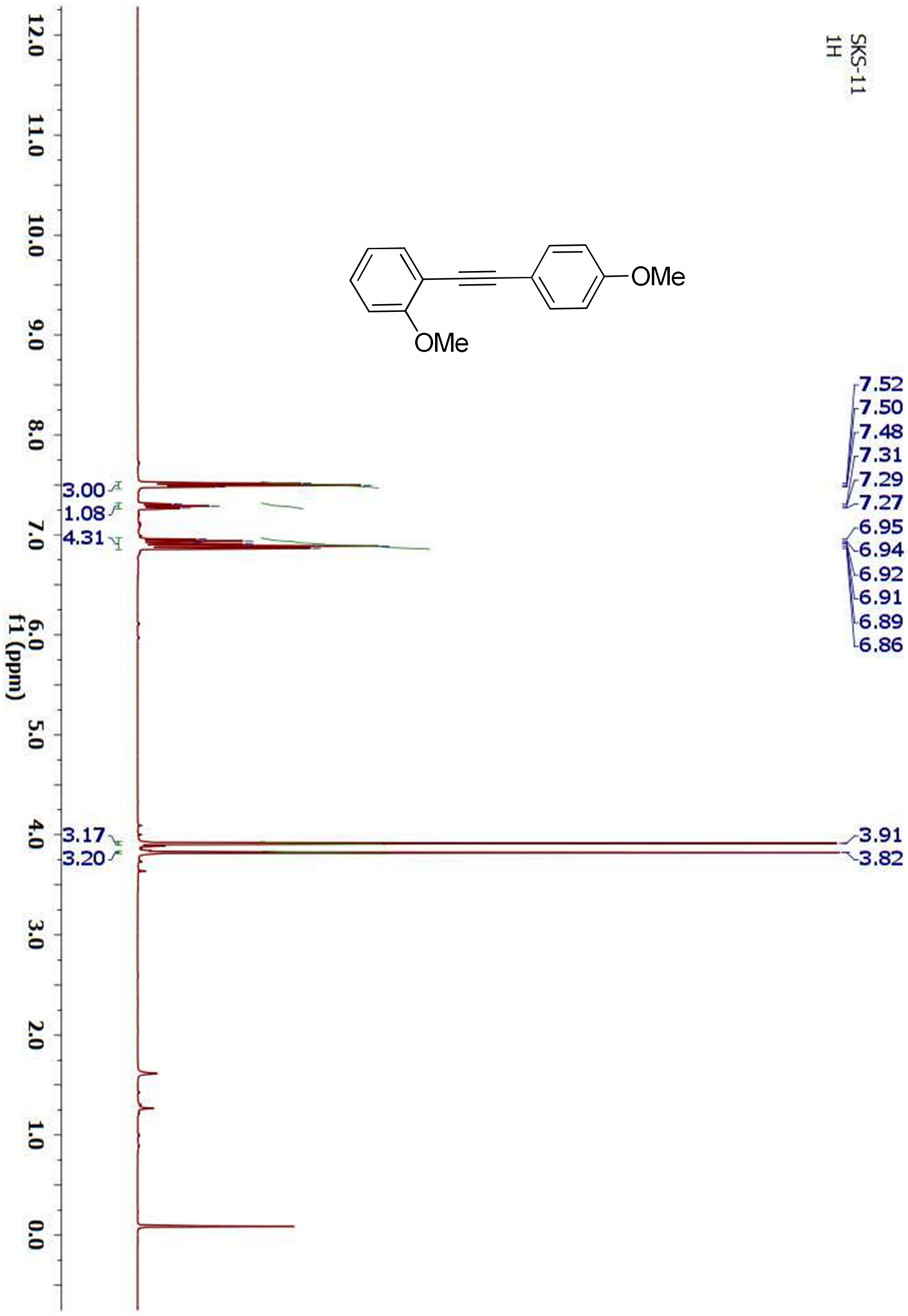

SKS-6
13C
OMe
159.55
137.95
133.02
132.03
128.83
128.51
128.19
127.66
115.49
113.97
89.00
88.21
77.32
77.00
76.68
55.29
21.23
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

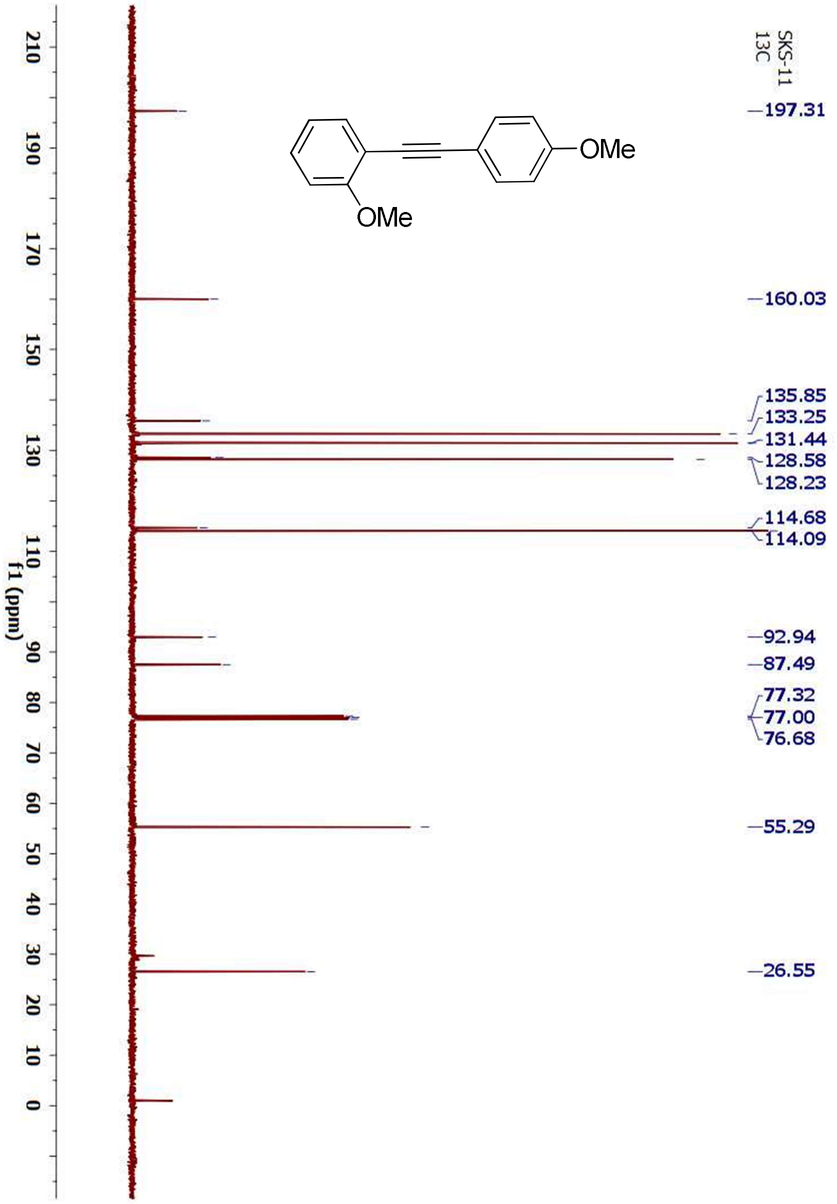

SKS-9
1H
OMe
7.58
7.57
7.56
7.51
7.49
7.34
7.33
7.31
7.26
6.96
6.94
6.92
6.90
3.92
1.96
1.00
4.03
2.03
3.17
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

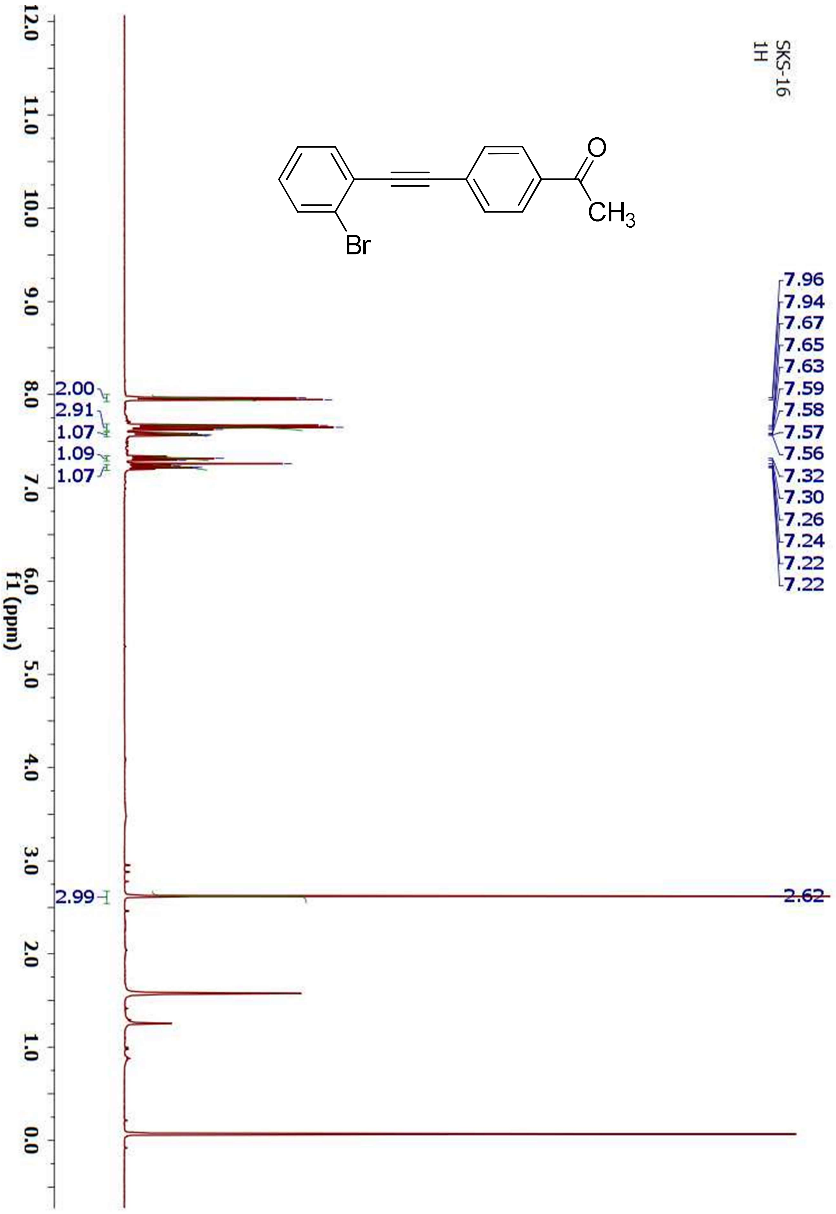

SKS-9
13C
OMe
159.93
133.57
131.65
129.73
128.22
128.08
123.57
120.48
110.73
93.41
85.70
77.32
77.00
76.68
55.85
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

