Supplementary Material

Surface Lewis Basic Site Enabled Proton Abstraction for the Regioselective Synthesis of Ynone and Flavone over Pd^0/Cs-ZSM-5 Catalyst: Mechanistic Understanding and Structure-Activity Correlation

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1. General information

All reagent chemicals were used analytical grade and as used without further purification. All solvents were dried and distilled by standard methods as described in the literature. Column chromatography was carried out using silica gel (100-200 and 60-120 mesh). ^{1}H NMR spectra were recorded by using Bruker VX NMR FT-300-500 MHz and ^{13}C NMR spectra were recorded by using Bruker VX NMR FT-75-125 MHz spectrometers instrument in $CDCl_3$ and DMSO-d_6. The chemical shifts (δ) are reported in ppm units relative to TMS as an internal standard for ^{1}H-NMR and $CDCl_3$ for ^{13}C NMR spectra. Coupling constants (J) are reported in hertz (Hz) and multiplicities are indicated as follows: s (singlet), d (doublet), dd (doublet of doublet), t(triplet), q (quartet), m (multiplet). Mass spectra were obtained at an ionisation potential of 70eV [scanned on VG 70-70H (micro mass)]. ^{29}Si and ^{27}Al SS-MAS NMR studies were conducted over Bruker AVANCE III 500WB NMR spectrometer with a spinning speed of 10 kHz using 3.2 mm triple resonance MASS probe. ^{29}Si NMR profiles are referenced to sodium trimethylsilyl propane sulfonate. The surface properties of Pd supported on different supports were measured by N_2 adsorption at -196 °C, in an Autosorb 3000 physical adsorption apparatus. The specific surface areas were calculated applying the BET method. The H_2-pulse chemisorption, H_2-TPR analysis and TPD of CO_2 and NH_3 were carried out using a Microtrac BEL Corp (Belcat-II, Japan). Hydrogen consumption was measured by analysing effluent gas using a calibration curve of TPR of Ag_2O under a similar protocol. The X-ray diffraction (XRD) patterns of the supported Pd fresh and used samples were characterized by powder XRD analysis using a Rigaku Miniflex X-ray diffractometer using Ni filtered CuKα radiation (λ= 0.15406 nm) from 2θ = 2°- 80°, at a scan rate of 2° min^{-1} with generator voltage and current of 30 kV and 15 mA, respectively. The XPS patterns were recorded using a Kratos Axis Ultra Imaging X-ray photoelectron spectrometer, equipped with Mg anode and a multichannel detector. Charge referencing was done against adventitious carbon (C 1s, 284.8 eV). A Shirley-type background was subtracted from the signals. The morphological analysis was carried out using transmission electron microscopy (TEM on a JEOL100S microscope at high resolution (HR) on a JEOL 2010 micro-scope). The nature of basic sites is investigated using formic acid adsorption in conjunction with FT-IR (Carry 660 equipped with mid-IR MCT detector; Agilent Technologies, USA). The spectra

were collected in the range of 2000-1200 cm^{-1} with a resolution of 4 cm^{-1} and 64 no. of scans. The experiments were carried out using a DRIFT (Harrick) cell connected to a vacuum-adsorption set-up. The catalyst samples were then pre-treated by heating them at 300 °C and maintained at the same temperature for 1 h. After cooling down to 125 °C, the spectrum was collected and used as a blank spectrum. Then the samples were exposed to formic acid (98%; Sigma-Aldrich) followed by vacuum for 30 minutes. The spectra obtained after formic acid adsorption subtracted from the blank spectrum. Finally, the resultant spectra were quantified using the Kubelka-Munk function. The inductively coupled plasma-optimal emission spectrophotometer (ICP-OES) analysis was carried out by using iCAP-6500 DUO, Thermo Fisher Scientifics UK.

Schematic representation of catalysts preparation

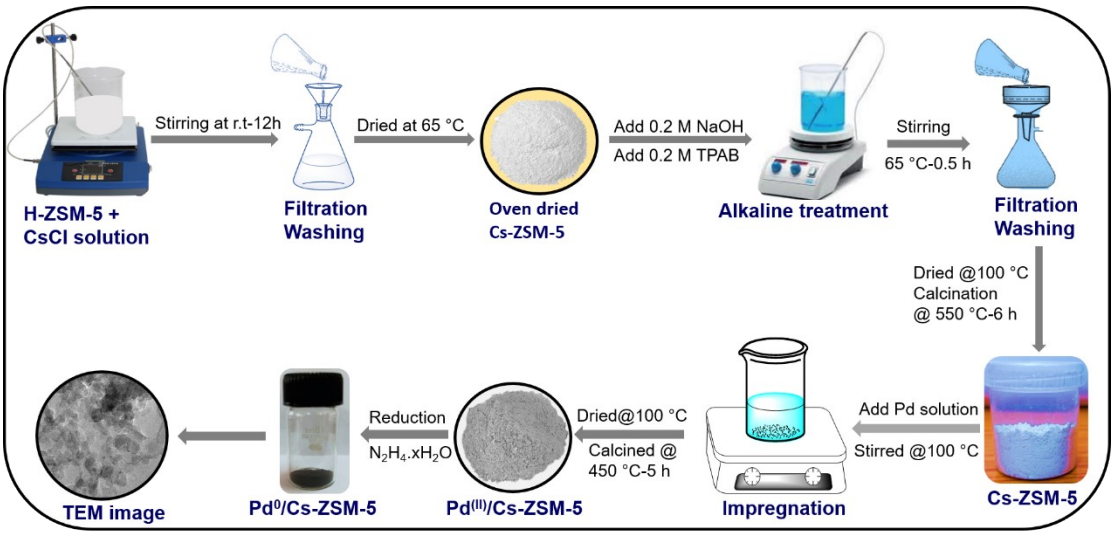


Figure S1: Preparation of Pd^0 supported Cs-ZSM-5 catalyst

Charactersation

2.1. BET-SA analysis

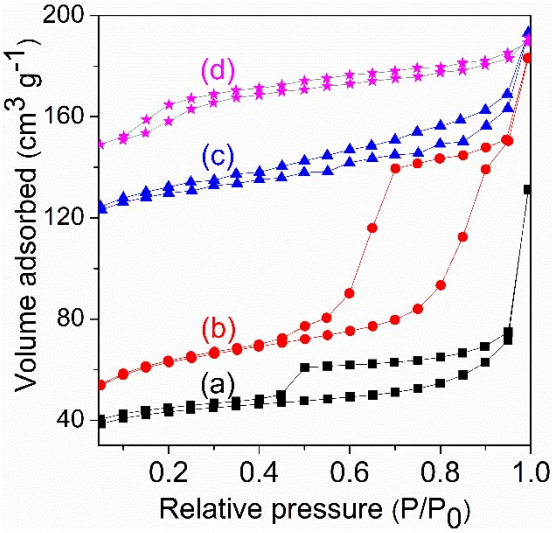


Figure S2: N_2-adsorption-desorption isotherms of a) Cs-ZSM-5(150), b) Cs-ZSM-5(80), c) Cs-ZSM-5(30), and d) 3wt%Pd/Cs-ZSM-5(30) samples.

Table S1: BET-surface and pore size distribution of catalysts

S. No	Catalyst (Si/Al) ratio	BET surface area [a] (m^2/g)	Average pore volume/(cm^3/g^{-1})[b]	Average pore diameter (nm)[b]
1	3wt%Pd/Cs-ZSM-5(30)	236	0.178	2.61
2	Cs-ZSM-5(30)	289	0.244	3.37
3	Cs-ZSM-5(80)	270	0.341	4.64
4	Cs-ZSM-5(150)	182	0.227	4.98
5	3wt%Pd/Fumed - SiO_2	149	-	-
6	3wt%Pd/Al_2O_3	168	-	-

a: Measured from BET surface are and b: evaluated by $p/p_0 = 0.99$.

2.2. X-ray diffraction (XRD) analysis

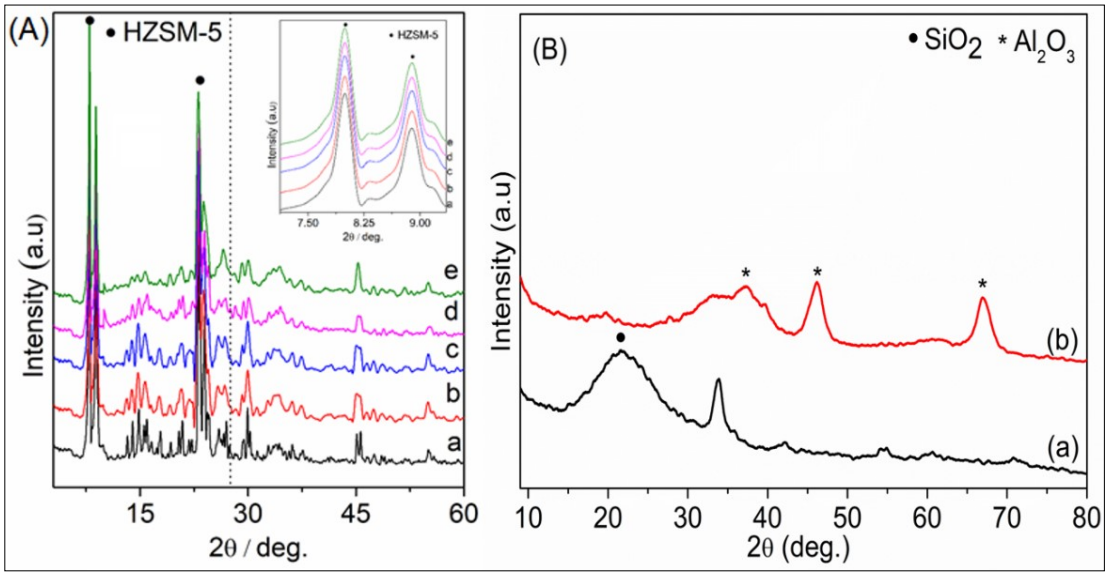


Figure S3: (A) XRD patterns of the 3wt%Pd supported on (a) H-ZSM-5 (b) Na-ZSM-5 (c) K-ZSM-5 (d) Cs-ZSM-5 fresh and e) used 3wt%Pd/Cs-ZSM-5 catalyst recovered after 4th cycle. **(B)** Calcined fresh 3wt%Pd supported on (a) fumed-SiO_2 and (b) γ-Al_2O_3 samples.

2.3. Acid-base properties of catalysts

Table S2: CO_2-TPD analysis and basic sites distribution on supported Pd catalysts.

3wt%Pd loading on	mmol g_{cat}^{-1}		
	Weak	Moderate	Strong
H-ZSM-5	0.671	0.00	0.00
Na-ZSM-5	0.893	0.680	0.00
K-ZSM-5	0.911	0.714	0.00
Cs-ZSM-5	0.945	1.022	0.642

Table S3: NH_3-TPD analysis and acidic sites distribution on supported Pd catalysts.

3wt%Pd loading on	mmol g_{cat}^{-1}			Total acidity
	Weak	Moderate	Strong	
H-ZSM-5	0.416	0.488	0.291	1.195
Na-ZSM-5	0.106	0.040	0.017	0.163
K-ZSM-5	0.073	0.018	0.005	0.096
Cs-ZSM-5	0.004	0.006	0.000	0.010

2.4. HR-TEM analysis

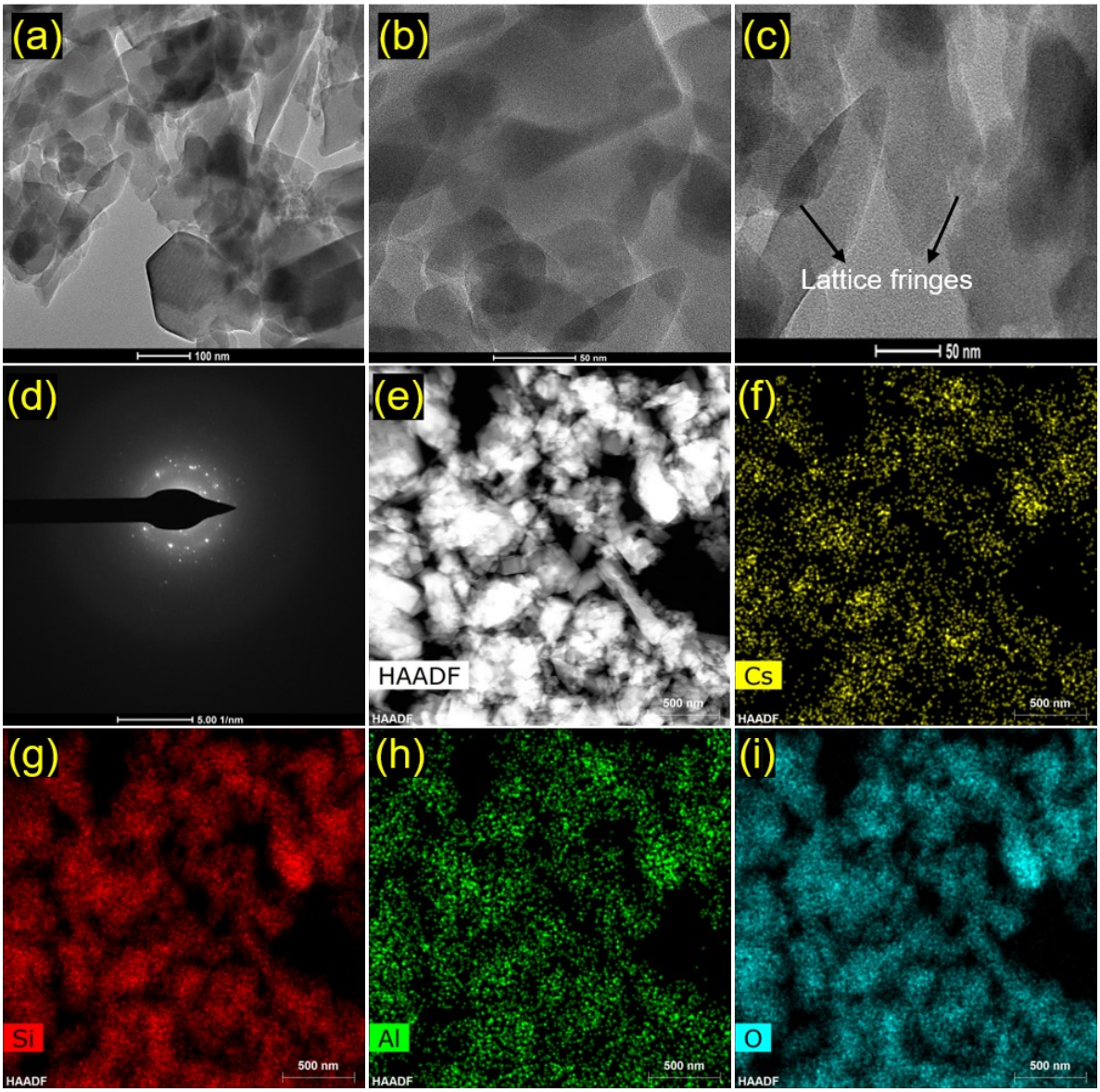


Figure S4: TEM analysis of Cs-ZSM-5(30) sample (a) TEM micrograph, (b-c) HR-TEM micrographs, (d) SAED patterns (e-i) HAADF-color mapping images of Cs, Si, Al, and O elements.

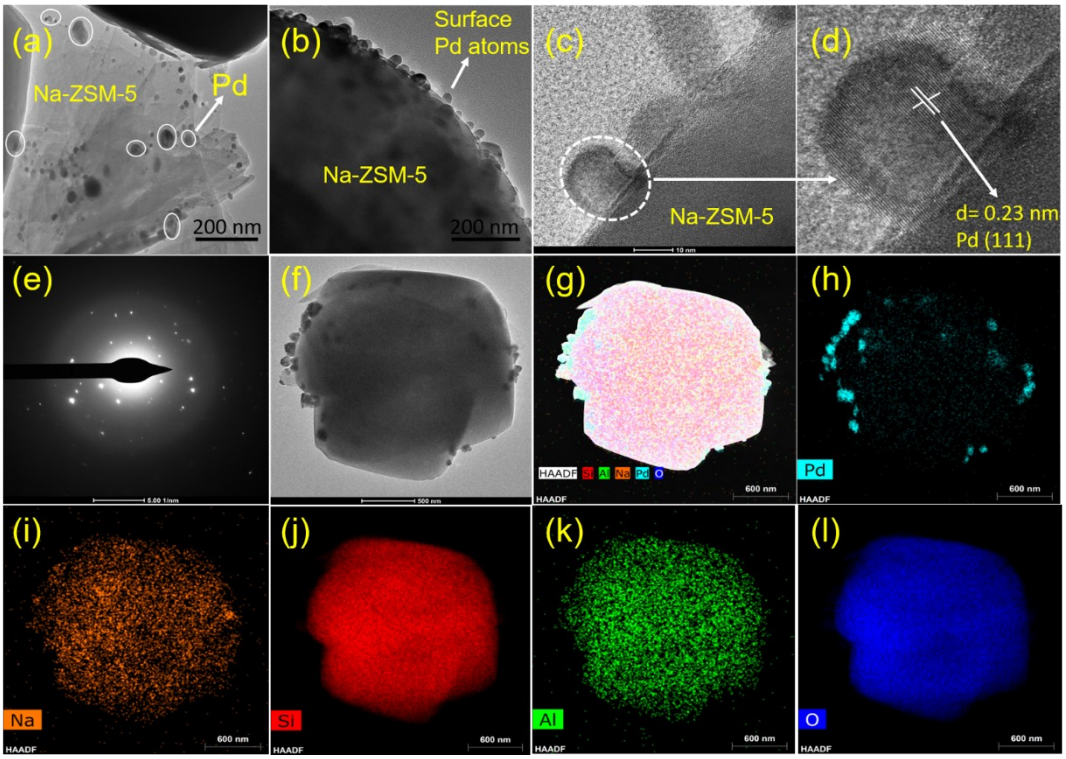


Figure S5: TEM analysis of 3wt%Pd/Na-ZSM-5(30) (a-b) TEM micrograph, (c-d) HR-TEM images, (e) SAED patterns, (f-l) HAADF-colour mapping images of Pd, Na, Si, Al, and O elements.

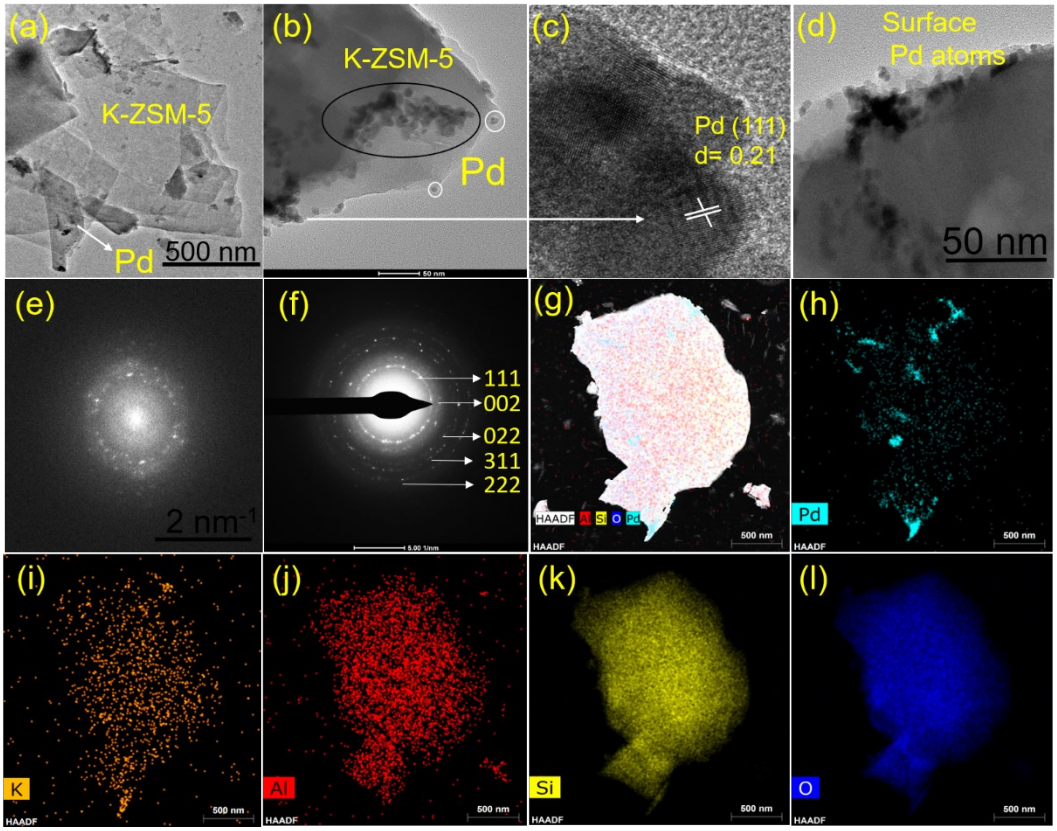


Figure S6: TEM analysis of 3wt%Pd/K-ZSM-5(30) (a-b) TEM micrograph, (c-d) HR-TEM images, (e-f) SAED patterns, (g-l) HAADF-colour mapping images of Pd, Na, Si, Al, and O elements.

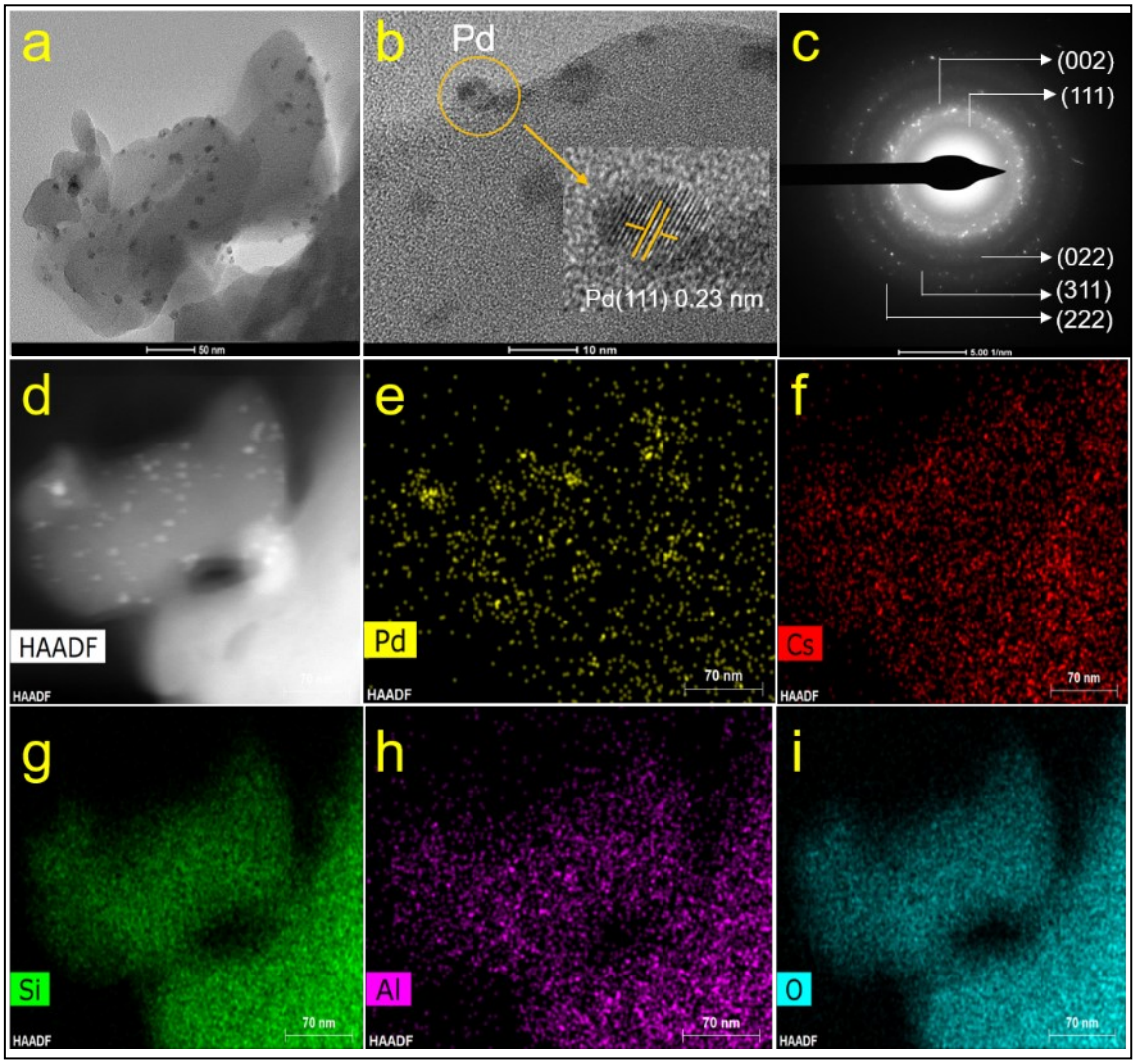


Figure S7: TEM analysis of 3wt%Pd/-ZSM-5(30) **used catalyst** (a) TEM micrograph, (b) HR-TEM micrograph, (c) SAED patterns, (d-i) HAADF-colour mapping images of Pd, Cs, Si, Al, and O elements.

2.5. XPS analysis

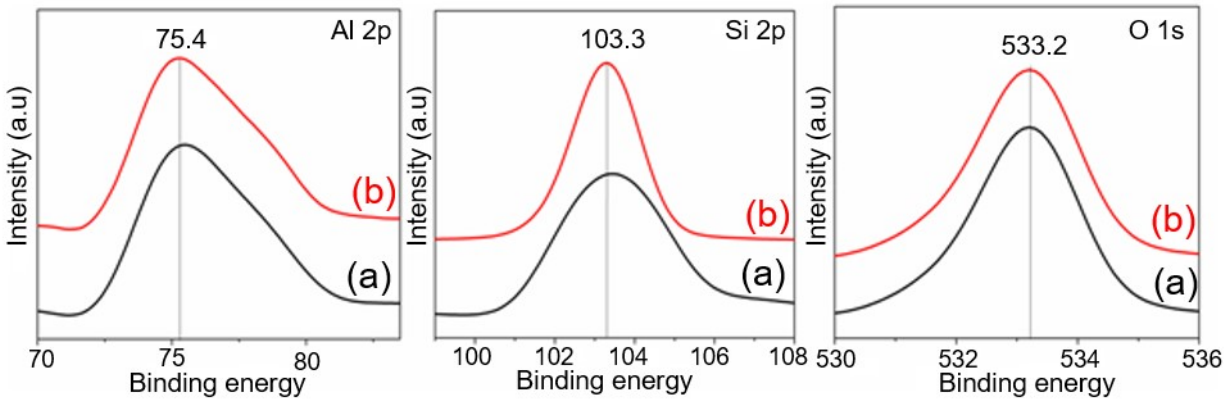


Figure S8: XPS spectra of Al 2p, Si 2p and O 1s of 3wt%Pd/Cs-ZSM-5 (a) fresh and (b) used catalysts.

2.6. ICP-OES analysis

Table S4: ICP-OES analysis of 3wt%Pd/Cs-ZSM-5 samples after each recycle

No. Cycles	Pd (wt%)
Fresh	2.83
1st	2.82
2nd	2.82
3rd	2.82
4th	2.82

2.7. X-ray Fluorescence spectroscopy (XRF) analysis

Table S5: Elemental composition of catalysts

S. No	Catalyst	Alkali metal (%)	Si (%)	Al (%)
1	Na-ZSM-5(30)	22.1	73.5	4.4
2	K-ZSM-5(30)	19.3	76.1	4.6
3	Cs-ZSM-5(30)	20.3	75.2	4.5
4	Cs-ZSM-5(80)	11.6	86.1	2.3
5	Cs-ZSM-5(150)	5.9	92.4	1.7
[a]6	3wt%Pd/Cs-ZSM-5(30)	19.1	76.6	4.3

a: Pd = 2.64%

2.8. Formic acid IR studies

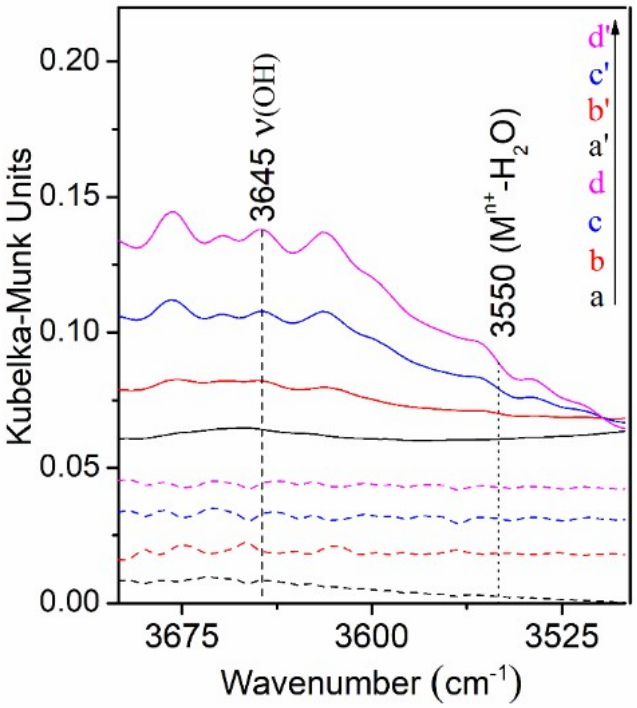


Figure S9: DRIFT spectra of 3wt%Pd supported on (a) H-ZSM-5; alkali metal (b) Na-, (c) K- and (d) Cs- exchanged ZSM-5 samples (background spectra) and their corresponding formic acid adsorbed DRIFT spectra of 3wt%Pd supported on (a') H-ZSM-5, (b') Na-ZSM-5, (c') K-ZSM-5 and (d') Cs-ZSM-5 samples.

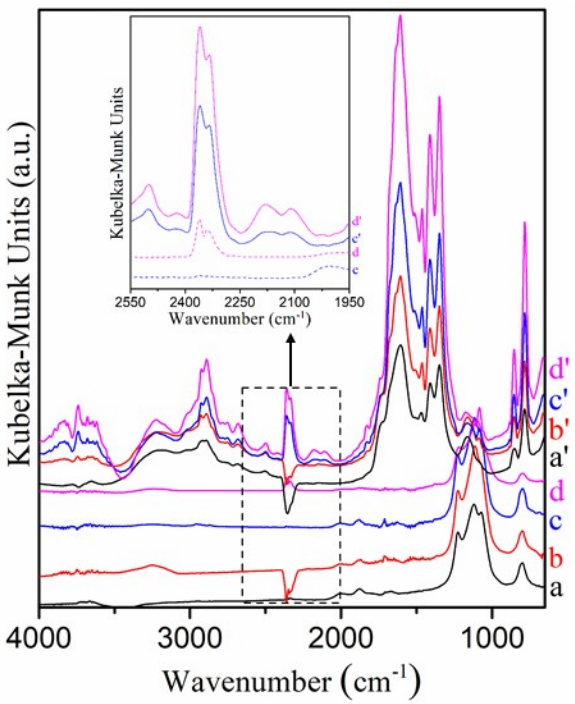


Figure S10: DRIFT spectra of 3wt%Pd supported on (a) H-ZSM-5; alkali metal (b) Na-, (c) K- and (d) Cs- exchanged ZSM-5 samples (background spectra) and their corresponding formic acid adsorbed DRIFT spectra of 3wt%Pd supported on (a') H-ZSM-5, (b') Na-ZSM-5, (c') K-ZSM-5 and (d') Cs-ZSM-5 samples in the CO and CO_2 region

2.9. Recyclable studies

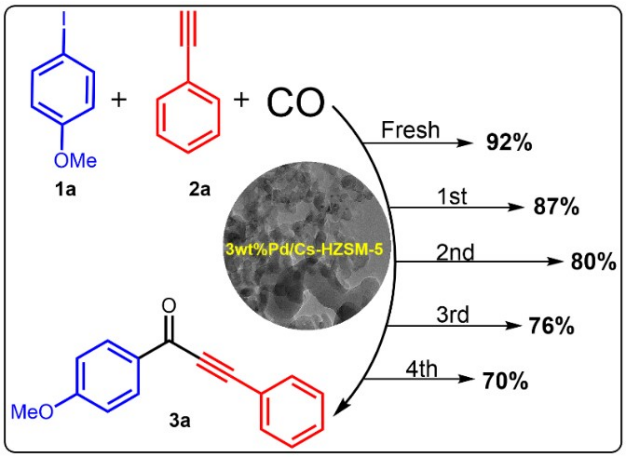


Figure S11: Recyclability of 3wt%Pd^0/Cs-ZSM-5 catalyst

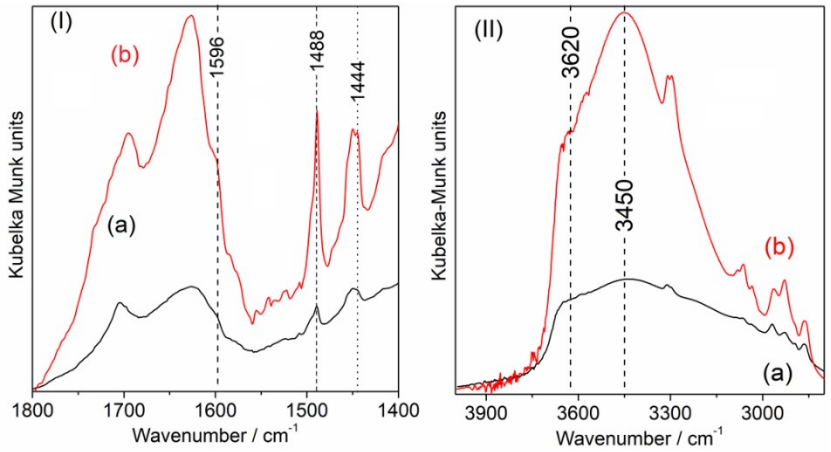


Figure S12: IR spectra of the alkyne adsorbed on (a) 3wt%Pd/H-ZSM-5 and (b) 3wt%Pd/Cs-ZSM-5 catalysts.

3. Experimental section

3.1. Preparation of catalysts

The 3wt%Cu supported on Cs-ZSM-5 catalysts were synthesized by a simple wet impregnation method. The required amount $Cu(NO_3)_2 \cdot 6H_2O$ was added to aqueous solutions of zeolite and then evaporated the water with constant stirring at 100 °C until the samples get dried. The resultant solids were oven dried at 120 °C for 12 h and subsequently calcined in static air at 300 °C for 5 h at a ramping rate of 5 °C/min. Finally, 3wt%Cu/Cs-ZSM-5 catalyst were reduced with H_2 flow (30mL/min) at 280 °C before performing the reaction.

3.2. Preparation of Cs modified H-ZSM-5 support

Prior to the alkali metal exchange, commercial H-ZSM-5 zeolite was calcined in air flow (30mL/min) at 550 °C for 6 h at a ramping rate of 5 °C/min. Alkali metal (Na, K and Cs)-modified zeolite samples were synthesized using the ion-exchange followed by alkaline treatment technique. For the ion-exchange process, a zeolite to liquid ratio of 20 g L^{-1} was used. Typically, 5 g of H-ZSM-5 (30) was mixed with 250 ml of 0.2 M CsCl solution and agitated for 12 h, at ambient temperature, filtered, washed twice with distilled water, and then dried at 65 °C. This procedure was repeated 3 times to achieve the alkali metal modified zeolite. The oven dried samples of (Na, K, Cs)- exchanged zeolites were then treated with 0.2 M NaOH and 0.2 M of tetrapropylammonium bromide at 65 °C for 0.5 h with continuous stirring, maintaining a zeolite to liquid ratio of 33 gL^{-1}. Subsequently, the alkali-exchanged H-ZSM-5 was filter and thoroughly washed with distilled water, after that oven-dried for 12 h followed by calcination of the sample in static air at 550 °C for 6 h at a ramping rate of 5 °C/min to obtain Cs-ZSM-5(30). The same procedure was followed to prepare the Cs-ZSM-5(80, 150), Na-ZSM-5 (30-150) and K-ZSM-5 (30-150) support with varied Si/Al ratios.

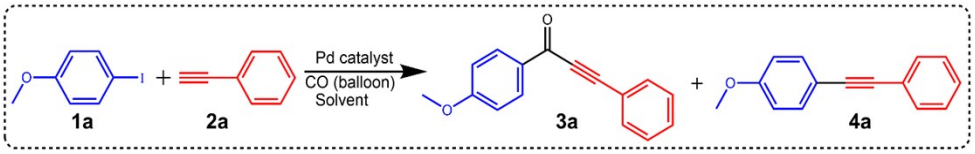
3.3. Preparation of Pd(0)/Cs-ZSM-5 catalyst

The alkali metal ion-exchanged ZSM-5 supported palladium catalyst was prepared by a simple wet impregnation method. In a typical procedure, the required amount of $Pd(NO_3)_2$ xH_2O was used to achieve the desired weight percent of Pd. This compound was dissolved in double-distilled H_2O and mixed with the Cs-ZSM-5(30) support. The excess H_2O was evaporated under stirring at 100 °C, followed by drying in an oven at 100 °C for 12 h. Subsequently, the oven dried sample was calcined in static air at 450 °C for 5 h at a ramping rate of 5 °C/min to get Pd(II)/Cs-ZSM-5(30). The calcined samples were treated with $N_2H_4.xH_2O$ and ethanol at room temperature to obtain the metallic Pd phase. Finally, the reduced solid catalyst was centrifuged, washed with anhydrous diethyl ether (2 x 5 mL), and then dried under vacuum at 45 °C to obtain the final catalyst. The catalyst samples are denoted as xPd(0)/Cs-ZSM-5(30), where 'x' represents the weight percentage of palladium, and (30) indicates the Si/Al ratio mole present in the zeolite. The same

procedure was employed for the preparation of Pd^0/H-ZSM-5, Pd^0/Na-ZSM-5, Pd^0/K-ZSM-5, 3wt%Pd^0/F-SiO_2, and 3wt%Pd^0/γ-Al_2O_3. A schematic representation of the process is provided in Figure S1.

3.2. Screening of reaction conditions

Table S6: Optimization of reaction conditions (conversion and selectivity)



Entry	Catalyst	Base	Solvent	**1a** Conv. (%)[b]	**3a Sel.** (%)[b]	**4a Sel.**(%)[b]
1	1wt%Pd^0/H-ZSM-5	-	DMF	0	0	0
2	1wt%Pd^0/Na-ZSM-5	-	DMF	10	20	80
3	1wt%Pd^0/K-ZSM-5	-	DMF	16	87.5	12.5
4	1wt%Pd^0/Cs-ZSM-5	-	DMF	27	100	0
5	2wt%Pd^0/Cs-ZSM-5	-	DMF	60	100	0
6	3wt%Pd^0/Cs-ZSM-5	-	DMF	92	100	00
7	3wt%Pd^0/Na-ZSM-5	-	DMF	28	57	43
8	3wt%Pd^0/K-ZSM-5		DMF	64	100	
9	Cs-ZSM-5	-	DMF	0	0	0
10	3wt%Pd^0/Cs-ZSM-5	-	DMSO	90	92	8
11	3wt%Pd^0/Cs-ZSM-5	-	DMA	19	100	0
12	3wt%Pd^0/Cs-ZSM-5	-	Toluene	35	28.5	71.5
13	3wt%Pd^0/Cs-ZSM-5	-	Dioxane	13	23	77
14	3wt%Pd^0/Cs-ZSM-5	-	H_2O	23	13	87
[c]15	3wt%Pd^0/Cs-ZSM-5	-	DMF	0	0	0
[d]16	3wt%Pd^0/Cs-ZSM-5	-	DMF	23	100	0
[e]17	3wt%Pd^0/Cs-ZSM-5	-	DMF	93	97	3
[f]18	3wt%Pd^0/Cs-ZSM-5	-	DMF	95	95	5
[g]19	3wt%Pd^0/Cs-ZSM-5	Et_3N	DMF	81	100	0
[g]20	3wt%Pd^0/Cs-ZSM-5	Et_2NH	DMF	79	100	0
[g]21	3wt%Pd^0/Cs-ZSM-5	DBU	DMF	63	86	14
[g]22	3wt%Pd^0/Cs-ZSM-5	DABCO	DMF	56	91	9
[g]23	3wt%Pd^0/Cs-ZSM-5	K_3PO_4	DMF	75	100	0
24	3wt%Pd^0/H-ZSM-5	-	DMF	10	60	40

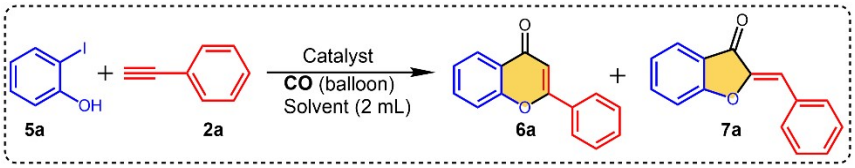
Reaction conditions: Iodobenzene **1a** (0.5 mmol), Phenylacetylene **2a** (0.7 mmol), catalyst weight: (0.050 g), Solvent (2 mL), Temperature: 70 °C, time: 9h. [b]conversion and selectivity (%) after silica gel column chromatography, [c] rt, [d]50 °C, [e]100, [f]120 °C, [g]6 h and Base (0.5 mmol). ZSM-5 with Si/Al ratio = 30.

Table S7: Experiments for optimization of reaction (conversion and selectivity)

Entry	Catalyst	Base	**1a** Conv. (%)[b]	**3a Sel.** (%)[b]	**4a Sel.**(%)[b]
[c]1	3wt%Pd^0/Cs-ZSM-5	-	47	100	0
[d]2	3wt%Pd^0/Cs-ZSM-5	-	32	100	0
[e]3	3wt%Pd^0/Cs-ZSM-5	-	54	100	0
4	3wt%Pd(II)/Cs-ZSM-5	-	0	100	0
[f]5	3wt%Pd^0/F-SiO_2	Et_3N	52	65	35
[f]6	3wt%Pd^0/γ-Al_2O_3	Et_3N	47	79	21
7	3wt%Cu^0/Cs-ZSM-5	-	7	0	100
[g]8	3wt%Pd^0/Cs-ZSM-5	-	92	100	0

[a] **Reaction conditions**: Iodobenzene **1a** (0.5 mmol), Phenylacetylene **2a** (0.7 mmol), catalyst weight: (0.050 g), Solvent: DMF (2 mL), Temperature: 70 °C, time: 9h. [b]conversion and selectivity (%) calculated after silica gel column chromatography, Si/Al ratio [c]80, [d]150, [e] Catalyst weight: 0.030 g, [f] Base (0.5 mmol), Si/Al ratio [g]30.

Table S8: Optimization of reaction conditions [a] (conversion and selectivity)



Entry	**Catalyst**	**Base**	**Solvent**	**5a** Conv. (%)[b]	**6a Selectivity** (%)[b]	**7a Selectivity** (%)[b]
1	3wt%Pd^0/Na-ZSM-5	-	DMF	10	>97	<3
2	3wt%Pd^0/K-ZSM-5	-	DMF	42	100	0
3	3wt%Pd^0/Cs-ZSM-5	-	DMF	81	100	0
4	3wt%Pd^0/Cs-ZSM-5	-	DMSO	69	100	0
5	3wt%Pd^0/Cs-ZSM-5	-	DCE	8	100	0
6	3wt%Pd^0/Cs-ZSM-5	-	Toluene	39	82	18
7	3wt%Pd^0/Cs-ZSM-5	Et_3N	DMF	90	100	0
8	3wt%Pd^0/Cs-ZSM-5	Et_2NH	DMF	95	100	0
9	3wt%Pd^0/Cs-ZSM-5	Piperazine	DMF	75	100	0
10	3wt%Pd^0/Cs-ZSM-5	piperidine	DMF	72	100	0
[d]11	3wt%Pd^0/Cs-ZSM-5	-	DMF	65	100	0
[e]12	3wt%Pd^0/Cs-ZSM-5	-	DMF	84	>96	<4

[a] **Reaction conditions**: Iodobenzene **1a** (0.5 mmol), Phenylacetylene **2a** (0.7 mmol), catalyst weight: (0.050 g), Solvent (2 mL), Base (0.5 mmol) Temperature: 90 °C, time: 24 h. [b]conversion and selectivity (%) calculated after silica gel column chromatography, [d]70 °C, [e]120 °C.

Table S9: Optimization of reaction conditions [a]

Entry	Catalyst	Base	Solvent	6a[b]	7a[b]	6a Rate / 10^{-9} mol s^{-1} m^{-2}
1	3wt%Pd^0/Na-ZSM-5	-	DMF	10	trace	0.04
2	3wt%Pd^0/K-ZSM-5	-	DMF	42	0	0.18
3	3wt%Pd^0/Cs-ZSM-5	-	DMF	81	0	0.39
4	3wt%Pd^0/Cs-ZSM-5	-	DMSO	69	0	0.33
5	3wt%Pd^0/Cs-ZSM-5	-	DCE	8	0	0.04
6	3wt%Pd^0/Cs-ZSM-5	-	Toluene	32	7	0.15
7	3wt%Pd^0/Cs-ZSM-5	Et_3N	DMF	90	0	0.44
8	3wt%Pd^0/Cs-ZSM-5	Et_2NH	DMF	95	0	0.46
9	3wt%Pd^0/Cs-ZSM-5	Piperazine	DMF	75	0	0.36
10	3wt%Pd^0/Cs-ZSM-5	piperidine	DMF	72	0	0.35
[d]11	3wt%Pd^0/Cs-ZSM-5	-	DMF	65	0	0.32
[e]12	3wt%Pd^0/Cs-ZSM-5	-	DMF	84	trace	0.41

[a] **Reaction conditions**: Iodobenzene **1a** (0.5 mmol), Phenylacetylene **2a** (0.7 mmol), catalyst weight: (0.050 g), Solvent (2 mL), Base (0.5 mmol) Temperature: 90 °C, time: 24 h. [b]conversion and selectivity (%) calculated after silica gel column chromatography, [d]70 °C, [e]120 °C.

3.3. Experimental procedures

General procedure (A) for the synthesis of alkynyl ketones

An oven dried 25 mL two necked round bottom flask was charged with aryl iodides **1** (0.5 mmol), aryl alkynes **2** (0.7 mmol), 3wt%Pd^0/Cs-ZSM-5 catalyst (0.050 g) in DMF (2 mL) at room temperature. Degassed and flushed the flask with CO gas at room temperature, followed by stirring the reaction mixture at 70 °C for 9 h under CO at balloon pressure. After the completion of the reaction, the temperature was brought down to room temperature. Then, the catalyst was separated from the reaction mixture by centrifugation, washed with EtOAc and Et_2O, and dried for the next use. The supernatant liquid was collected and added to H_2O, subsequently extracted with ethyl acetate (3x20 mL), dried over Na_2SO_4, and concentrated in a rotary evaporator. Finally, the crude product was purified by column chromatography (silica

gel, 100–200 mesh) using hexane/ethyl acetate as the eluents to afford the desired products and characterized by ^{1}H-NMR and ^{13}C-NMR.

General procedure (B) for the synthesis of flavones

In a typical method the completely dried two necked round bottom flask (25 mL) was charged with 2-iodophenol **5** (0.5 mmol), aryl alkynes **2** (0.7 mmol), 3wt%Pd^{0}/Cs-ZSM-5 catalyst (0.050 g) in DMF (2 mL) at room temperature. Degassed and flushed the flask with CO gas at room temperature, followed by stirring the reaction mixture at 90 °C for 24 h under CO balloon pressure. After the completion of the reaction, cooled the reaction mixture to room temperature. Then, the catalyst was separated from the reaction mixture by filtration/centrifugation, washed with ethyl acetate and ether, and dried for next use. The supernatant was collected and added to H_2O, subsequently extracted with ethyl acetate (3 × 20 mL), dried over Na_2SO_4, and concentrated in a rotary evaporator. Then, the crude product was purified by column chromatography (silica gel, 60–120 mesh) using hexane: ethyl acetate as the eluents to afford the desired products and characterized by ^{1}H-NMR and ^{13}C-NMR.

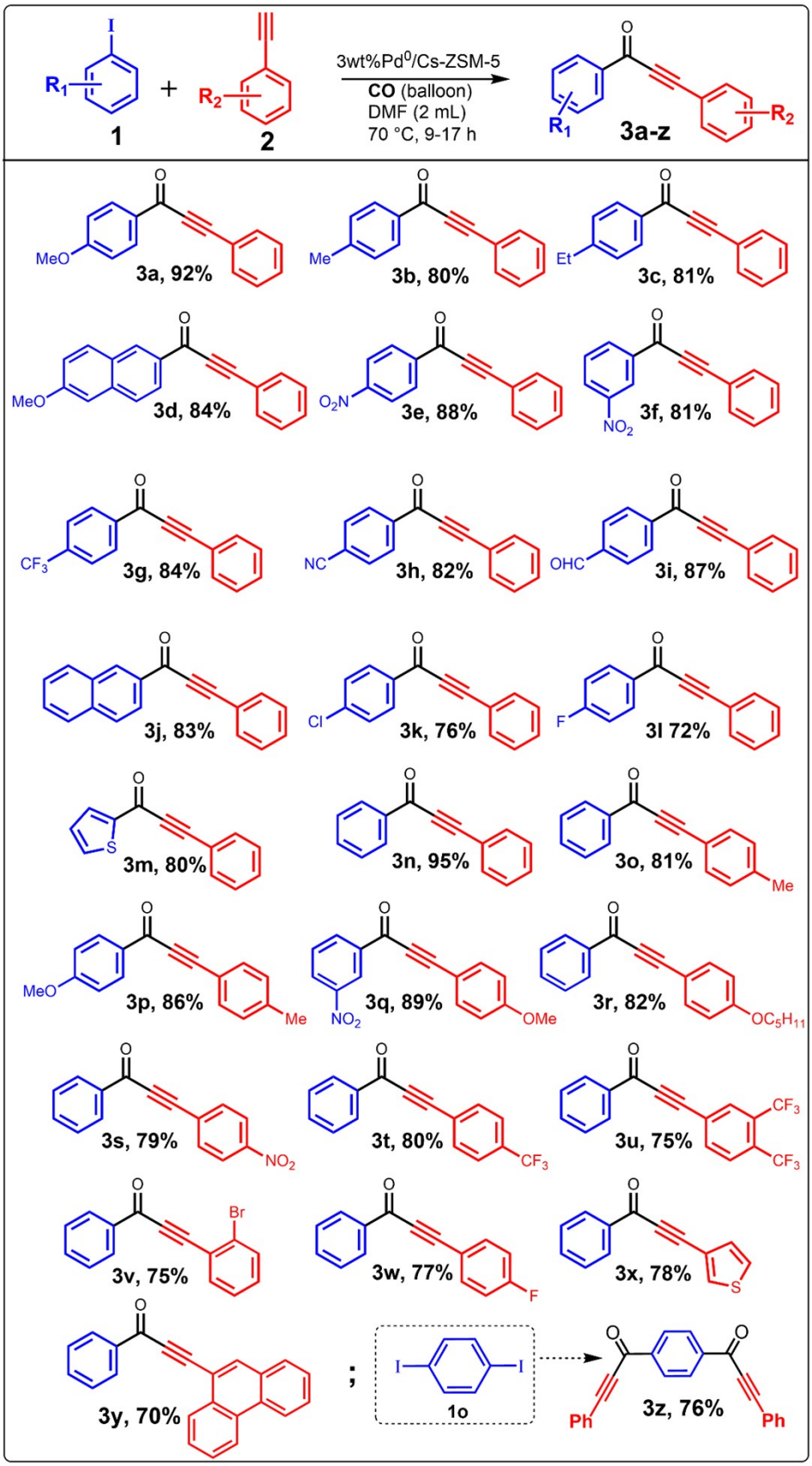


Figure S12: Substrate scope of various aryl iodides and alkynes over 3wt%Pd^0/Cs-ZSM-5

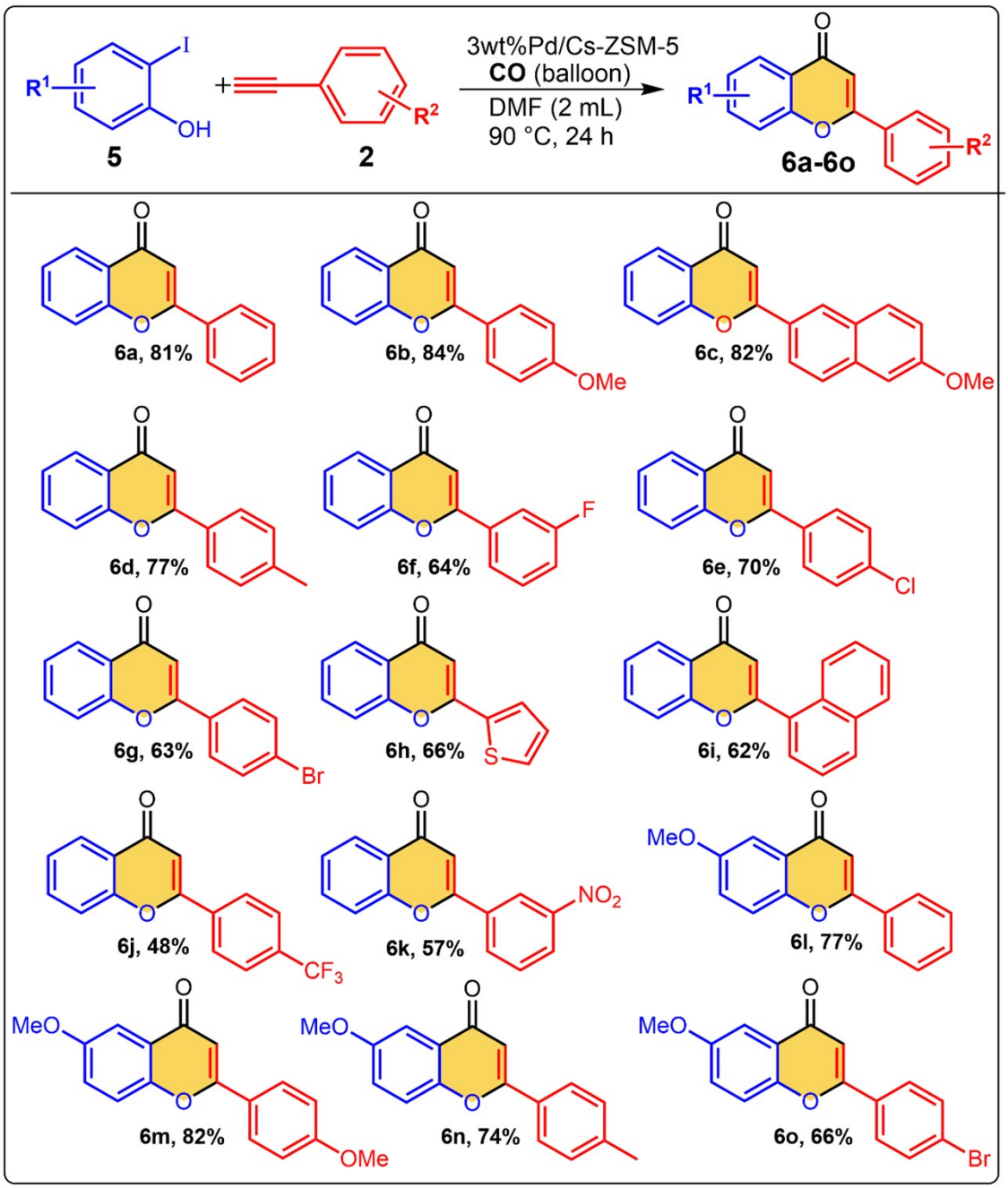
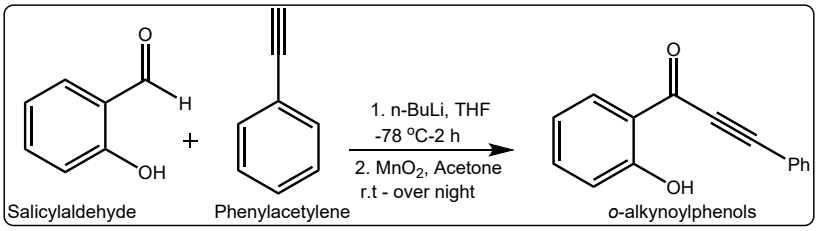


Figure S13: Substrate scope of various 2-iodophenols and alkynes over 3wt%Pd^0/Cs-ZSM-5.

Preparation of *o*-alkynoylphenol (3zb)[S1]



To a solution of aryl acetylene or alkyl acetylene derivative (2.5 mmol, 2.5 eq) in anhydrous THF (2 mL) was dropwise added n-BuLi (2 mmol, 2 eq, 2.5 M in THF) at -78 °C under nitrogen

atmosphere. After 1 h stirring, a solution of corresponding salicylaldehyde (1.5 mmol, 1 eq, in 2 mL anhydrous THF) was dropwise added at -78 °C. The reaction mixture was stirred at -78 °C for 2 h and followed by 30 min at 0 °C then quenched with saturated aqueous NH_4Cl at 0 °C. The THF was removed by rotary evaporator and extracted with EtOAc twice. The collected EtOAc layer was washed with brine, dried over magnesium sulfate, filtered, and concentrated. The afforded crude was further oxidation MnO_2 (699 mg, 8.03 mmol, 5 equiv) was dissolved in acetone (10 mL) at room temperature. The reaction mixture was stirred for 12h at the same temperature. Upon completion of the reactions (TLC showed complete consumption of starting material), the reaction mixture was filtered using Buckner funnel and washed with Dichloromethane. The filtrate was concentrated in vacuo. The crude product was used for the next step without further purification.

Various aryl iodides and alkynes used in the synthesis of ynones and flavones:

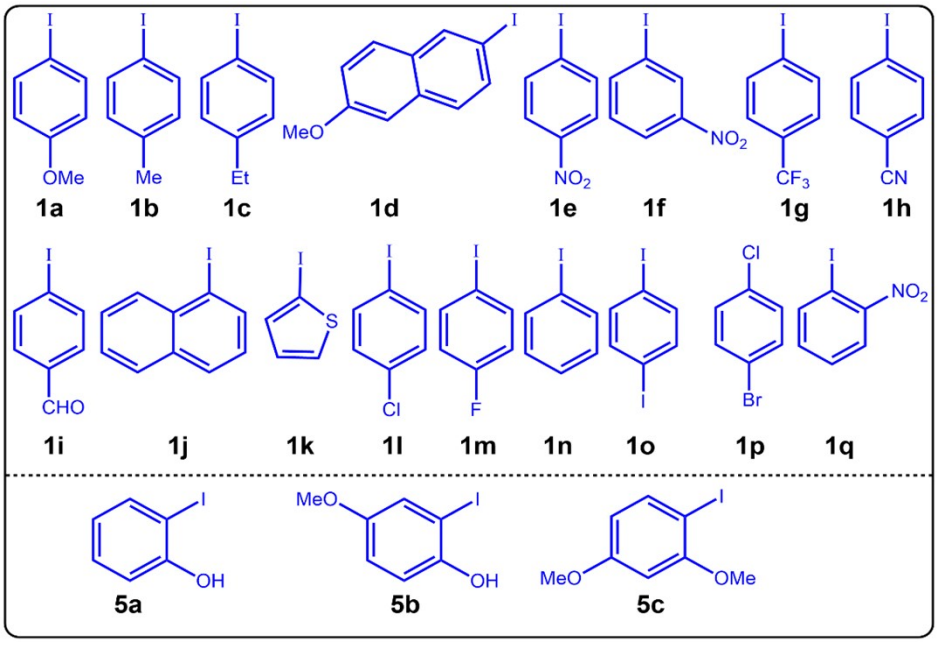


Figure S14: Various aryl iodides used for the synthesis of ynones and flavones

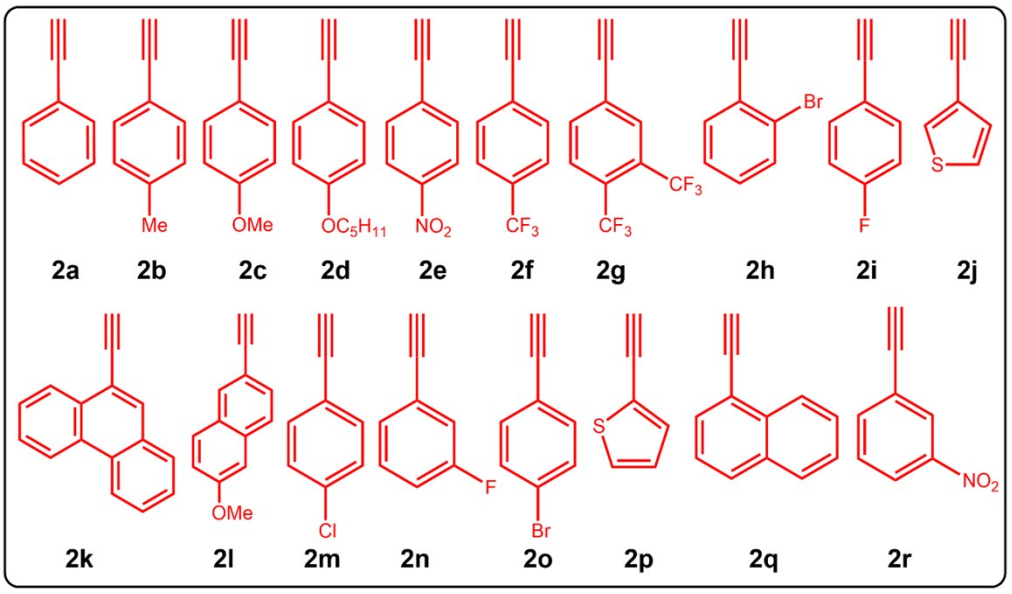


Figure S15: Various aryl alkynes used for the synthesis of ynones and flavones

Comparative analysis of the normalized rates (*ca.* with respect to the applied CO pressure) during the synthesis of Ynones

$$\text{Rate} = \frac{Fractional\ yield\ x\ Substrate\ concentration}{Weight\ of\ catalyst} \times \frac{1}{Reaction\ time} \times \frac{1}{(CO)\ Pressure}$$

Table S10: Comparison the activity of 3wt%Pd^0/Cs-ZSM-5 catalyst with literature data in carbonylation of aryl iodides and aryl alkynes to ynones

Ref.	Catalyst	CO (bar)	Base	Ligands/ additives	Yield (%)	Reaction conditions	r_{3a} /10^{-6} × mol g^{-1} s^{-1}
[1]	IPr-Pd-dmba-Cl	20	Et_3N	-	60	100°C, 18 h	0.071
[2]	Pd–NHC-Py	13.78	Et_3N	-	93	120°C, 6 h	0.558
[3]	Polysalen-Pd	20	Et_3N	-	95	130°C, 6 h	0.073
[4]	Pd-NHC_2@M	13.78	Et_3N	-	98	100°C, 12 h	0.283
[5]	[(cinnamyl)PdCl]$_2$	10	K_2CO_3	$BuPAd_2$	76	100°C, 20 h	0.102
[6]	$Pd(acac)_2$	10	Et_3N	TBAAc	78	90°C, 12 h	0.059
[7]	$PdCl_2(PPh_3)_2$	1	Et_3N	-	93	25°C, 24 h	0.364

[8]	Pd/Fe_3O_4 (BET-SA not reported by authors)	20	Et_3N	-	95	130°C, 4 h	0.165
Present work	**3%Pd/Cs-ZSM-5**	**Balloon**	**-**	**-**	**92**	**70°C, 9 h**	**0.289**

Comparative analysis of the normalized rates (*ca.* with respect to the applied CO pressure and the respective BET-surface areas of the catalysts) during the synthesis of Ynones.

$$\text{Rate} = \frac{Fractional\ yield\ x\ Substrate\ concentration}{Weight\ of\ catalyst} \times \frac{1}{Reaction\ time} \times \frac{1}{(CO)\ Pr} \times \frac{1}{BET - SA}$$

Ref.	Catalyst	CO (bar)	Base	Ligands/ additives	Yield (%)	Reaction conditions	r_{3a} /10^{-9} × mol s^{-1} m^{-2}
[9]	Pd(II)APTES@K10 BET-SA: 134 m^2/g^{-1}	4	Et_3N	-	90	80°C, 7 h	2.22
[10]	5%Pd/C (BET-SA: 983 m^2/g^{-1})	20	Et_3N		97	130°C, 4 h	0.85
Present work	**3wt%Pd/Cs-ZSM-5** (BET-SA: 236 m^2/g^{-1})	**Balloon**	**-**	**-**	**92**	**70°C, 9 h**	**1.23**

Comparative analysis of the normalized rates (*ca.* with respect to the applied CO pressure) during the synthesis of Flavone

Table S11: Comparison the activity of 3wt%Pd^0/Cs-ZSM-5 catalyst with literature data in carbonylation-cyclization of 2-iodophenol and aryl alkynes to flavones.

Ref.	Catalyst	CO (bar)	Base	Ligands/ additives	Yield (%)	Reaction conditions	r_{3a} /10^{-6} × mol g^{-1} s^{-1}
[11]	$PdCl_2(PPh_3)_2$	20	Et_2NH	Benzimidazolium	78	130°C, 24 h	0.012
[12]	Dibromidobis (NHC)Pd(II)	6.89	Et_2NH	-	96	100°C, 16 h	0.806
[13]	trans-($PdBr_2$(iPr_2-bimy)	4	Et_2NH	N-phenyl Imidazole	98	80°C, 24 h	0.945
[14]	10%Pd/C	20	Et_2NH	-	95	110°C, 20 h	0.065
[15]	$Pd(OAc)_2$	3.5	Piperazine	Dppf	83	50°C, 24 h	0.12
[16]	$PdCl_2(PPh_3)_2$	1	Et_2NH/DBU	Thiourea/dppp	79	40°C, 48 h	0.13
[17]	$PdCl_2$	1	Et_3N	PSIL102	95	110°C, 24 h	1.24

Present work	**3wt%Pd/Cs-ZSM-5**	**Balloon**	**-**	**-**	**81**	**90°C, 24 h**	**0.102**

Comparative analysis of the normalized rates (*ca*. with respect to the applied CO pressure and the respective BET-surface areas of the catalysts) during the synthesis of Flavone.

Ref.	Catalyst	CO (bar)	Base	Ligands/additives	Yield (%)	Reaction conditions	r_{3a} /10^{-9} × mol s^{-1} m^{-2}
[18]	Pd^0APTES @K10; 99.92 m^2/g^{-1}	4	Et_2NH	-	68	90°C, 24 h	0.381
Present work	**3wt%Pd/Cs-ZSM-5** (BET-SA: 236 m^2/g^{-1})	**Balloon**	**-**	**-**	**81**	**90°C, 24 h**	**0.432**

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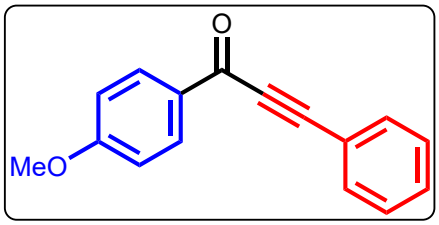
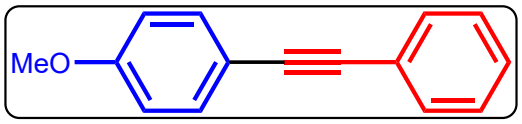
4. NMR spectral data of all synthesized compounds

1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-one (3a)[S2]



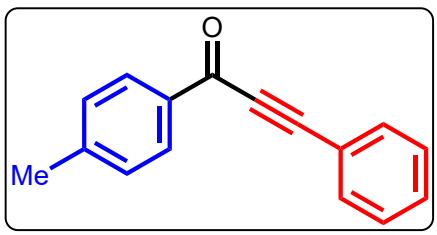
The title compound was prepared by following the general procedure (**A**) from **1a** and **2a**, white solid, 92% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 8.23 – 8.17 (m, 2H), 7.71 – 7.65 (m, 2H), 7.51 – 7.44 (m, 1H), 7.44 – 7.39 (m, 2H), 7.02 – 6.96 (m, 2H), 3.90 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 176.71, 164.52, 132.99, 132.02, 130.61, 130.36, 128.68, 120.41, 113.92, 92.34, 86.96, 55.64.

1-(4-Methoxyphenyl)-3-phenylprop-2-yn (4a)



The title compound was prepared by following the general procedure (**A**) from **1a** and **2a**, white solid. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 7.51 (dd, *J* = 8.0, 1.6 Hz, 2H), 7.48 – 7.45 (m, 2H), 7.35 – 7.29 (m, 1H), 6.91 – 6.84 (m, 2H), 3.81 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 159.66, 133.09, 131.49, 128.35, 127.97, 123.64, 115.42, 114.04, 89.42, 88.12, 55.34.

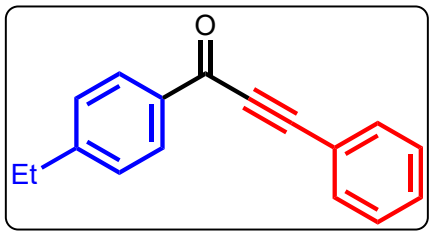
3-Phenyl-1-(*p*-tolyl)prop-2-yn-1-one (3b)[S2]



The title compound was prepared by following the general procedure (**A**) from **1b** and **2a**, yellow solid, 80% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.12 (d, *J* = 8.2 Hz, 2H), 7.74 – 7.61 (m, 2H), 7.47 (dd, *J* = 5.1, 3.7 Hz, 1H), 7.45 –

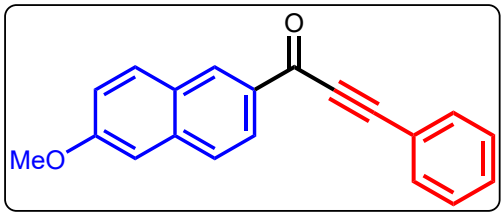
7.40 (m, 2H), 7.31 (d, J = 8.0 Hz, 2H), 2.45 (s, 3H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 177.77, 145.28, 134.66, 133.06, 130.71, 129.76, 129.39, 128.70, 120.31, 92.65, 87.02, 21.89.

1-(4-Ethylphenyl)-3-phenylprop-2-yn-1-one (3c)[S3]



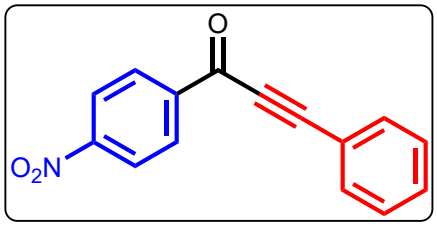
The title compound was prepared by following the general procedure (**A**) from **1c** and **2a**, pale yellow oil, 81% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.18 – 8.12 (m, 2H), 7.72 – 7.64 (m, 2H), 7.51 – 7.45 (m, 1H), 7.45 – 7.39 (m, 2H), 7.37 – 7.32 (m, 2H), 2.74 (q, J = 7.6 Hz, 2H), 1.29 (d, J = 7.6 Hz, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.81, 151.43, 134.85, 133.07, 130.71, 129.88, 128.70, 128.21, 120.31, 92.67, 87.04, 29.74, 15.21.

1-(6-Methoxynaphthalen-2-yl)-3-phenylprop-2-yn-1-one (3d)[S4]



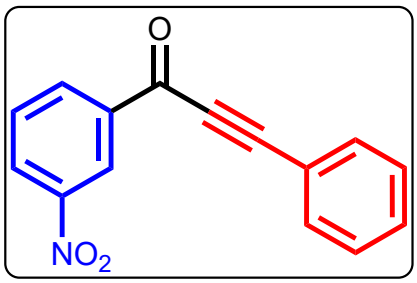
The title compound was prepared by following the general procedure (**A**) from **1d** and **2a**, pale green solid, 84% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.27 (dd, J = 8.3, 1.2 Hz, 2H), 8.17 (s, 1H), 7.76 (dd, J = 8.6, 5.8 Hz, 2H), 7.69 – 7.61 (m, 2H), 7.53 (dd, J = 10.6, 4.7 Hz, 2H), 7.21 (dd, J = 9.0, 2.5 Hz, 2H), 7.14 (d, J = 2.2 Hz, 1H), 3.94 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.06, 159.43, 137.09, 135.63, 134.30, 134.05, 129.86, 129.60, 129.24, 128.65, 128.24, 127.31, 120.04, 114.76, 105.97, 94.48, 87.13, 55.47.

1-(4-Nitrophenyl)-3-phenylprop-2-yn-1-one (3e)[S2]



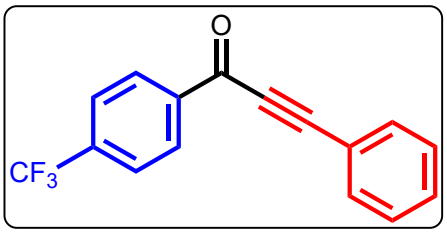
The title compound was prepared by following the general procedure (**A**) from **1e** and **2a**, yellow solid, 88% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.34 – 8.28 (m, 2H), 8.21 (dt, J = 8.5, 1.7 Hz, 2H), 7.88 – 7.82 (m, 2H), 7.71 – 7.65 (m, 1H), 7.59 – 7.51 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 175.92, 150.91, 141.05, 133.32, 131.49, 130.47, 128.90, 123.90, 119.43, 95.46, 86.56.

1-(3-Nitrophenyl)-3-phenylprop-2-yn-1-one (3f)[S3]



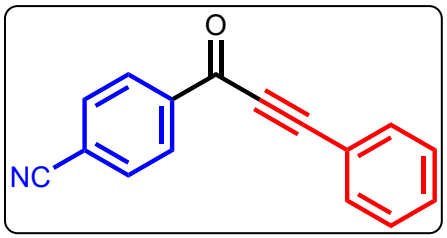
The title compound was prepared by following the general procedure (**A**) from **1f** and **2a**, yellow solid, 81% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 9.06 (t, *J* = 1.9 Hz, 1H), 8.58 – 8.51 (m, 1H), 8.49 (ddd, *J* = 8.2, 2.3, 1.1 Hz, 1H), 7.76 – 7.70 (m, 3H), 7.58 – 7.51 (m, 1H), 7.47 (ddd, *J* = 6.8, 4.5, 1.2 Hz, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 175.47, 148.50, 138.15, 134.61, 133.40, 131.50, 129.97, 128.91, 128.21, 124.59, 119.41, 95.39, 86.26.

3-Phenyl-1-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (3g)[S5]



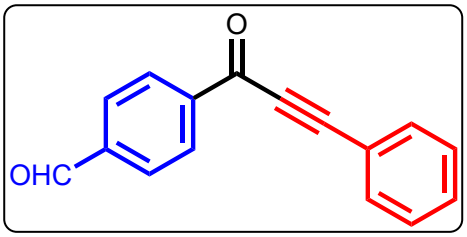
The title compound was prepared by following the general procedure (**A**) from **1g** and **2a**, light yellow solid, 84% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.34 (s, 1H), 8.32 (s, 1H), 7.79 (d, *J* = 8.2 Hz, 2H), 7.73 – 7.68 (m, 2H), 7.52 (ttt, *J* = 6.6, 5.0, 1.4 Hz, 1H), 7.47 – 7.41 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 176.74, 139.41, 133.23, 131.23, 129.83, 128.83, 125.76, 125.72, 123.57 (d, *J* = 272.9 Hz), 119.70, 94.52, 86.61. ^{19}F-NMR (377 MHz, $CDCl_3$) δ = -63.13 (s, 3F).

4-(3-Phenylpropioloyl)benzonitrile (3h)[S5]



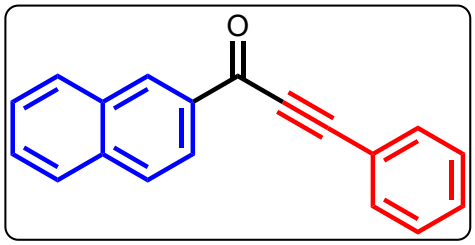
The title compound was prepared by following the general procedure (**A**) from **1h** and **2a**, yellow solid, 82% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.30 (dd, *J* = 7.5, 1.1 Hz, 2H), 7.82 (dd, *J* = 7.4, 1.2 Hz, 2H), 7.69 (dd, *J* = 8.2, 1.1 Hz, 2H), 7.56 – 7.49 (m, 1H), 7.48 – 7.42 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 176.22, 139.67, 133.29, 132.54, 131.41, 129.84, 128.88, 119.49, 117.91, 117.19, 95.17, 86.46.

4-(3-Phenylpropioloyl)benzaldehyde (3i)[S6]



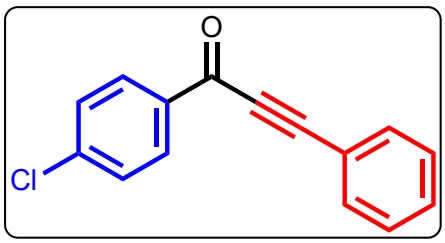
The title compound was prepared by following the general procedure (**A**) from **1i** and **2a**, yellow solid, 87% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 10.13 (s, 1H), 8.42 – 8.24 (m, 2H), 8.06 – 7.92 (m, 2H), 7.82 – 7.60 (m, 2H), 7.59 – 7.47 (m, 1H), 7.48 – 7.38 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 191.58, 177.02, 140.89, 139.66, 133.25, 131.26, 130.04, 129.78, 128.83, 119.69, 94.66, 86.82.

1-(Naphthalen-1-yl)-3-phenylprop-2-yn-1-one (3j)[S2]



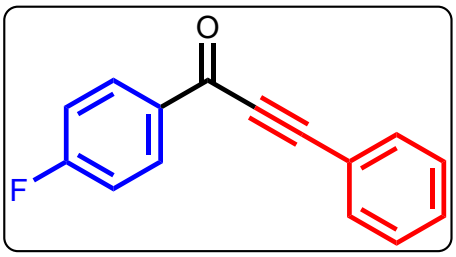
The title compound was prepared by following the general procedure (**A**) from **1j** and **2a**, yellow solid, 83% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 9.24 (d, *J* = 8.7 Hz, 1H), 8.65 (dd, *J* = 7.3, 1.3 Hz, 1H), 8.10 (d, *J* = 8.2 Hz, 1H), 7.95 – 7.87 (m, 1H), 7.69 (m, 3H), 7.62 – 7.56 (m, 2H), 7.48 (m, 1H), 7.43 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 179.78, 135.14, 134.55, 132.99, 130.79, 130.65, 129.78, 129.00, 128.70, 128.61, 126.81, 126.04, 124.52, 120.40, 91.75, 88.53.

1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-one (3k)[S2]



The title compound was prepared by following the general procedure (**A**) from **1k** and **2a**, white solid, 76% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.18-816 (t, *J* = 2.1 Hz, 1H), 8.15-8.14 (t, *J* = 2.1 Hz, 1H), 7.51 (t, *J* = 2.1 Hz, 1H), 7.49 – 7.48 (m, 2H), 7.46 – 7.41 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 176.70, 140.75, 135.34, 133.14, 131.01, 130.90, 129.04, 128.77, 119.93, 93.68, 86.62.

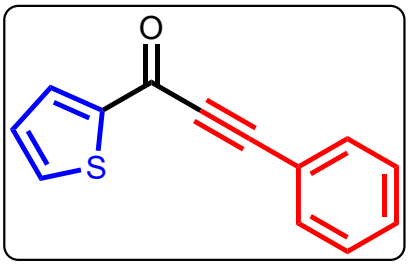
1-(4-Fluorophenyl)-3-phenylprop-2-yn-1-one (3l)[S2]



The title compound was prepared by following the general procedure (**A**) from **1l** and **2a**, yellow solid, 72% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 8.27 – 8.23 (m, 2H), 7.68 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.49 (d, *J* = 7.5 Hz,

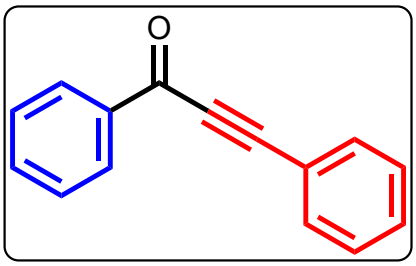
1H), 7.46 – 7.41 (m, 2H), 7.23 – 7.17 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 176.36, 167.72, 165.17, 133.39 (d, *J* = 2.2 Hz), 133.04, 132.22 (d, *J* = 9.6 Hz), 130.88, 128.70, 119.95, 115.85 (d, *J* = 22.2 Hz), 93.34, 86.58. ^{19}F-NMR (377 MHz, $CDCl_3$) δ = -103.18 (s, 1F).

3-Phenyl-1-(thiophen-2-yl)prop-2-yn-1-one (3m)[S5]



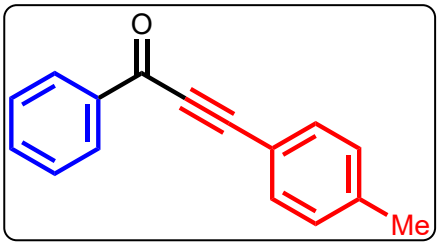
The title compound was prepared by following the general procedure (**A**) from **1m** and **2a**, brown solid, 80% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.04 – 7.98 (m, 1H), 7.74 – 7.72 (m, 1H), 7.70 – 7.64 (m, 2H), 7.52 – 7.46 (m, 1H), 7.45 – 7.39 (m, 2H), 7.19 (dd, *J* = 4.9, 3.8 Hz, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 169.83, 144.98, 135.28, 135.12, 133.08, 130.89, 128.73, 128.38, 119.98, 91.78, 86.52.

1,3-diphenylprop-2-yn-1-one (3n)[S2]



The title compound was prepared by following the general procedure (**A**) from **1n** and **2a**, pale yellow solid, 95% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 8.24 – 8.21 (m, *J* = 8.4 2H), 7.70 – 7.67 (m, 1H), 7.65 – 7.60 (m, 1H), 7.54 – 7.46 (m, 2H), 7.41 (3, 1H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 178.05, 136.92, 134.18, 133.11, 130.87, 129.61, 128.75, 128.69, 120.15, 93.18, 86.96.

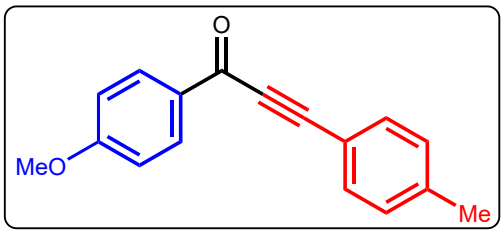
1-phenyl-3-(*p*-tolyl)prop-2-yn-1-one (3o)[S2]



The title compound was prepared by following the general procedure (**A**) from **1n** and **2b**, yellow solid, 81% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.28 – 8.19 (m, 2H), 7.68 – 7.56 (m, 3H), 7.55 – 7.48 (m, 2H), 7.23 (d, *J* = 7.9 Hz,

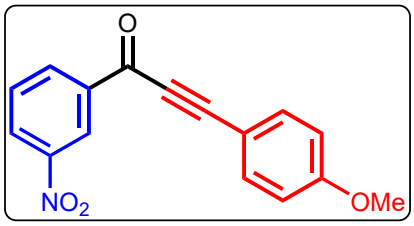
2H), 2.41 (s, 3H). **^{13}C-NMR** (100 MHz, $CDCl_3$) 178.16, 141.62, 137.12, 134.02, 133.20, 129.66, 129.54, 128.69, 117.12, 93.94, 86.86, 20.85.

1-(4-methoxyphenyl)-3-(*p*-tolyl)prop-2-yn-1-one (3p)[S7]



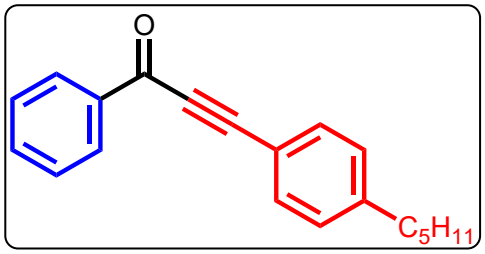
The title compound was prepared by following the general procedure (**A**) from **1a** and **2b**, white solid, 86% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.22 – 8.15 (m, 2H), 7.60 – 7.53 (m, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.03 – 6.94 (m, 2H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 176.79, 164.43, 141.33, 133.02, 131.97, 130.43, 129.48, 117.26, 113.88, 93.03, 86.80, 55.62, 21.78.

3-(4-methoxyphenyl)-1-(3-nitrophenyl)prop-2-yn-1-one (3q)



The title compound was prepared by following the general procedure (**A**) from **1f** and **2c**, yellow solid, 89% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 9.04 (s, 1H), 8.47 (ddd, *J* = 10.9, 8.1, 4.5 Hz, 2H), 7.84 – 7.62 (m, 3H), 7.06 – 6.90 (m, 2H), 3.88 (s, 3H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 175.35, 162.32, 148.46, 138.35, 135.57, 134.48, 129.87, 127.96, 124.52, 114.68, 111.11, 96.84, 86.52, 55.55. HRMS (ESI-TOF): *m/z* calcd. for $C_{16}H_{12}NO_4$ $[M + H]^+$ = 282.0766; Found: 282.0775.

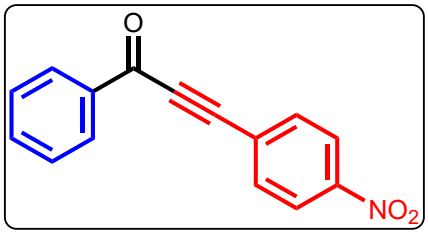
3-(4-(Pentyl)phenyl)-1-phenylprop-2-yn-1-one (3r)[S8]



The title compound was prepared by following the general procedure (**A**) from **1n** and **2d**, light yellow oil, 82% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 8.23 (dd, *J* = 8.2, 1.2 Hz, 2H), 7.64 – 7.57 (m, 3H), 7.51 (dd, *J* = 10.7, 4.8 Hz, 2H), 7.23 (d, *J* = 8.1 Hz, 2H), 2.64 (t, *J* = 7.7 Hz,2H), 1.63 (dt, *J* = 15.0, 7.6 Hz, 2H), 1.39 – 1.26 (m, 4H), 0.90 (t, *J* = 7.0 Hz, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ =

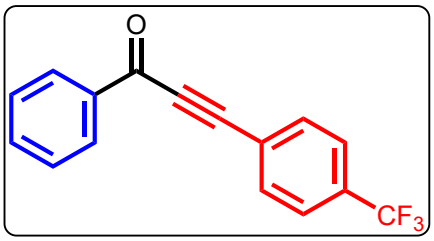
178.08, 146.59, 137.04, 134.04, 133.20, 129.58, 128.88, 128.63, 117.22, 93.94, 86.84, 36.11, 31.45, 30.82, 22.54, 14.05.

3-(4-Nitrophenyl)-1-phenylprop-2-yn-1-one (3s)[S3]



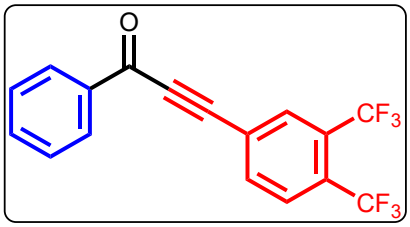
The title compound was prepared by following the general procedure (**A**) from **1n** and **2e**, yellow solid, 79% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.33 – 8.27 (m, 2H), 8.23 – 8.19 (m, 2H), 7.87 – 7.82 (m, 2H), 7.71 – 7.64 (m, 1H), 7.59 – 7.52 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.42, 148.56, 136.42, 134.71, 133.70, 129.69, 128.86, 126.83, 123.88, 89.89, 89.21.

1-Phenyl-3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (3t)[S5]



The title compound was prepared by following the general procedure (**A**) from **1n** and **2f**, pale yellow oil, 80% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.24 – 8.19 (m, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.72 – 7.63 (m, 3H), 7.59 – 7.50 (m, 2H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 177.71, 136.59, 134.51, 133.20, 129.67, 128.79, 125.68, 125.66, 124.67, 123.98, 123.59 (q, *J* = 273.1 Hz), 122.50, 90.51, 88.11. ^{19}F-NMR (377 MHz, $CDCl_3$) δ = -63.13 (s, 3F).

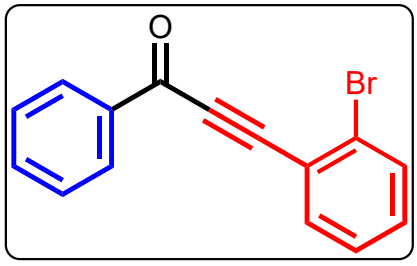
3-(3,4-Bis(trifluoromethyl)phenyl)-1-phenylprop-2-yn-1-one (3u)



The title compound was prepared by following the general procedure (**A**) from **1n** and **2g**, yellow solid, 75% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.23 – 8.18 (m, 1H), 8.10 (s, 2H), 7.97 (s, 1H), 7.73 – 7.62 (m, 1H), 7.55 (t, *J* = 7.7 Hz, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.14, 136.26, 134.71, 132.65, 132.61, 132.32, 129.63, 128.83, 125.27 (q, *J* = 284.0 Hz), 123.97, 122.65, 122.56 (q, *J* = 262.2 Hz), 121.26, 88.52,

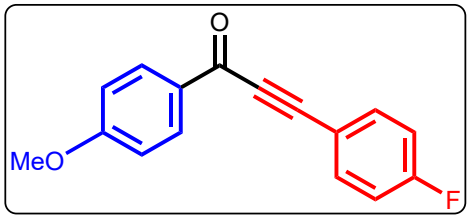
87.90. ^{19}F-NMR (377 MHz, $CDCl_3$) δ = -63.22 (s, 6F). HRMS (ESI-TOF): *m/z* calcd. for $C_{17}H_9OF_6$ $[M + H]^+$ = 343.0558; Found: 343.0554.

3-(2-Bromophenyl)-1-phenylprop-2-yn-1-one (3v)[S9]



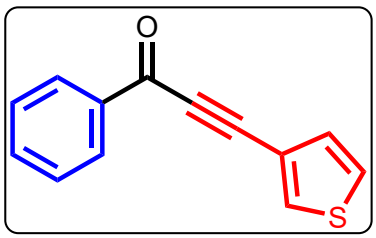
The title compound was prepared by following the general procedure (**A**) from **1n** and **2h**, light yellow solid, 75% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 8.35 – 8.31 (m, 2H), 7.72 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.68 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.67 – 7.62 (m, 1H), 7.56 – 7.51 (m, 2H), 7.36 – 730 (m, 2H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.87, 136.86, 135.35, 134.28, 132.86, 131.87, 129.90, 128.69, 127.42, 126.80, 122.78, 90.58, 90.40.

3-(4-fluorophenyl)-1-(4-methoxyphenyl)prop-2-yn-1-one (3w)[S5]



The title compound was prepared by following the general procedure (**A**) from **1a** and **2i**, pale yellow solid, 77% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.22 – 8.13 (m, 2H), 7.71 – 7.63 (m, 2H), 7.18 – 7.08 (m, 2H), 7.04 – 6.95 (m, 2H), 3.90 (s, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 176.56, 164.88 (d, *J* = 62.1 Hz), 162.67, 135.28 (d, *J* = 8.9 Hz), 131.99, 130.26, 116.53 (d, *J* = 3.5 Hz), 116.11, 116.09, 113.94, 91.22, 86.86, 55.64. ^{19}F-NMR (377 MHz, $CDCl_3$) δ = -106.55 (s, 1F).