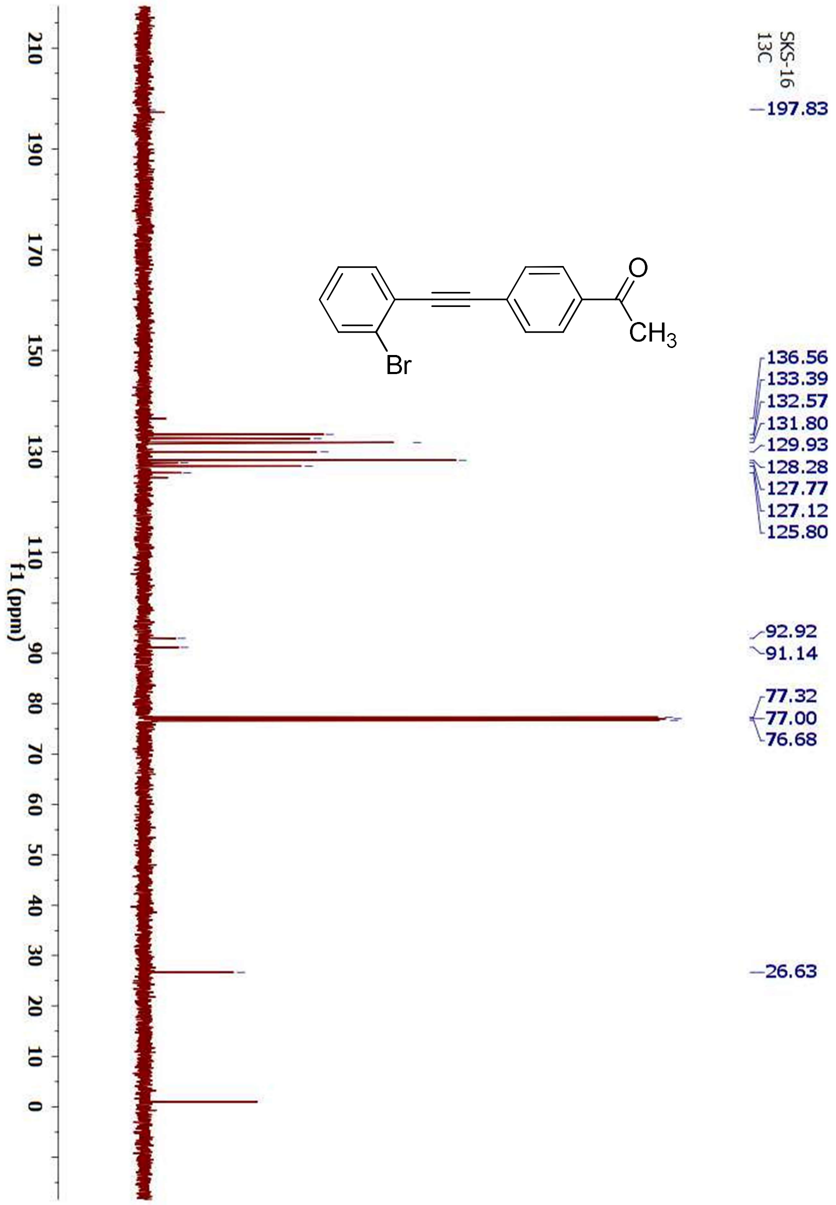

SKS-12
1H
CH3
OCH3
7.52
7.50
7.48
7.46
7.32
7.30
7.29
7.17
7.15
6.96
6.95
6.93
6.92
6.90
3.92
2.37
2.91
1.00
2.07
2.10
3.09
3.27
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

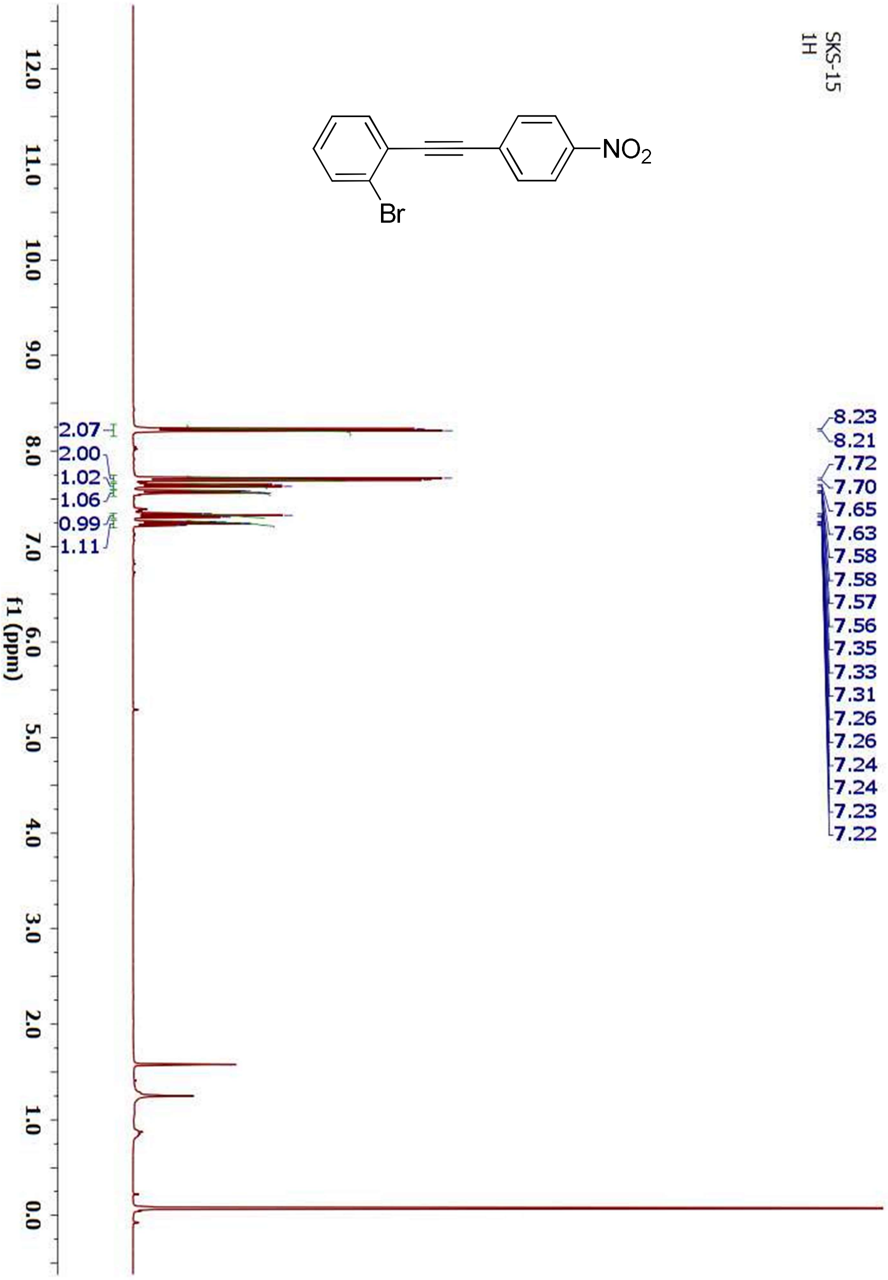

SKS-12
13C
OCH$_3$
CH$_3$
159.83
138.15
133.50
131.52
129.52
128.97
120.44
112.64
110.67
93.60
84.99
77.32
77.00
76.68
55.80
21.46
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