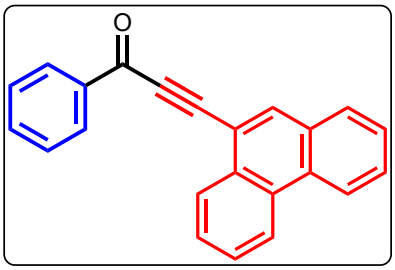
1-Phenyl-3-(thiophen-3-yl)prop-2-yn-1-one (3x)[S8]



The title compound was prepared by following the general procedure (**A**) from **1n** and **2j**, brown oil, 78% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.23 – 8.18 (m, 2H), 7.85 (dd, *J* = 2.9, 1.1 Hz, 1H), 7.66 – 7.60 (m, 1H), 7.51 (dd, *J* = 10.5, 4.7 Hz, 2H), 7.38 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.33 (dd, *J* = 5.0, 1.1 Hz, 1H). **^{13}C-NMR** (101 MHz,

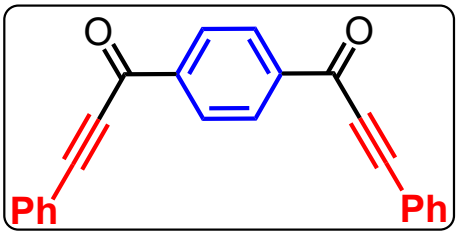
$CDCl_3$) δ = 178.04, 136.88, 134.13, 133.95, 130.32, 129.57, 128.65, 126.31, 119.43, 88.55, 87.21.

3-(Phenanthren-9-yl)-1-phenylprop-2-yn-1-one (3y)[S4]



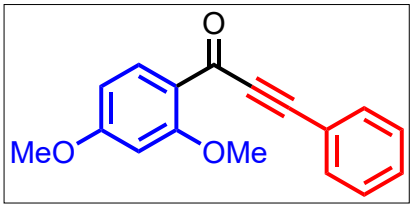
The title compound was prepared by following the general procedure (**A**) from **1n** and **2k**, yellow solid, 70% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.73 – 8.64 (m, 1H), 8.50 (dd, *J* = 5.9, 3.5 Hz, 1H), 8.38 – 8.33 (m, 1H), 8.27 (s, 1H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.77 – 7.70 (m, 1H), 7.70 – 7.55 (m, 2H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 178.02, 137.12, 135.69, 134.23, 133.79, 131.33, 130.73, 130.67, 130.24, 130.10, 129.70, 129.18, 128.89, 128.79, 128.52, 127.64, 127.32, 126.66, 123.02, 122.81, 116.68, 91.75, 91.24.

1,1'-(1,4-Phenylene)bis(3-phenylprop-2-yn-1-one) (3z)[S5]



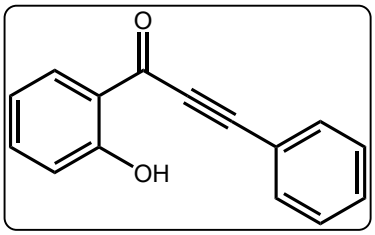
The title compound was prepared by following the general procedure (**A**) from **1o** and **2a** for 17 hours, pale yellow solid, 76% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.36 (s, 1H), 7.76 – 7.64 (m, 4H), 7.58 – 7.49 (m, 2H), 7.48 – 7.41 (m, 4H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.11, 140.55, 133.25, 131.20, 129.69, 128.82, 119.78, 94.56, 86.89.

1-(2,4-Dimethoxyphenyl)-3-phenylprop-2-yn-1-one (3za)



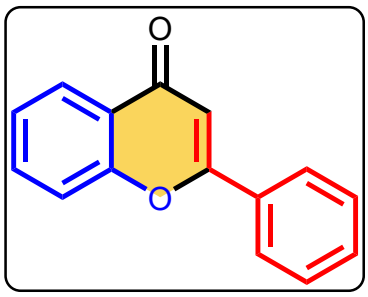
The title compound was prepared by following the general procedure (**B**) from **5c** and **2a**, light yellow solid, 67% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.14 (d, *J* = 8.8 Hz, 1H), 7.66 – 7.56 (m, 2H), 7.46 – 7.35 (m, 3H), 6.57 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.49 (d, *J* = 2.3 Hz, 1H), 3.94 (s, 3H), 3.89 (s, 3H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 175.17, 165.57, 162.10, 135.48, 132.87, 130.24, 128.58, 120.98, 120.25, 105.13, 98.71, 90.84, 89.13, 55.94, 55.68. HRMS (ESI-TOF): *m/z* calcd. for $C_{17}H_{15}O_3$ $[M + H]^+$ = 267.1021; Found: 267.1009.

1-(2-Hydroxyphenyl)-3-phenylprop-2-yn-1-one (3zb)[S11]



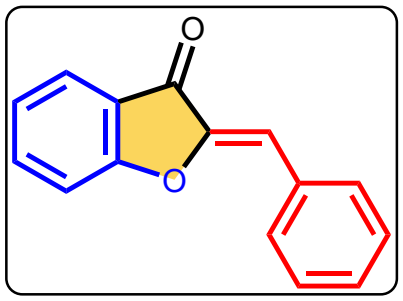
^{1}H-NMR (400 MHz, $CDCl_3$) δ = 11.74 (s, 1H), 8.12 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.72 – 7.66 (m, 2H), 7.55 – 7.49 (m, 2H), 7.45 – 7.40 (m, 2H), 7.00 (d, *J* = 7.8 Hz, 2H). NMR data matched with previous report.

2-Phenyl-4*H*-chromen-4-one (6a)[S10]



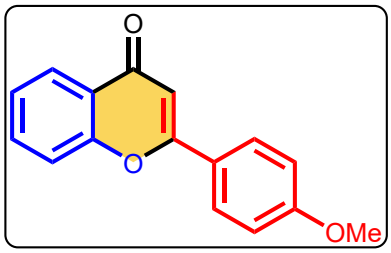
The title compound was prepared by following the general procedure (**B**) from **5a** and **2a**, white solid, 81% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 8.07 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.74 (dd, *J* = 7.7, 1.7 Hz, 2H), 7.56 – 7.50 (m, 1H), 7.41 – 7.34 (m, 4H), 7.28 – 7.23 (m, 1H), 6.65 (s, 1H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 177.27, 162.22, 155.11, 132.69, 130.59, 130.53, 127.95, 125.16, 124.55, 124.13, 122.84, 117.02, 106.42.

(*Z*)-2-Benzylidenebenzofuran-3(2*H*)-one (7a)[S10]



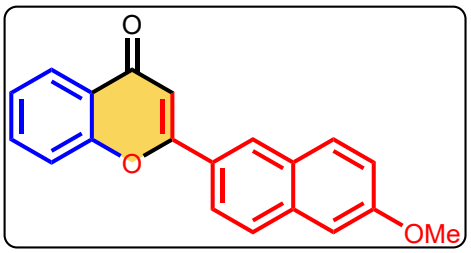
The title compound was prepared by following the general procedure (**B**) from **5a** and **2a**, pale yellow solid, **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.94 – 7.88 (m, 2H), 7.83 – 7.77 (m, 1H), 7.64 (ddd, *J* = 8.5, 7.4, 1.4 Hz, 1H), 7.49 – 7.42 (m, 2H), 7.42 – 7.36 (m, 1H), 7.32 (d, *J* = 8.3 Hz, 1H), 7.24 – 7.18 (m, 1H), 6.89 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 184.68, 166.05, 146.79, 136.81, 132.21, 131.46, 129.82, 128.81, 124.57, 123.39, 121.54, 112.96, 112.86.

2-(4-Methoxyphenyl)-4*H*-chromen-4-one (6b)[S11]



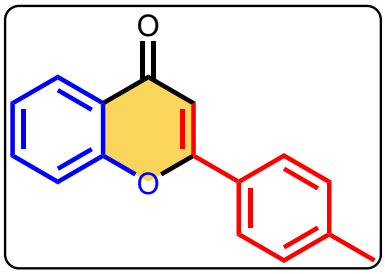
The title compound was prepared by following the general procedure (**B**) from **5a** and **2c**, white solid, 84% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.22 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.94 – 7.85 (m, 1H), 7.68 (ddd, *J* = 8.6, 7.1, 1.7 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.44 – 7.37 (m, 1H), 7.07 – 6.99 (m, 1H), 6.74 (s, 1H), 3.89 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.38, 163.41, 162.42, 156.19, 133.57, 128.01, 125.67, 125.08, 124.03, 123.95, 117.97, 114.48, 106.19, 55.52.

2-(6-Methoxynaphthalen-2-yl)-4*H*-chromen-4-one (6c)[S12]

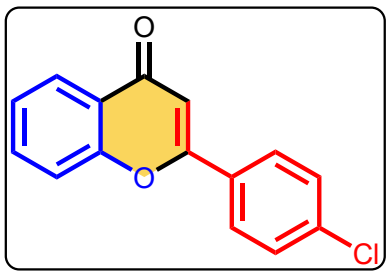


The title compound was prepared by following the general procedure (**B**) from **5a** and **2l**, pale yellow solid, 82% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.29 (s, 1H), 8.21 – 8.09 (m, 1H), 7.82 – 7.70 (m, 3H), 7.68 – 7.60 (m, 1H), 7.53 (d, *J* = 8.3 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.13 (dd, *J* = 8.9, 2.4 Hz, 1H), 7.07 (d, *J* = 2.2 Hz, 1H), 6.82 (s, 1H), 3.87 (s, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.44, 162.57, 158.38, 155.29, 135.25, 132.68, 129.60, 127.32, 126.62, 125.69, 125.58, 124.69, 124.14, 123.01, 122.12, 119.00, 117.04, 106.17, 104.77, 54.43.

2-(*p*-Tolyl)-4*H*-chromen-4-one (6d)[S10]



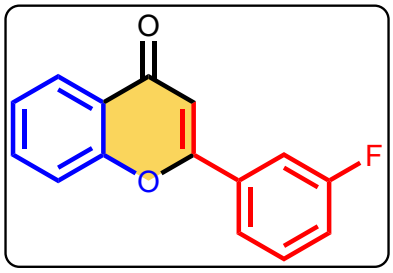
The title compound was prepared by following the general procedure (**B**) from **5a** and **2b**, pale yellow solid, 77% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.23 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.83 (d, *J* = 8.3 Hz, 2H), 7.69 (ddd, *J* = 8.6, 7.2, 1.7 Hz, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.47 – 7.37 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 6.80 (s, 1H), 2.44 (s, 3H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 178.54, 163.66, 156.28, 142.29, 133.69, 129.80, 128.99, 126.27, 125.71, 125.17, 124.01, 118.08, 107.01, 21.58.



2-(4-Chlorophenyl)-4*H*-chromen-4-one (6e)[S12]

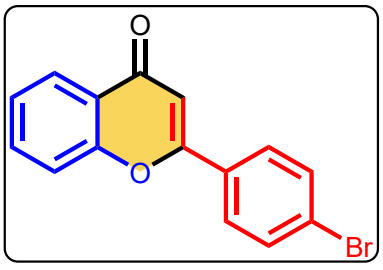
The title compound was prepared by following the general procedure (**B**) from **5a** and **2m**, white solid, 70% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.24 (dd, *J* = 7.9, 1.6 Hz, 1H), 8.00 – 7.89 (m, 2H), 7.71 (ddd, *J* = 8.7, 7.2, 1.7 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.49 – 7.39 (m, 1H), 7.24 (dd, *J* = 15.8, 7.3 Hz, 3H), 6.78 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.82, 158.98, 155.84, 135.05, 133.74, 130.31, 128.51, 128.48, 125.60, 125.24, 123.92, 117.92, 106.09.

2-(3-Fluorophenyl)-4*H*-chromen-4-one (6f)[S11]



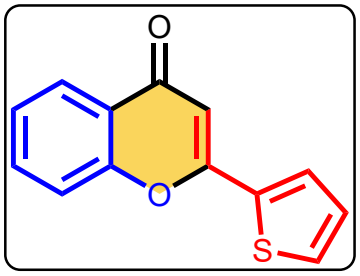
The title compound was prepared by following the general procedure (**B**) from **5a** and **2n**, pale yellow solid, 64% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.22 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.65 – 7.59 (m, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.49 (td, *J* = 8.1, 5.7 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.23 (tdd, *J* = 8.3, 2.6, 0.8 Hz, 1H), 6.80 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.15, 164.13, 161.74, 156.02, 133.90, 133.79, 130.76 (d, *J* = 8.1 Hz), 125.58 (d, *J* = 29.3 Hz), 123.79, 121.87, 121.85, 118.52 (d, *J* = 21.2 Hz), 113.33 (d, *J* = 23.9 Hz), 117.98, 107.98. ^{19}F-NMR (376 MHz, $CDCl_3$) δ = -111.26 (s, 1F).

2-(4-Bromophenyl)-4*H*-chromen-4-one (6g)[S10]



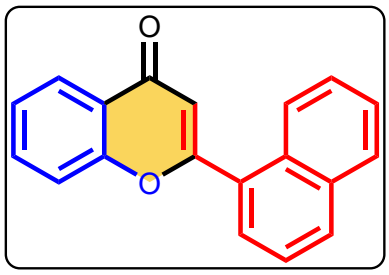
The title compound was prepared by following the general procedure (**B**) from **5a** and **2o**, yellow solid, 63% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.21 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.80 – 7.75 (m, 2H), 7.73 – 7.63 (m, 3H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.46 – 7.39 (m, 1H), 6.79 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.26, 162.29, 156.17, 133.96, 132.37, 130.71, 127.72, 126.34, 125.77, 125.42, 123.93, 118.07, 107.72.

2-(Thiophen-2-yl)-4*H*-chromen-4-one (6h)[S13]



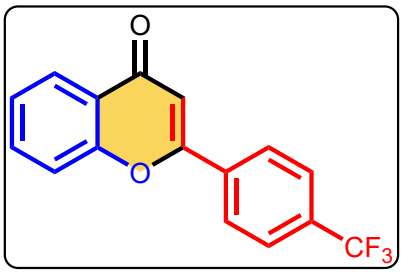
The title compound was prepared by following the general procedure (**B**) from **5a** and **2p**, white solid, 66% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 8.15 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.69 – 7.61 (m, 2H), 7.52 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.46 (d, *J* = 8.1 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.13 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.64 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 177.82, 158.98, 155.84, 135.05, 133.74, 130.31, 128.51, 128.48, 125.60, 125.24, 123.92, 117.92, 106.09.

2-(Naphthalen-1-yl)-4*H*-chromen-4-one (6i)[S13]



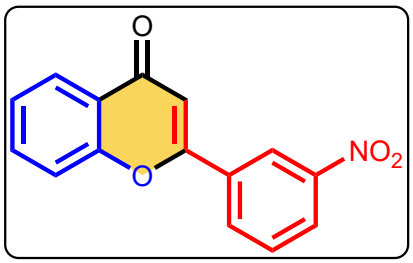
The title compound was prepared by following the general procedure (**B**) from **5a** and **2q**, pale yellow solid, 62% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.32 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.17 – 8.11 (m, 1H), 8.03 (d, *J* = 8.3 Hz, 1H), 7.97 – 7.93 (m, 1H), 7.77 (dd, *J* = 7.1, 1.2 Hz, 1H), 7.72 (ddd, *J* = 8.6, 7.2, 1.7 Hz, 1H), 7.59 – 7.51 (m, 4H), 7.50 – 7.45 (m, 1H), 6.70 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.32, 165.48, 156.76, 143.74, 133.92, 133.78, 131.56, 130.67, 130.42, 128.78, 127.99, 127.48, 126.62, 125.90, 125.42, 125.10, 124.91, 124.06, 118.28, 113.11.

2-(4-(Trifluoromethyl)phenyl)-4*H*-chromen-4-one (6j)[S12]



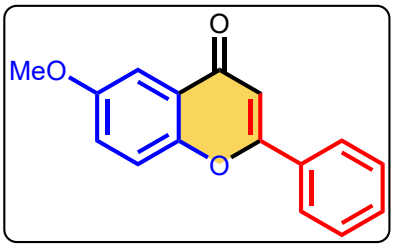
The title compound was prepared by following the general procedure (**B**) from **5a** and **2f**, pale yellow solid, 48% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 8.25 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.06 (d, *J* = 8.2 Hz, 2H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.78 – 7.71 (m, 1H), 7.60 (d, *J* = 7.7 Hz, 1H), 7.49 – 7.43 (m, 1H), 6.88 (s, 1H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.21, 161.65, 156.22, 135.22, 134.12, 126.66, 126.08, 126.04, 125.83, 125.57, 123.95, 123.60 (q, *J* = 272.8 Hz), 118.12, 108.77. ^{19}F-NMR (376 MHz, $CDCl_3$) δ = -63.03 (s, 3F).

4-Nitrophenyl)-4*H*-chromen-4-one (6k)[S13]



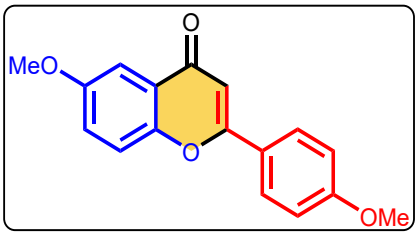
The title compound was prepared by following the general procedure (**B**) from **5a** and **2s**, pale yellow solid, 57% yield. **^{1}H-NMR** (400 MHz, DMSO-d_6) δ = 9.91 (s, 1H), 8.05 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.84 (ddd, *J* = 8.6, 7.0, 1.7 Hz, 1H), 7.80 – 7.74 (m, 1H), 7.56 – 7.47 (m, 2H), 7.46 – 7.43 (m, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.01 (ddd, *J* = 8.1, 2.4, 0.7 Hz, 1H), 6.92 (s, 1H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 182.33, 167.96, 163.13, 160.89, 139.58, 137.66, 135.51, 130.77, 130.03, 128.57, 124.10, 123.73, 122.44, 118.07, 112.14.

6-Methoxy-2-phenyl-4*H*-chromen-4-one (6l)[S11]



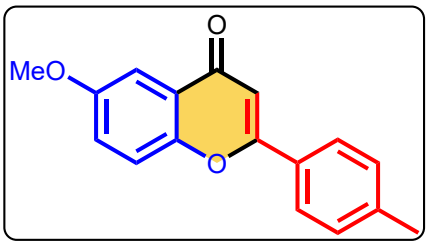
The title compound was prepared by following the general procedure (**B**) from **5b** and **2a**, pale yellow solid, 77% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.94 – 7.87 (m, 2H), 7.58 (d, *J* = 3.1 Hz, 1H), 7.51 (ddd, *J* = 15.7, 7.4, 5.1 Hz, 4H), 7.27 (dd, *J* = 9.1, 3.1 Hz, 1H), 6.80 (s, 1H), 3.89 (s, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.28, 163.13, 157.00, 151.06, 131.85, 131.50, 129.02, 126.23, 124.55, 123.79, 119.52, 106.80, 104.84, 55.93.

6-Methoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one (6m)[S14]



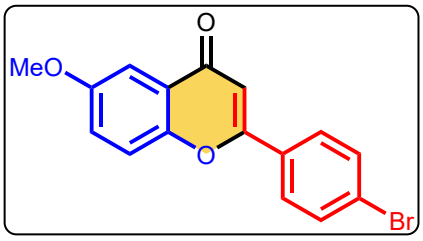
The title compound was prepared by following the general procedure (**B**) from **5b** and **2c**, white solid, 82% yield. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ = 7.87 (d, *J* = 8.9 Hz, 2H), 7.59 (d, *J* = 3.1 Hz, 1H), 7.48 (d, *J* = 9.1 Hz, 1H), 7.27 (dd, *J* = 9.6, 2.6 Hz, 2H), 7.02 (d, *J* = 8.9 Hz, 1H), 6.74 (s, 3H), 3.91 (s, 1H), 3.89 (s, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.29, 163.25, 162.35, 156.94, 151.03, 127.97, 124.54, 124.17, 123.58, 119.41, 114.47, 105.53, 104.91, 55.97, 55.53.

6-**Methoxy-2-(p-tolyl)-4*H*-chromen-4-one (6n)**[S14]



The title compound was prepared by following the general procedure (**B**) from **5b** and **2b**, yellow solid, 74% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 8.3 Hz, 2H), 7.57 (d, *J* = 3.1 Hz, 1H), 7.46 (d, *J* = 9.1 Hz, 1H), 7.34 – 7.23 (m, 3H), 6.76 (s, 1H), 3.89 (s, 3H), 2.41 (s, 3H). **^{13}C-NMR** (101 MHz, $CDCl_3$) δ = 178.30, 163.33, 156.92, 151.02, 142.10, 129.73, 128.98, 126.14, 124.53, 123.64, 119.46, 106.17, 104.82, 55.91, 21.53.

6-**Bromo-2-(*p*-tolyl)-4*H*-chromen-4-one (6o)**[S14]



The title compound was prepared by following the general procedure (**B**) from **5b** and **2o**, yellow solid, 66% yield. **^{1}H-NMR** (500 MHz, $CDCl_3$) δ = 7.79 – 7.74 (m, 2H), 7.68 – 7.61 (m, 2H), 7.57 (d, *J* = 3.1 Hz, 1H), 7.48 (d, *J* = 9.1 Hz, 1H), 7.28 (dd, *J* = 9.1, 3.1 Hz, 1H), 6.77 (s, 1H), 3.90 (s, 3H). **^{13}C-NMR** (126 MHz, $CDCl_3$) δ = 178.13, 162.05, 157.14, 150.99, 132.35, 130.81, 127.66, 126.20, 124.55, 123.98, 119.50, 106.95, 104.88, 55.98.

5. References

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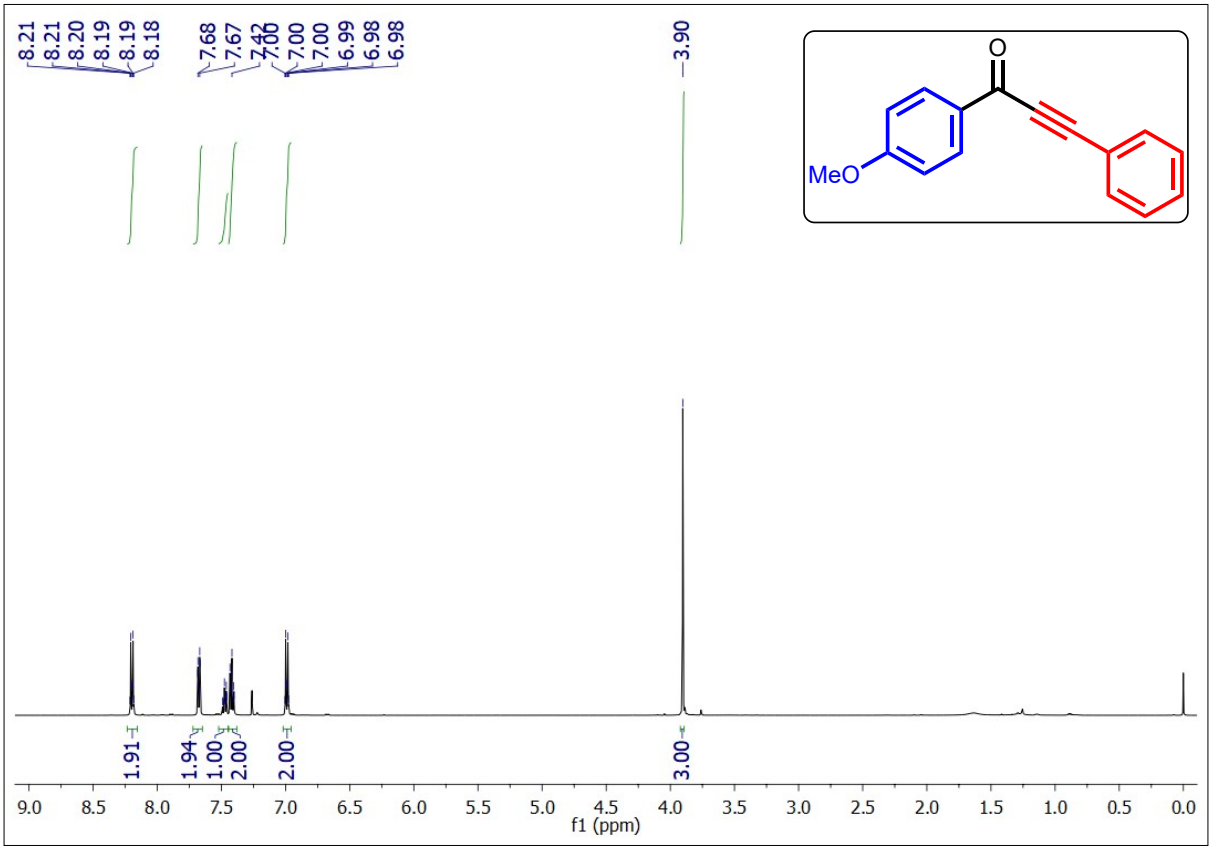
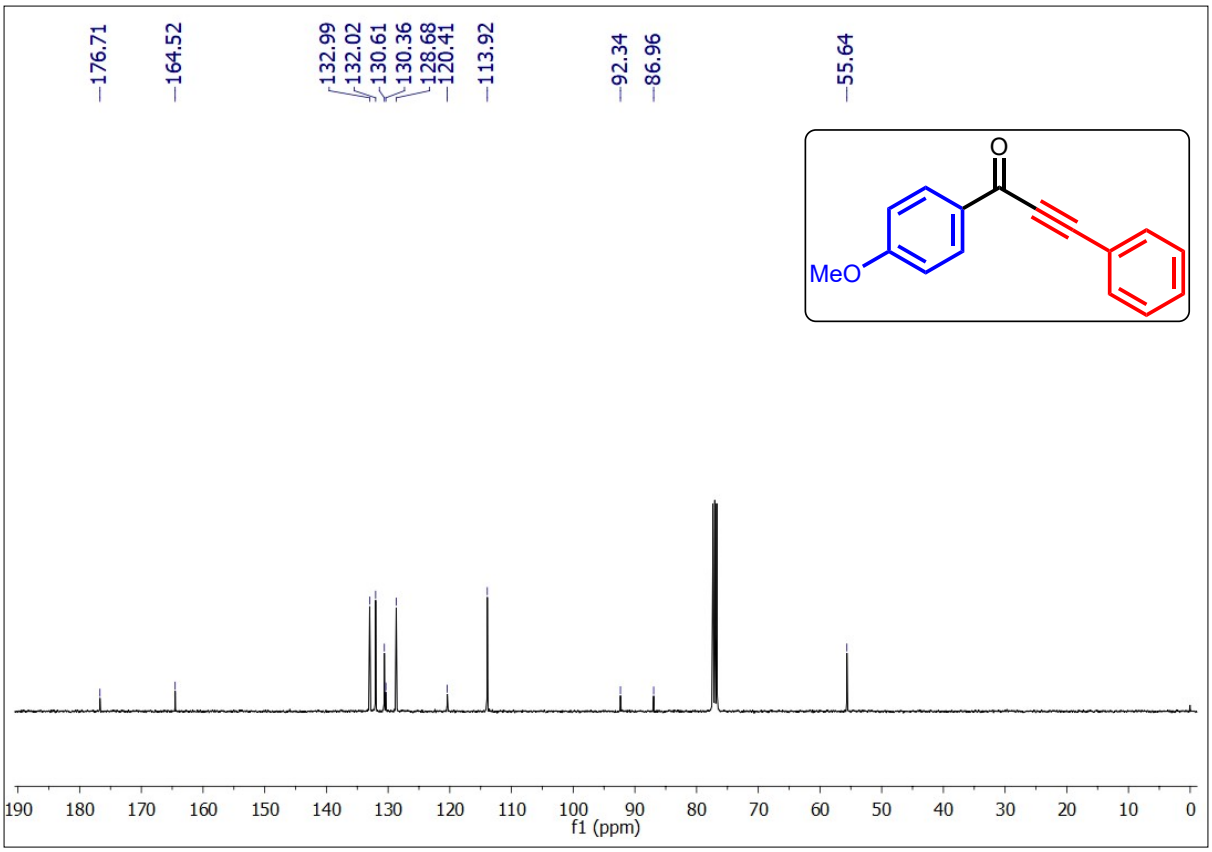
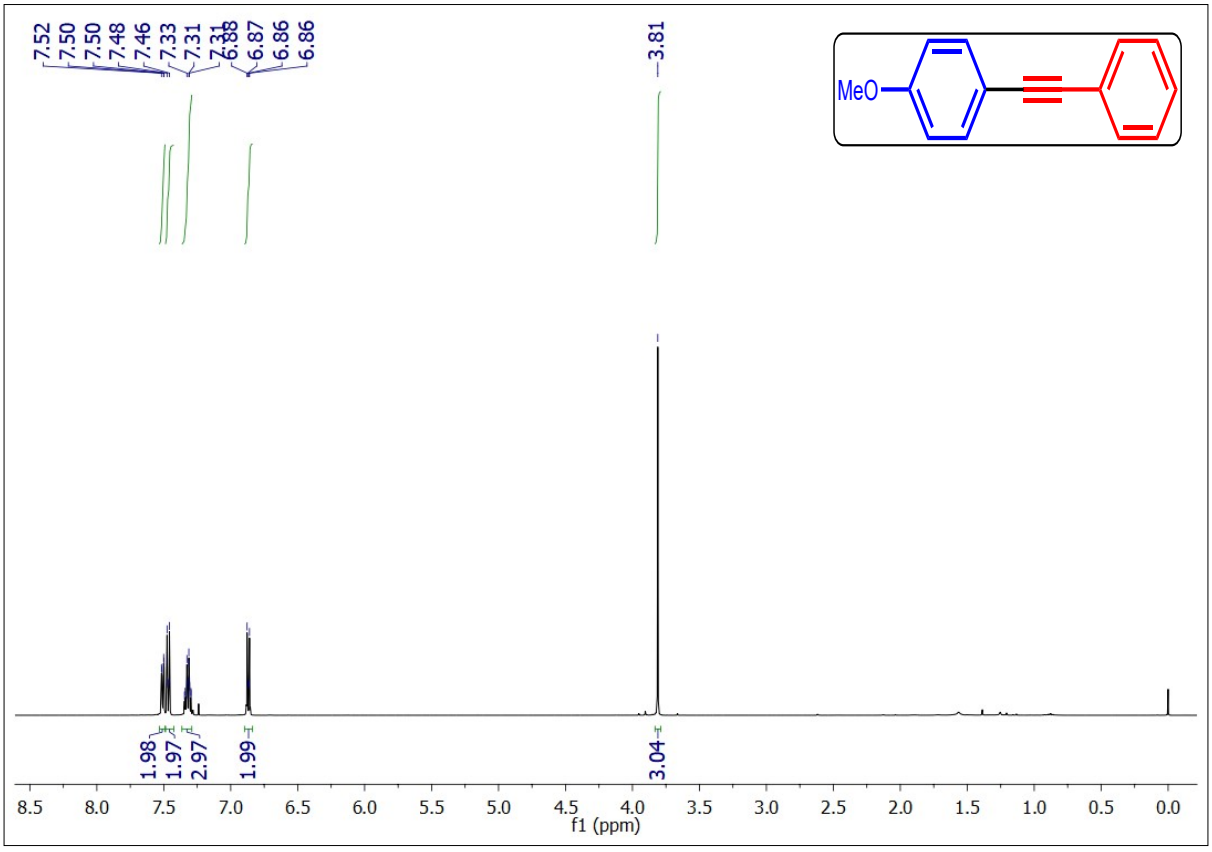
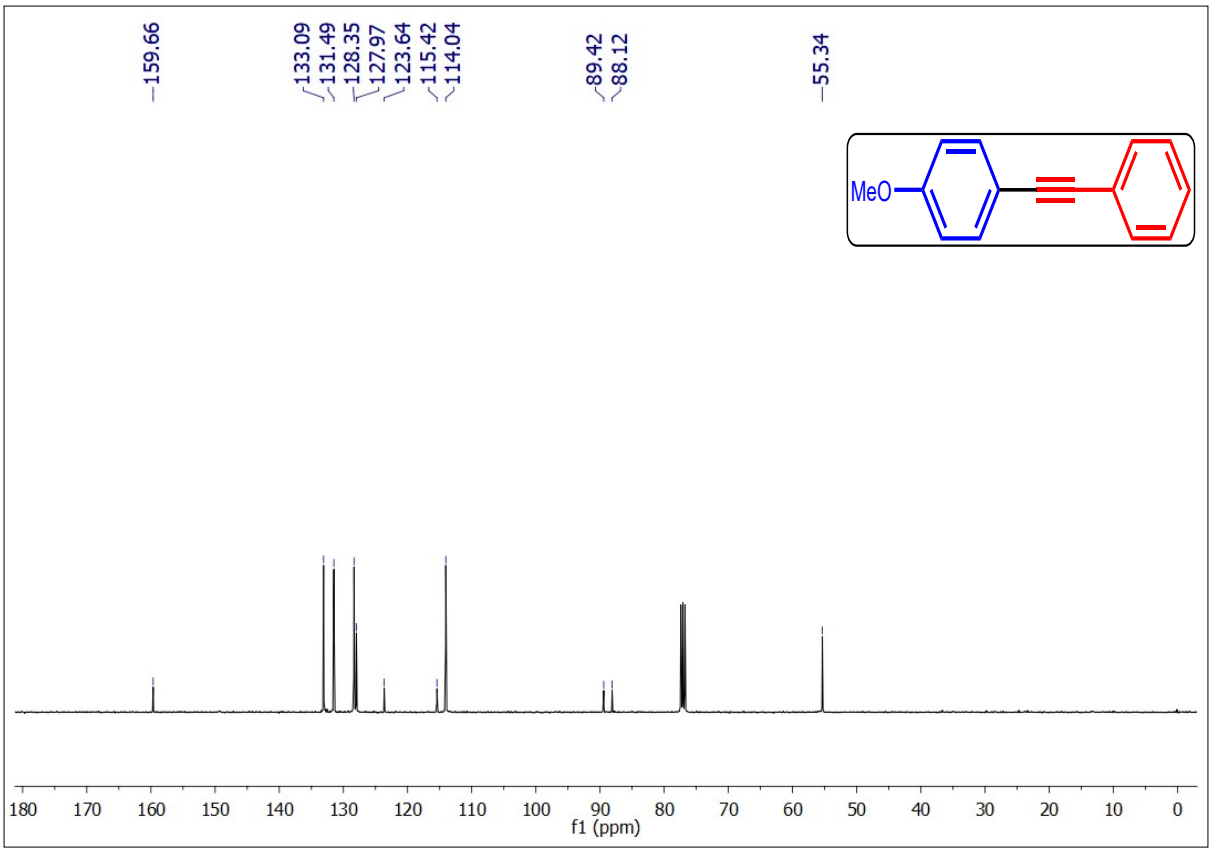
^{1}H and ^{13}C NMR spectra of 1-(4-Methoxyphenyl)-3-phenylprop-2-yn-1-one (3a)



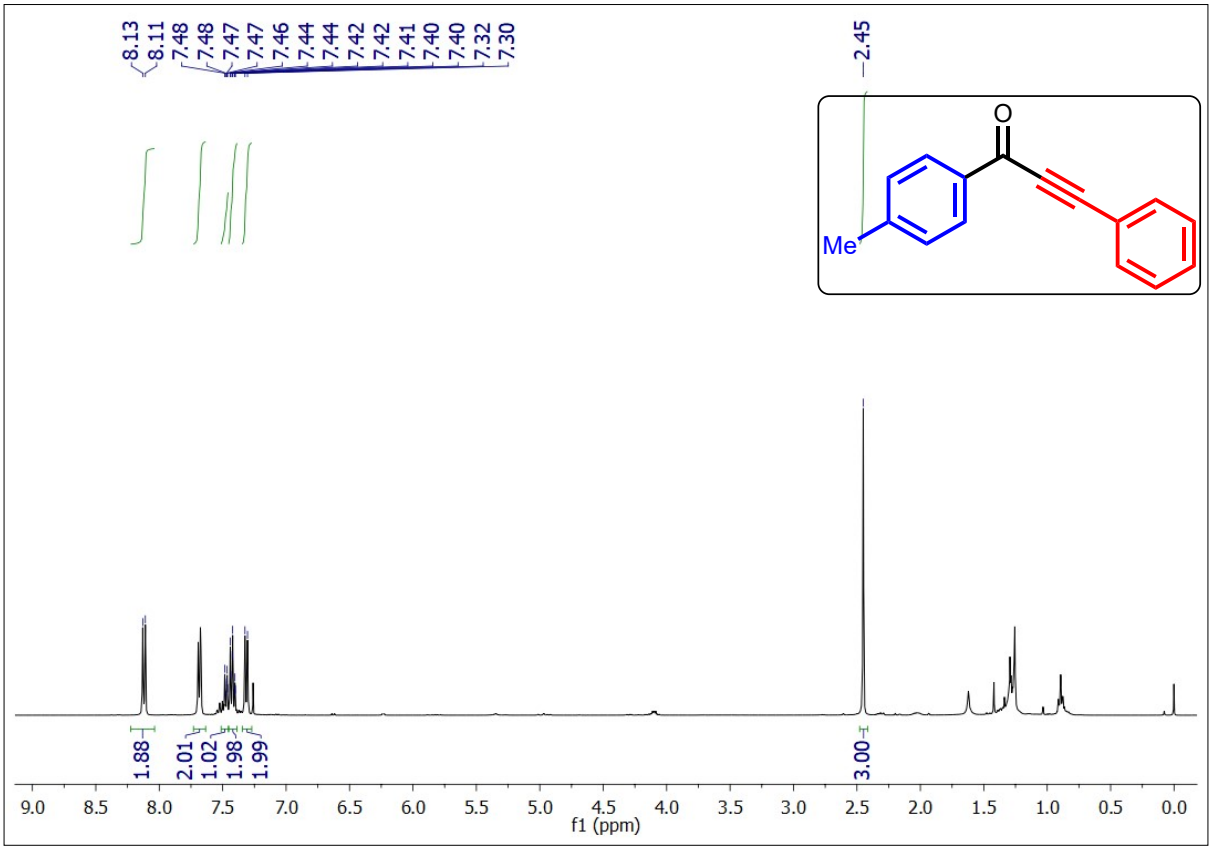


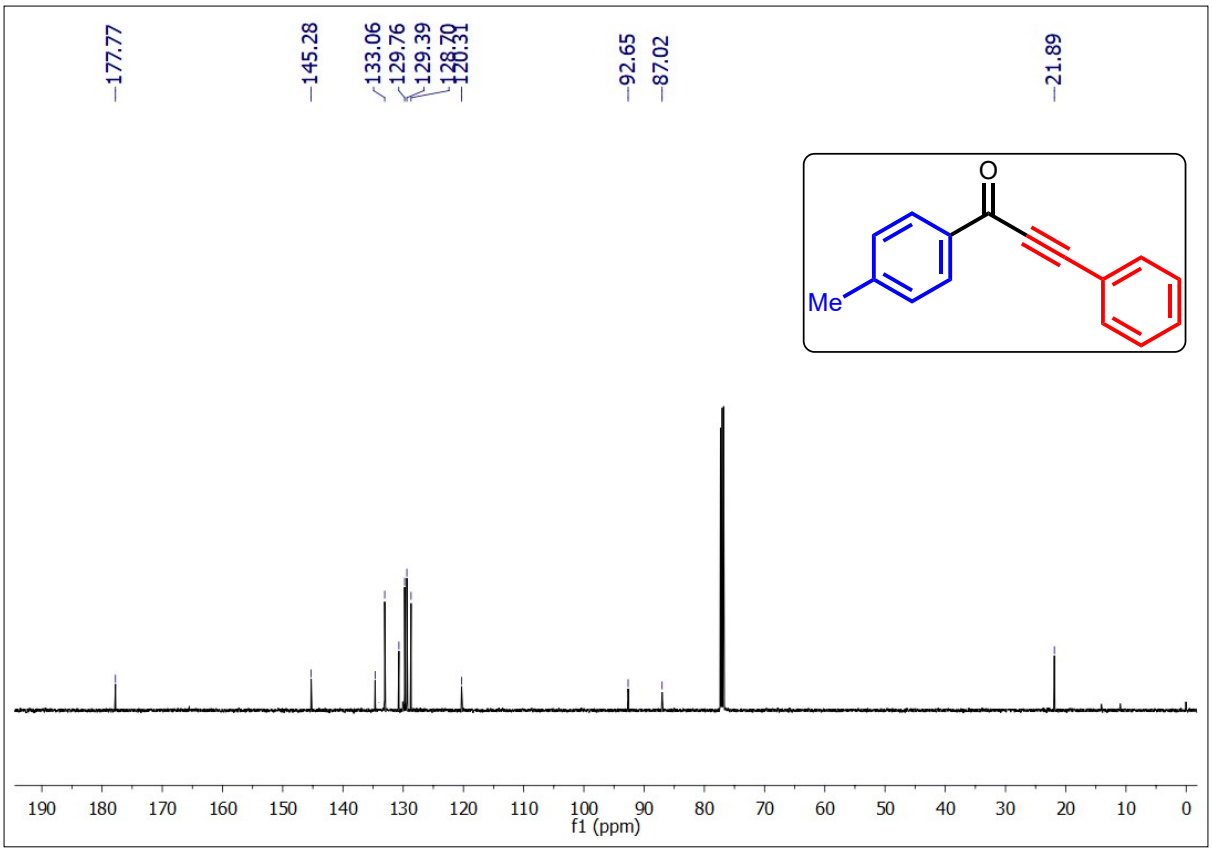
^{1}H and ^{13}C NMR spectra of 1-(4-Methoxyphenyl)-3-phenylprop-2-yn (4a)



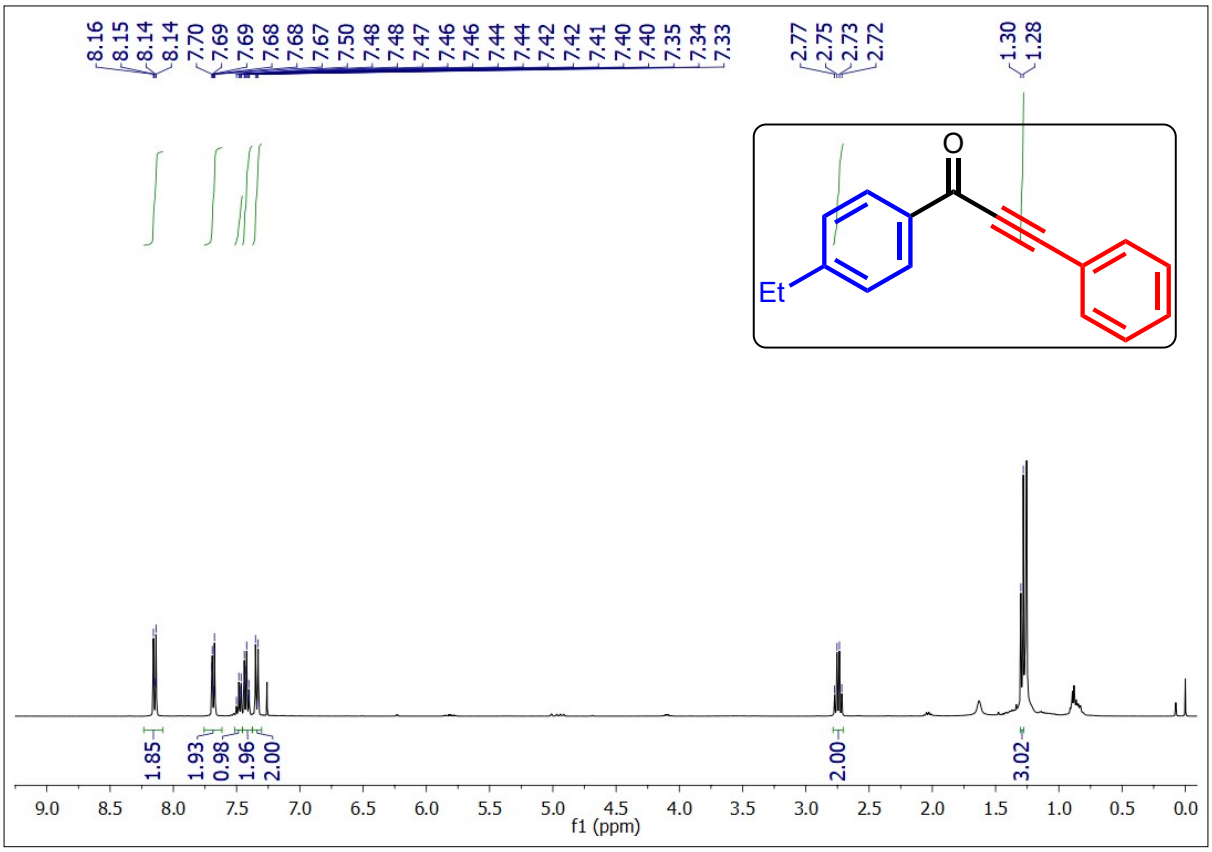


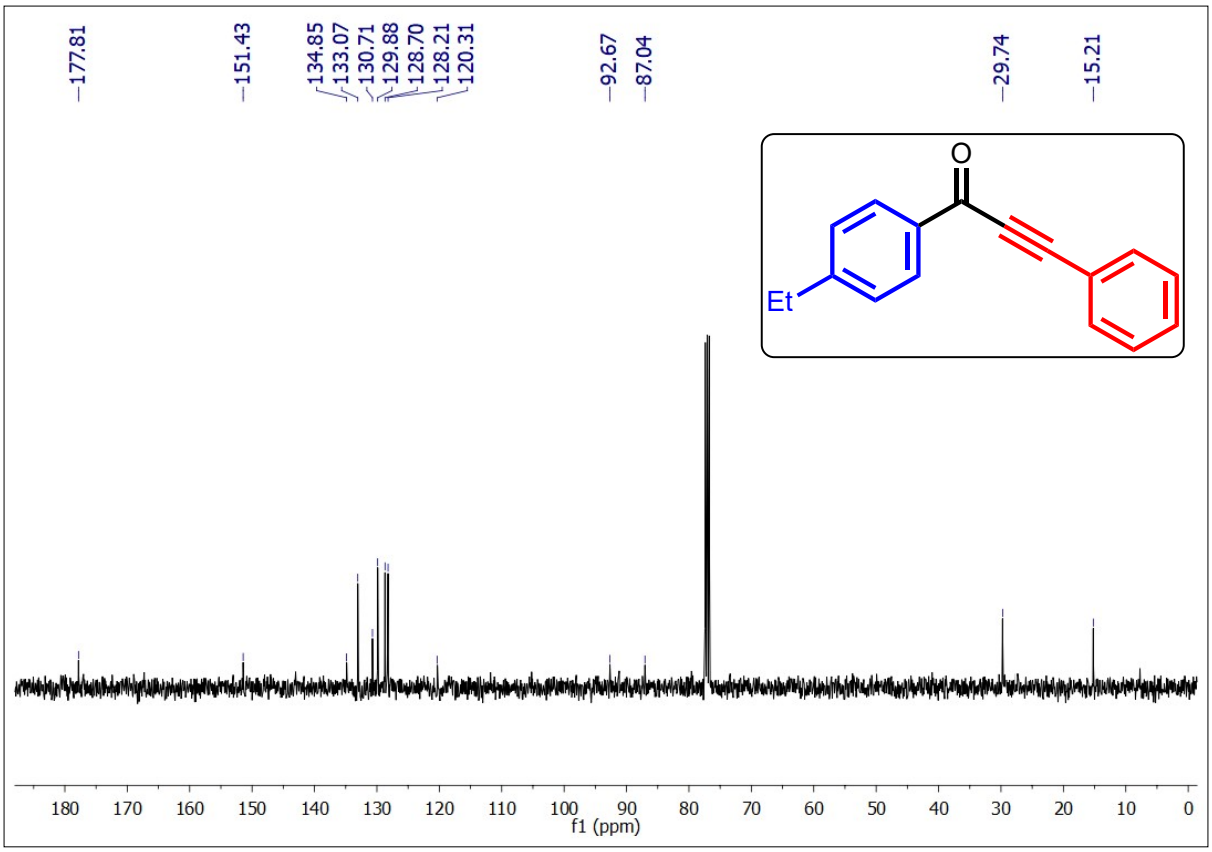
^{1}H and ^{13}C NMR spectra of 3-Phenyl-1-(p-tolyl)prop-2-yn-1-one (3b)



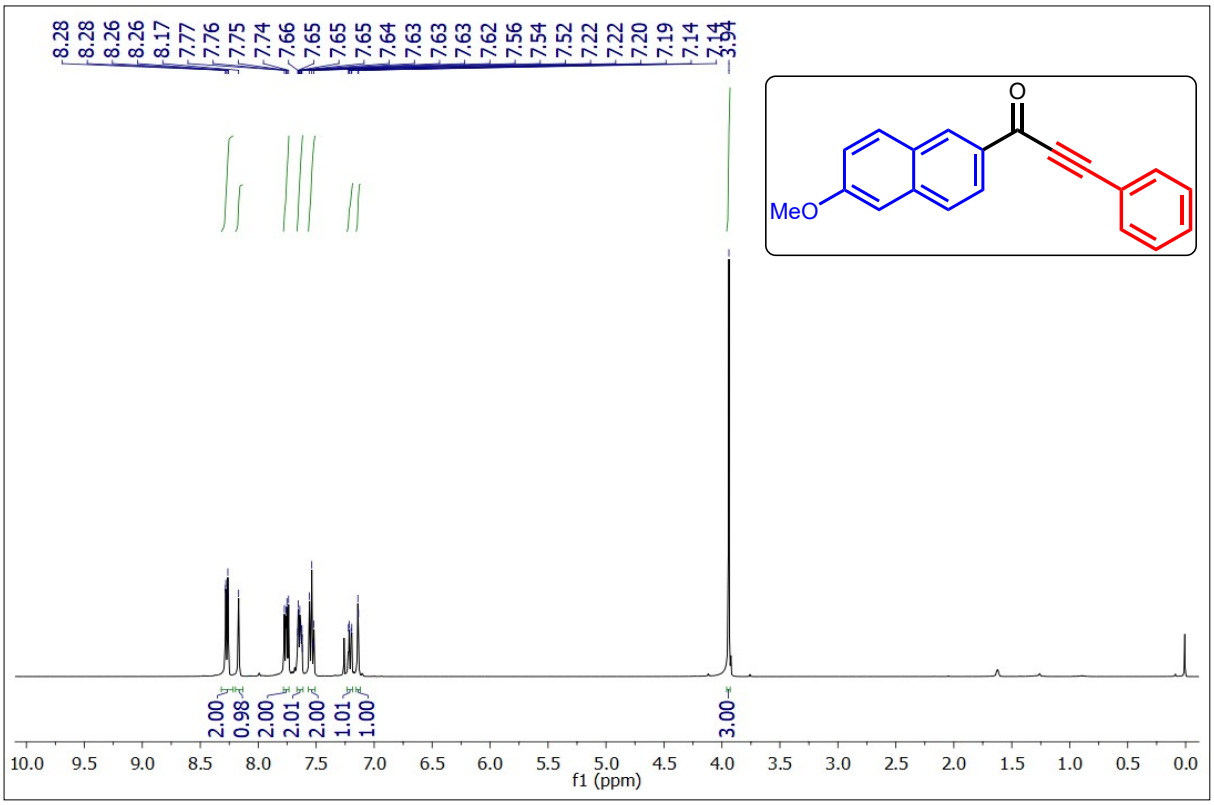


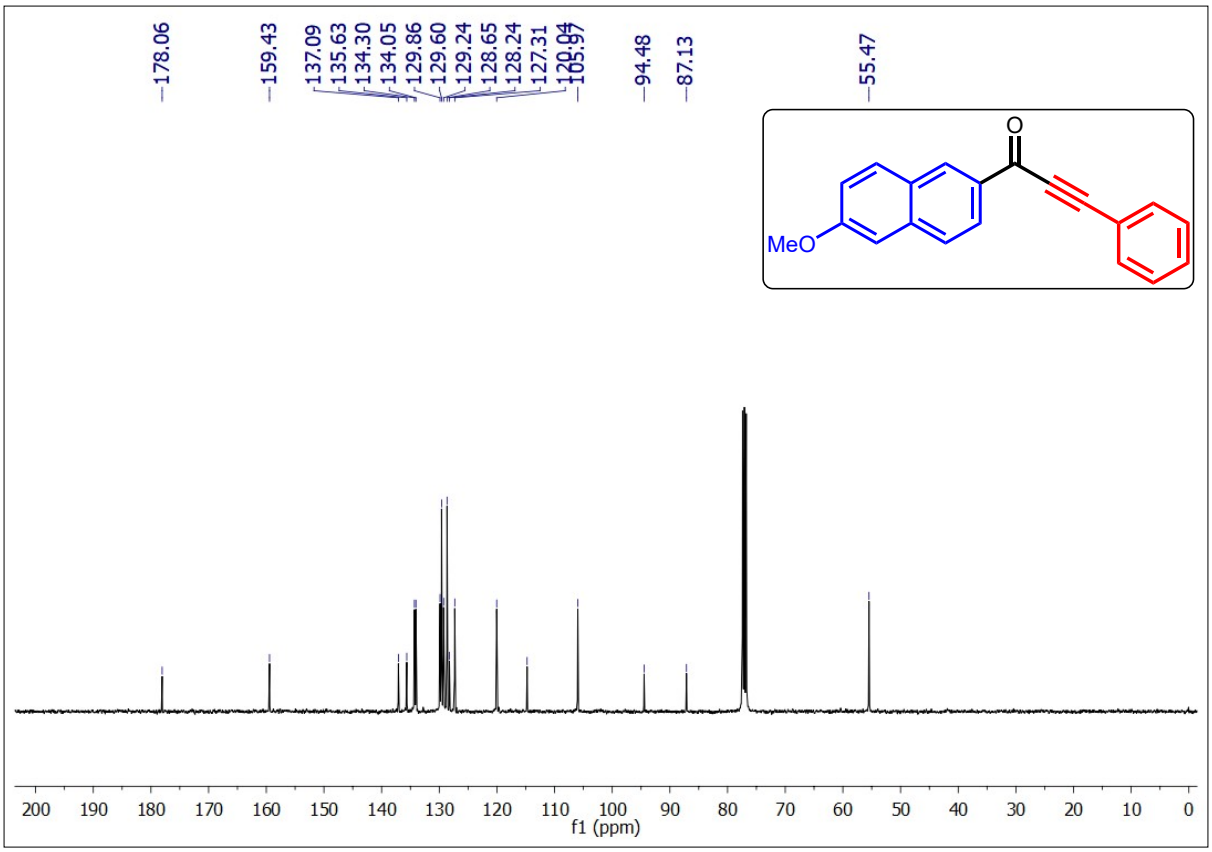
^{1}H and ^{13}C NMR spectra of 1-(4-Ethylphenyl)-3-phenylprop-2-yn-1-one (3c)



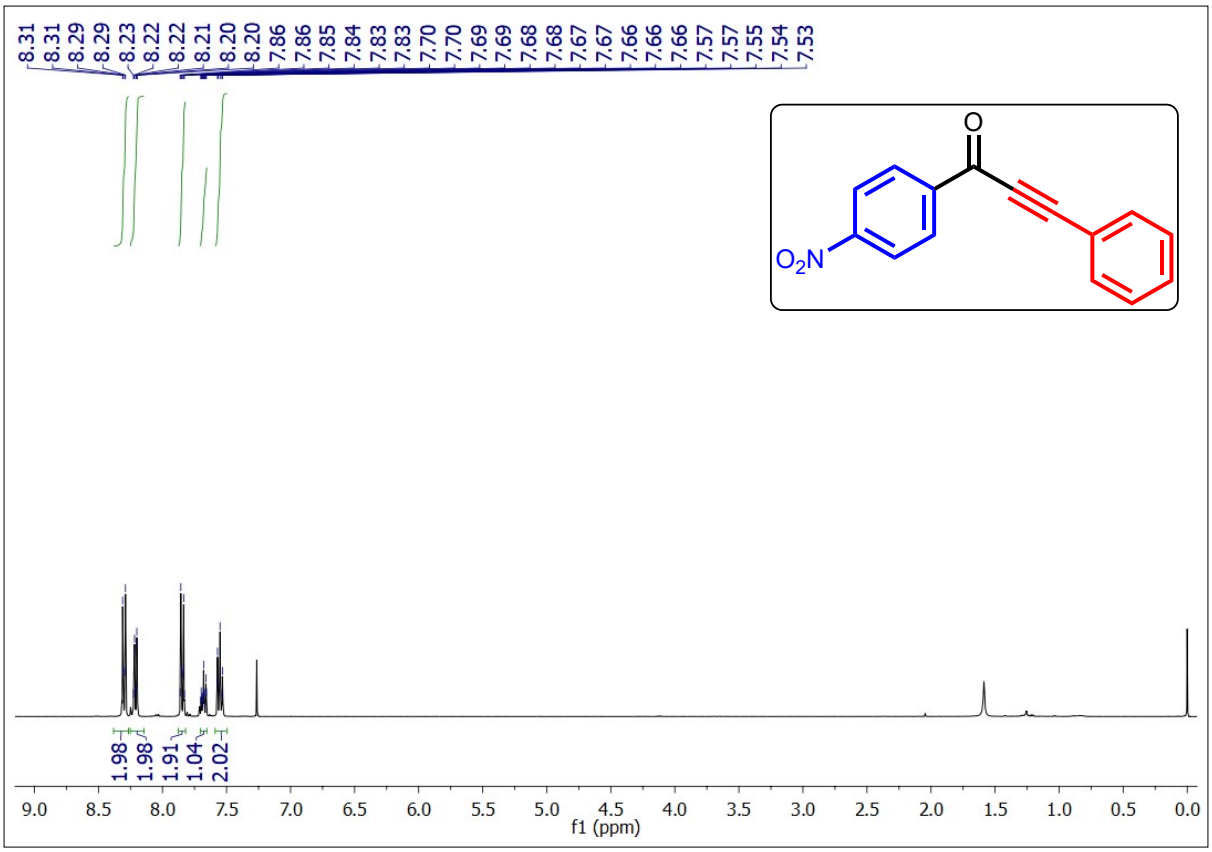


^{1}H and ^{13}C NMR spectra of 1-(6-Methoxynaphthalen-2-yl)-3-phenylprop-2-yn-1-one (3d)





^{1}H and ^{13}C NMR spectra of 1-(4-Nitrophenyl)-3-phenylprop-2-yn-1-one (3e)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8.29
8.29
8.23
8.22
8.22
8.21
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8.20
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7.86
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7.84
7.83
7.83
7.70
7.70
7.69
7.69
7.68
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7.67
7.67
7.66
7.66
7.66
7.57
7.57
7.55
7.54
7.53
O
O2N
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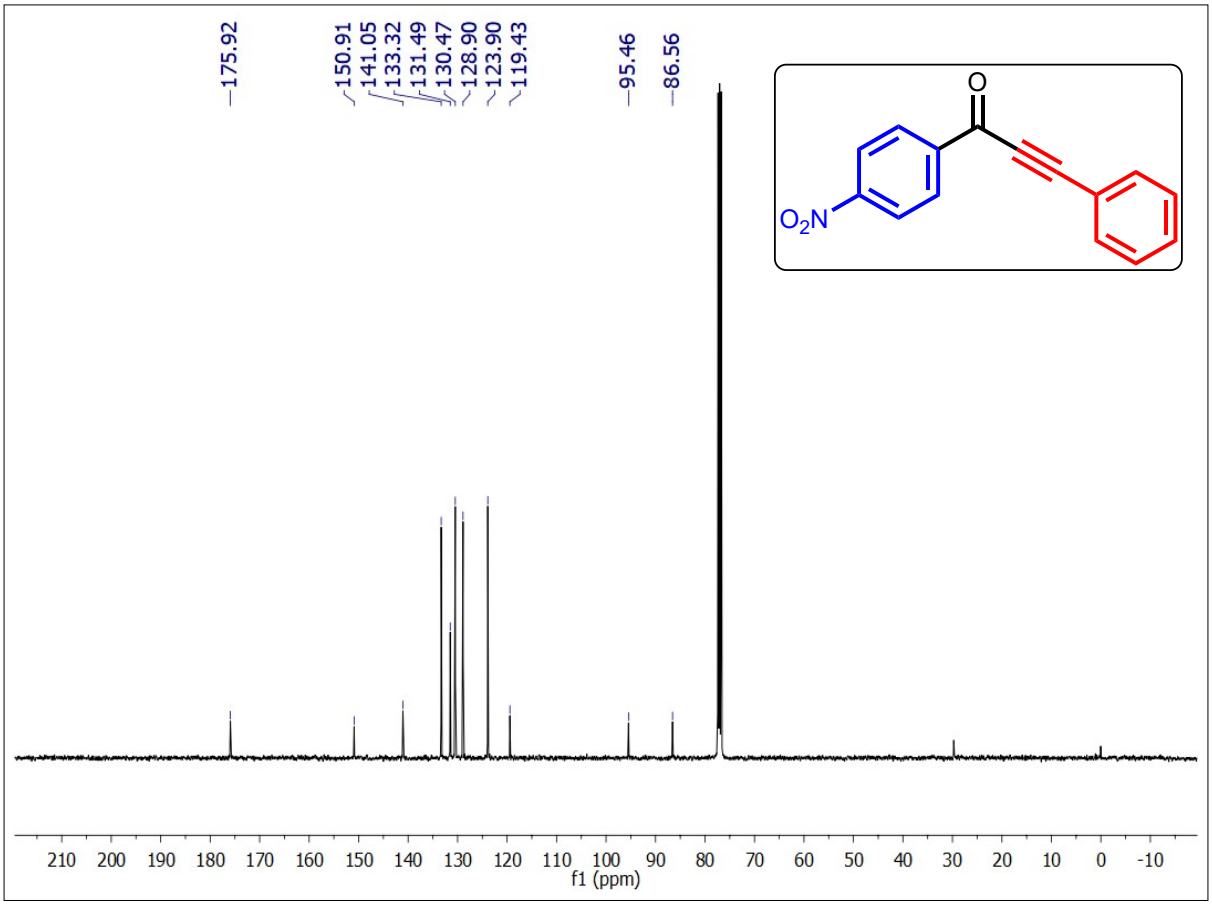
1.98
1.91
1.04
2.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.49
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128.90
123.90
119.43
95.46
86.56
O
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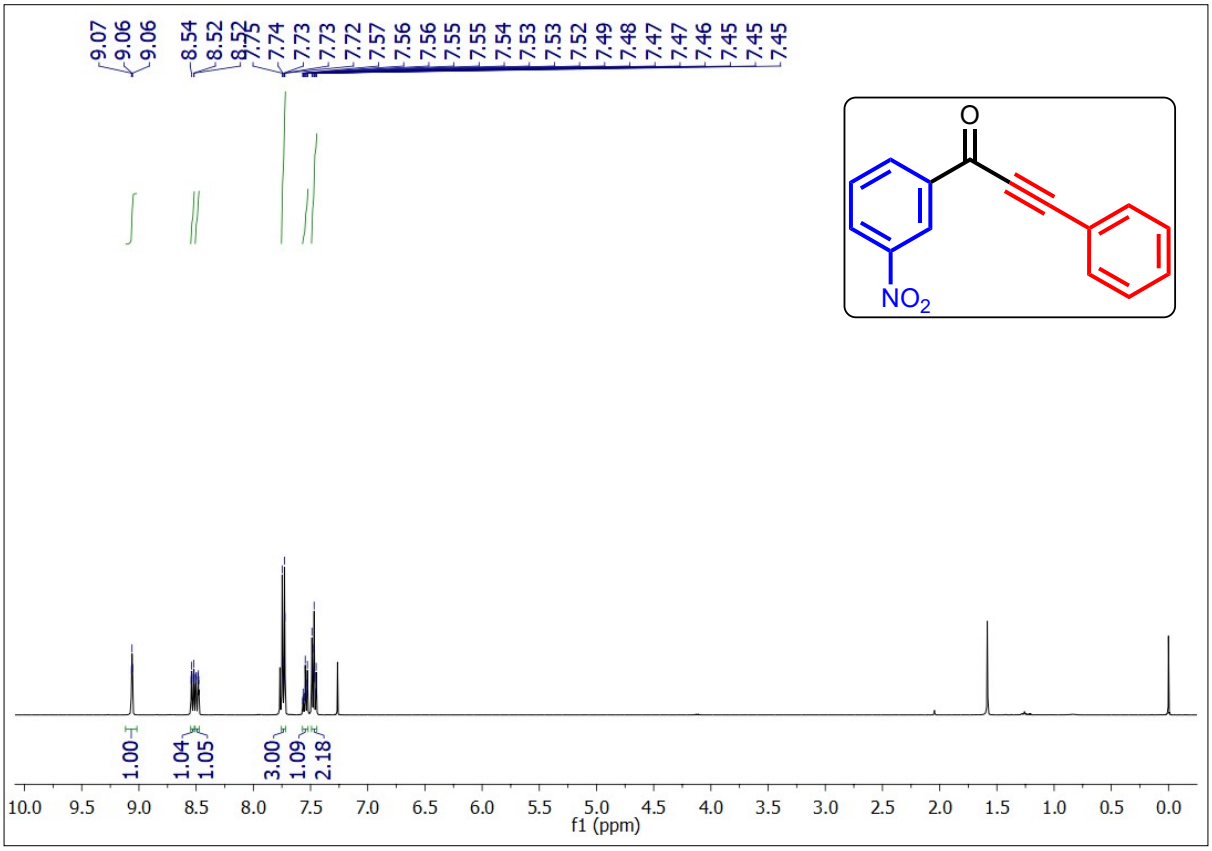
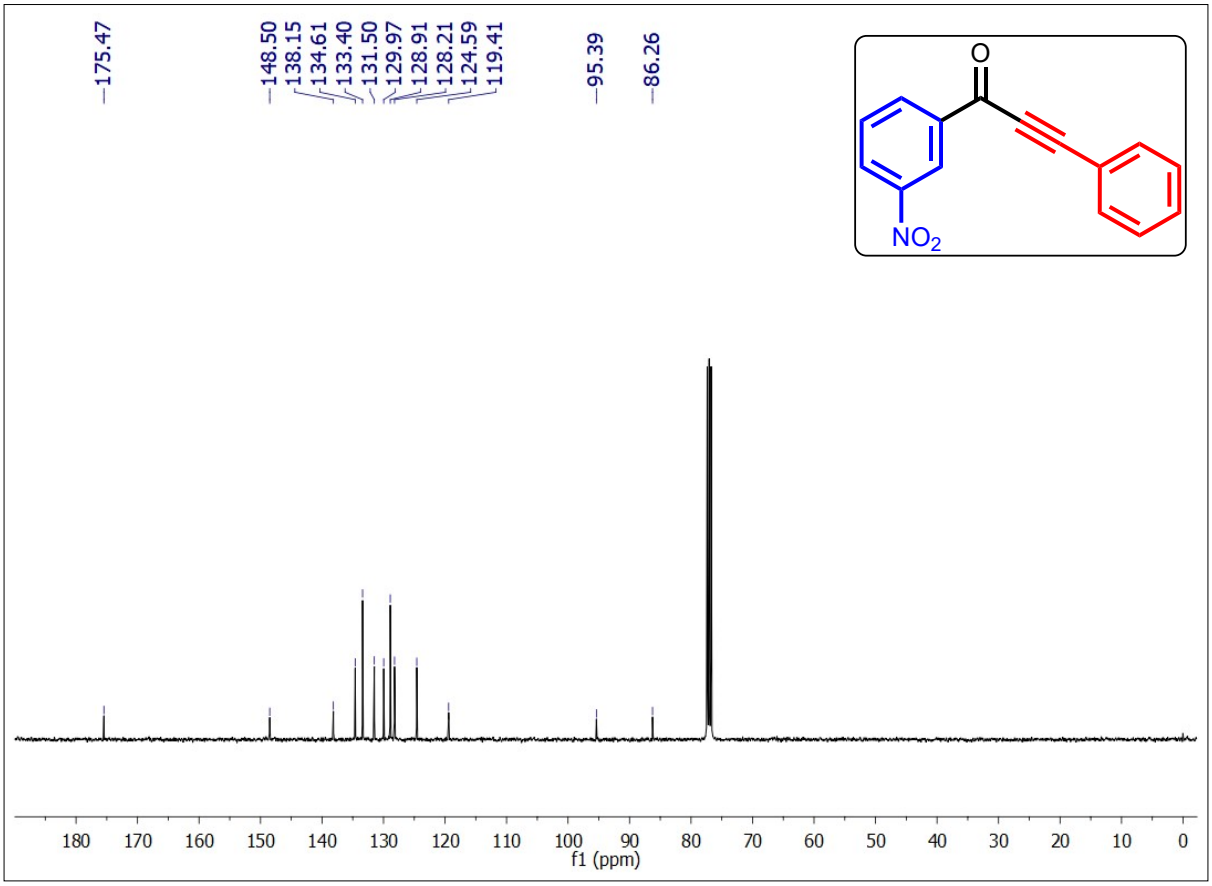
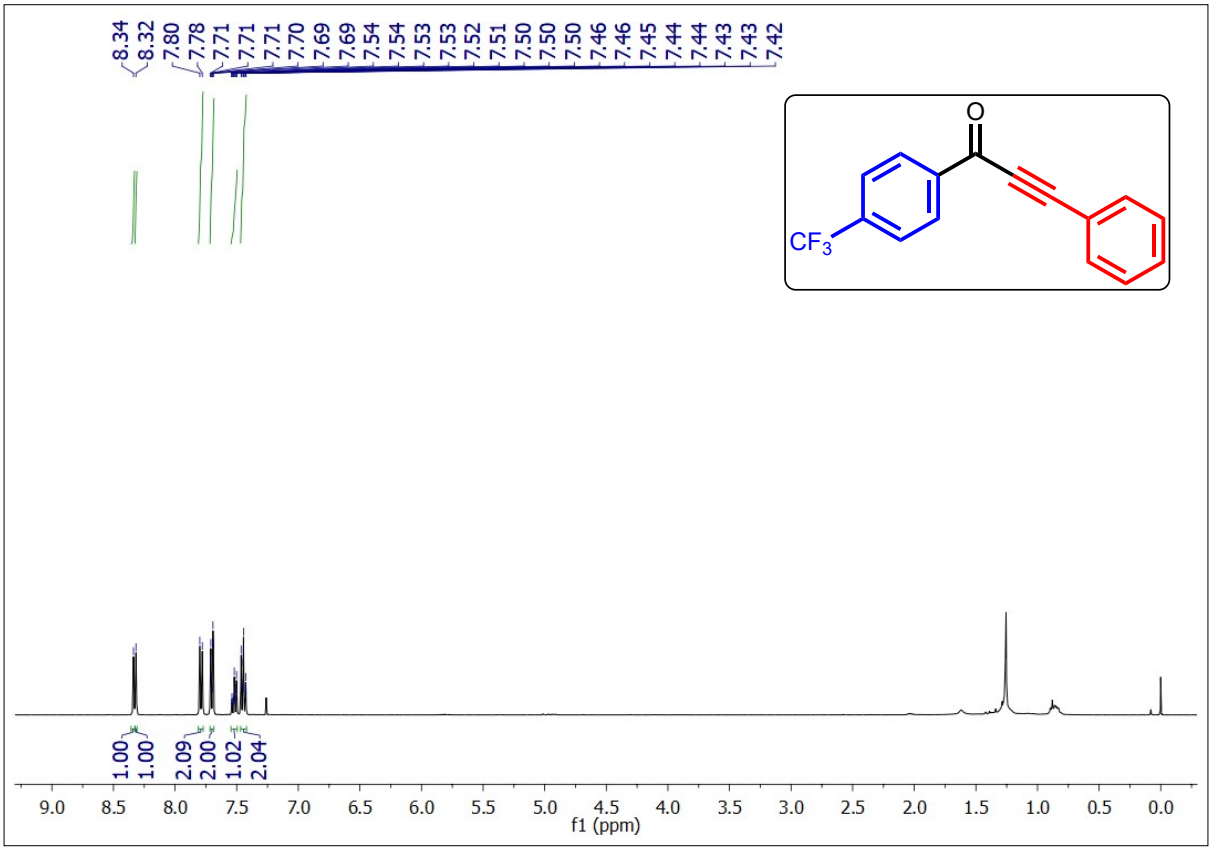
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

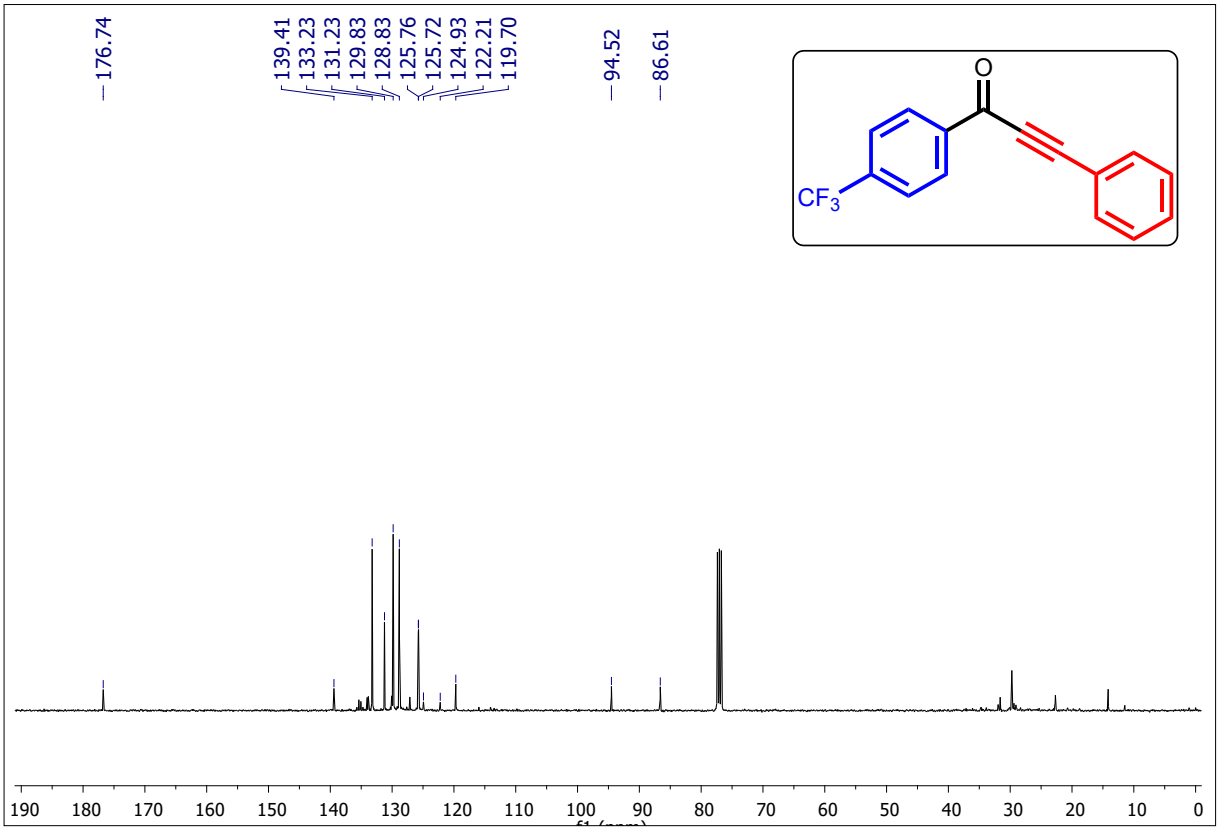
^{1}H and ^{13}C NMR spectra of 1-(3-Nitrophenyl)-3-phenylprop-2-yn-1-one (3f)



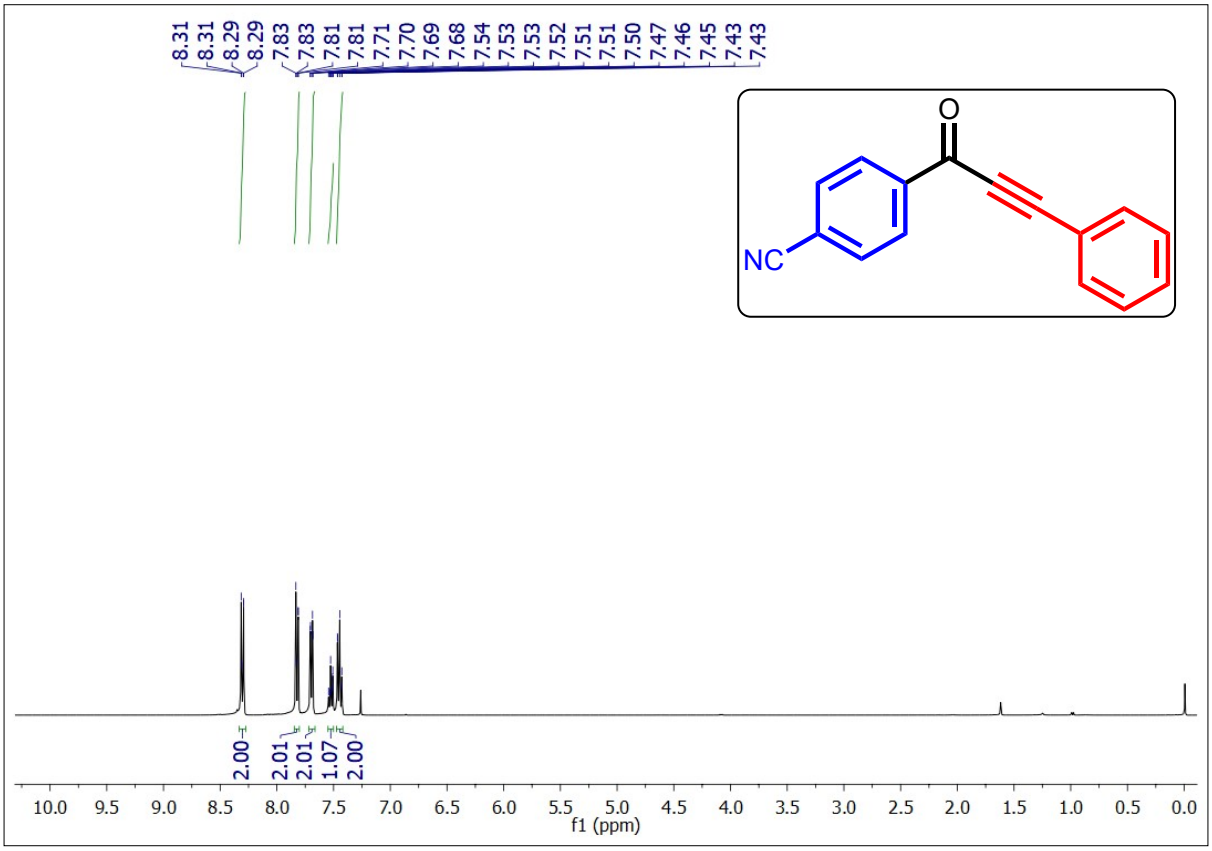


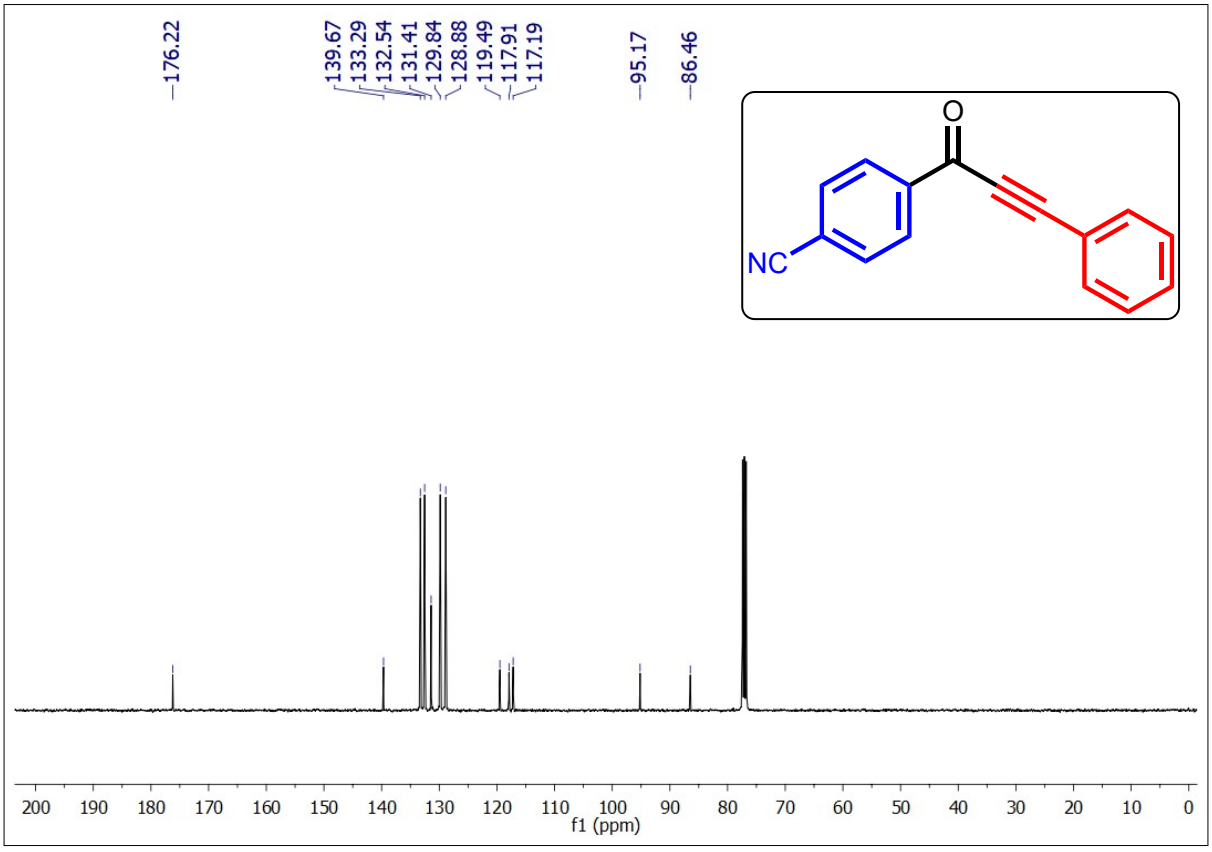
^{1}H and ^{13}C NMR spectra of 3-Phenyl-1-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (3g)



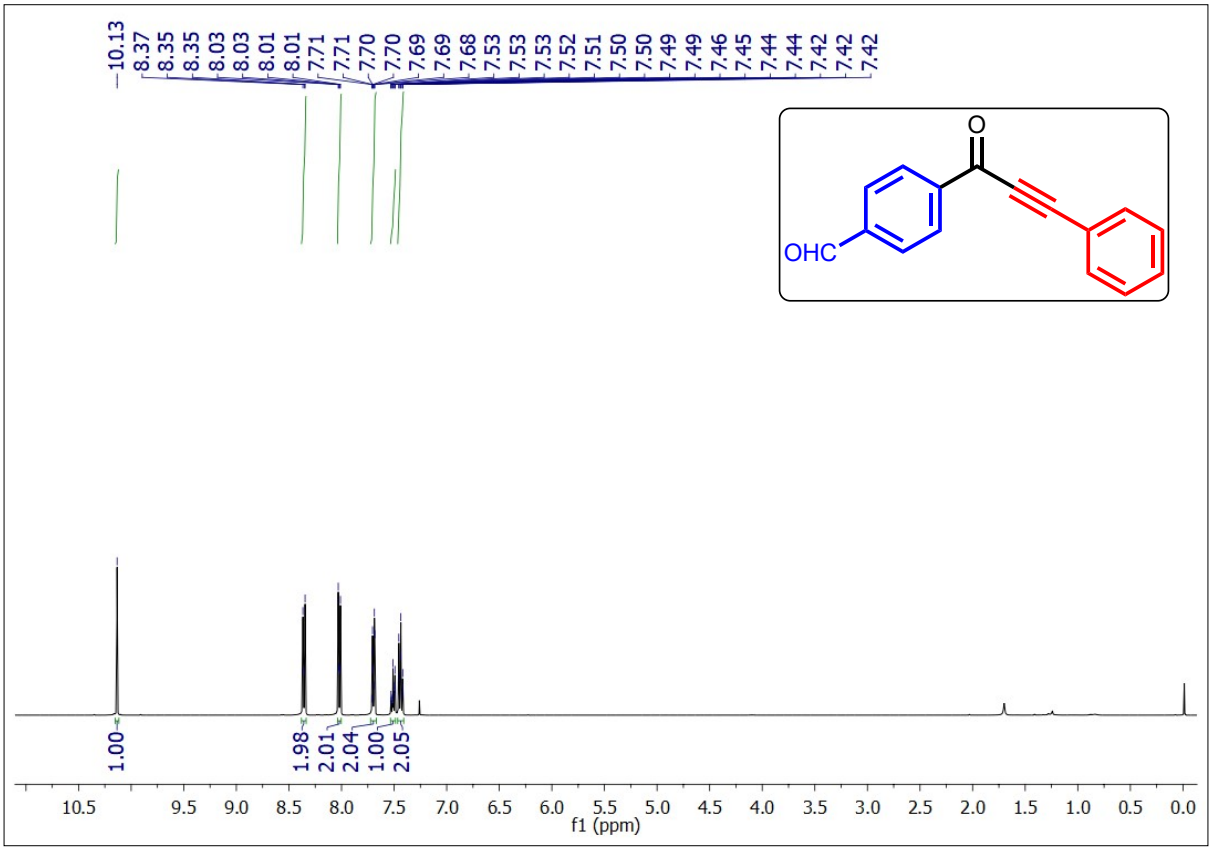


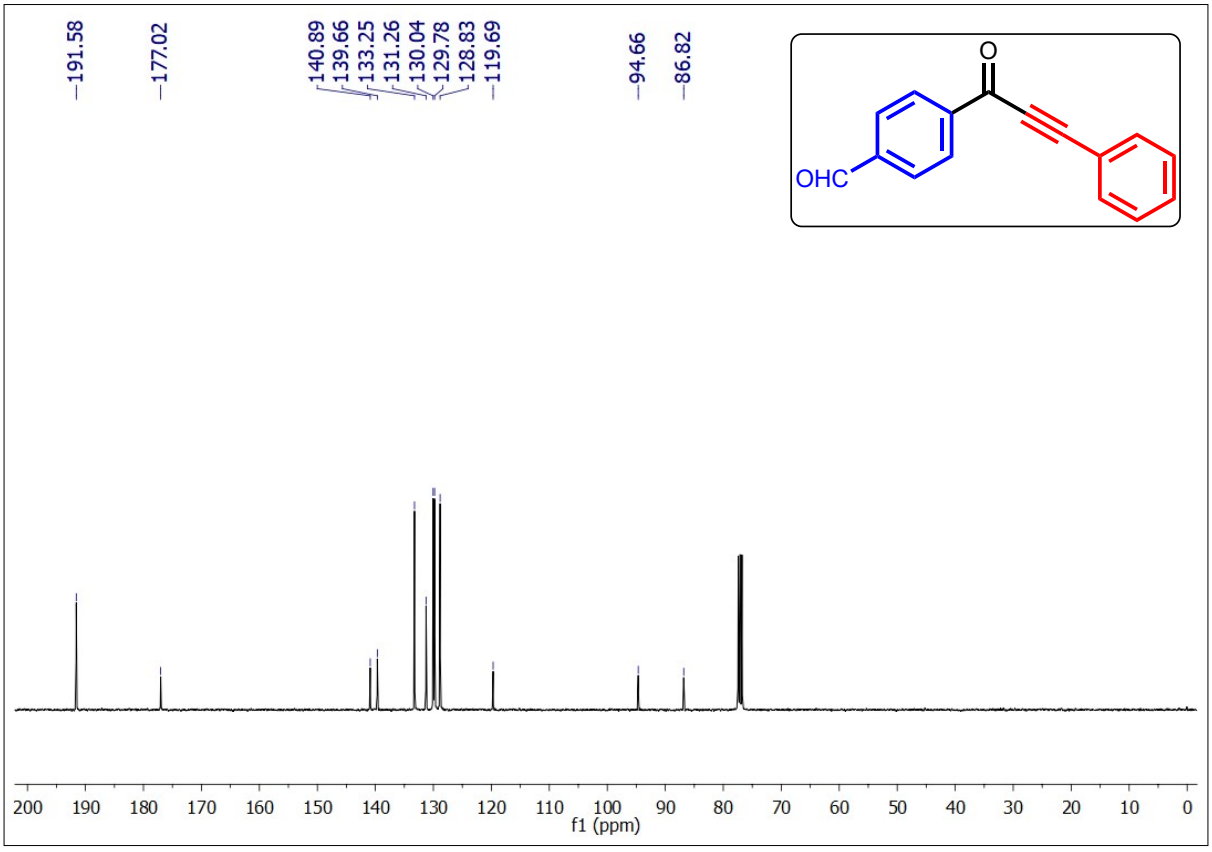
^{1}H and ^{13}C NMR spectra of 4-(3-Phenylpropioloyl)benzonitrile (3h)