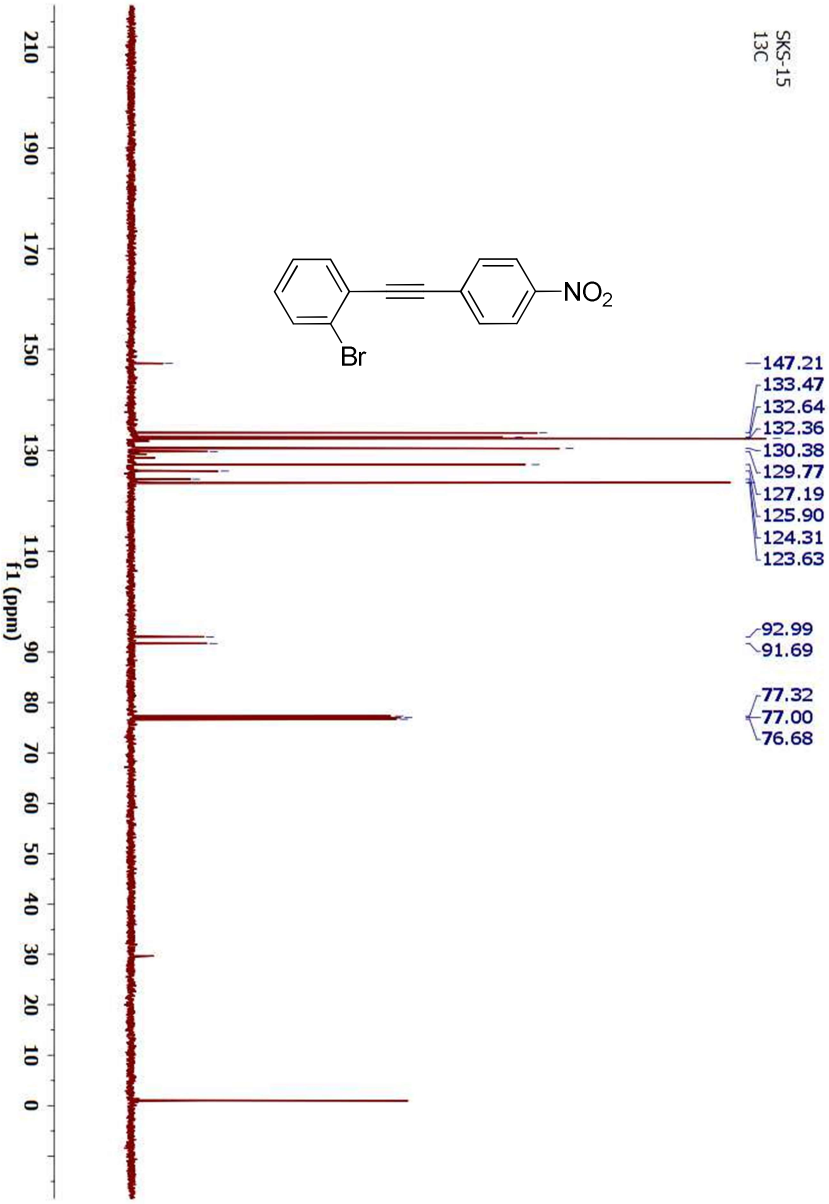

SKS-11
1H
OMe
OMe
7.52
7.50
7.48
7.31
7.29
7.27
6.95
6.94
6.92
6.91
6.89
6.86
3.91
3.82
3.00
1.08
4.31
3.17
3.20
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

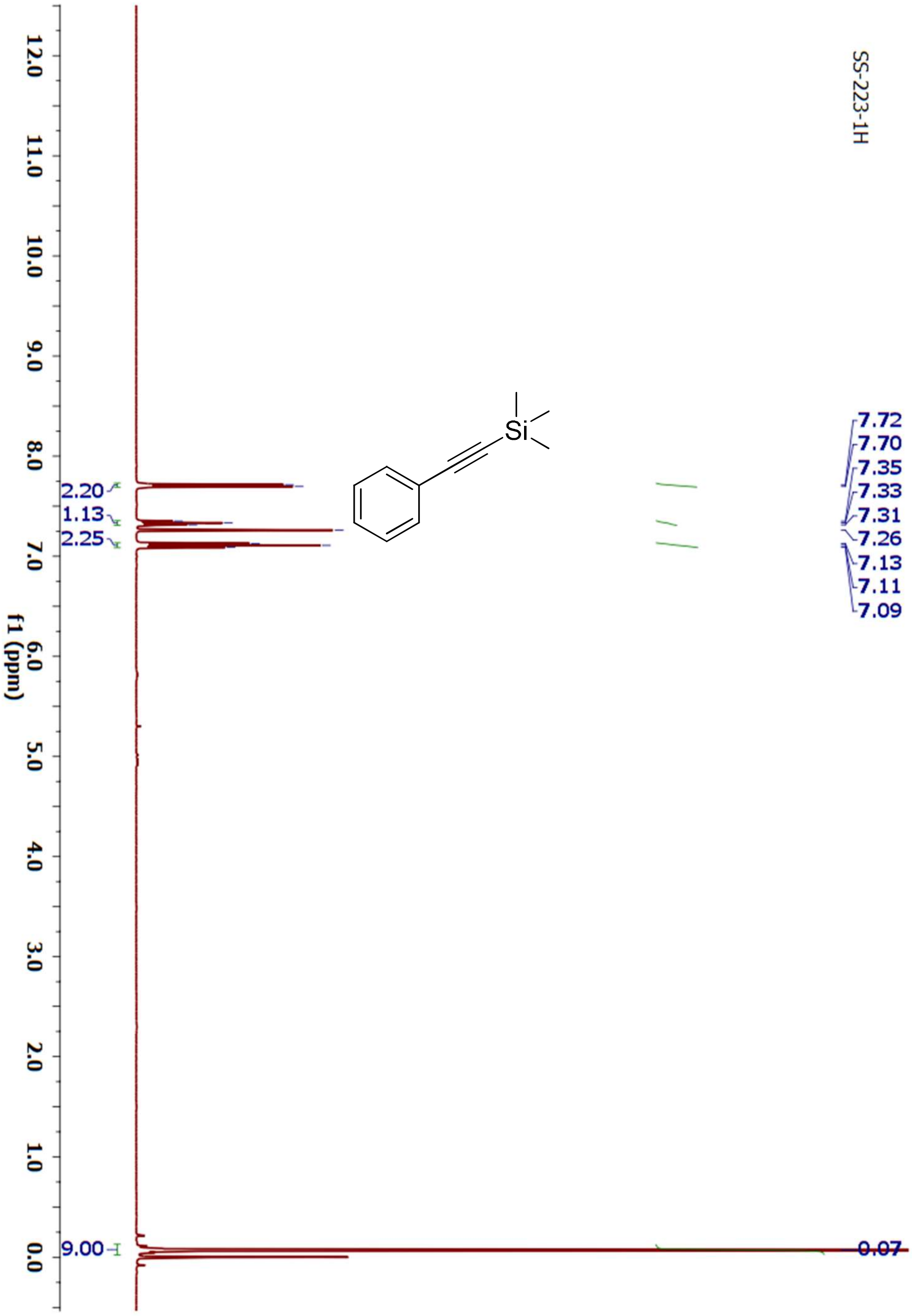

SKS-11
13C
197.31
160.03
135.85
133.25
131.44
128.58
128.23
114.68
114.09
92.94
87.49
77.32
77.00
76.68
55.29
26.55
OMe
OMe
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

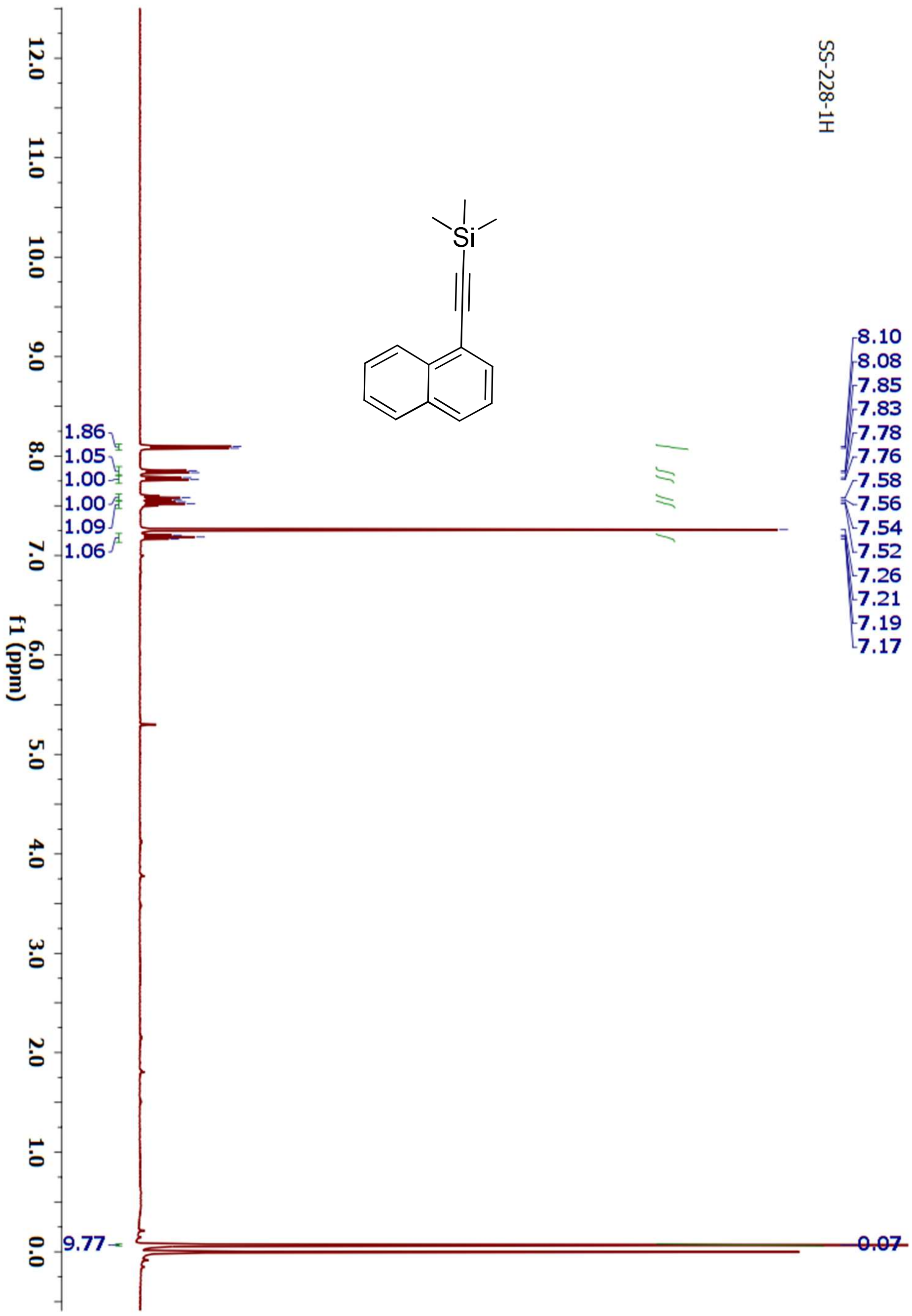

SKS-16
1H
O
CH3
Br
7.96
7.94
7.67
7.65
7.63
7.59
7.58
7.57
7.56
7.32
7.30
7.26
7.24
7.22
7.22
2.62
2.00
2.91
1.07
1.09
1.07
2.99
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