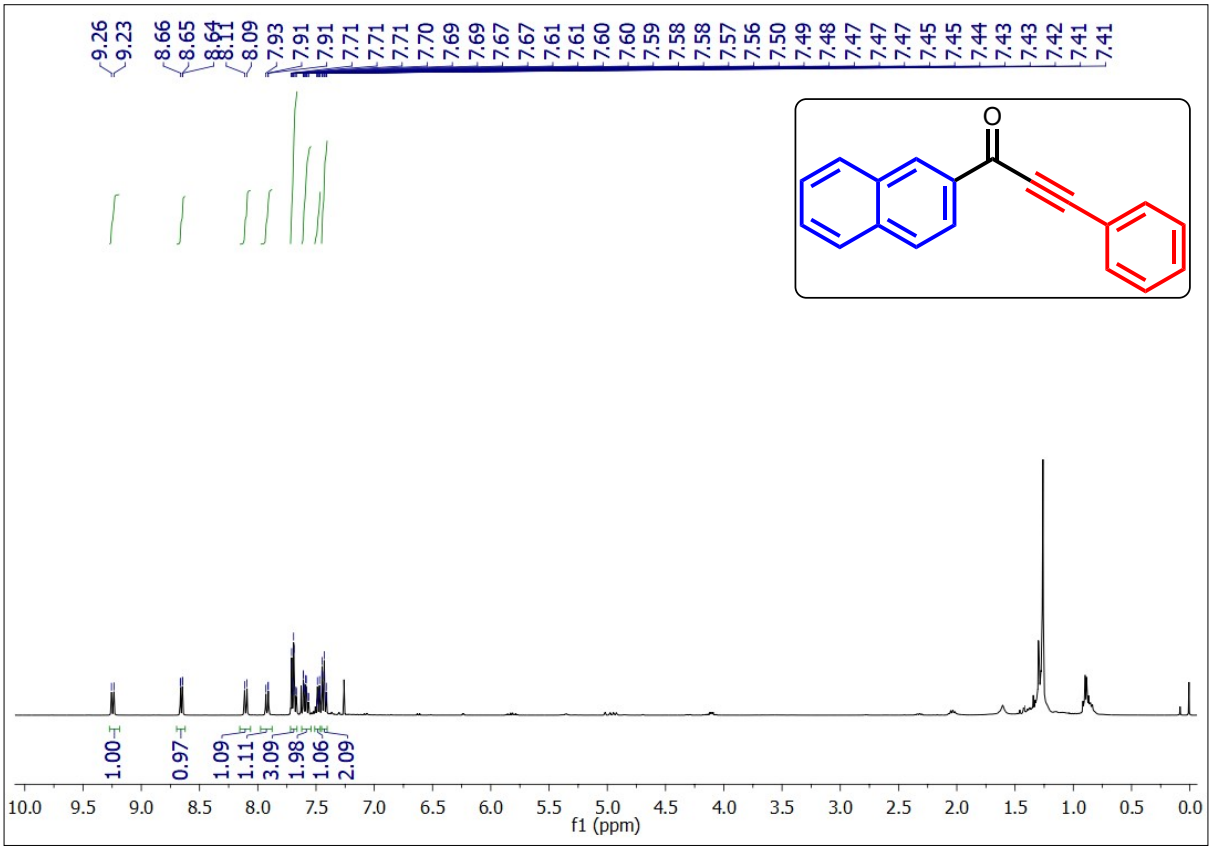


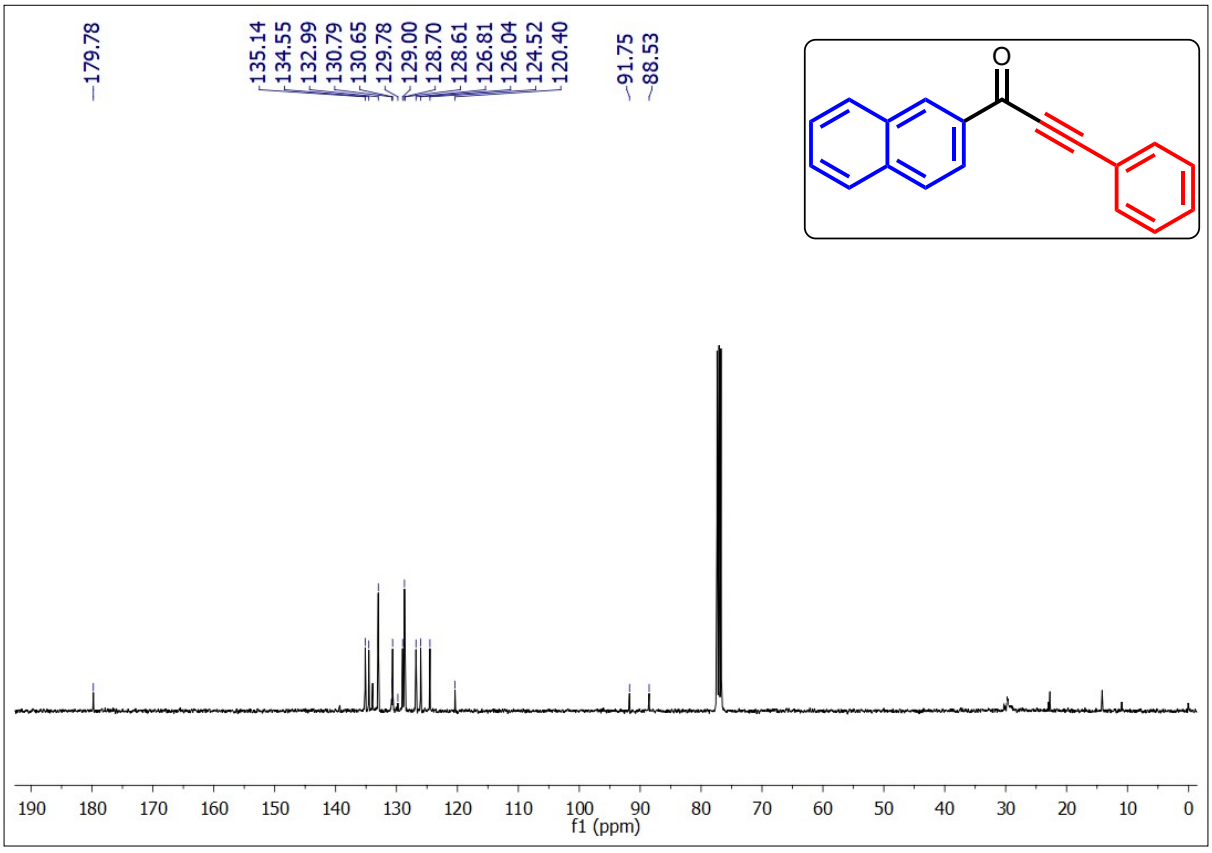
^{1}H and ^{13}C NMR spectra of 4-(3-Phenylpropioloyl)benzaldehyde (3i)



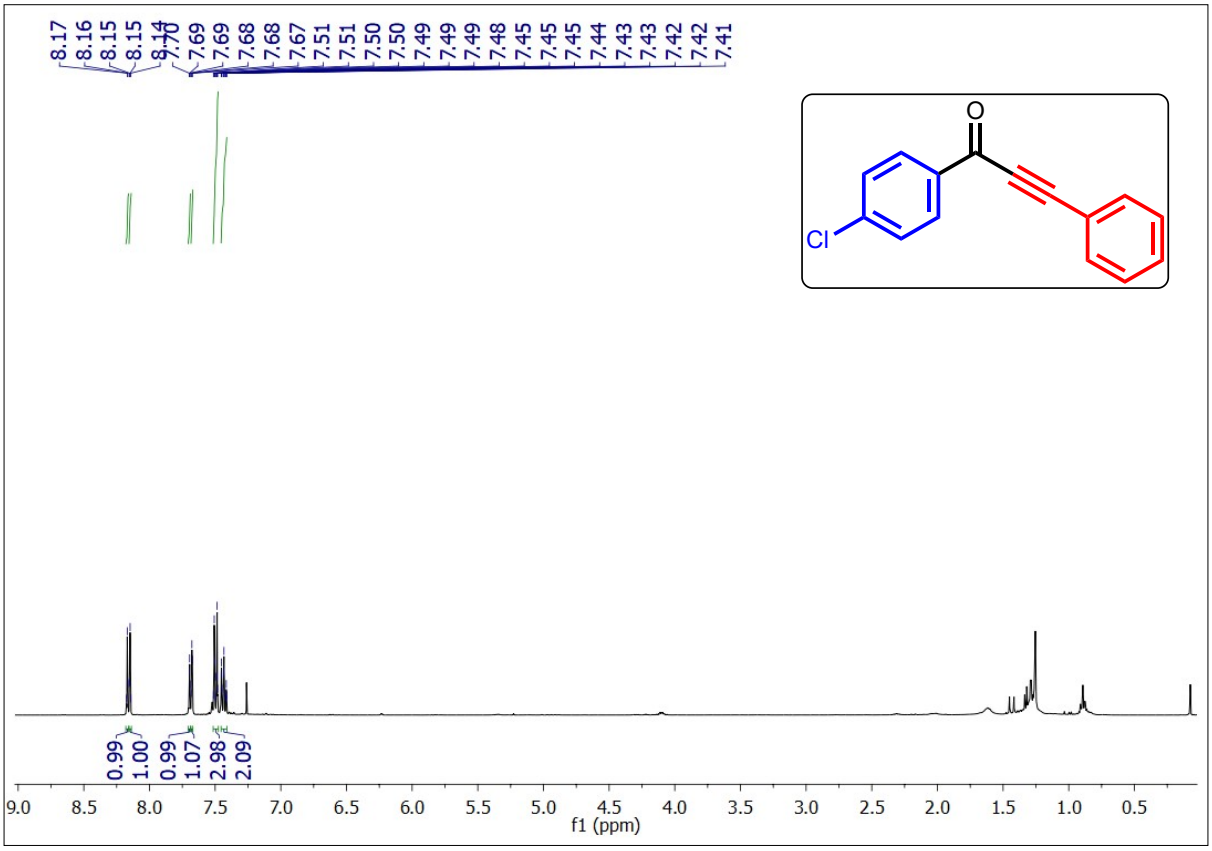


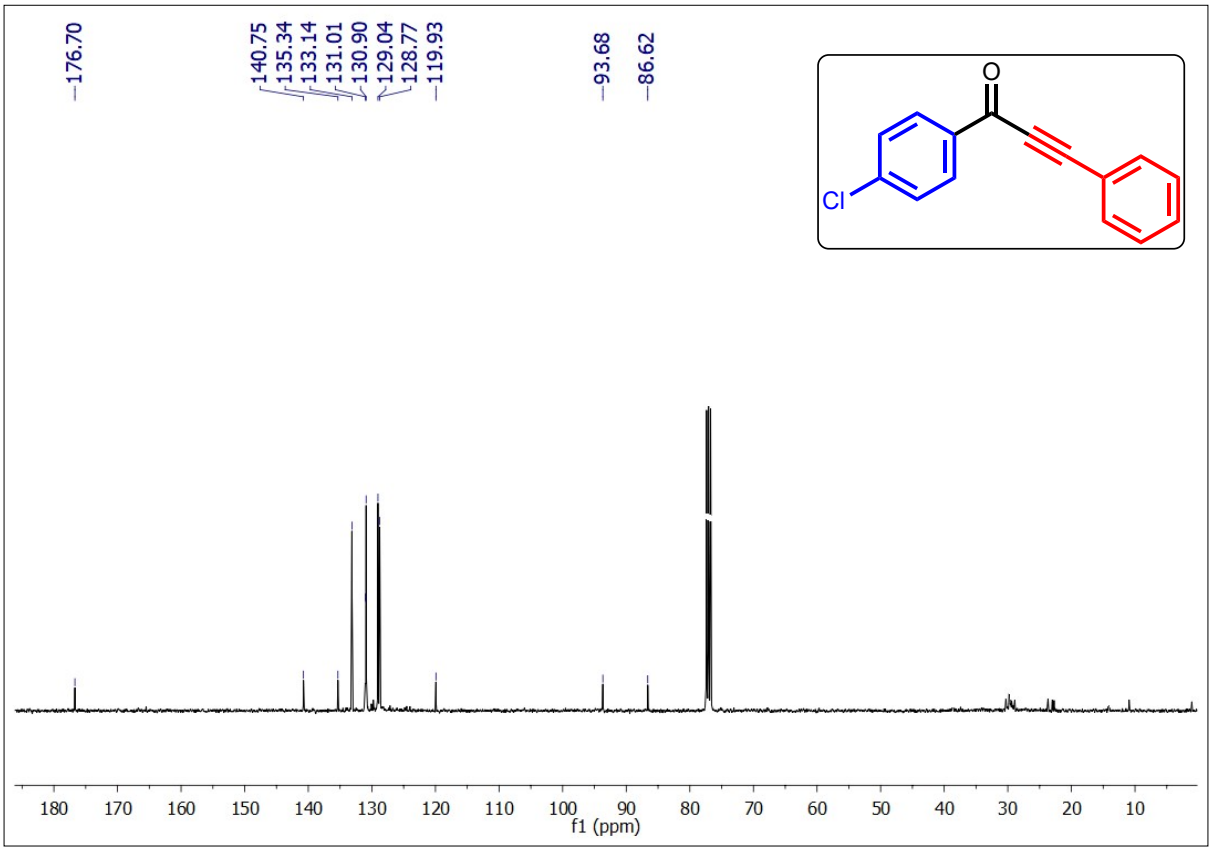
^{1}H and ^{13}C NMR spectra of 1-(Naphthalen-1-yl)-3-phenylprop-2-yn-1-one (3j)



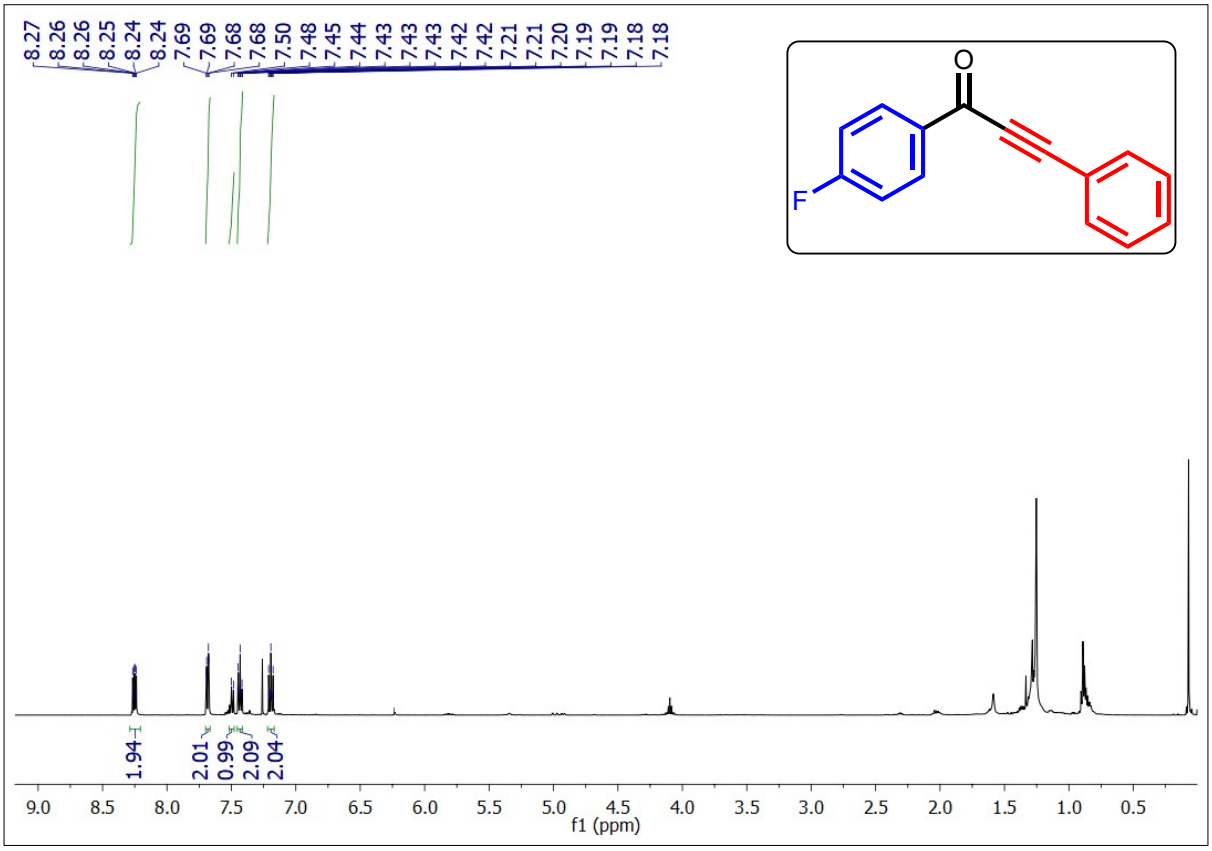


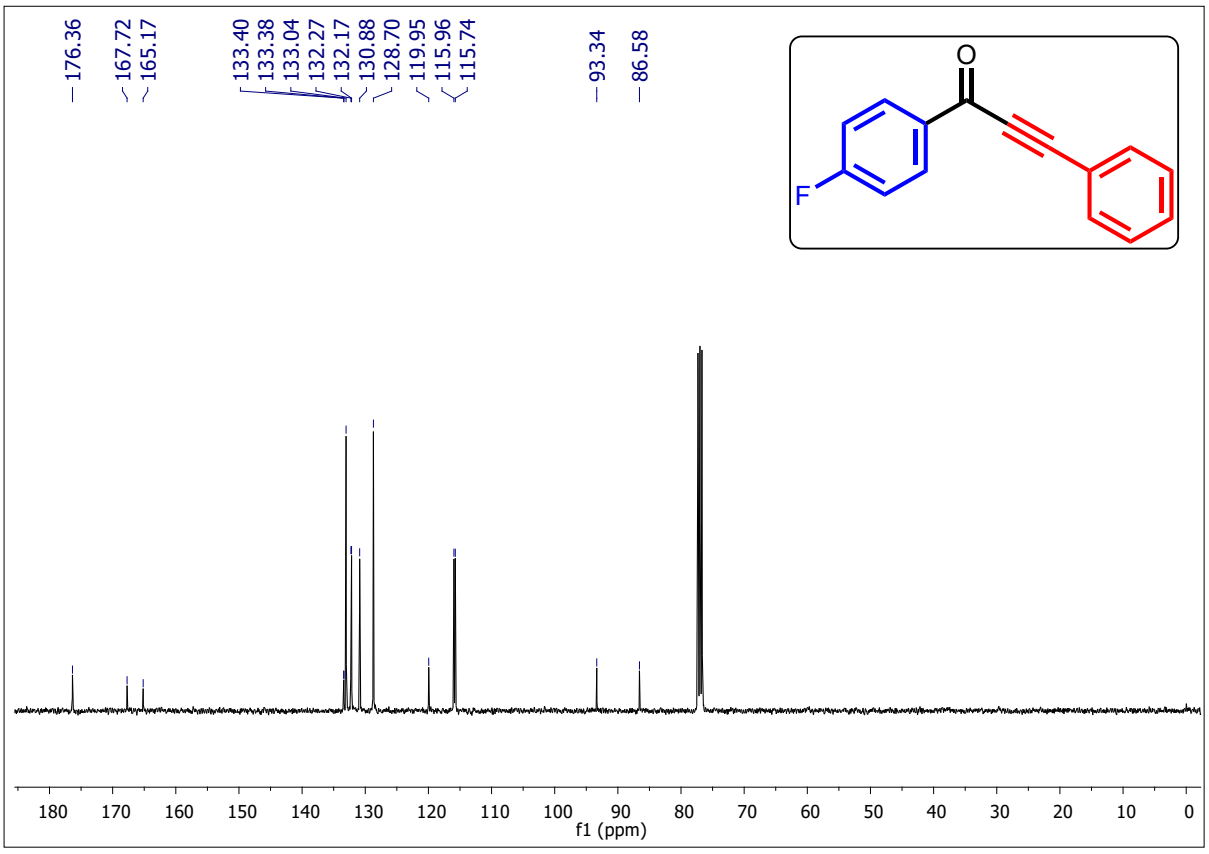
^{1}H and ^{13}C NMR spectra of 1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-one (3k)



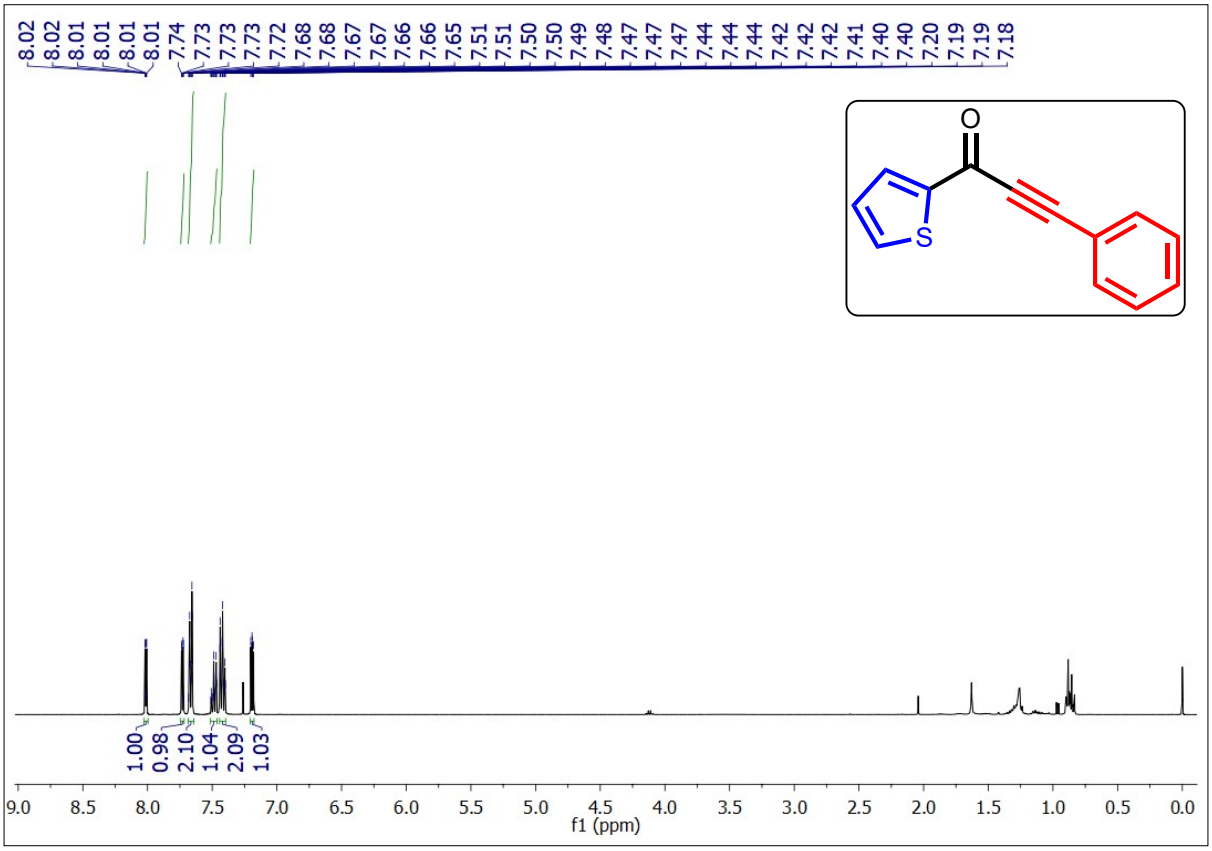


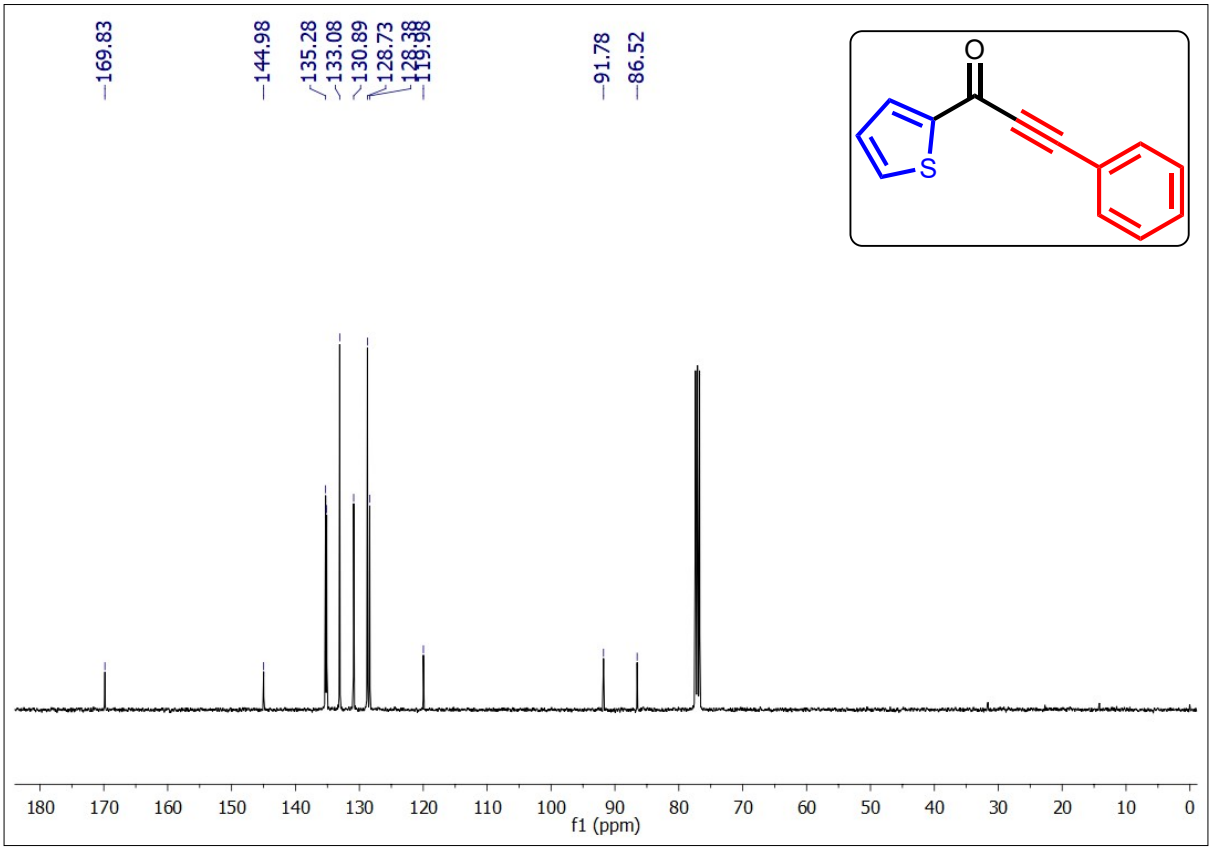
^{1}H and ^{13}C NMR spectra of 1-(4-Fluorophenyl)-3-phenylprop-2-yn-1-one (3l)



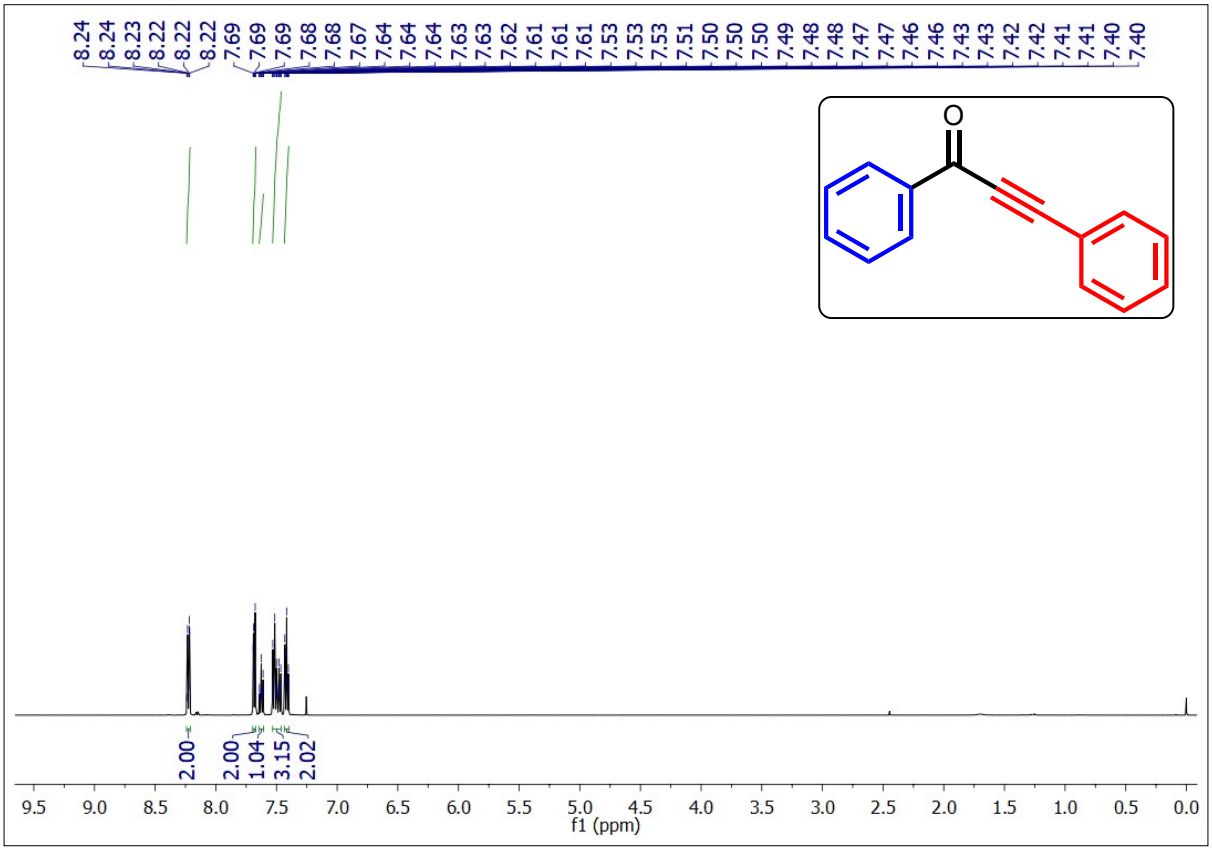


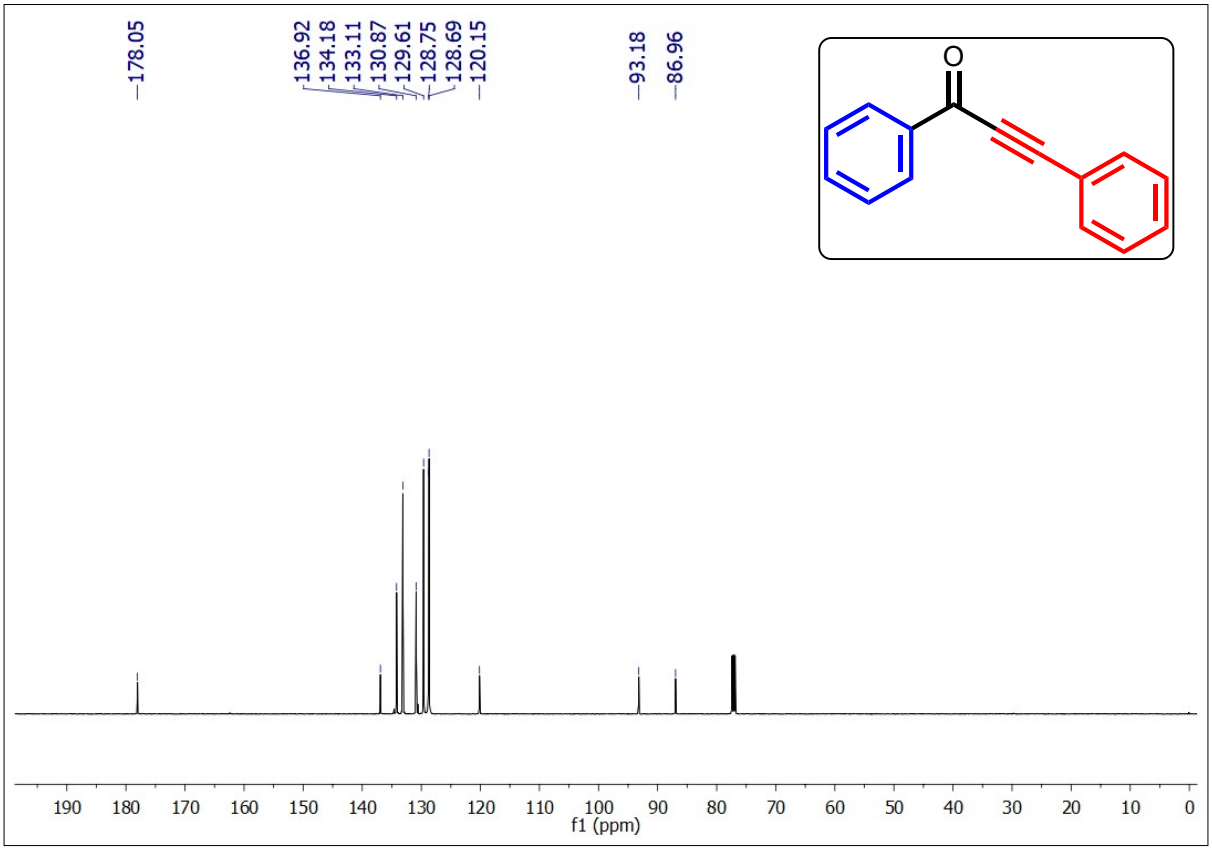
^{1}H and ^{13}C NMR spectra of 3-Phenyl-1-(thiophen-2-yl)prop-2-yn-1-one (3m)



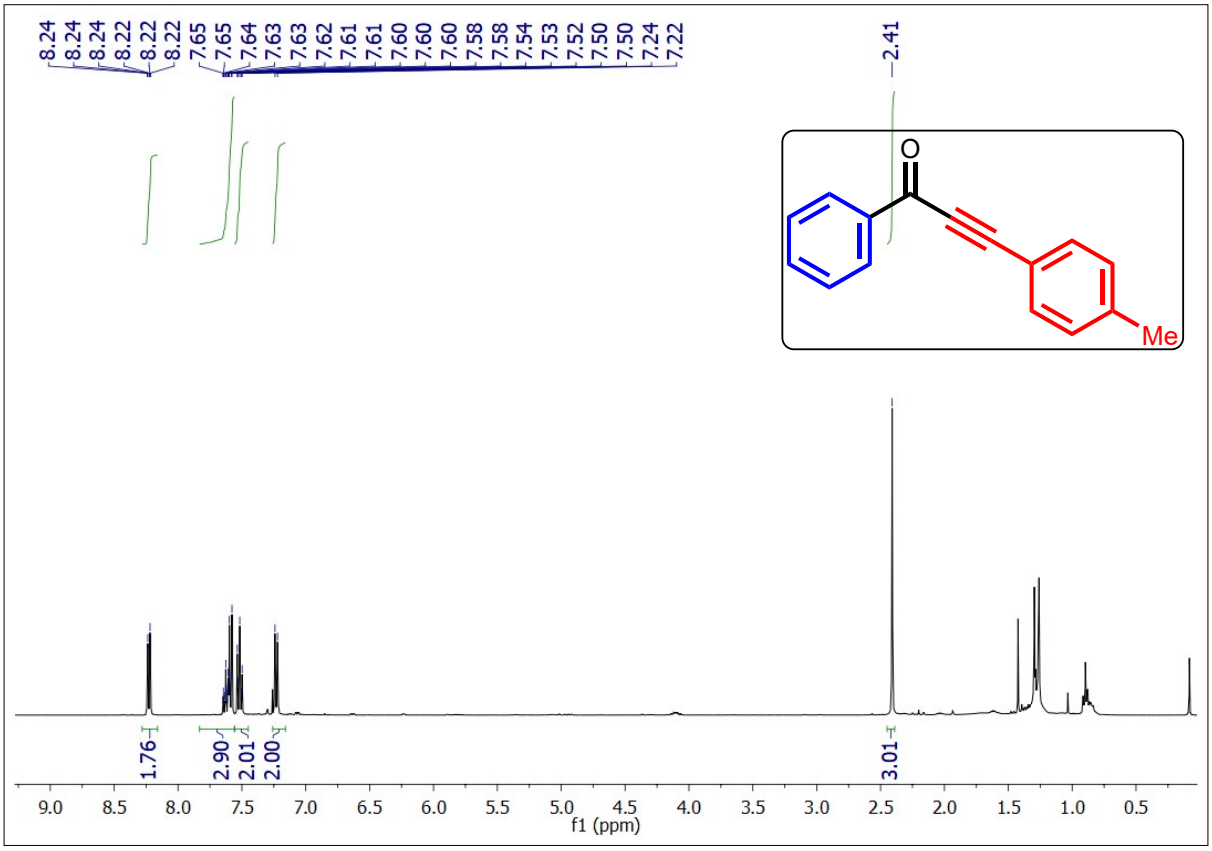


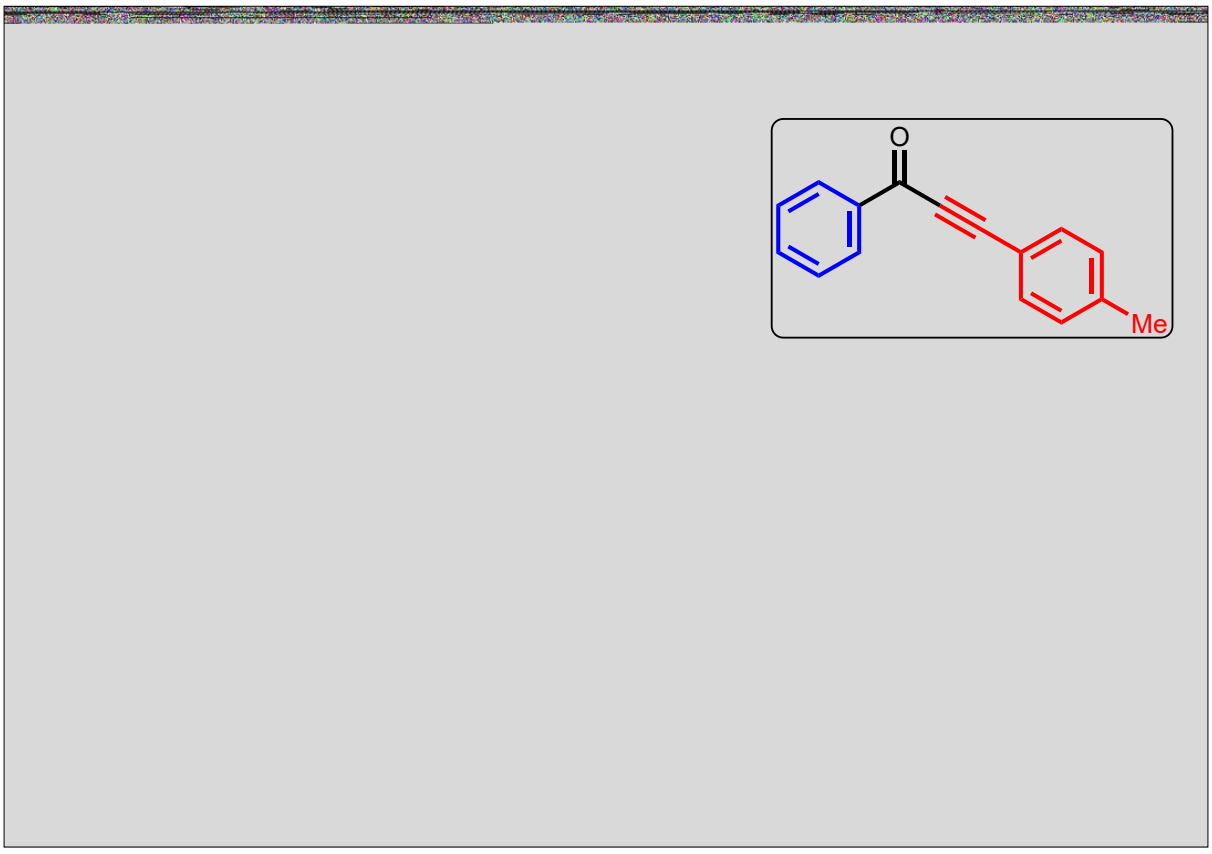
^{1}H and ^{13}C NMR spectra of 1,3-Diphenylprop-2-yn-1-one (3n)



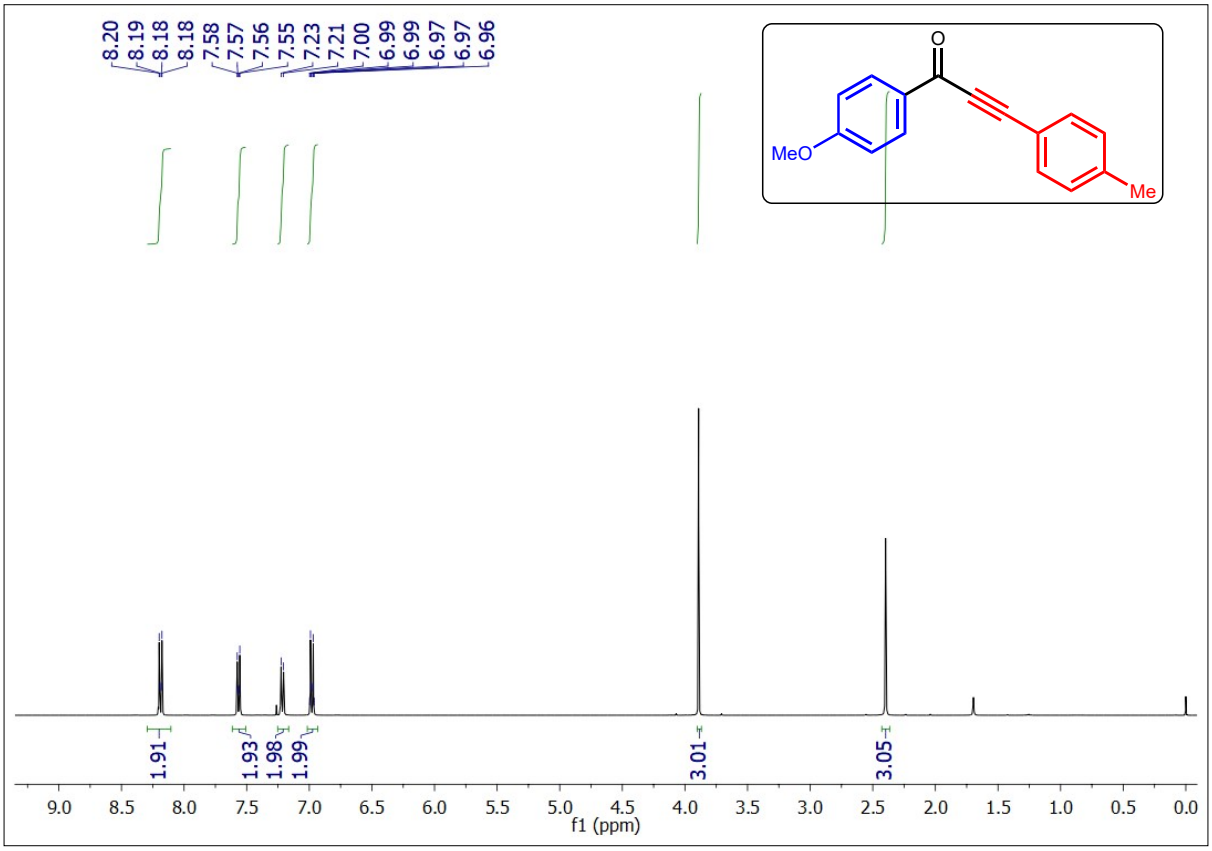


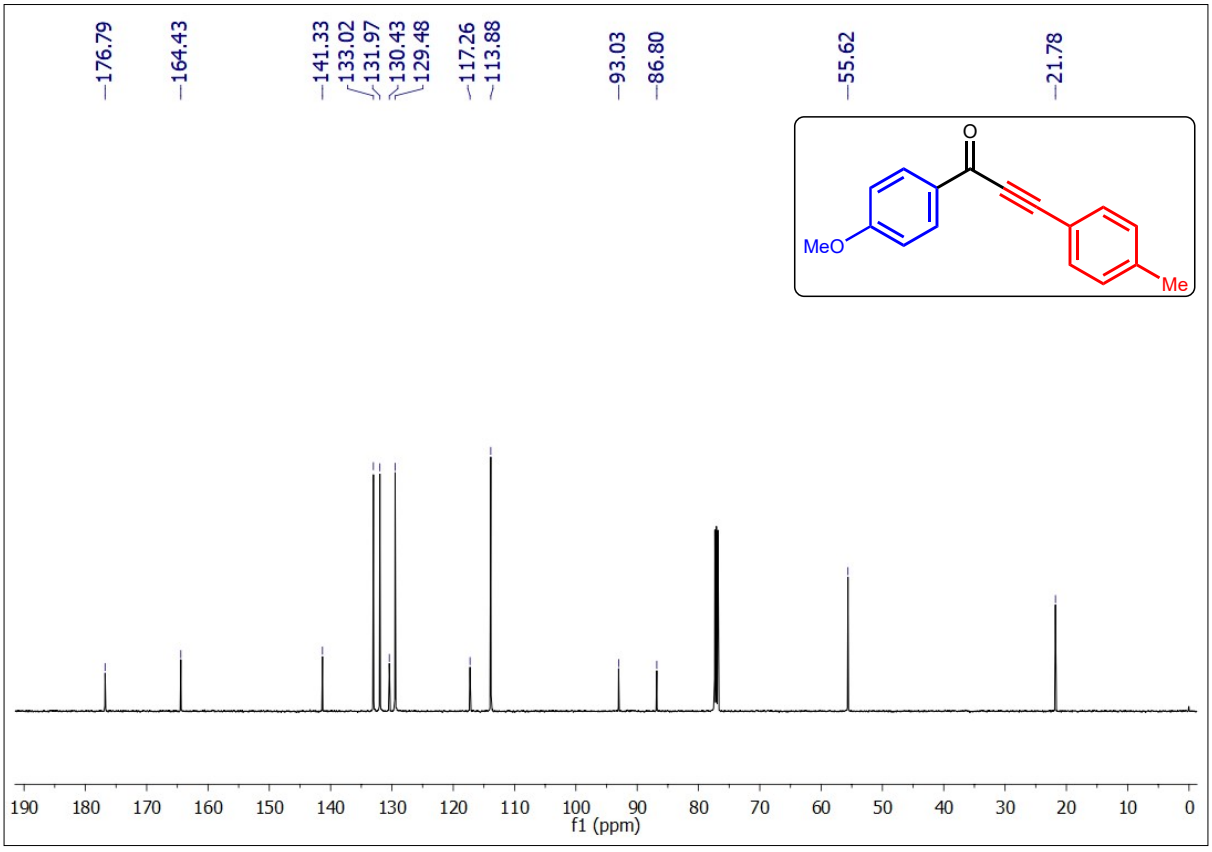
^{1}H and ^{13}C NMR spectra of 1-Phenyl-3-(*p*-tolyl)prop-2-yn-1-one (3o)



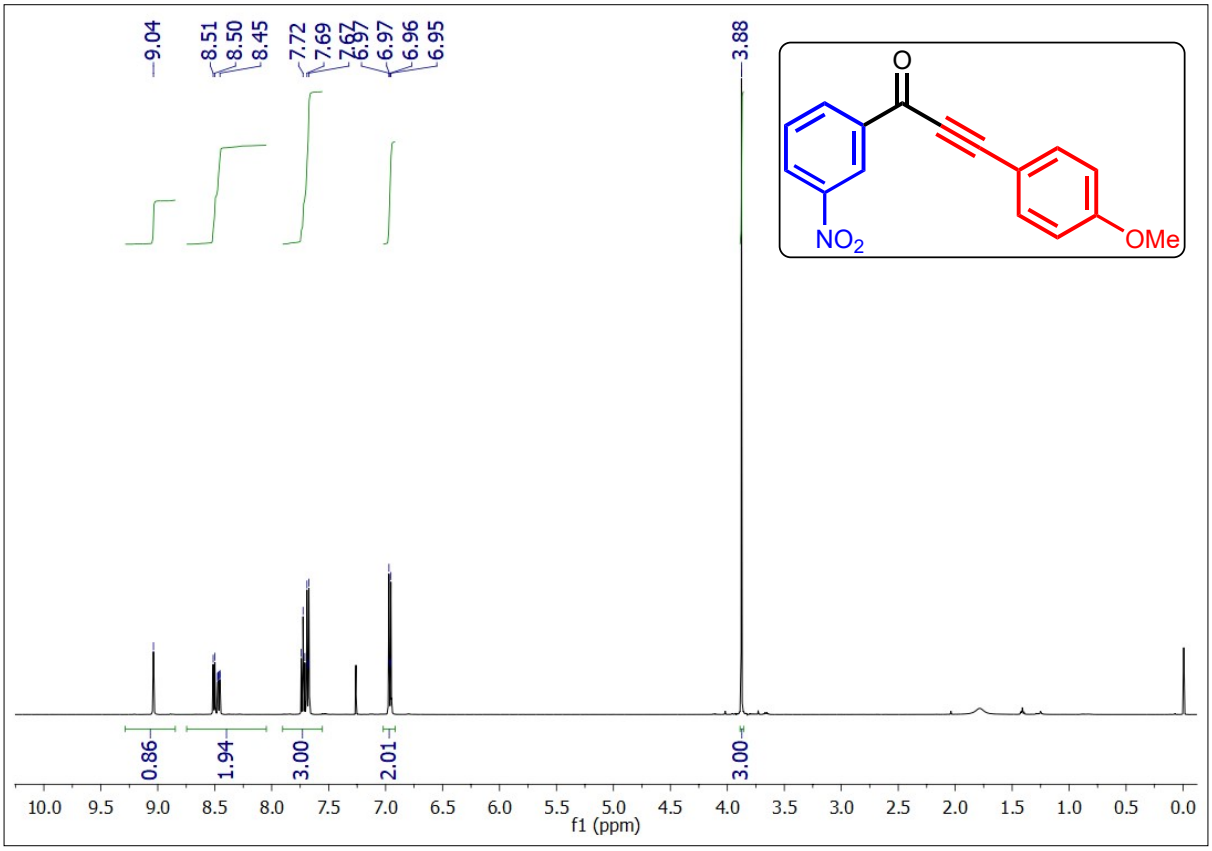


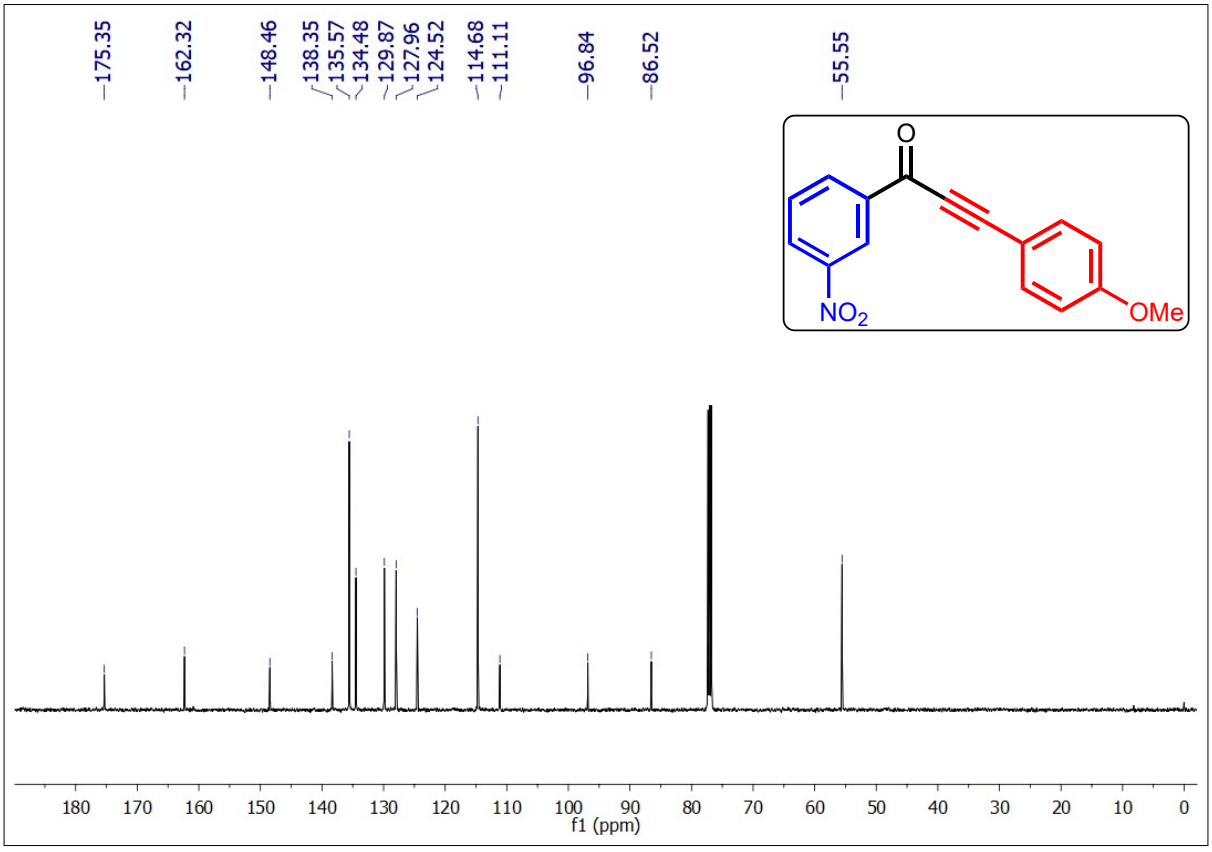
^{1}H and ^{13}C NMR spectra of 1-(4-methoxyphenyl)-3-(p-tolyl)prop-2-yn-1-one (3p)



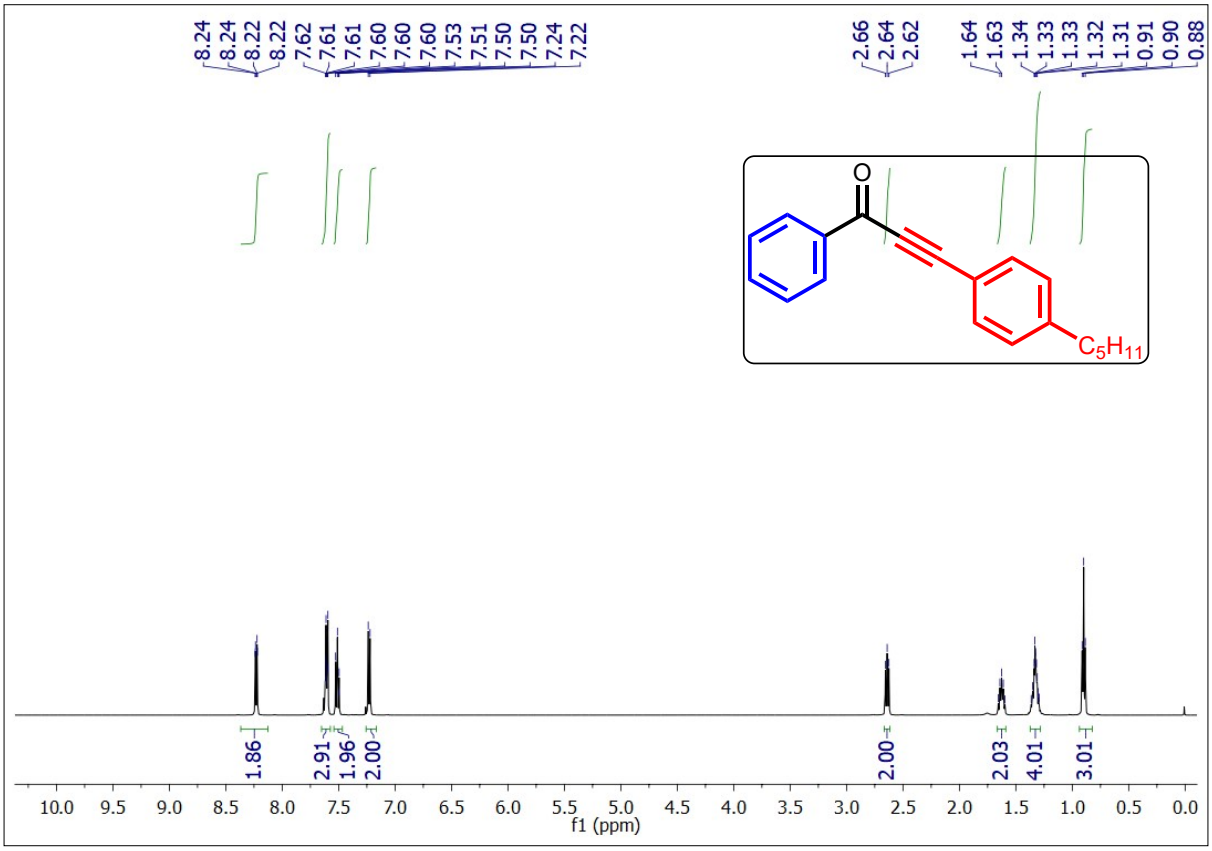


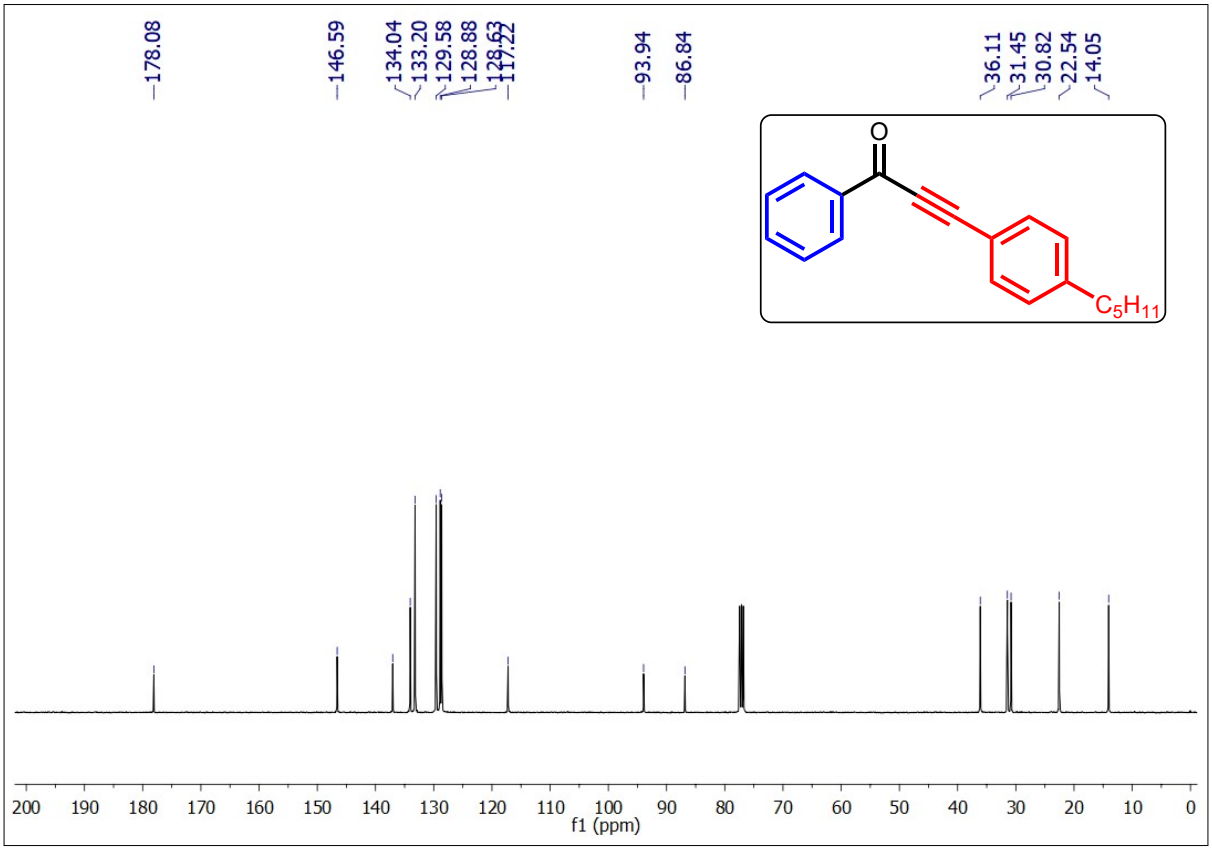
^{1}H and ^{13}C NMR spectra of 3-(4-Methoxyphenyl)-1-(3-nitrophenyl)prop-2-yn-1-one (3q)



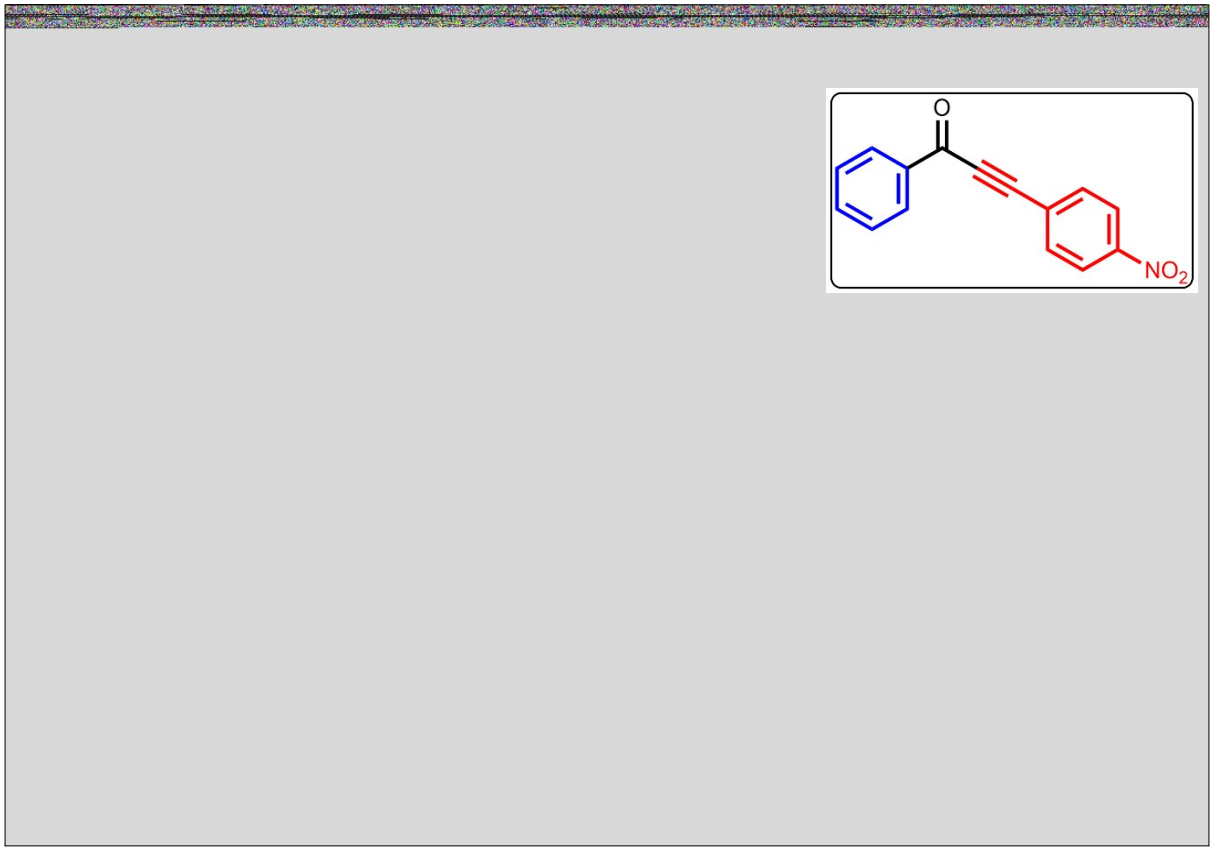


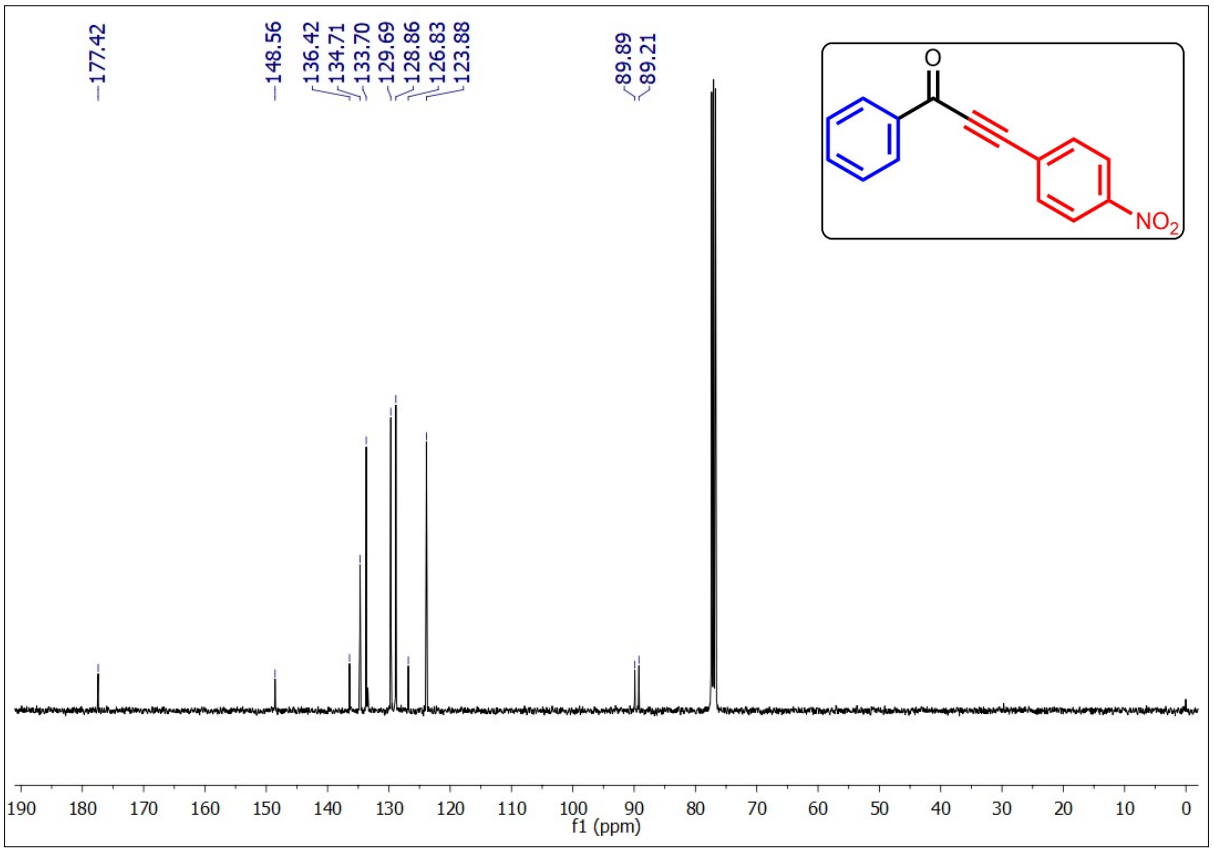
^{1}H and ^{13}C NMR spectra of 3-(4-(Pentyl)phenyl)-1-phenylprop-2-yn-1-one (3r)



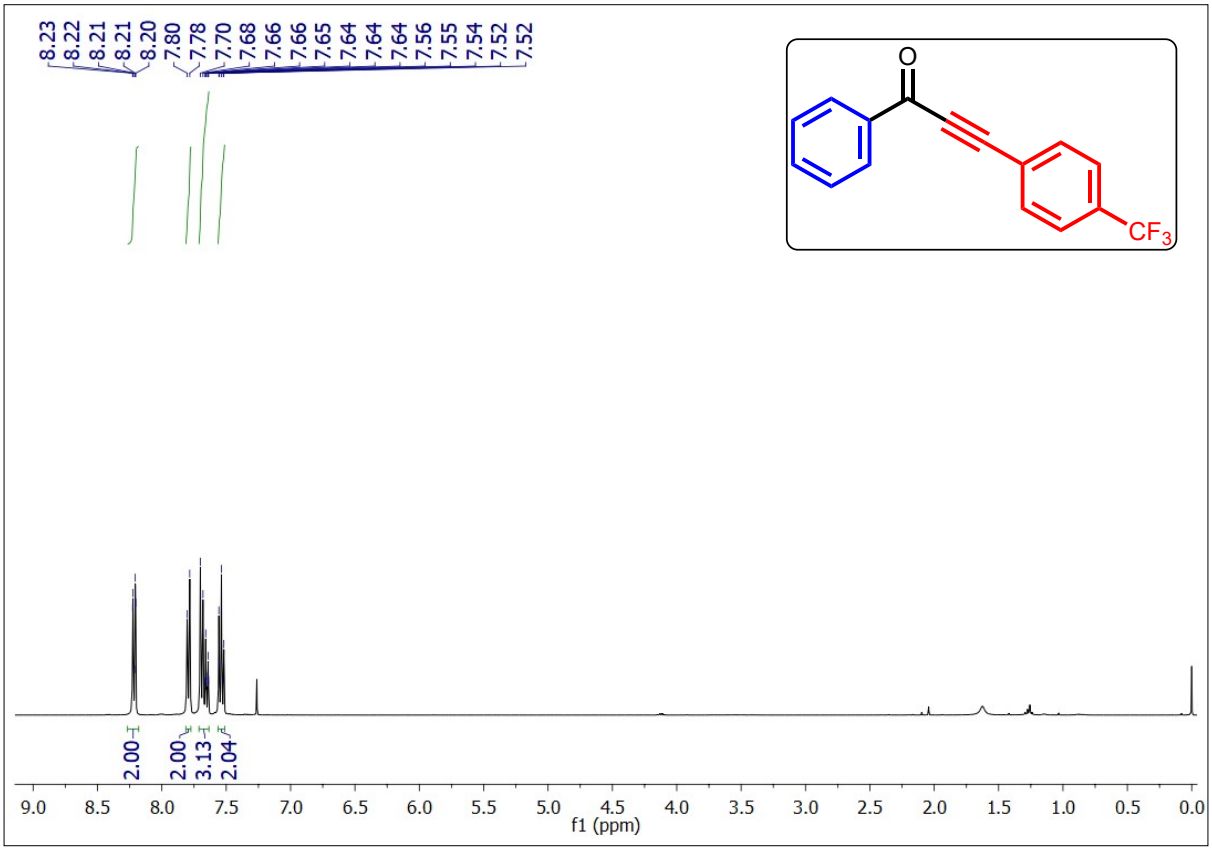


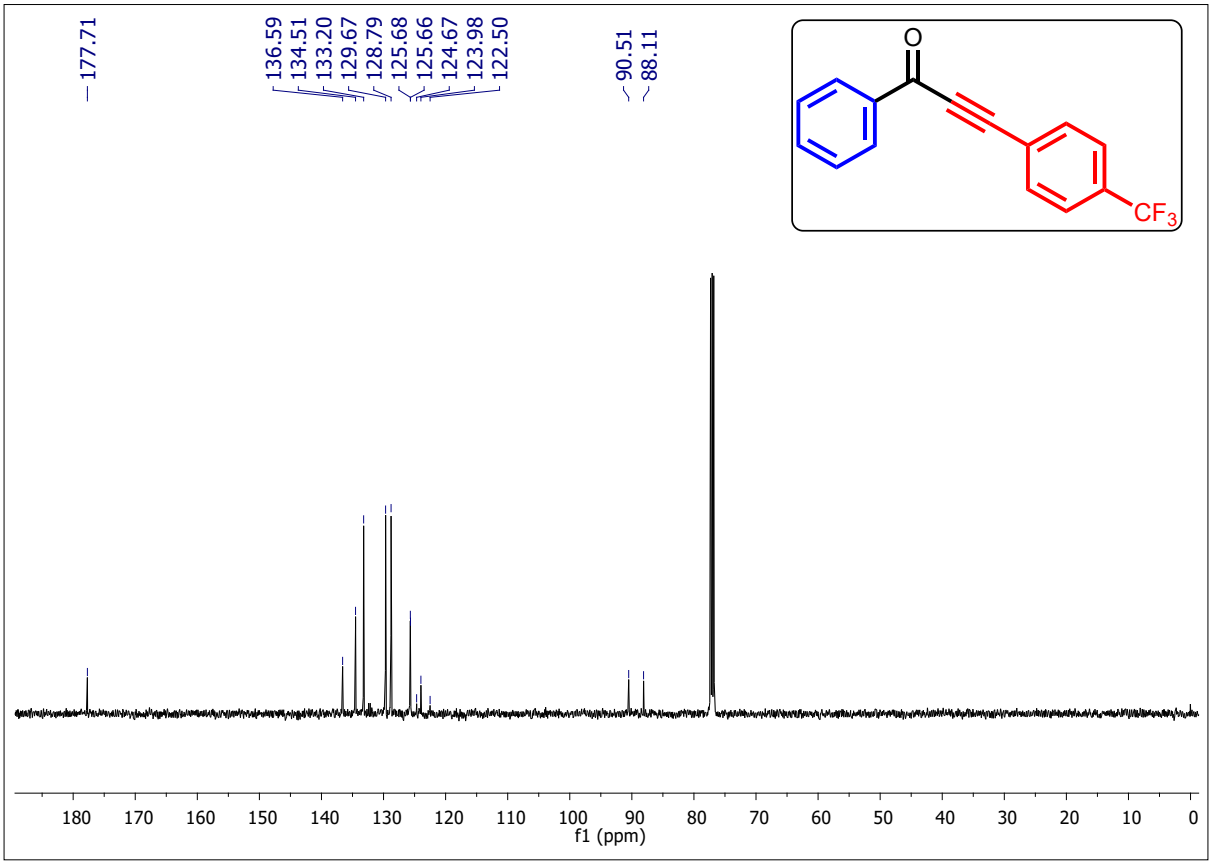
^{1}H and ^{13}C NMR spectra of 3-(4-Nitrophenyl)-1-phenylprop-2-yn-1-one (3s)



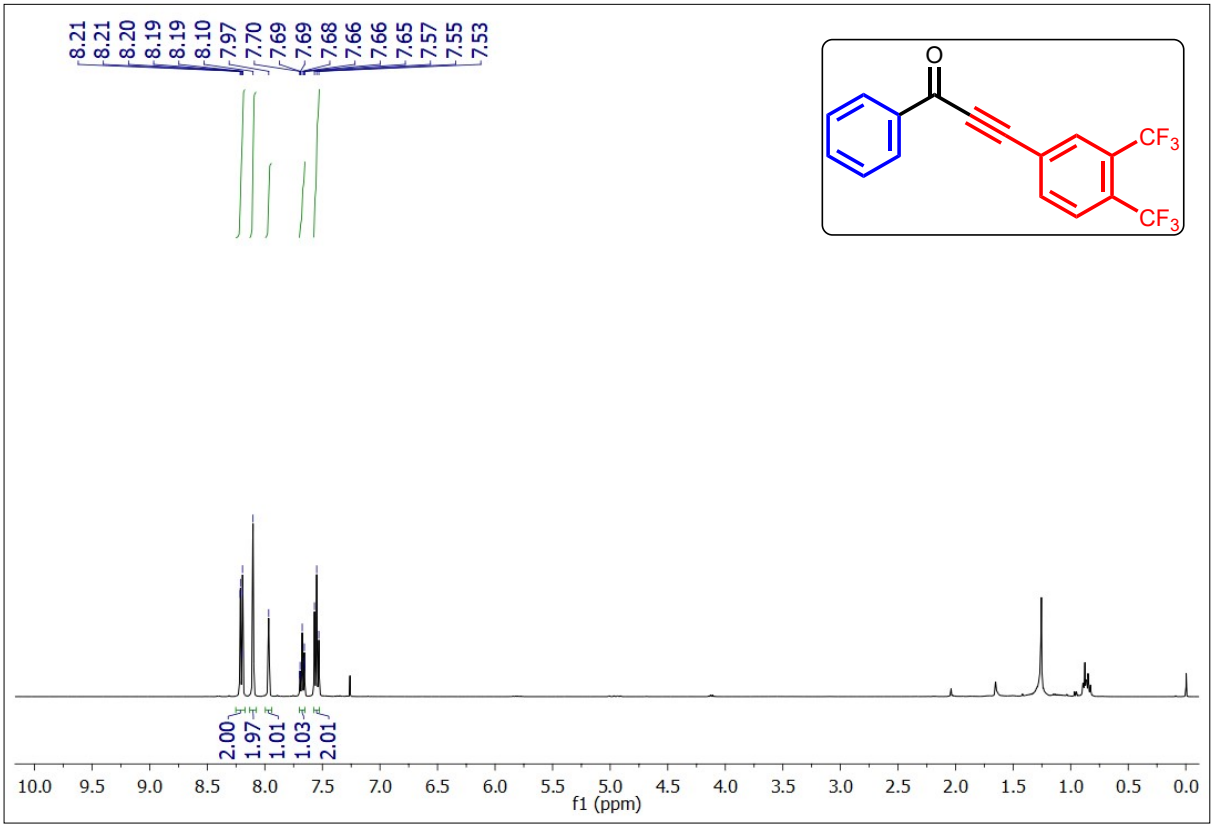


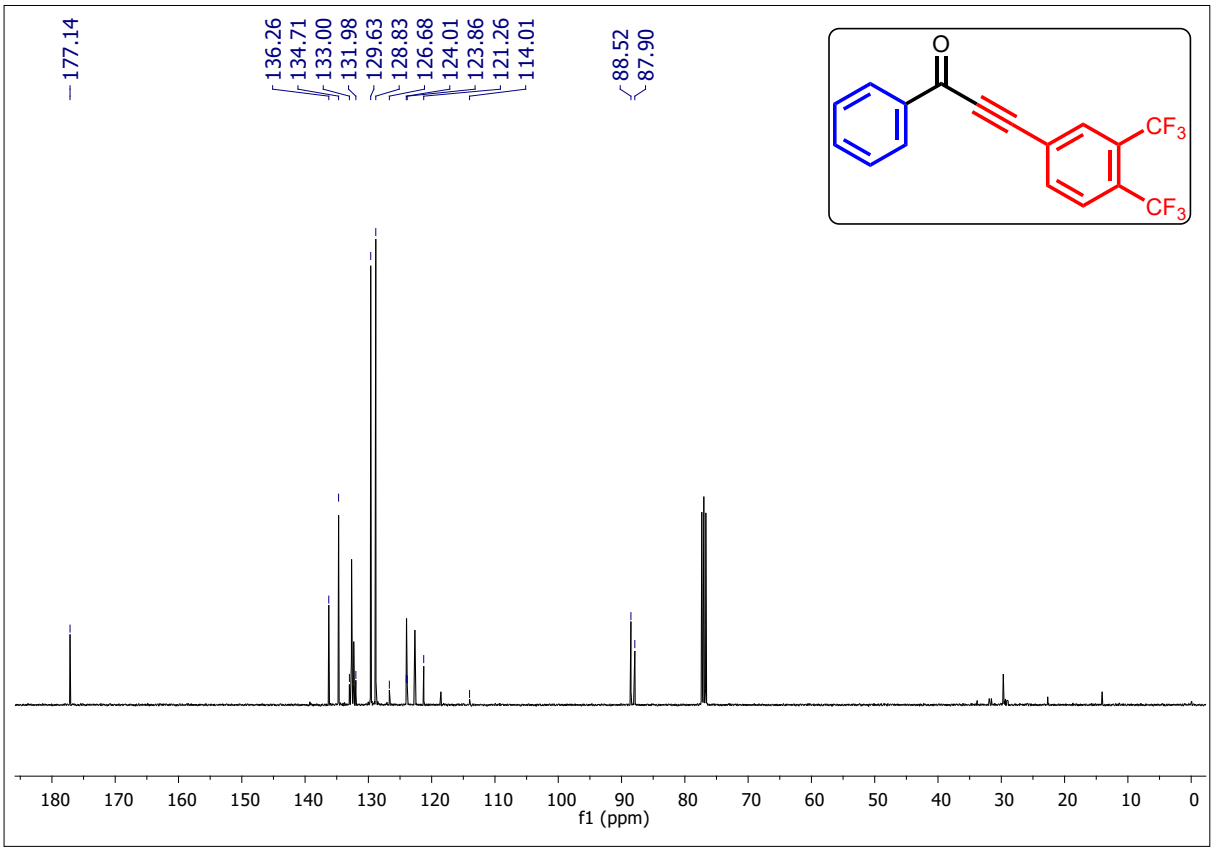
^{1}H and ^{13}C NMR spectra of 1-Phenyl-3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (3t)



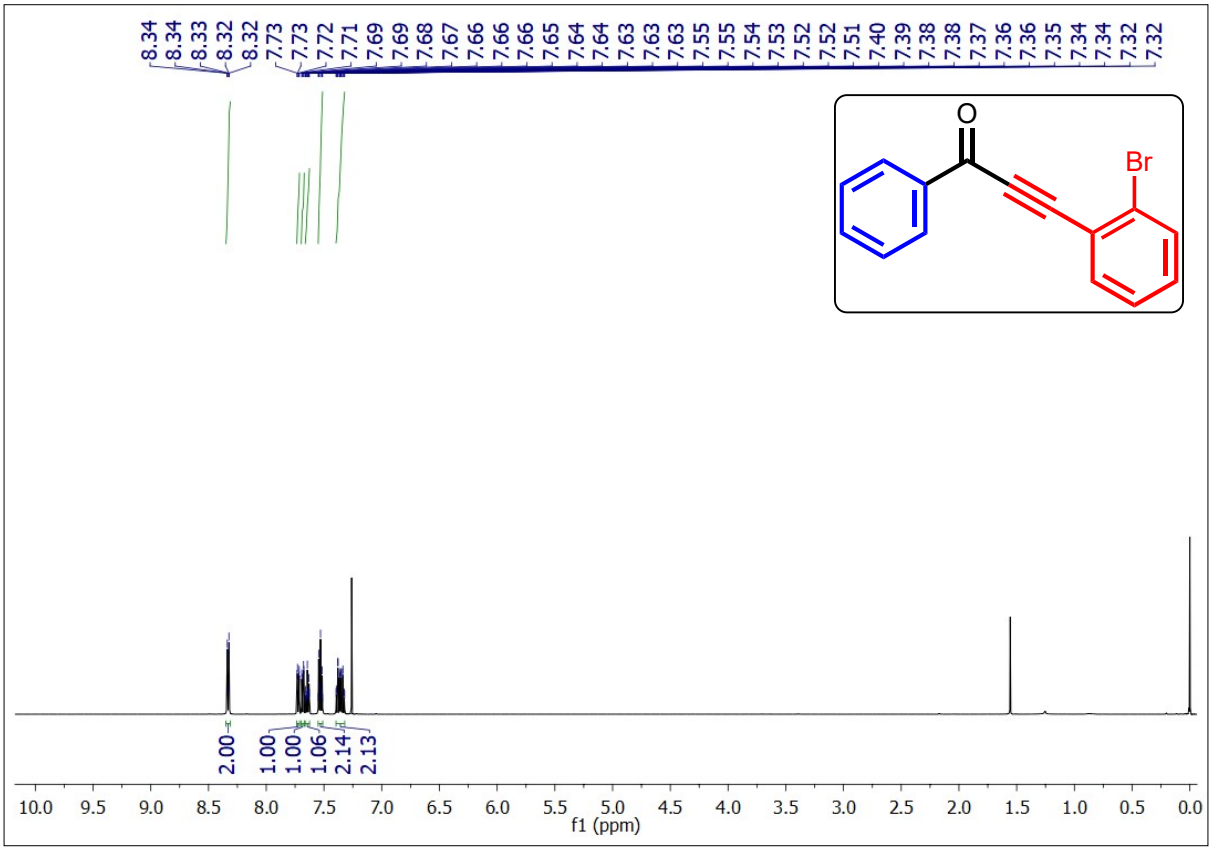


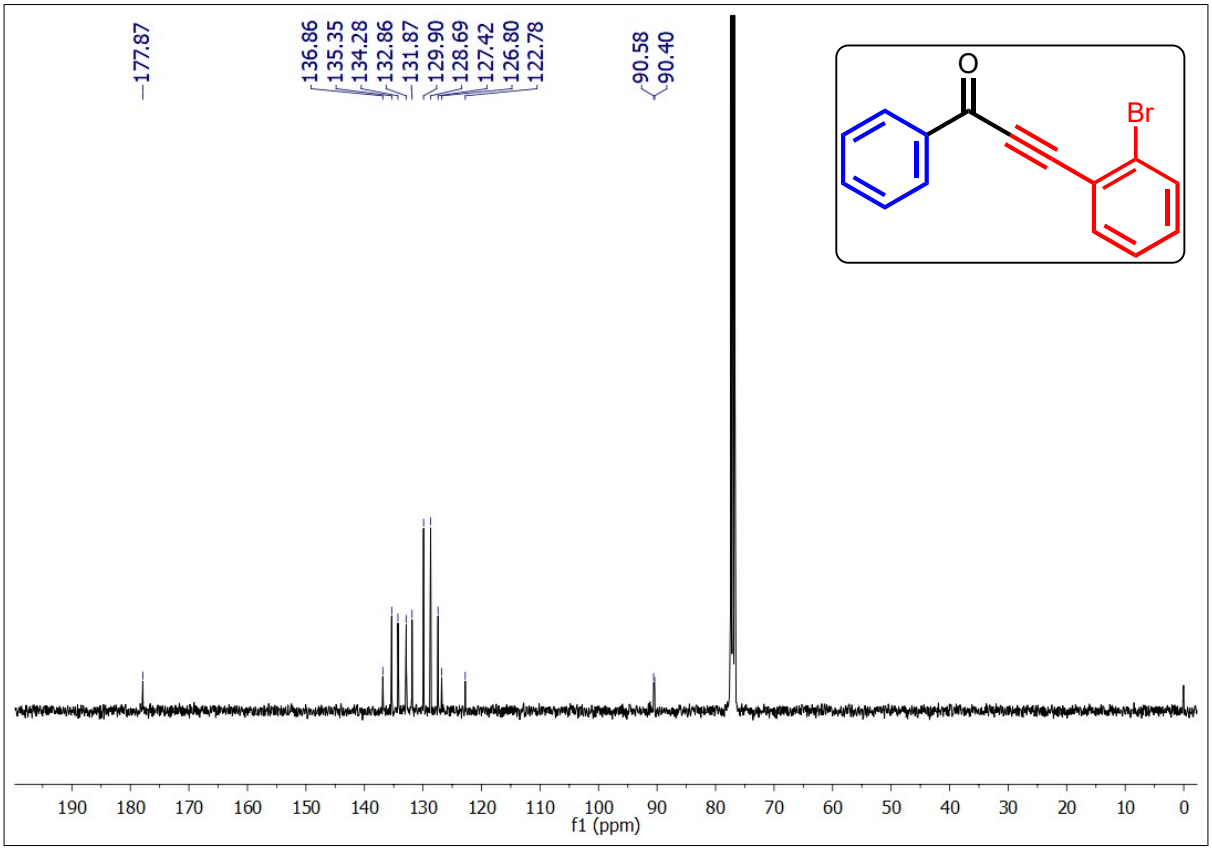
^{1}H and ^{13}C NMR spectra of 3-(3,4-Bis(trifluoromethyl)phenyl)-1-phenylprop-2-yn-1-one (3u)



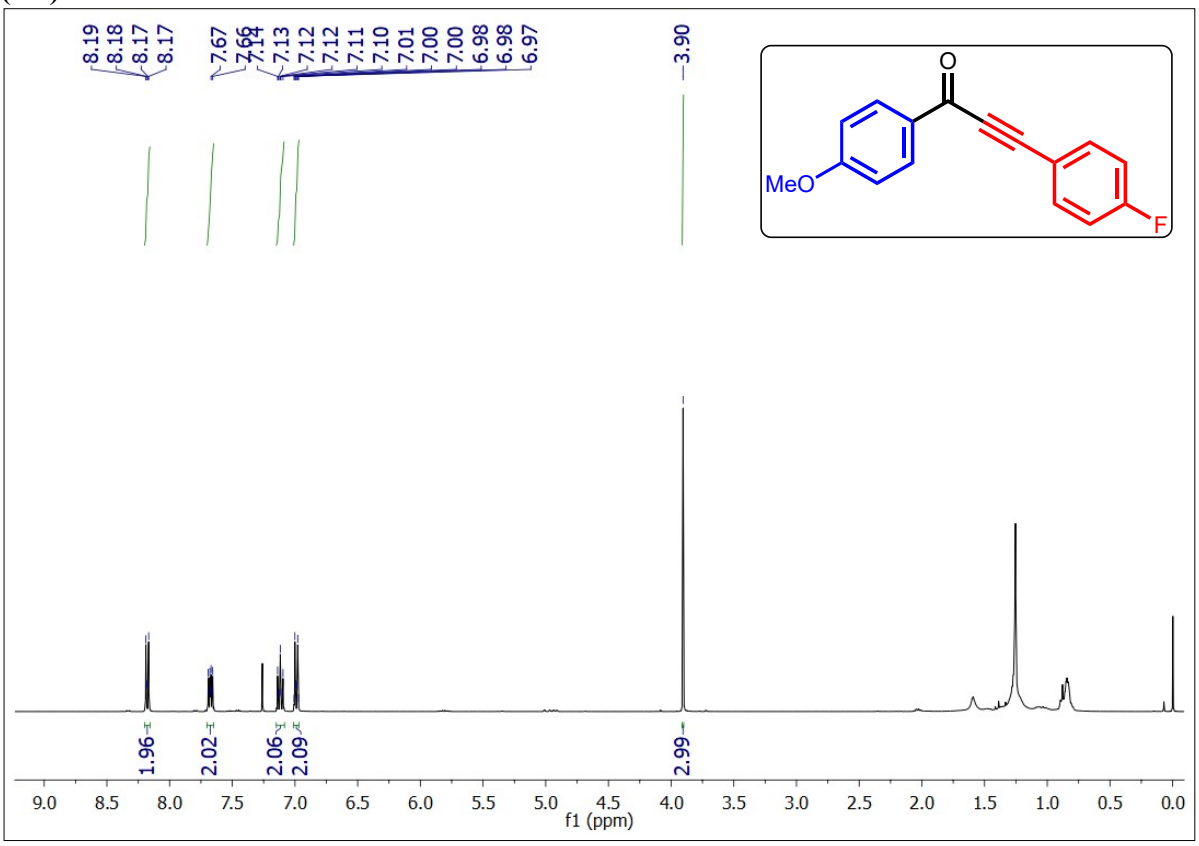


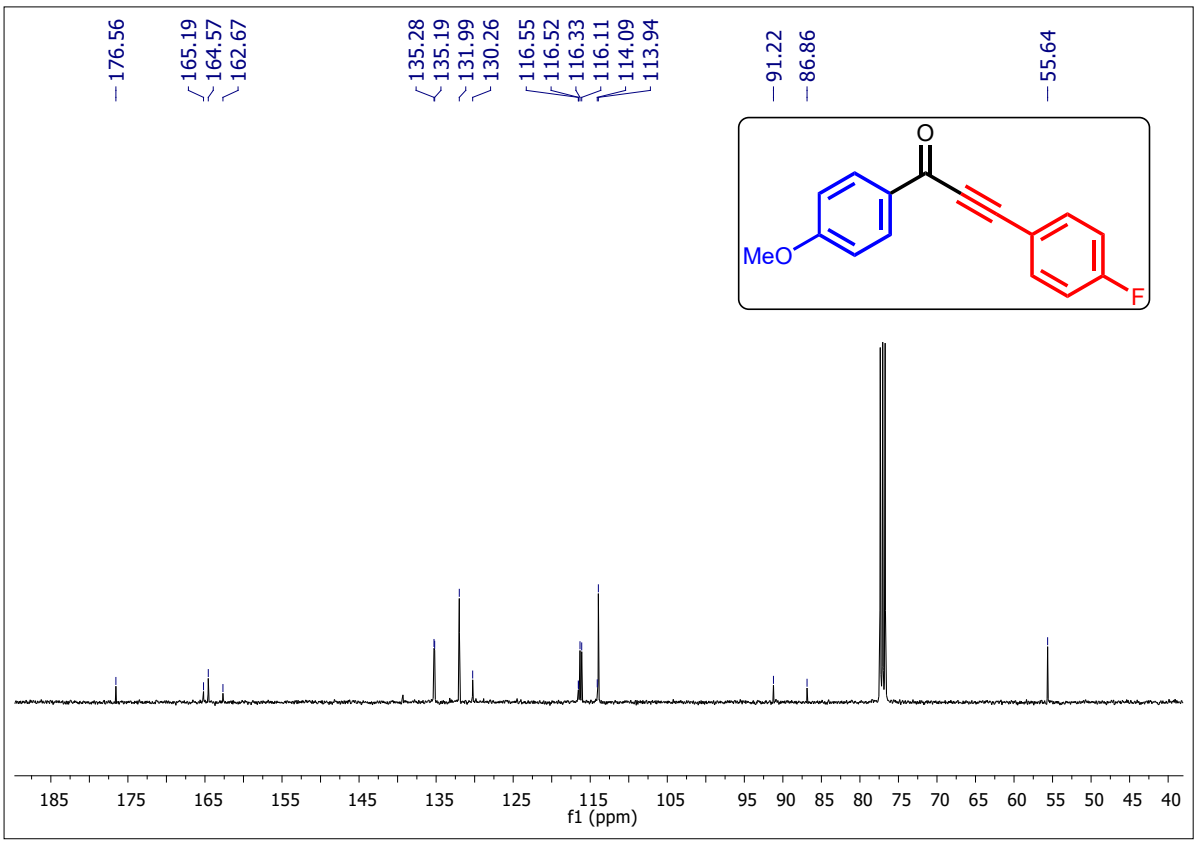
^{1}H and ^{13}C NMR spectra of 3-(2-Bromophenyl)-1-phenylprop-2-yn-1-one (3v)