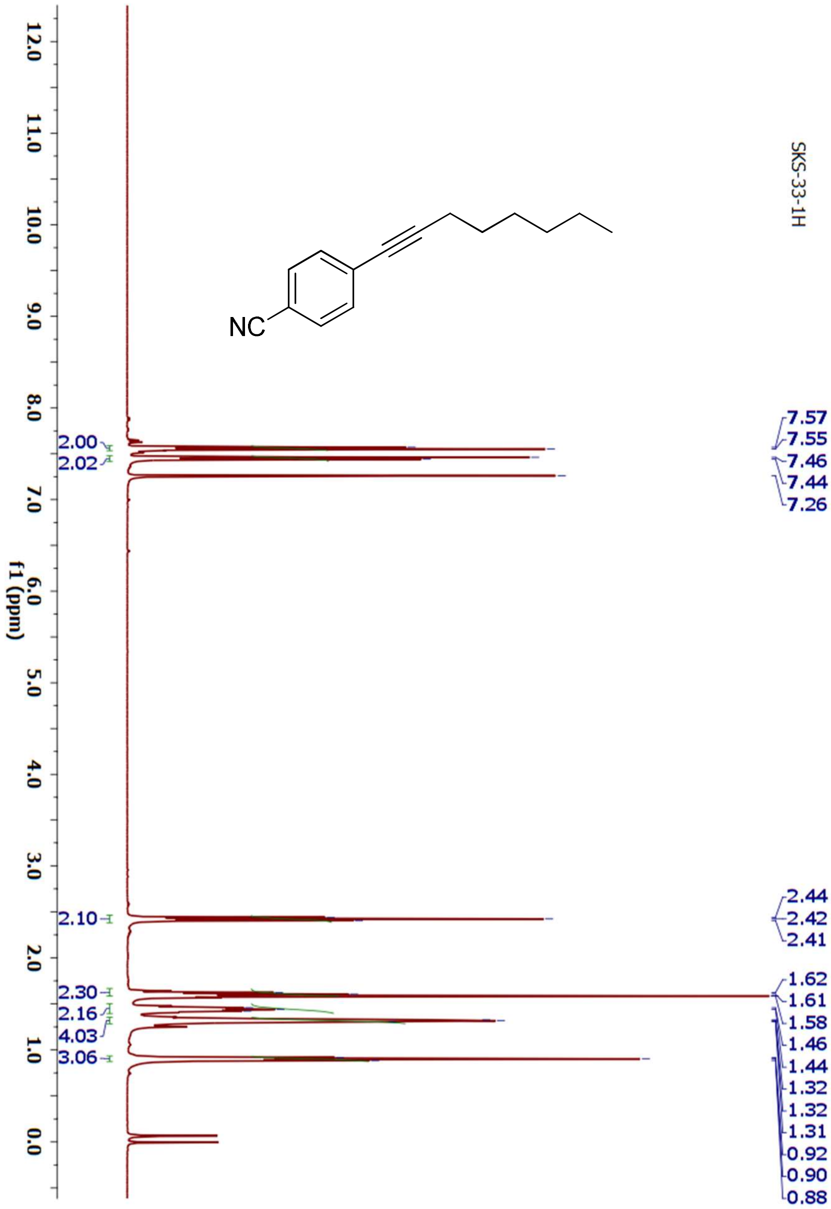

SKS-16
13C
197.83
136.56
133.39
132.57
131.80
129.93
128.28
127.77
127.12
125.80
92.92
91.14
77.32
77.00
76.68
26.63
Br
O
CH3
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

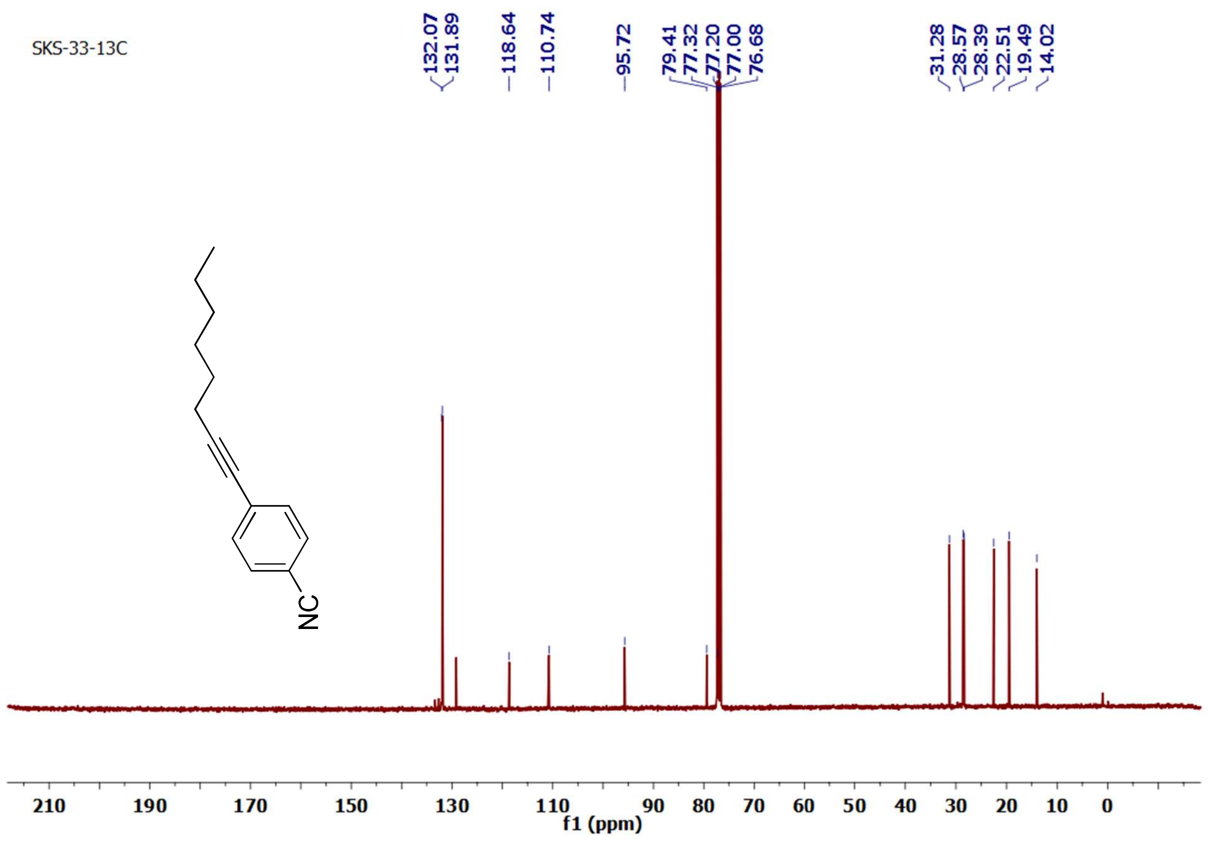

SKS-15
1H
NO2
Br
8.23
8.21
7.72
7.70
7.65
7.63
7.58
7.58
7.57
7.56
7.35
7.33
7.31
7.26
7.26
7.24
7.24
7.23
7.22
2.07
2.00
1.02
1.06
0.99
1.11
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

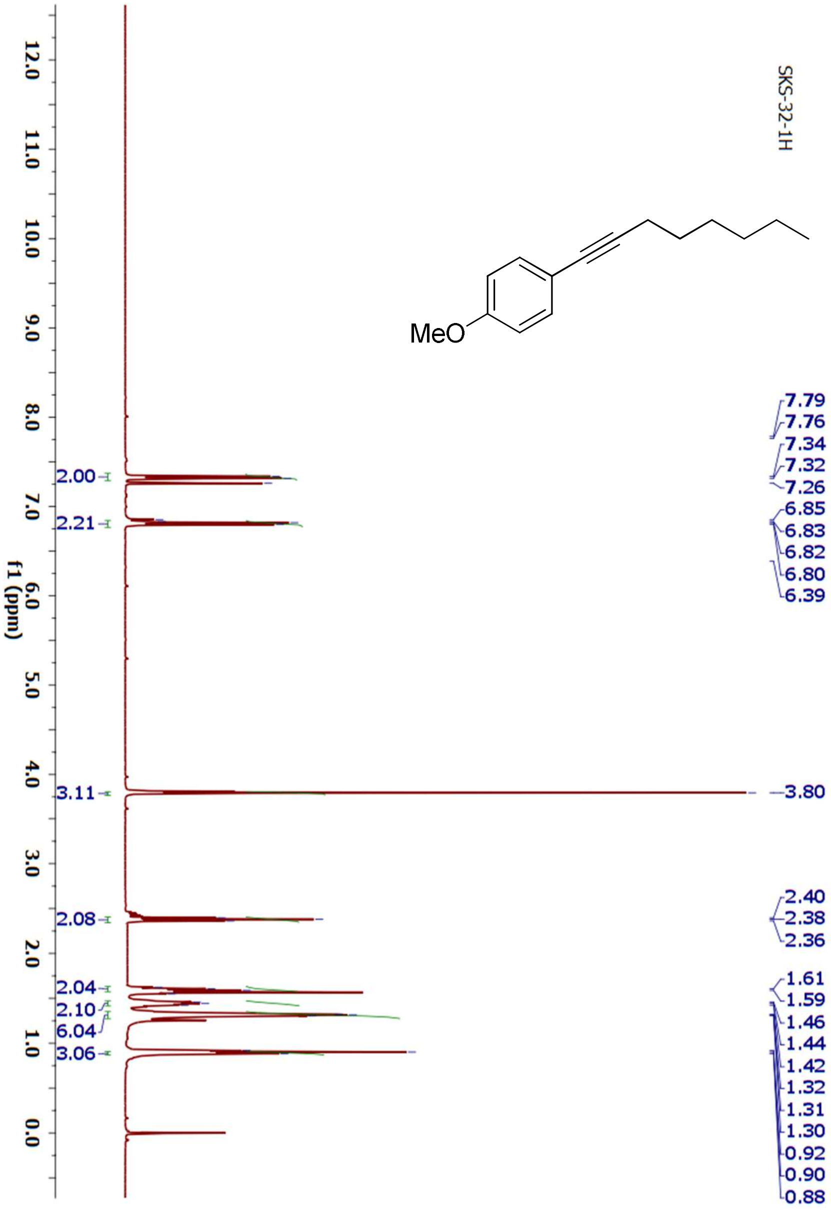

SKS-15
13C
Br
NO$_2$
147.21
133.47
132.64
132.36
130.38
129.77
127.19
125.90
124.31
123.63
92.99
91.69
77.32
77.00
76.68
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

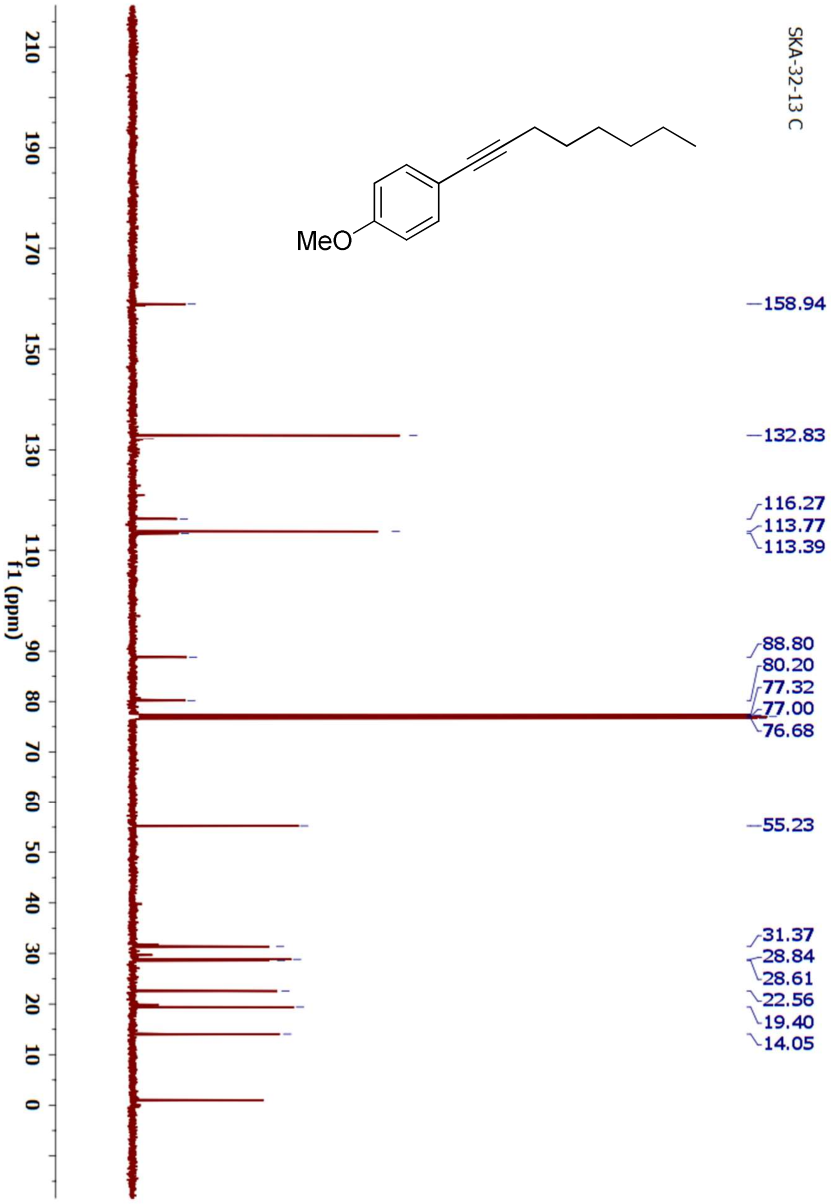

SS-223-1H
7.72
7.70
7.35
7.33
7.31
7.26
7.13
7.11
7.09
0.07
2.20
1.13
2.25
9.00
Si
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

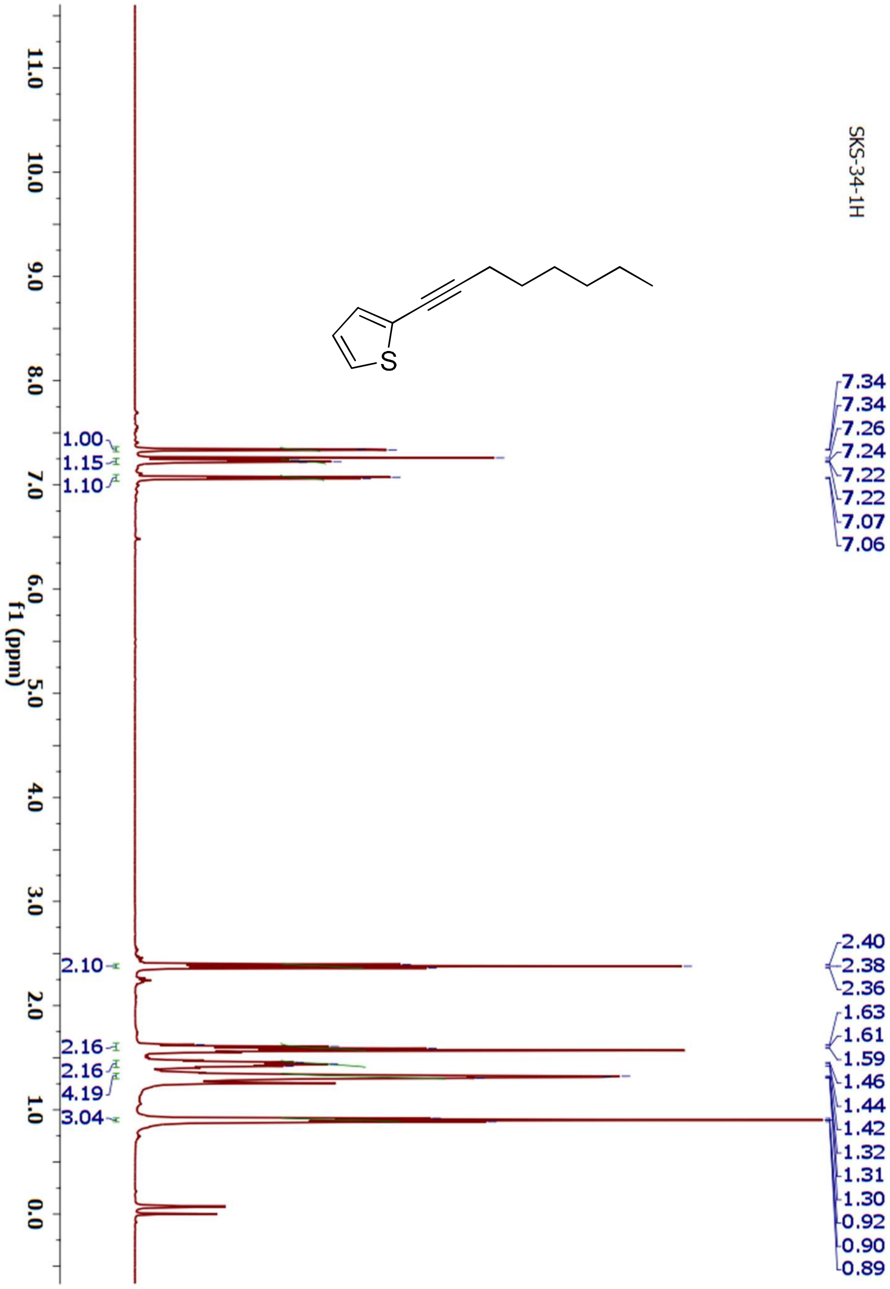

SS-228-1H
Si
8.10
8.08
7.85
7.83
7.78
7.76
7.58
7.56
7.54
7.52
7.26
7.21
7.19
7.17
0.07
1.86
1.05
1.00
1.00
1.09
1.06
9.77
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

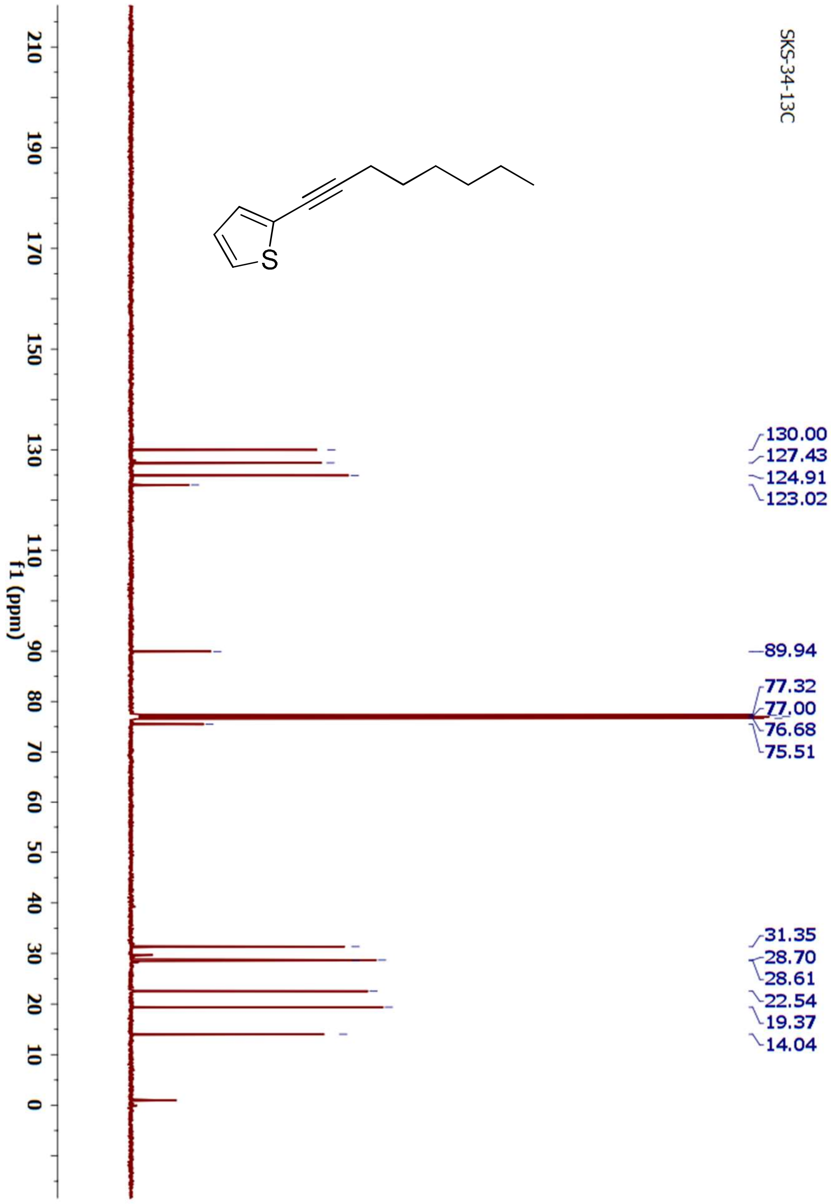

SKS-33-1H
NC
12.0
11.0
10.0
9.0
8.0
7.0
6.0
f1 (ppm)
5.0
4.0
3.0
2.0
1.0
0.0
2.00
2.02
2.10
2.30
2.16
4.03
3.06
7.57
7.55
7.46
7.44
7.26
2.44
2.42
2.41
1.62
1.61
1.58
1.46
1.44
1.32
1.32
1.31
0.92
0.90
0.88