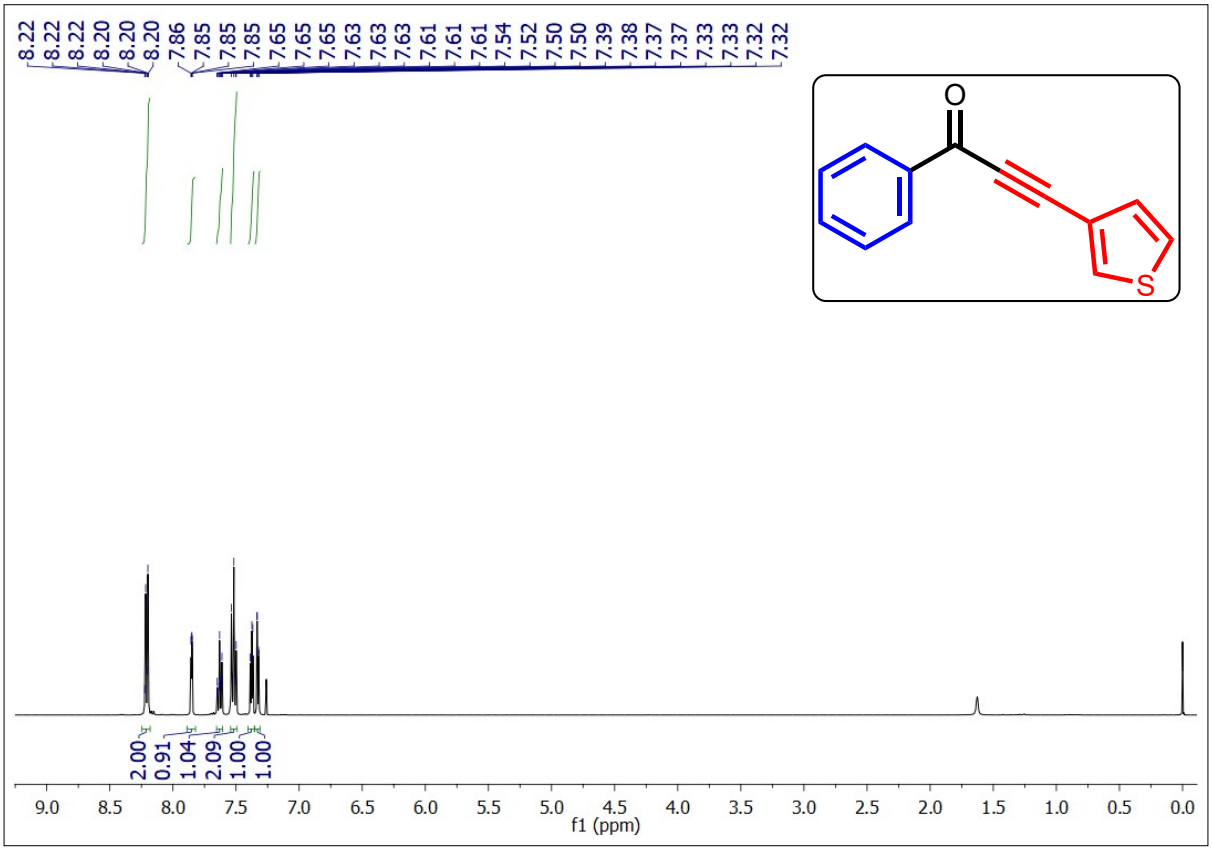


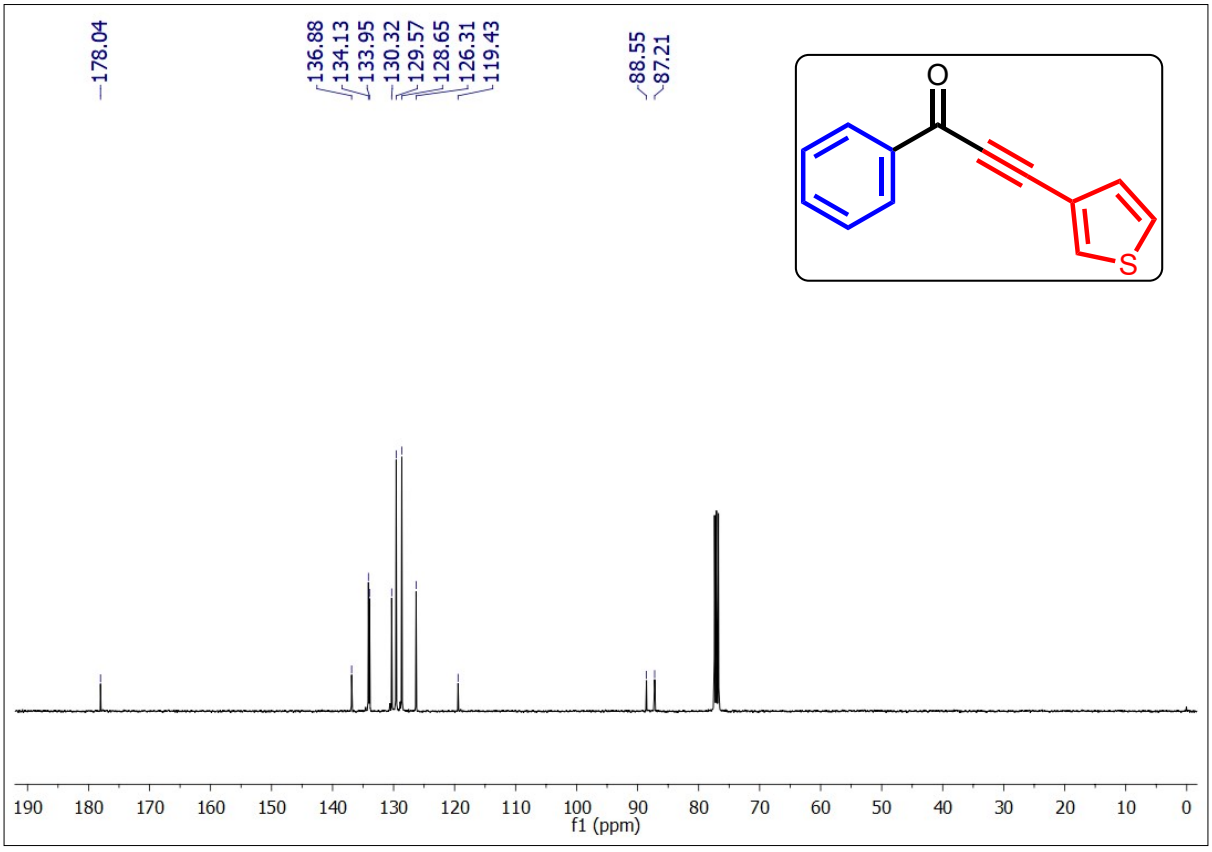
^{1}H and ^{13}C NMR spectra of 3-(4-fluorophenyl)-1-(4-methoxyphenyl)prop-2-yn-1-one (3w)



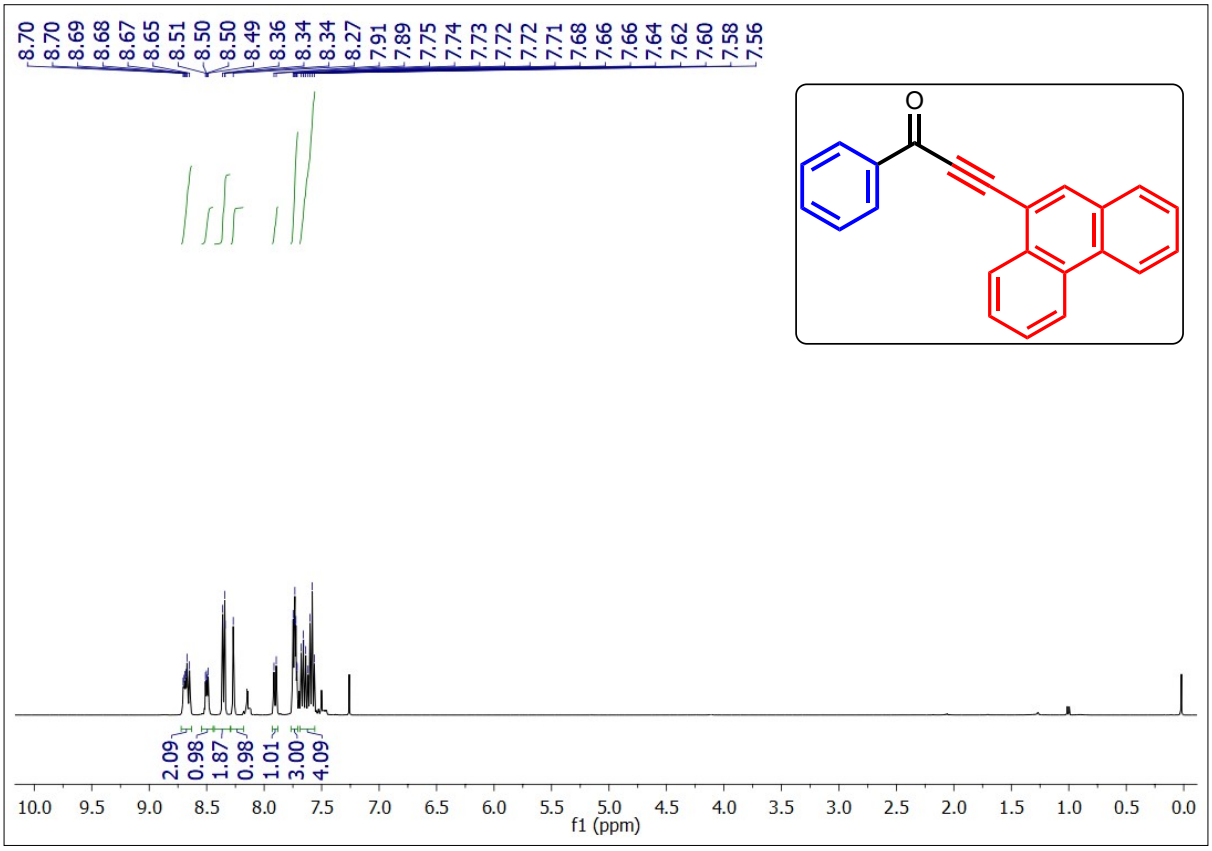


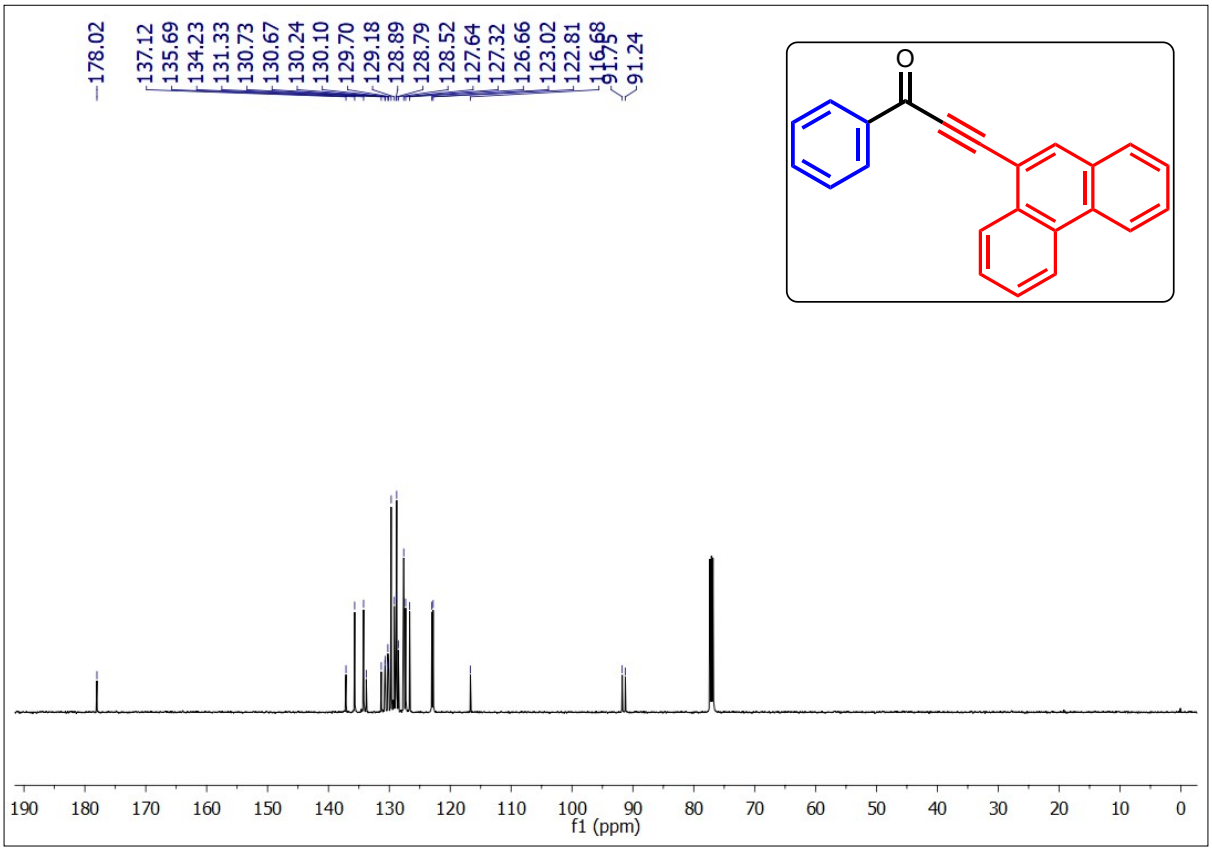
^{1}H and ^{13}C NMR spectra of 1-Phenyl-3-(thiophen-3-yl)prop-2-yn-1-one (3x)



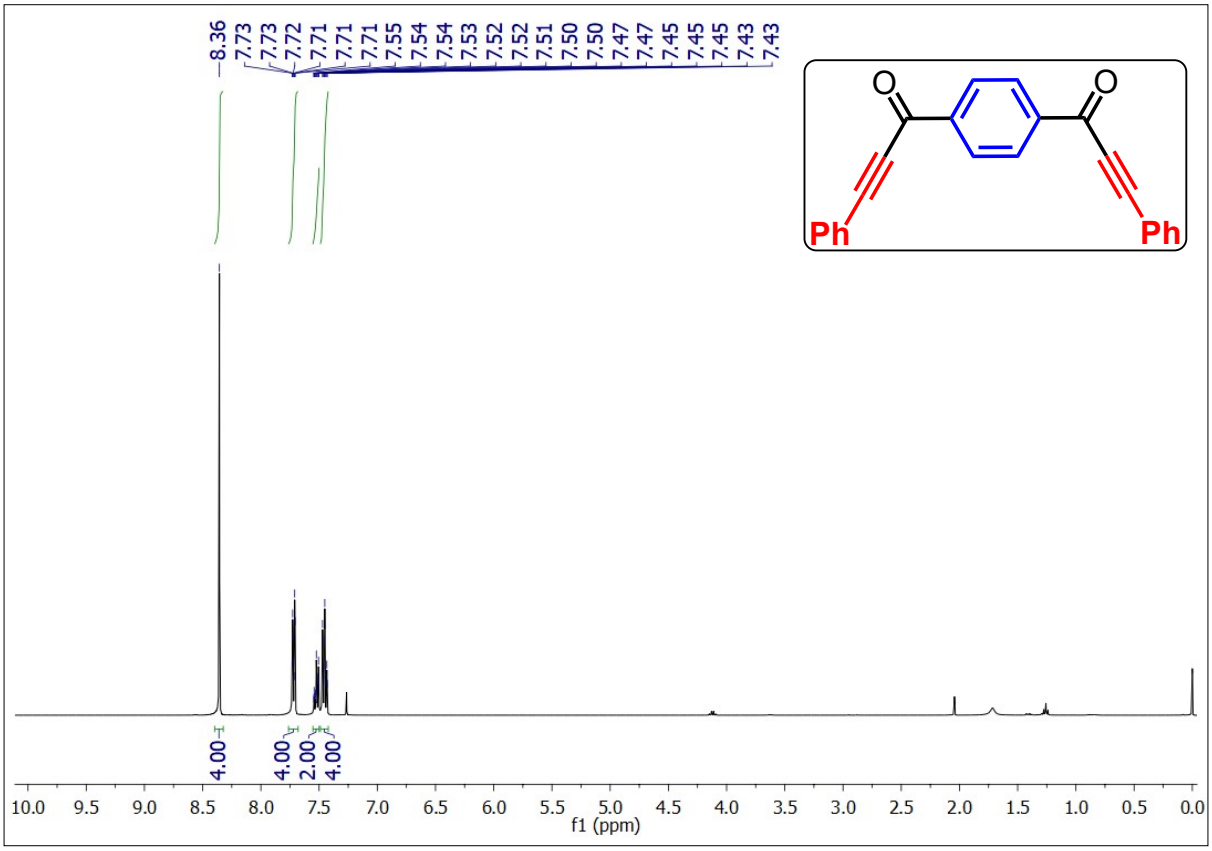


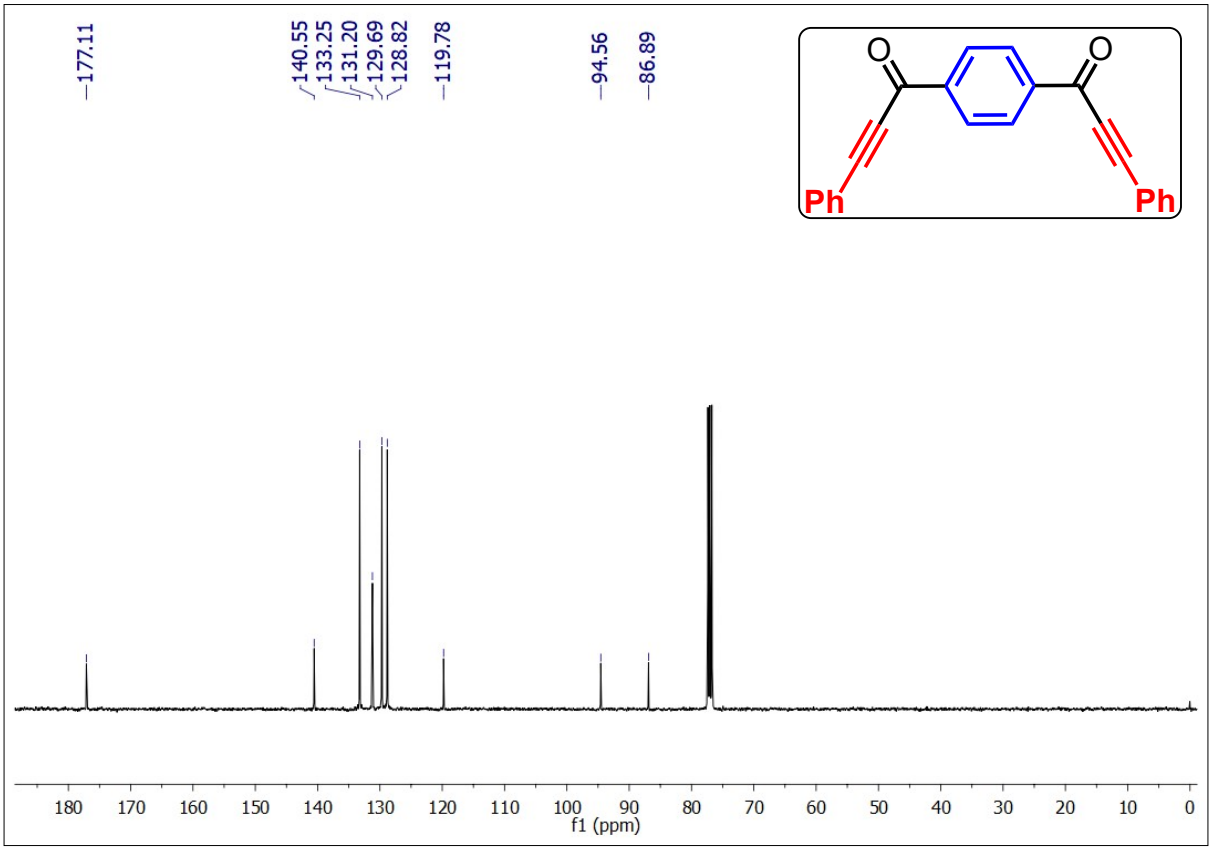
^{1}H and ^{13}C NMR spectra of 3-(Phenanthren-9-yl)-1-phenylprop-2-yn-1-one (3y)



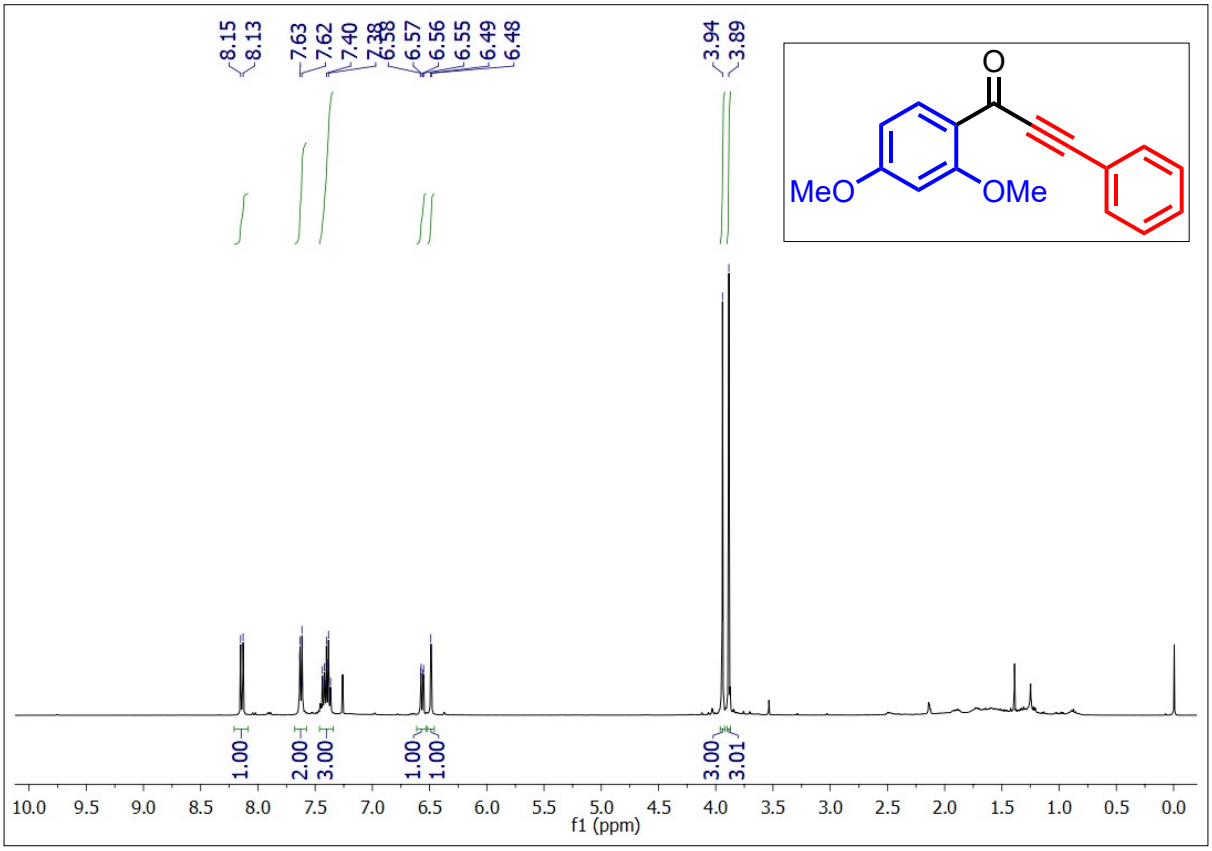


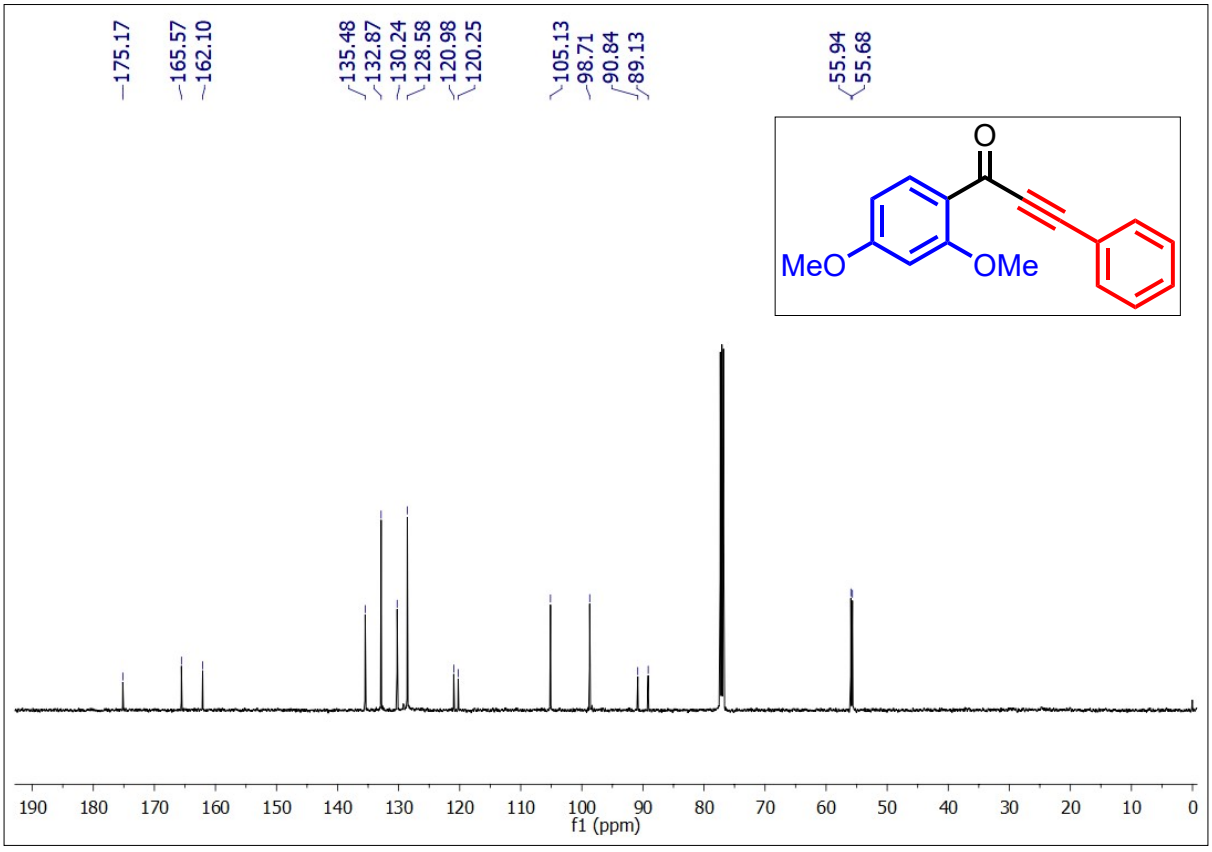
^{1}H and ^{13}C NMR spectra of 1,1'-(1,4-Phenylene)bis(3-phenylprop-2-yn-1-one) (3z)



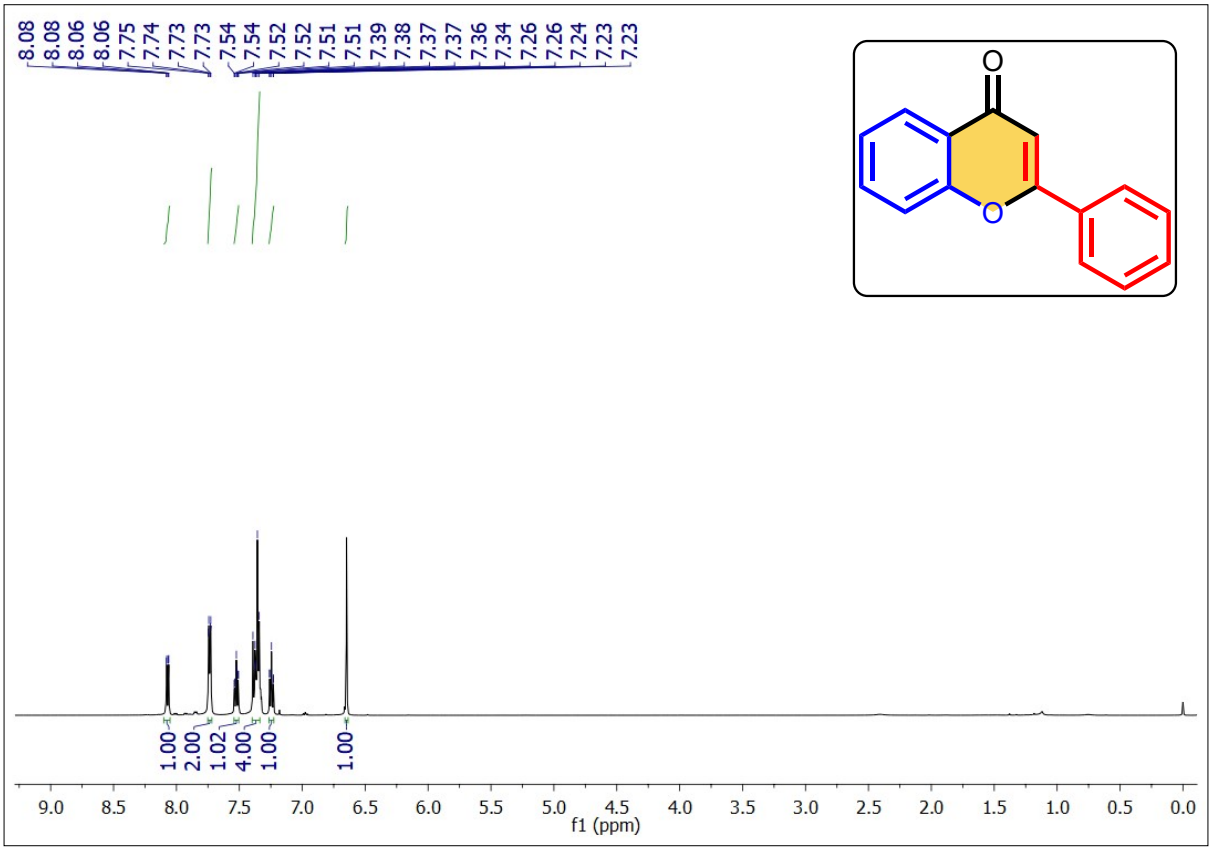


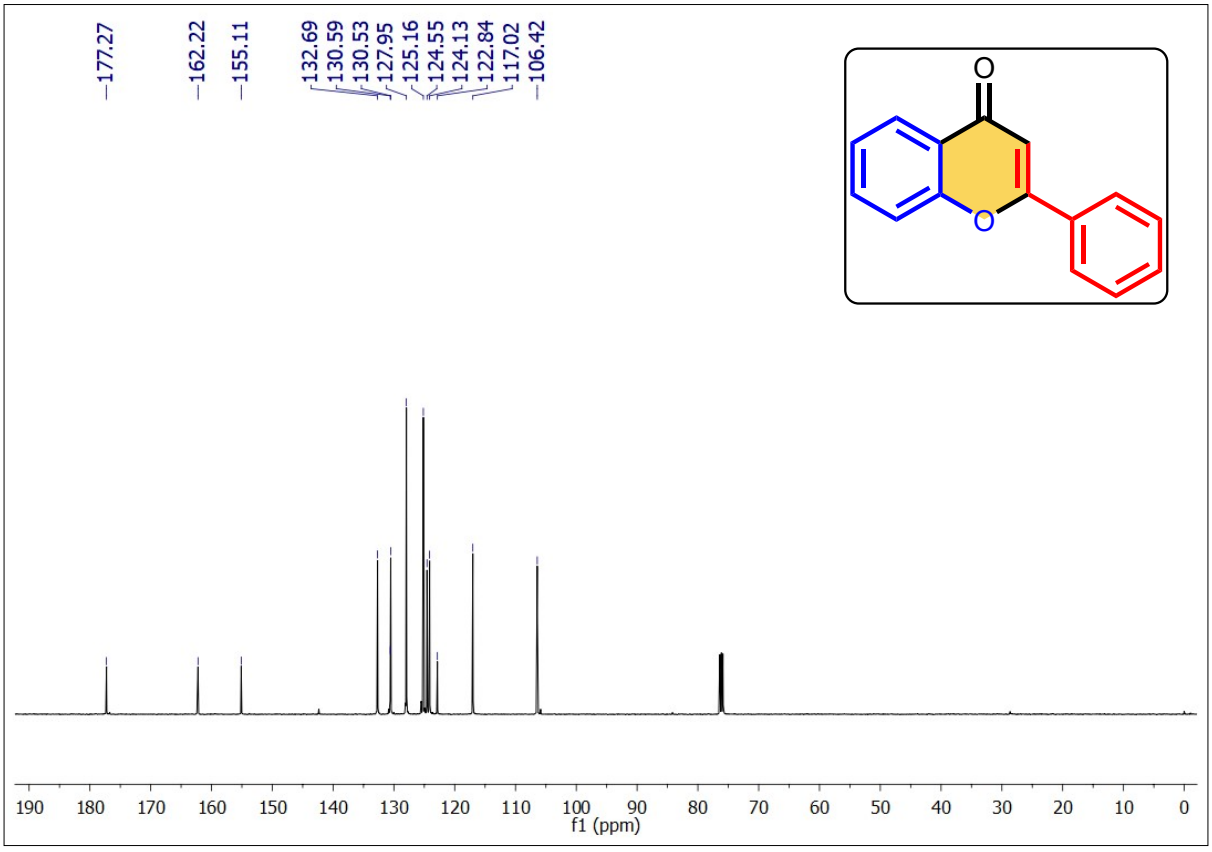
^{1}H and ^{13}C NMR spectra of 1-(2,4-Dimethoxyphenyl)-3-phenylprop-2-yn-1-one (3za)



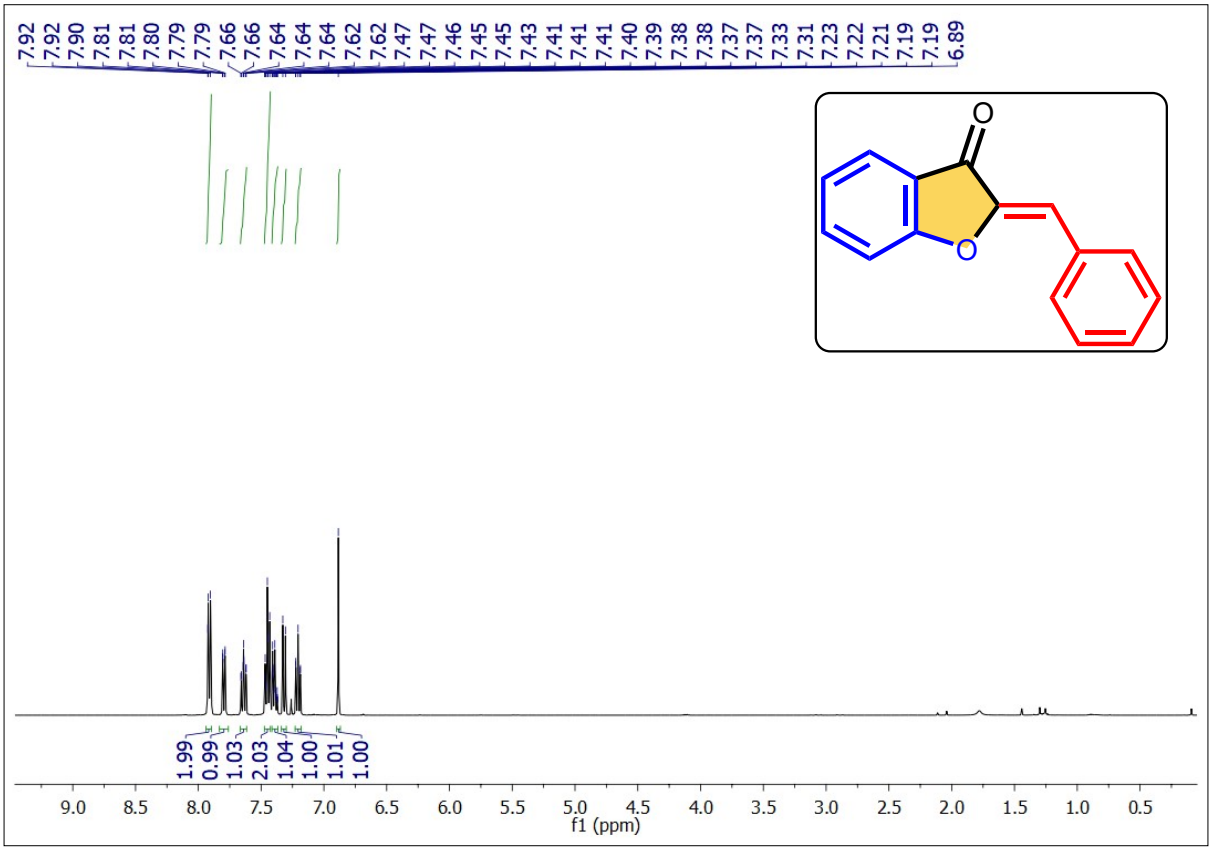


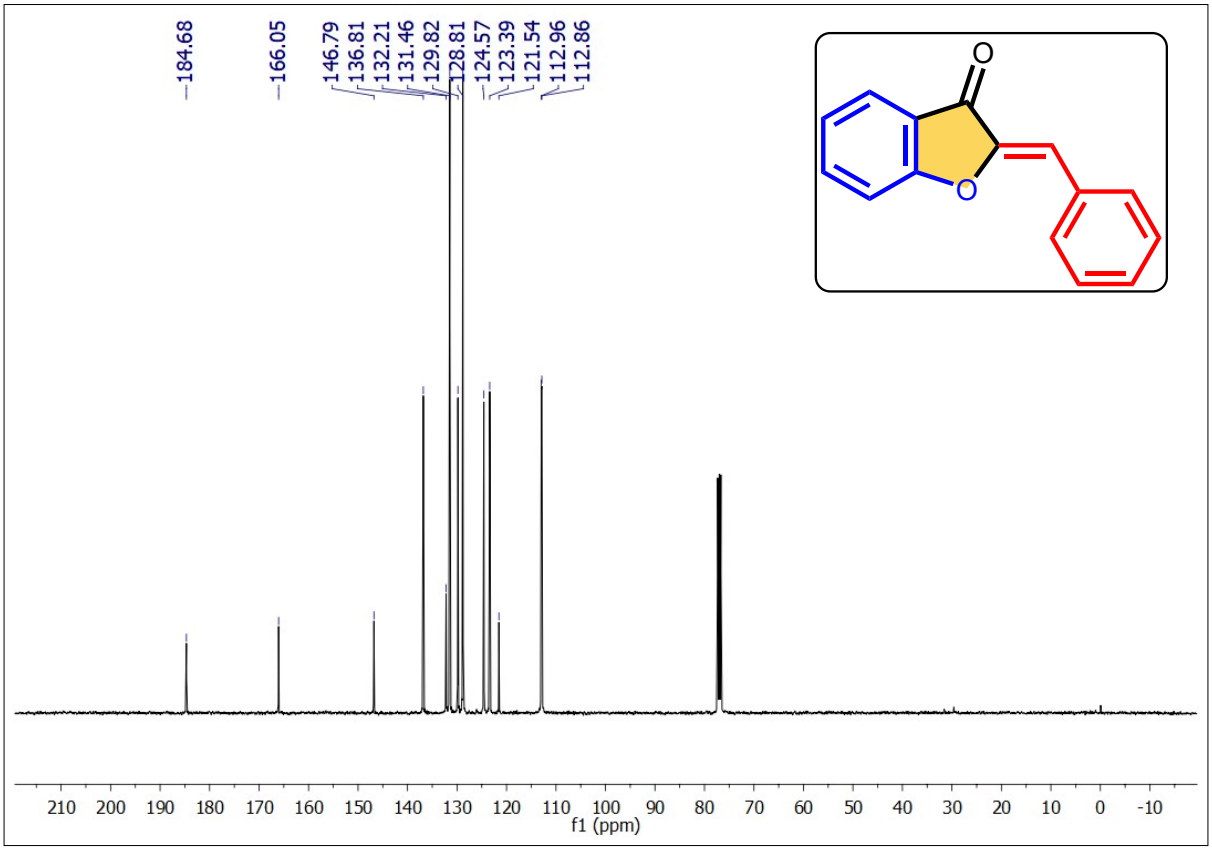
^{1}H and ^{13}C NMR spectra of 2-Phenyl-4*H*-chromen-4-one (6a)



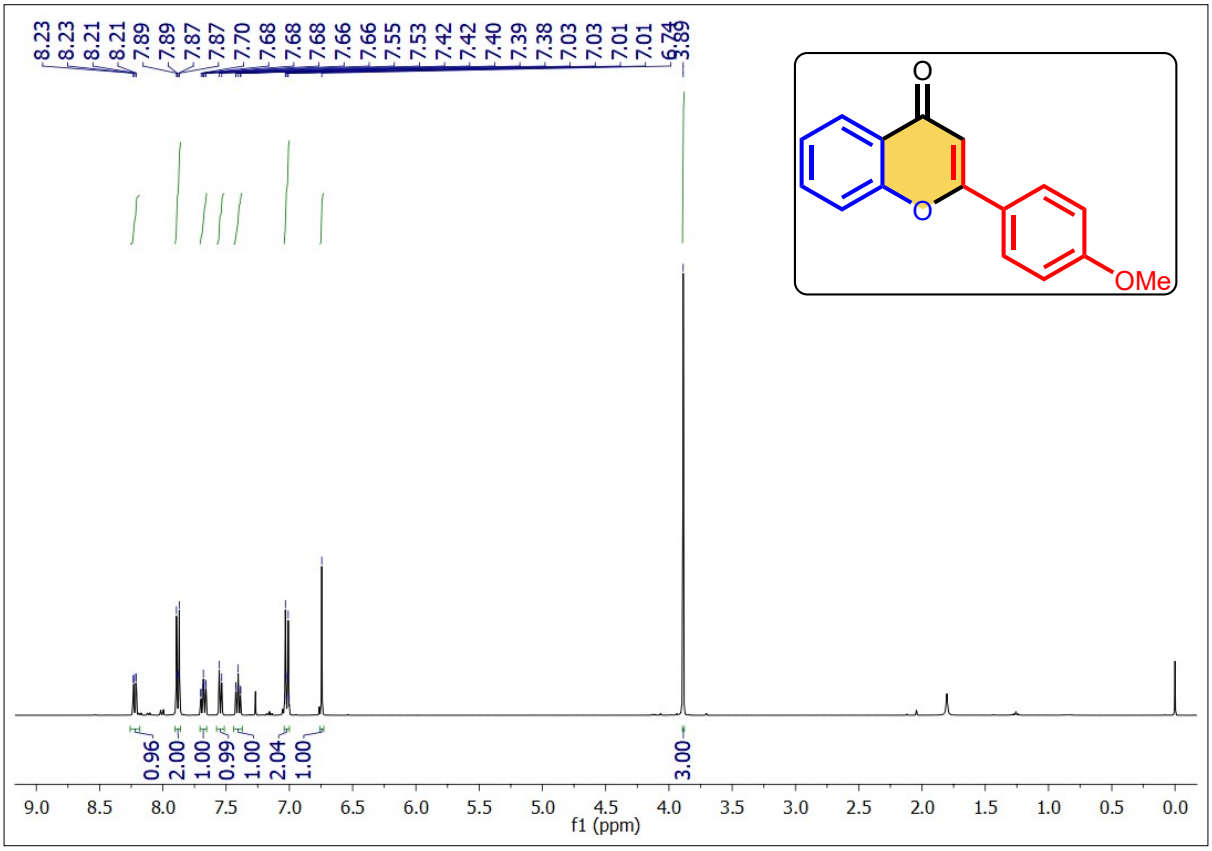


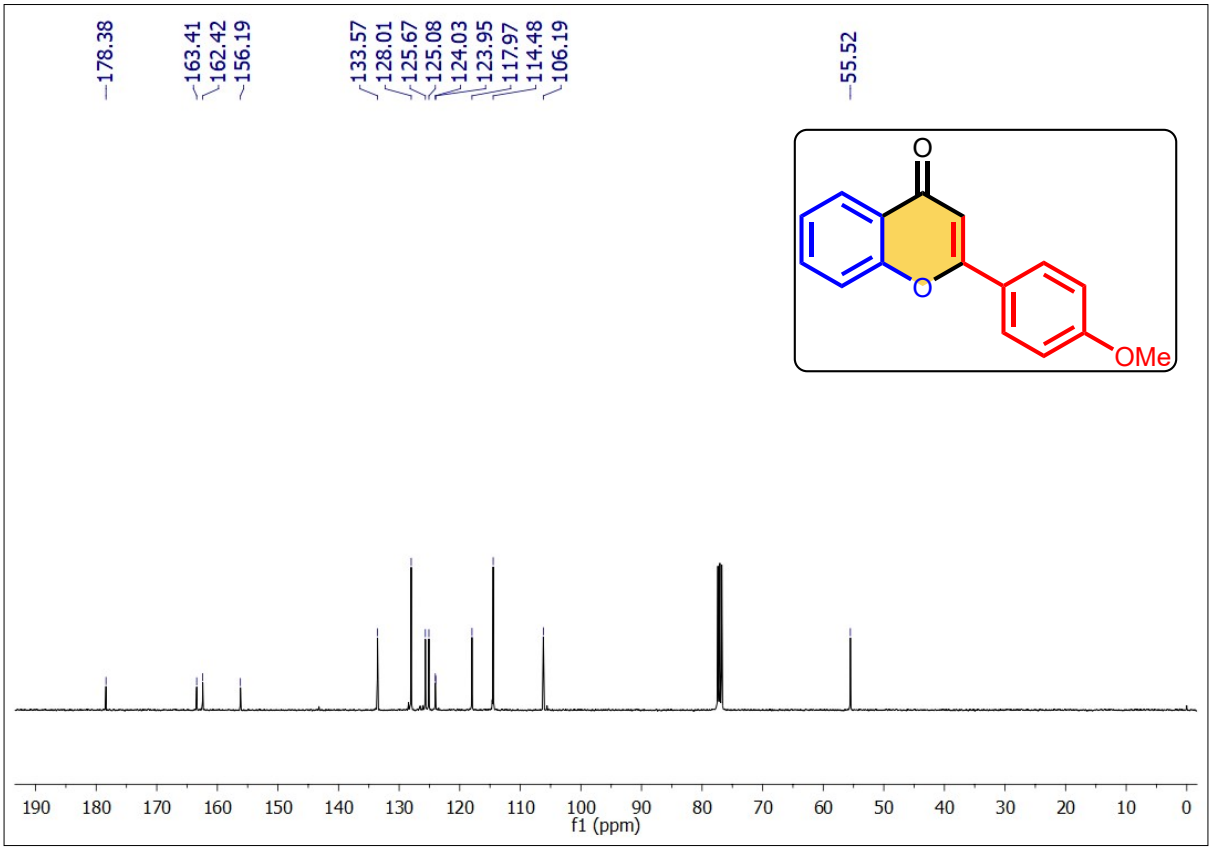
^{1}H and ^{13}C NMR spectra of (Z)-2-Benzylidenebenzofuran-3(2*H*)-one (7a)