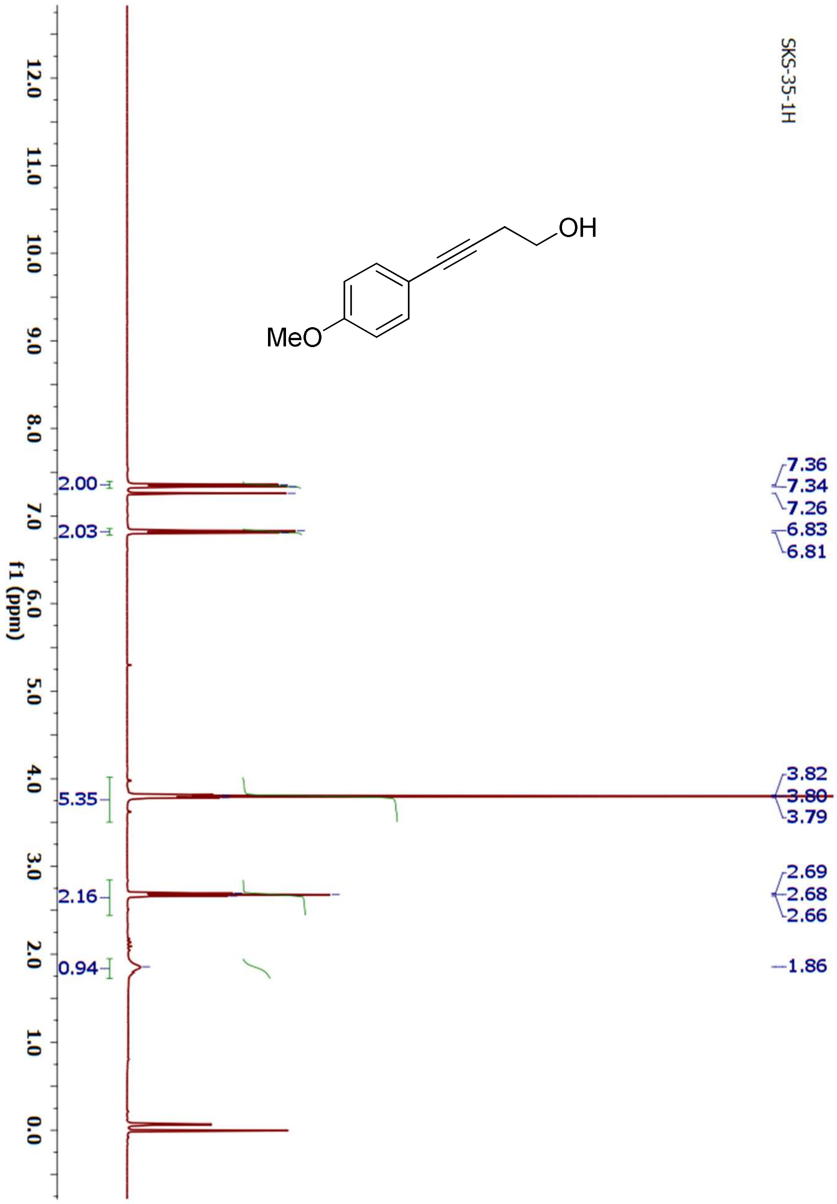

SKS-33-13C
NC
132.07
131.89
118.64
110.74
95.72
79.41
77.32
77.20
77.00
76.68
31.28
28.57
28.39
22.51
19.49
14.02
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

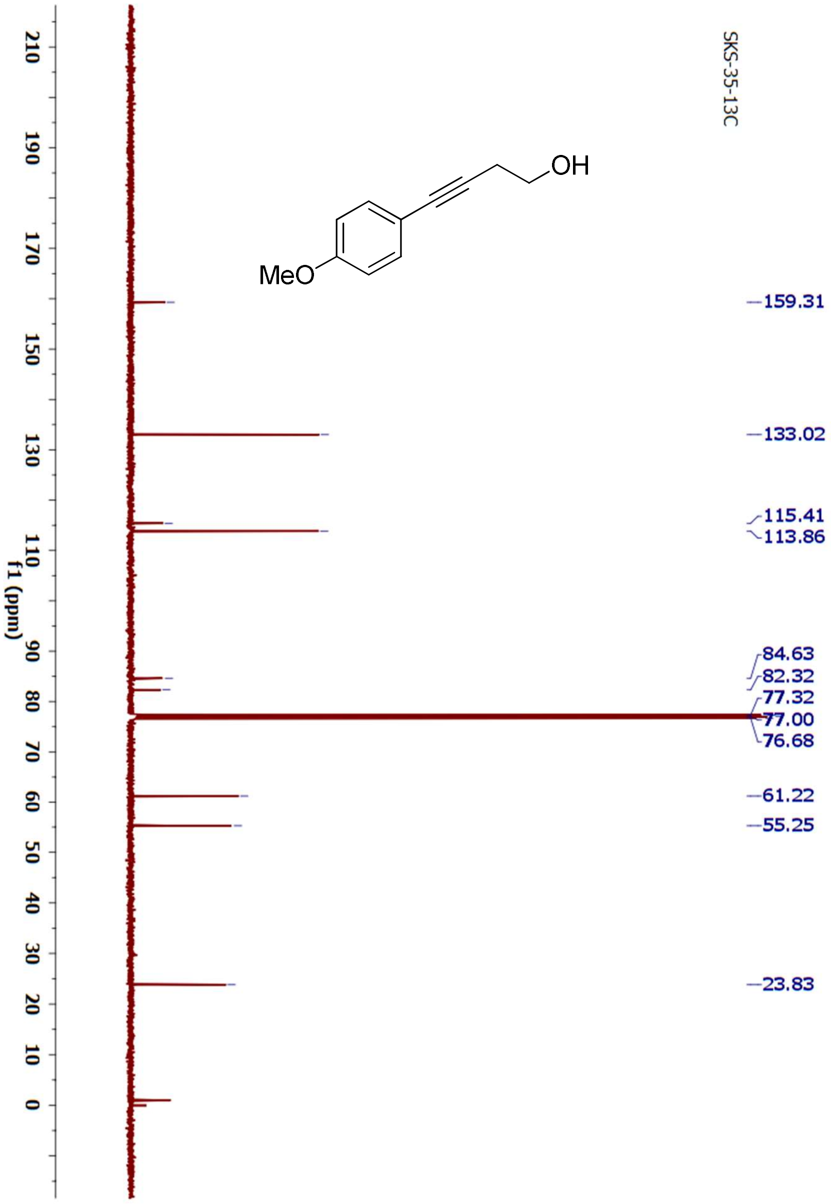

SKS-32-1H
MeO
7.79
7.76
7.34
7.32
7.26
6.85
6.83
6.82
6.80
6.39
3.80
2.40
2.38
2.36
1.61
1.59
1.46
1.44
1.42
1.32
1.31
1.30
0.92
0.90
0.88
2.00
2.21
3.11
2.08
2.04
2.10
6.04
3.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

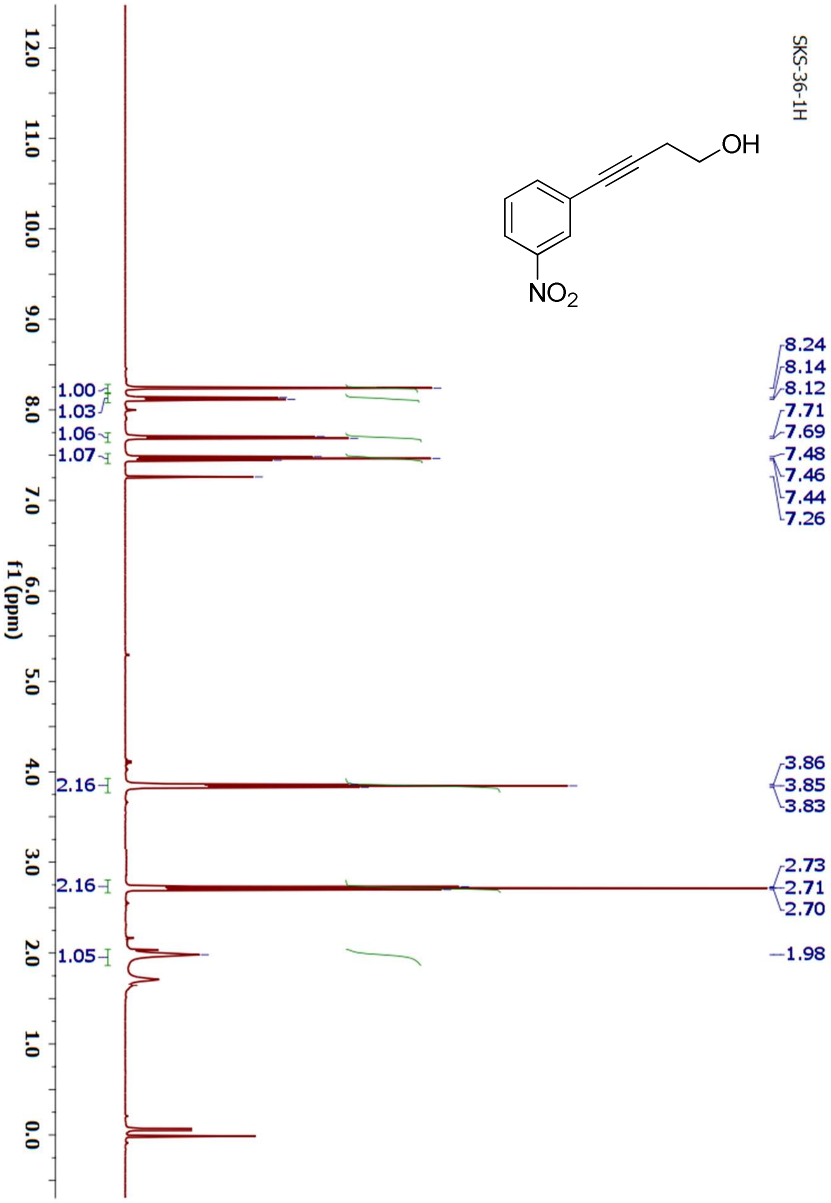

SKA-32-13 C
MeO
158.94
132.83
116.27
113.77
113.39
88.80
80.20
77.32
77.00
76.68
55.23
31.37
28.84
28.61
22.56
19.40
14.05
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

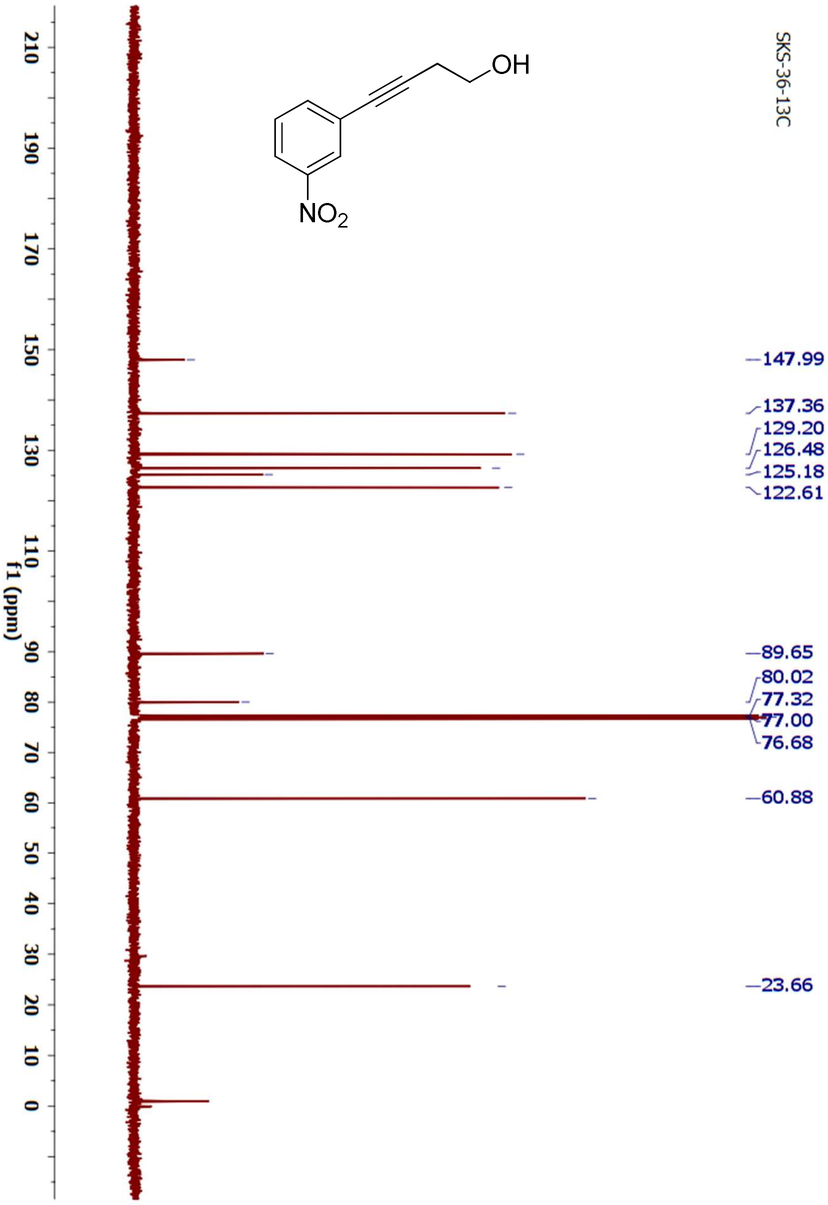

SKS-34-1H
S
7.34
7.34
7.26
7.24
7.22
7.22
7.07
7.06
2.40
2.38
2.36
1.63
1.61
1.59
1.46
1.44
1.42
1.32
1.31
1.30
0.92
0.90
0.89
1.00
1.15
1.10
2.10
2.16
2.16
4.19
3.04
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

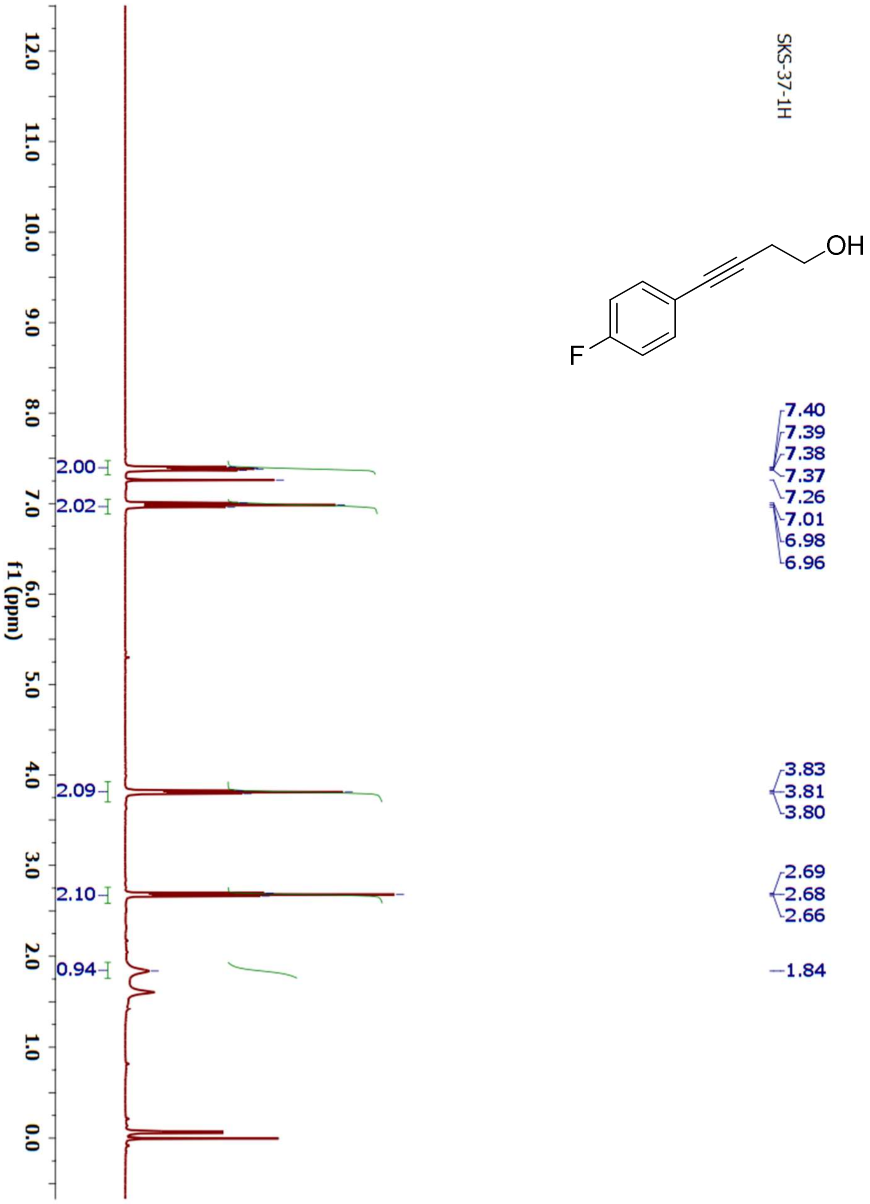

SKS-34-13C
S
130.00
127.43
124.91
123.02
89.94
77.32
77.00
76.68
75.51
31.35
28.70
28.61
22.54
19.37
14.04
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

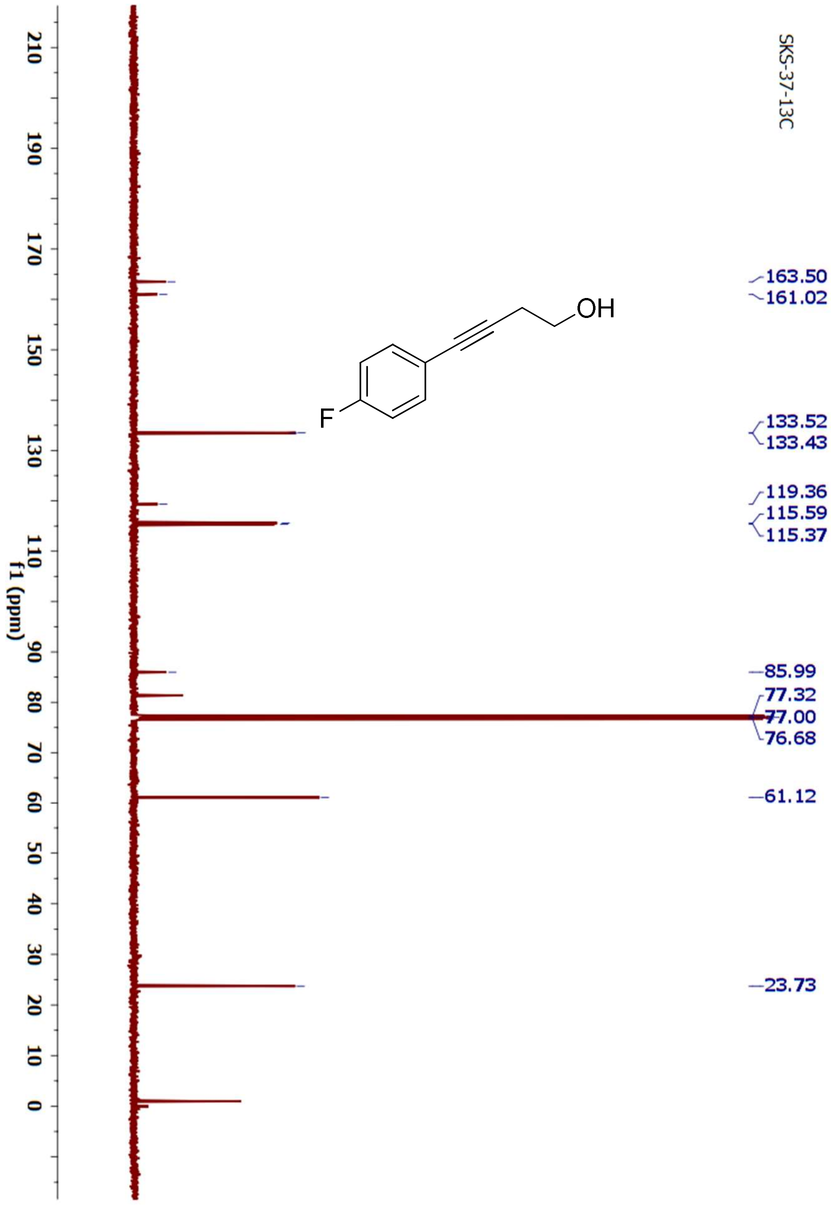

SKS-35-1H
MeO
OH
7.36
7.34
7.26
6.83
6.81
3.82
3.80
3.79
2.69
2.68
2.66
1.86
2.00
2.03
5.35
2.16
0.94
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

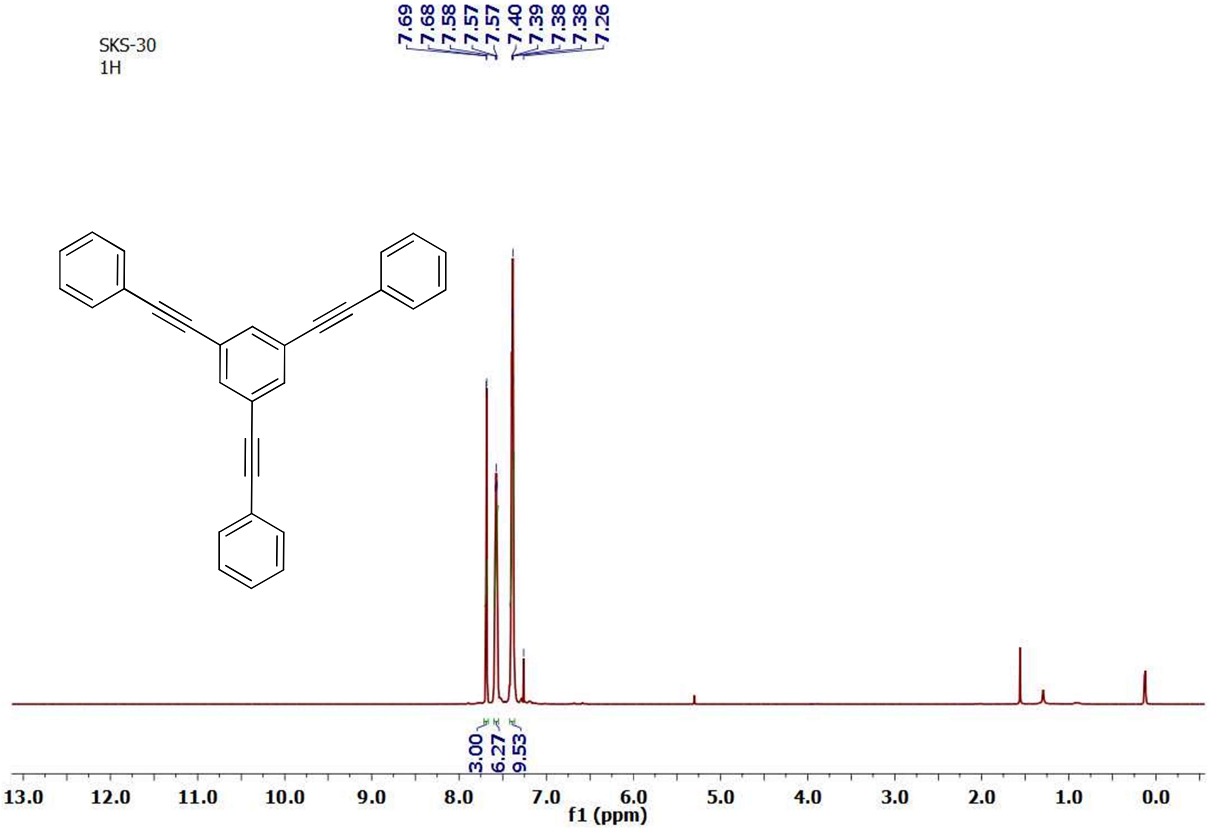

SKS-35-13C
MeO
OH
159.31
133.02
115.41
113.86
84.63
82.32
77.32
77.00
76.68
61.22
55.25
23.83
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

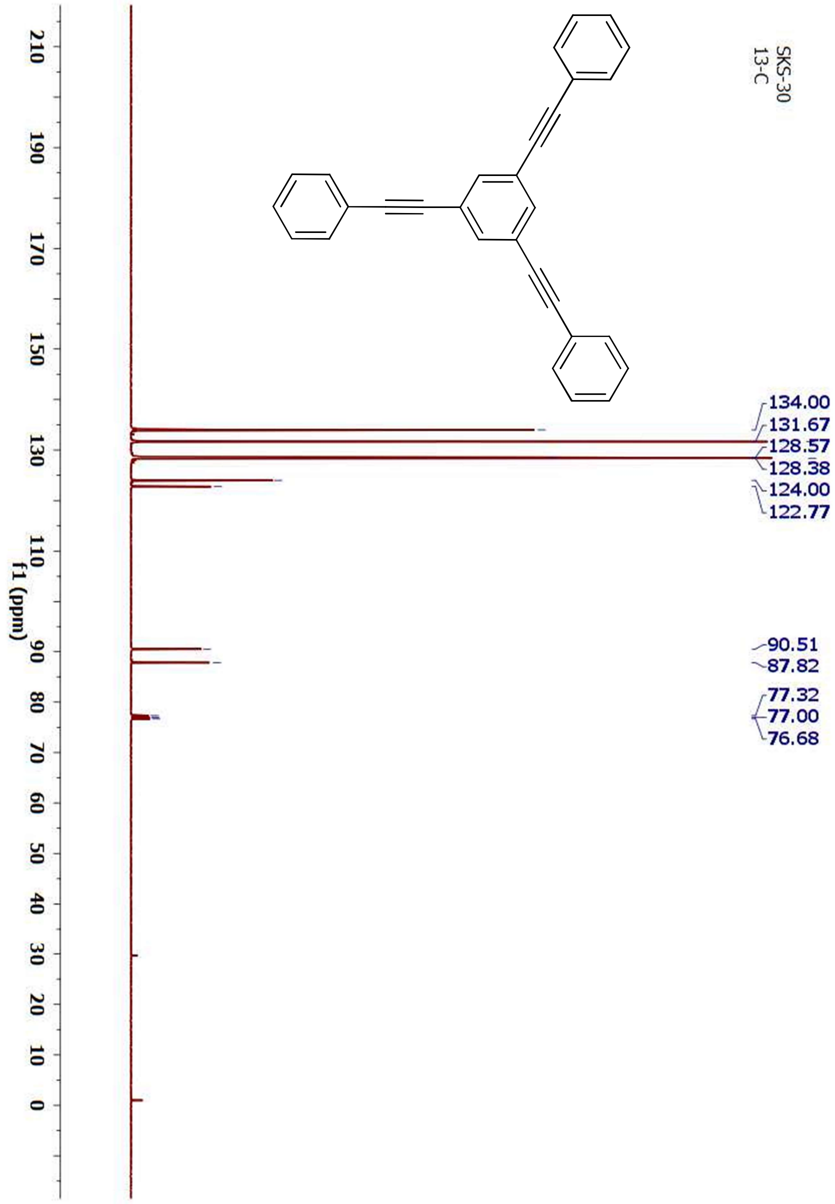

SKS-36-1H
OH
NO2
8.24
8.14
8.12
7.71
7.69
7.48
7.46
7.44
7.26
3.86
3.85
3.83
2.73
2.71
2.70
1.98
1.00
1.03
1.06
1.07
2.16
2.16
1.05
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


SKS-36-13C
OH
NO2
147.99
137.36
129.20
126.48
125.18
122.61
89.65
80.02
77.32
77.00
76.68
60.88
23.66
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SKS-37-1H
F
OH
7.40
7.39
7.38
7.37
7.26
7.01
6.98
6.96
3.83
3.81
3.80
2.69
2.68
2.66
1.84
2.00
2.02
2.09
2.10
0.94
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


SKS-37-13C
163.50
161.02
133.52
133.43
119.36
115.59
115.37
85.99
77.32
77.00
76.68
61.12
23.73
F
OH
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


SKS-30
1H
7.69
7.68
7.58
7.57
7.57
7.40
7.39
7.38
7.38
7.26
3.00
6.27
9.53
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


SKS-30
13-C
134.00
131.67
128.57
128.38
124.00
122.77
90.51
87.82
77.32
77.00
76.68
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)