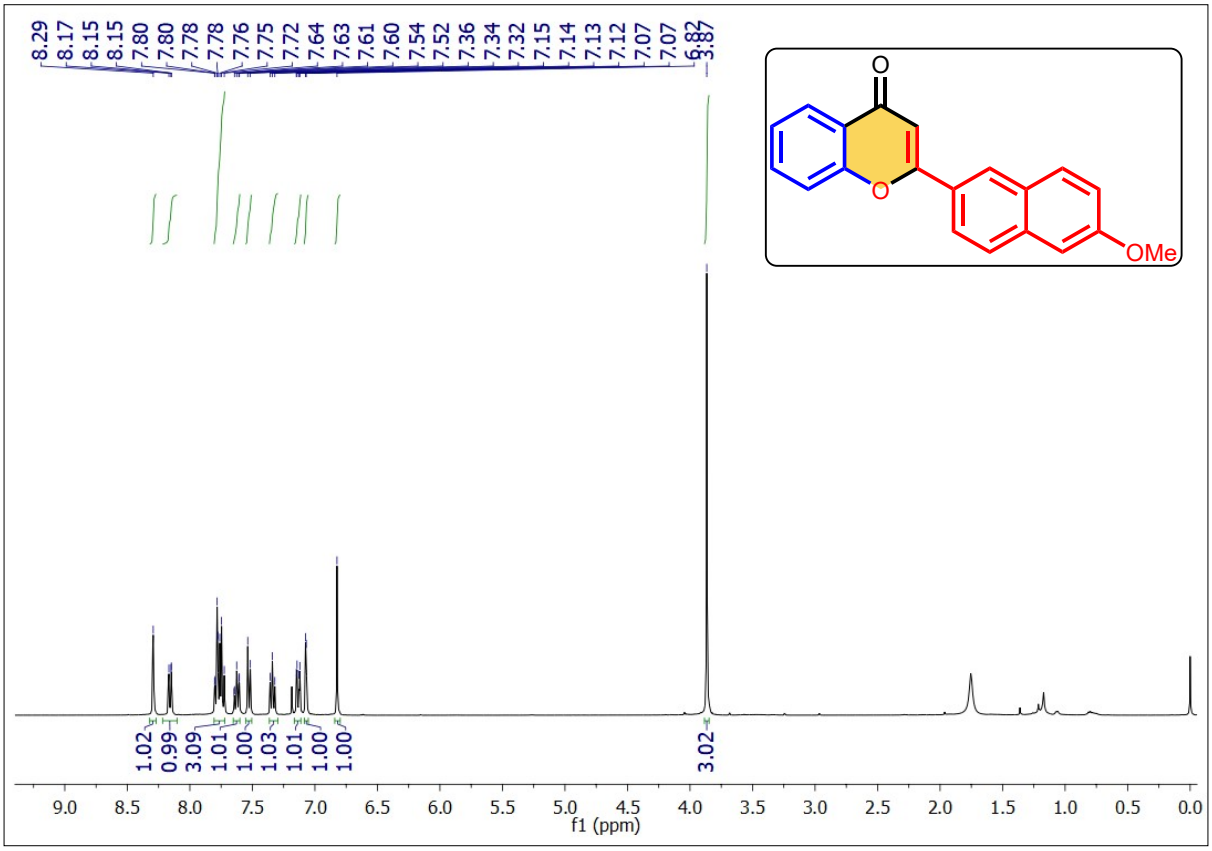


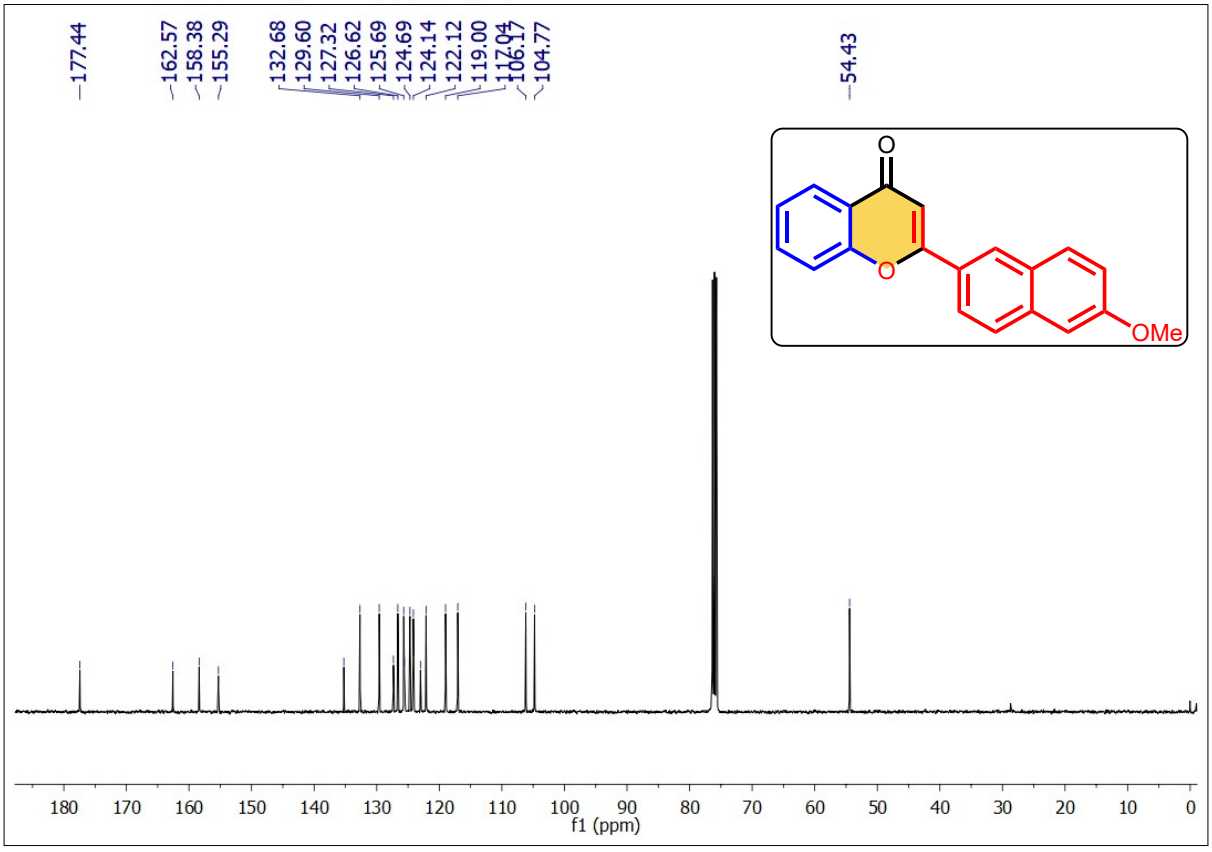
^{1}H and ^{13}C NMR spectra of 2-(4-Methoxyphenyl)-4*H*-chromen-4-one (6b)



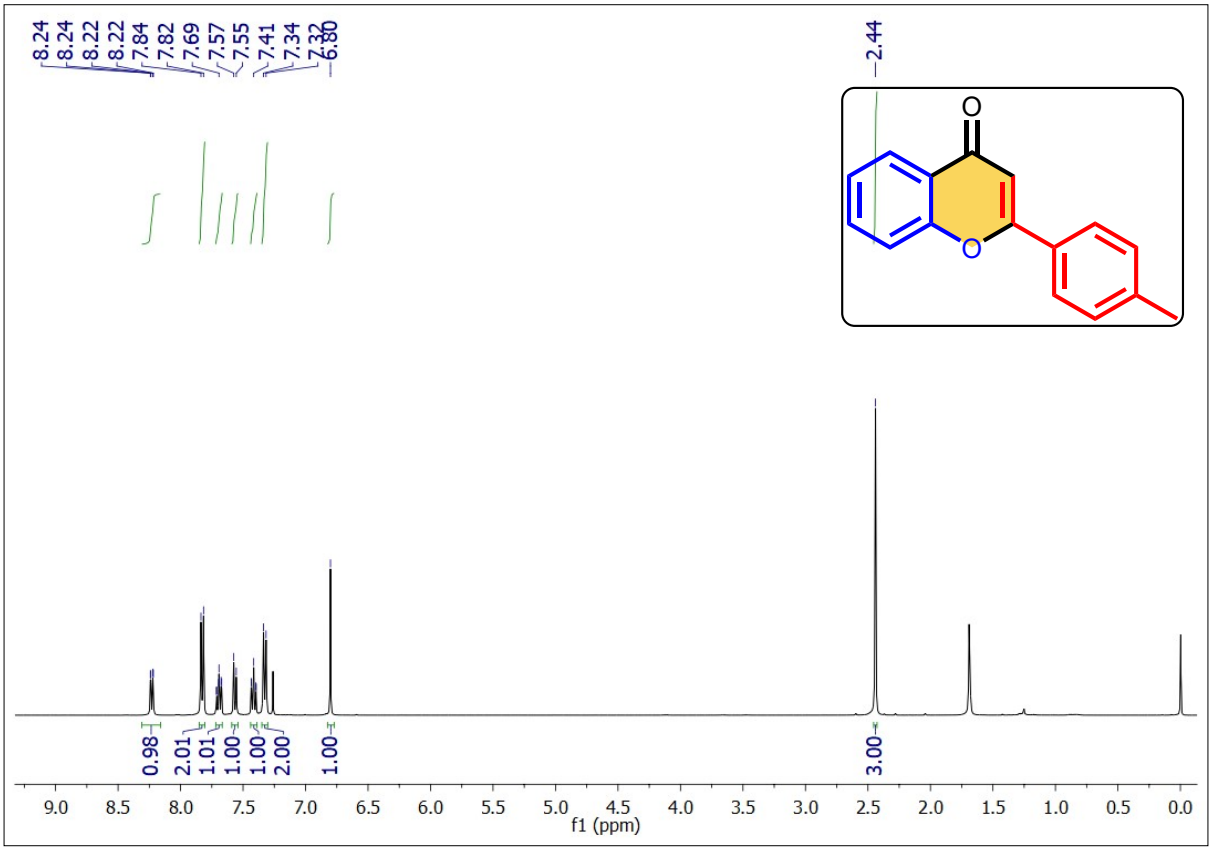


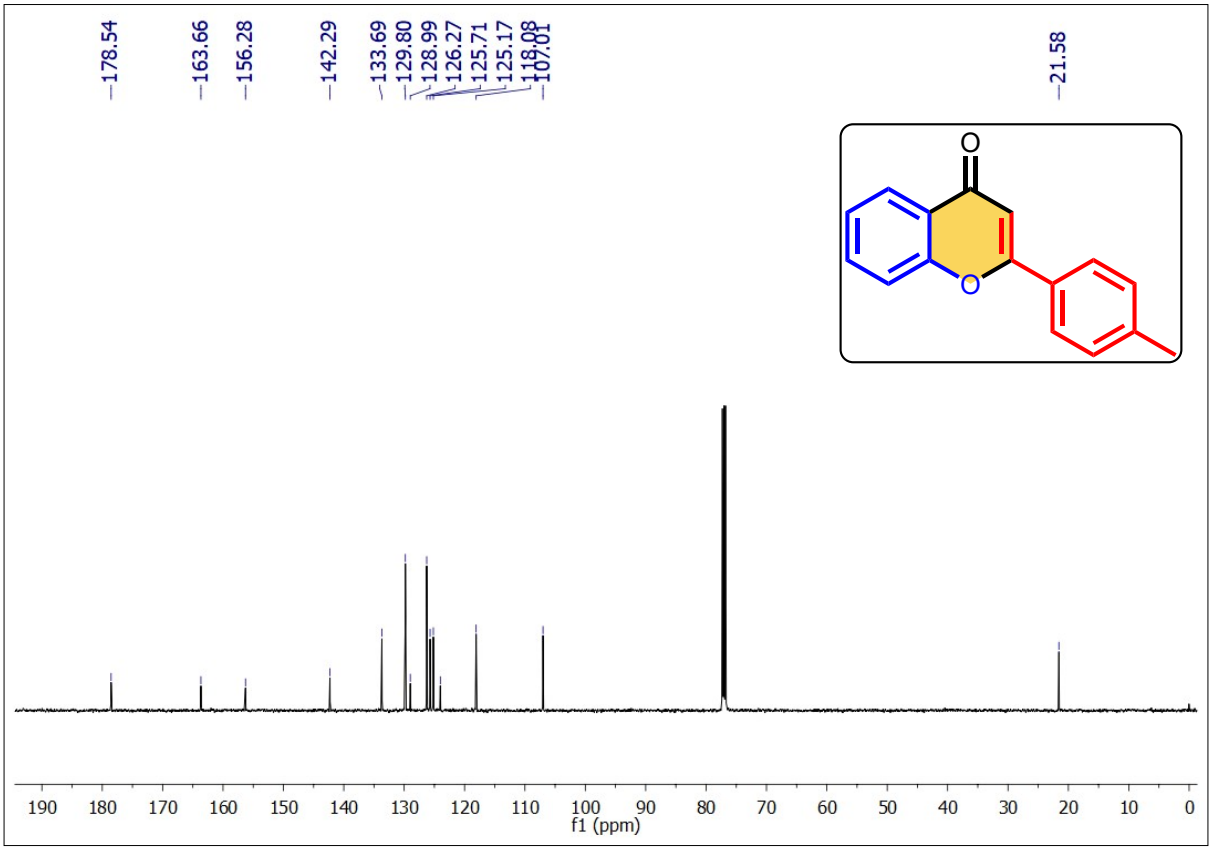
^{1}H and ^{13}C NMR spectra of 2-(6-Methoxynaphthalen-2-yl)-4*H*-chromen-4-one (6c)



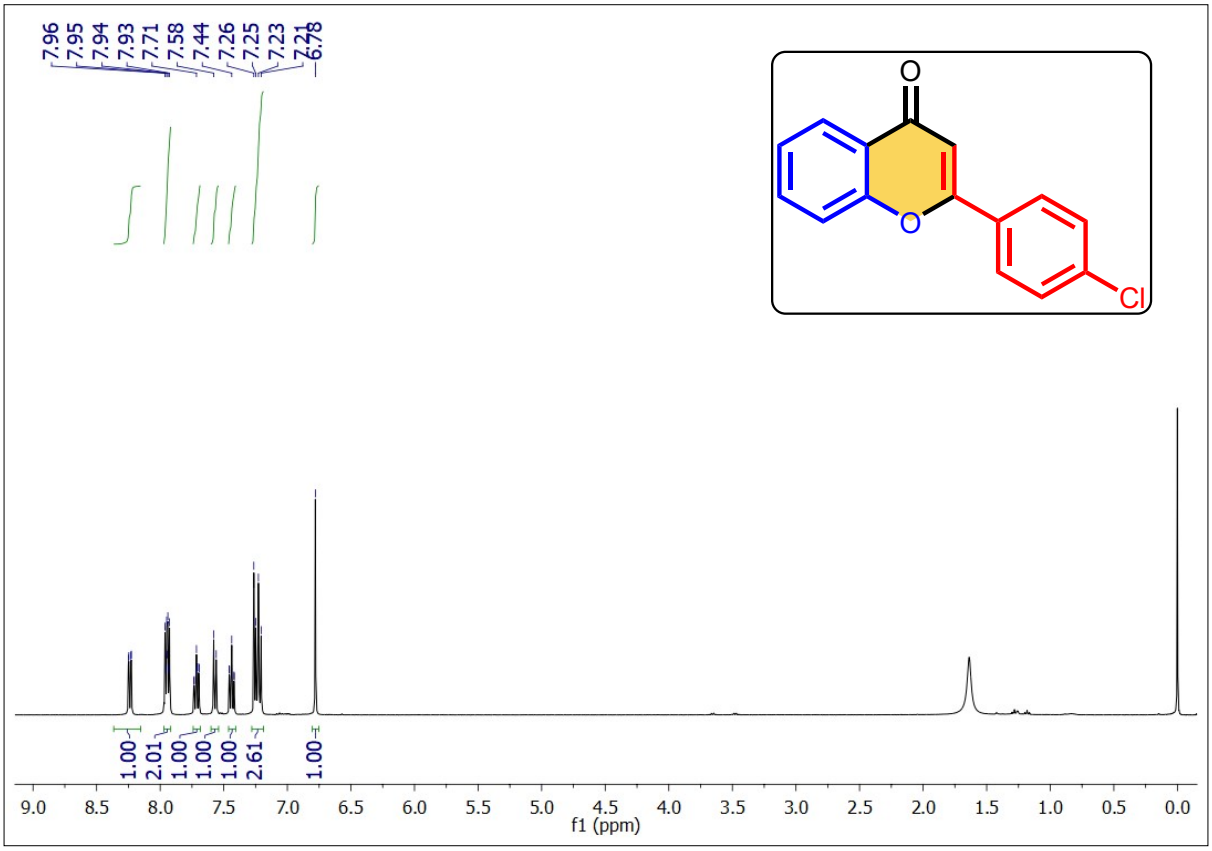


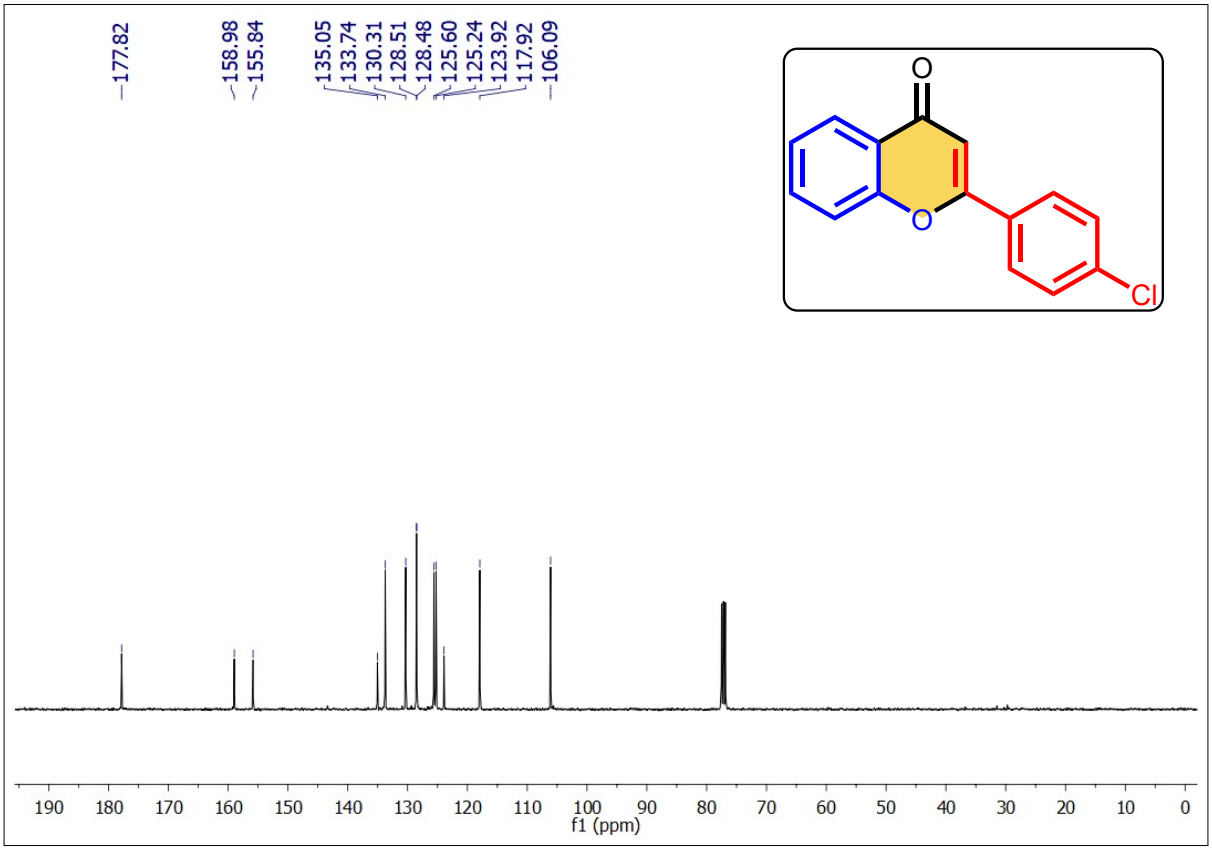
^{1}H and ^{13}C NMR spectra of 2-(*p*-Tolyl)-4*H*-chromen-4-one (6d)



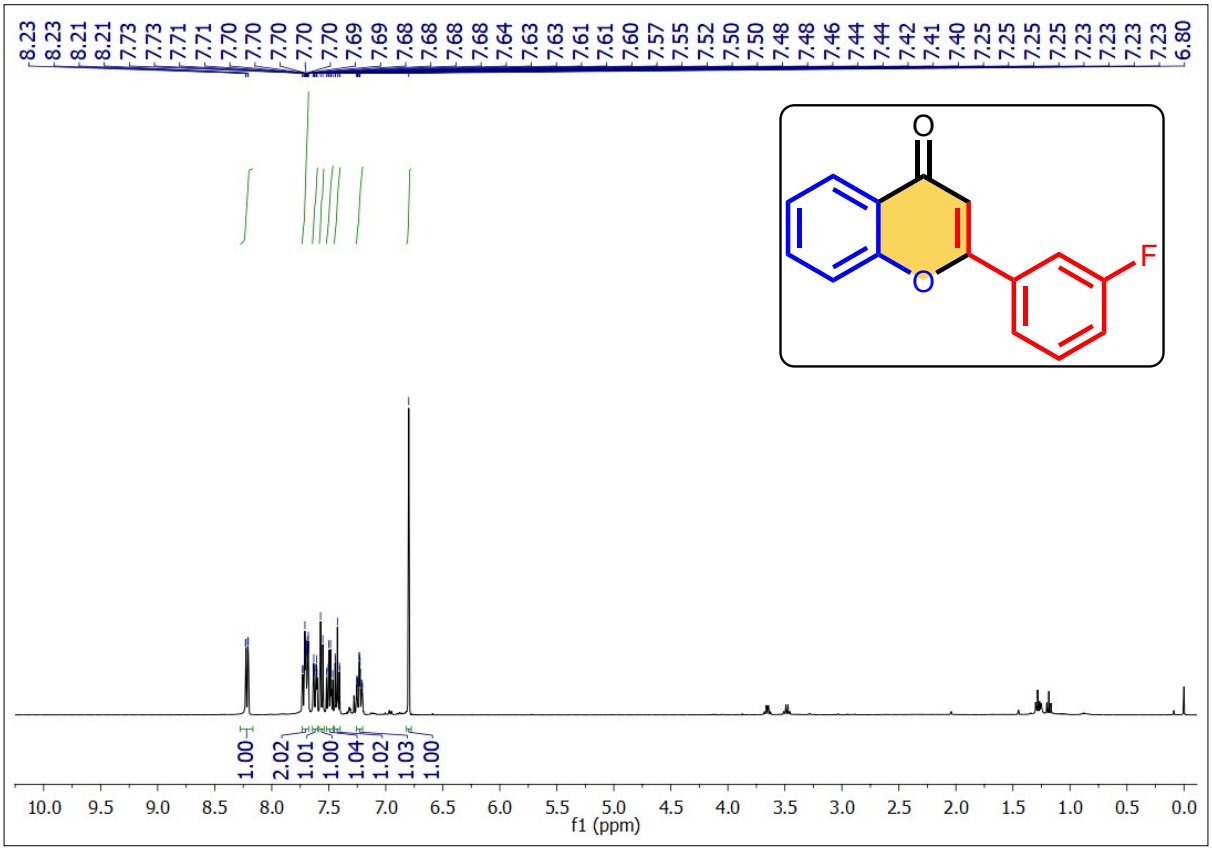


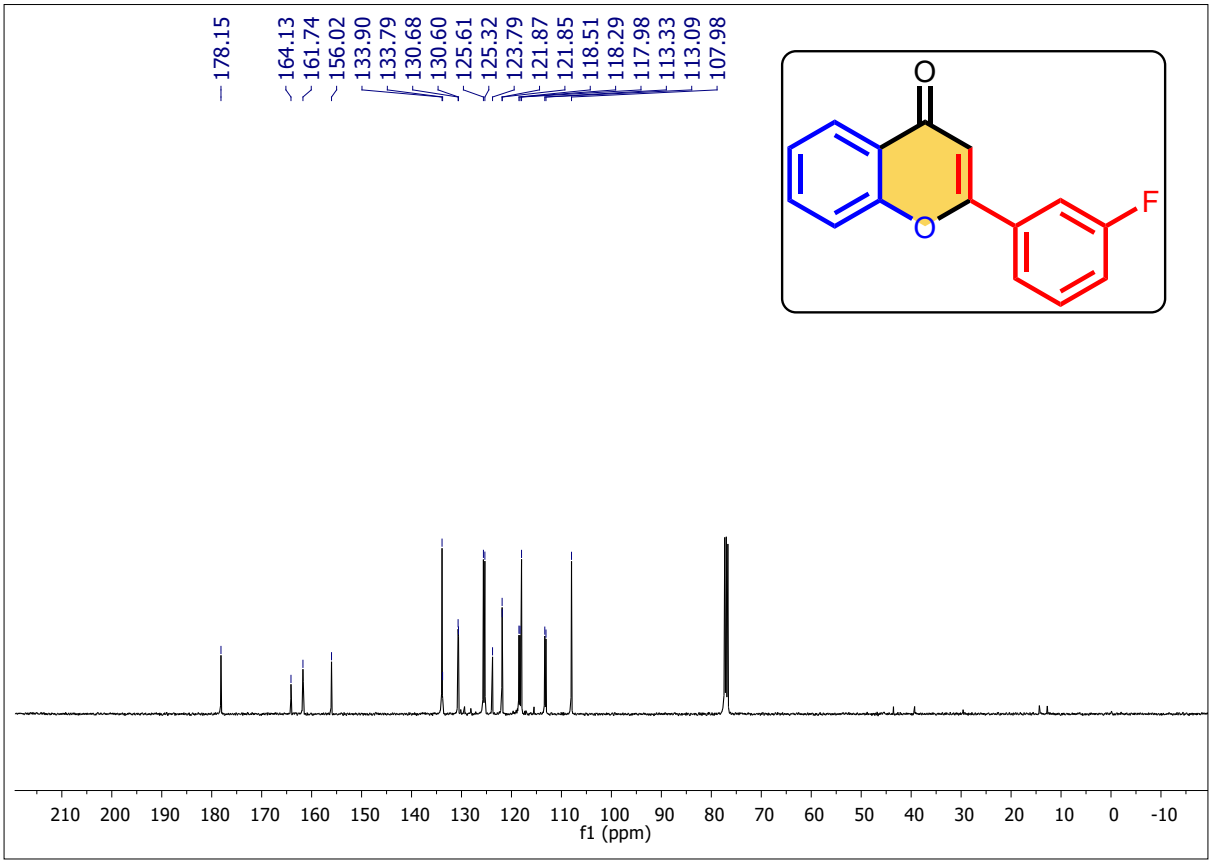
^{1}H and ^{13}C NMR spectra of 2-(4-Chlorophenyl)-4*H*-chromen-4-one (6e)



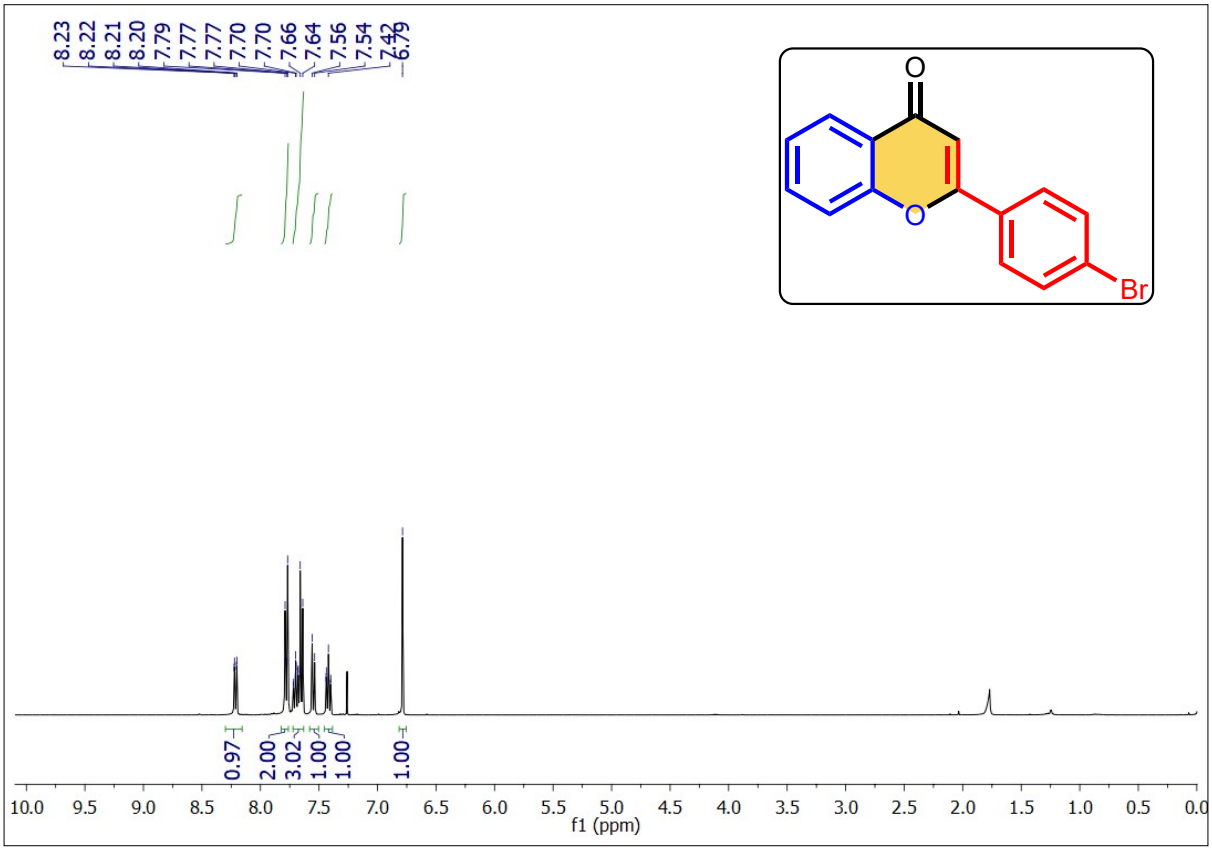


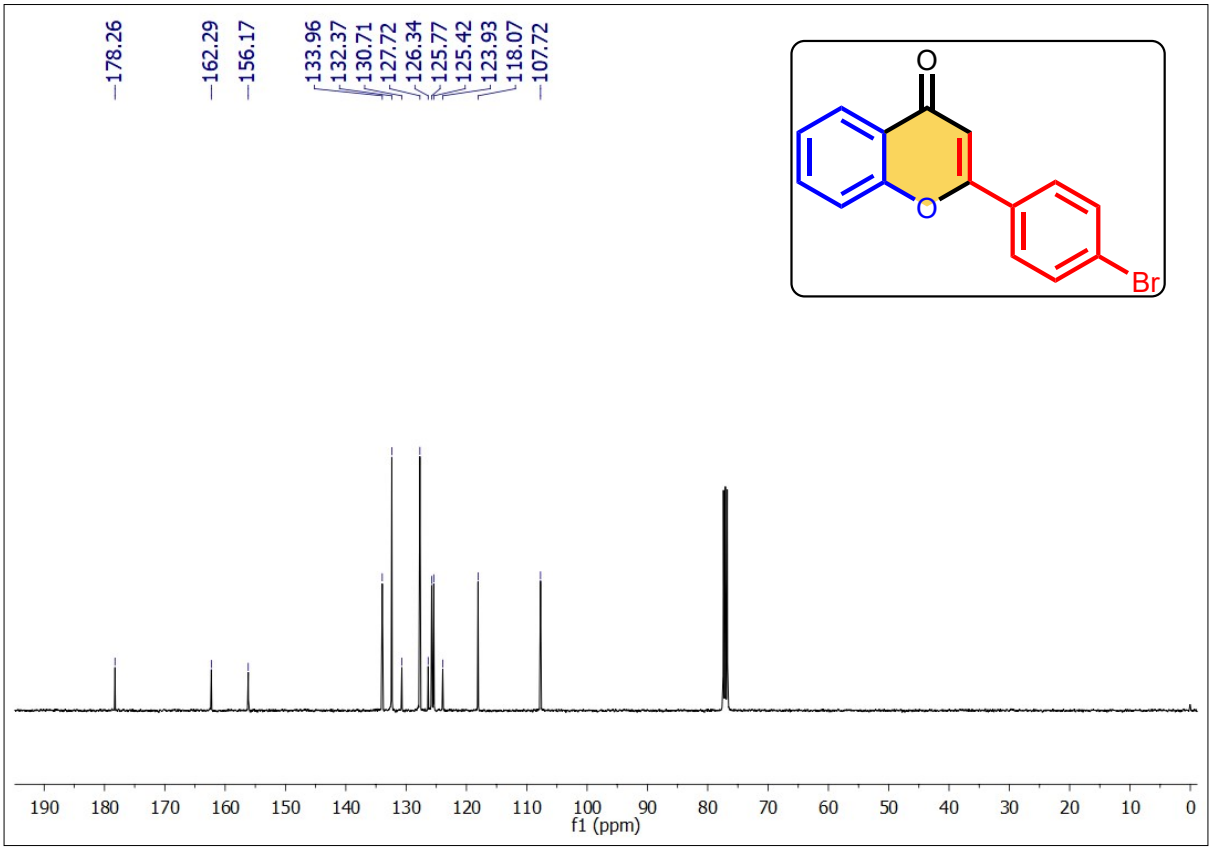
^{1}H and ^{13}C NMR spectra of 2-(3-Fluorophenyl)-4*H*-chromen-4-one (6f)



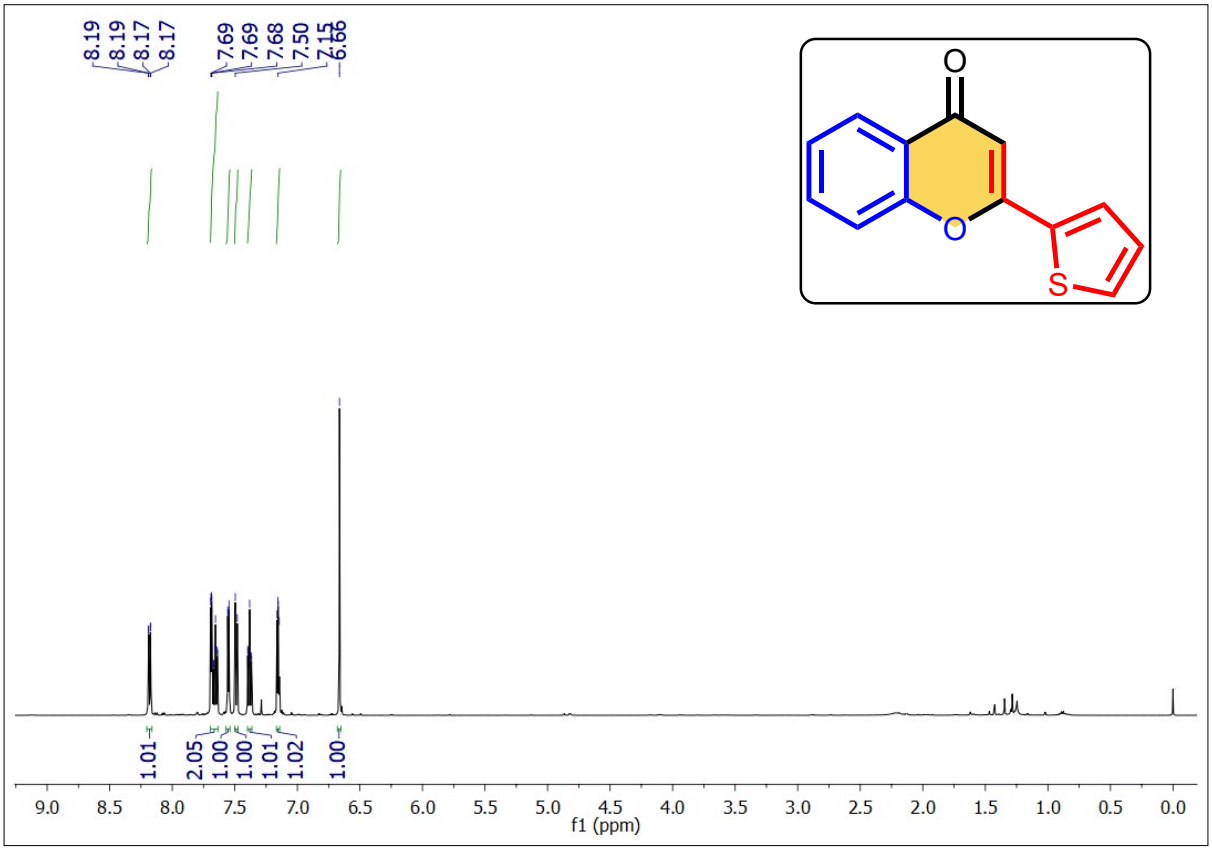


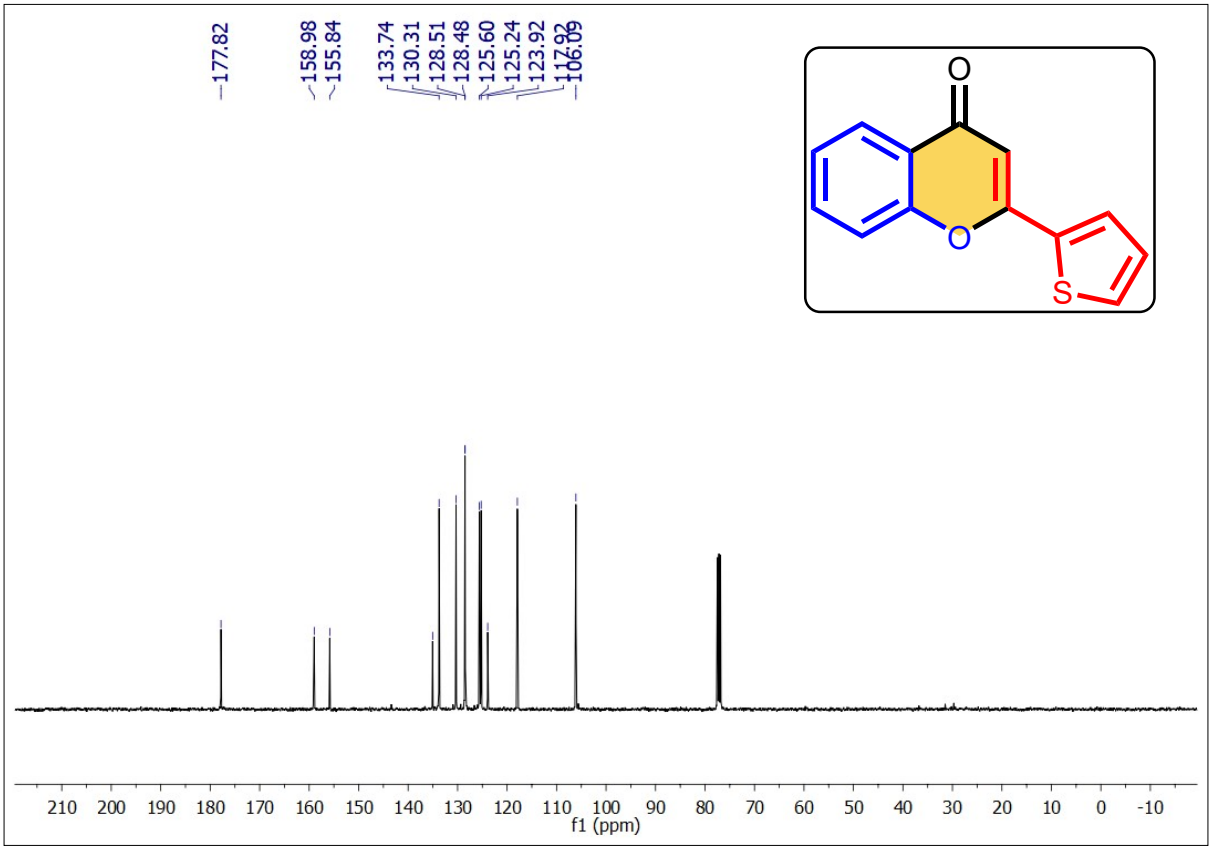
^{1}H and ^{13}C NMR spectra of 2-(4-Bromophenyl)-4*H*-chromen-4-one (6g)



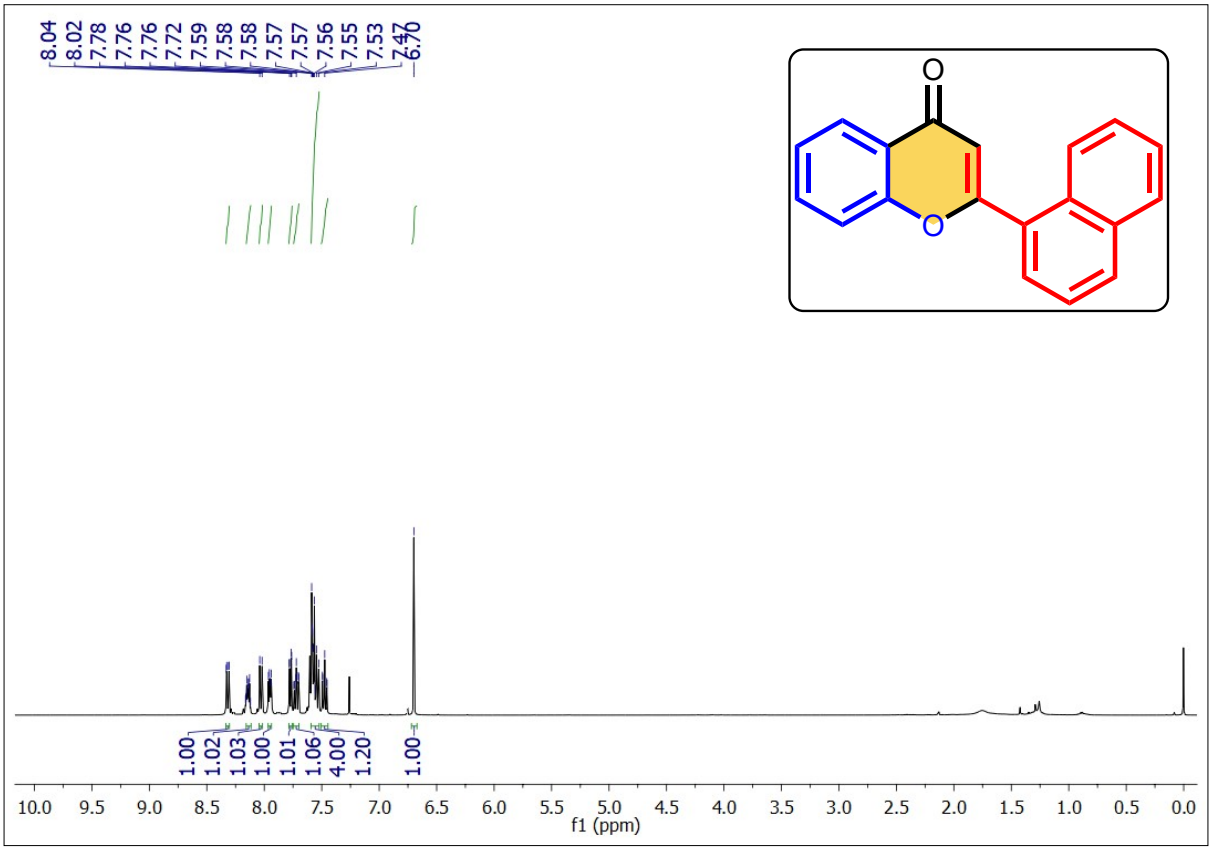


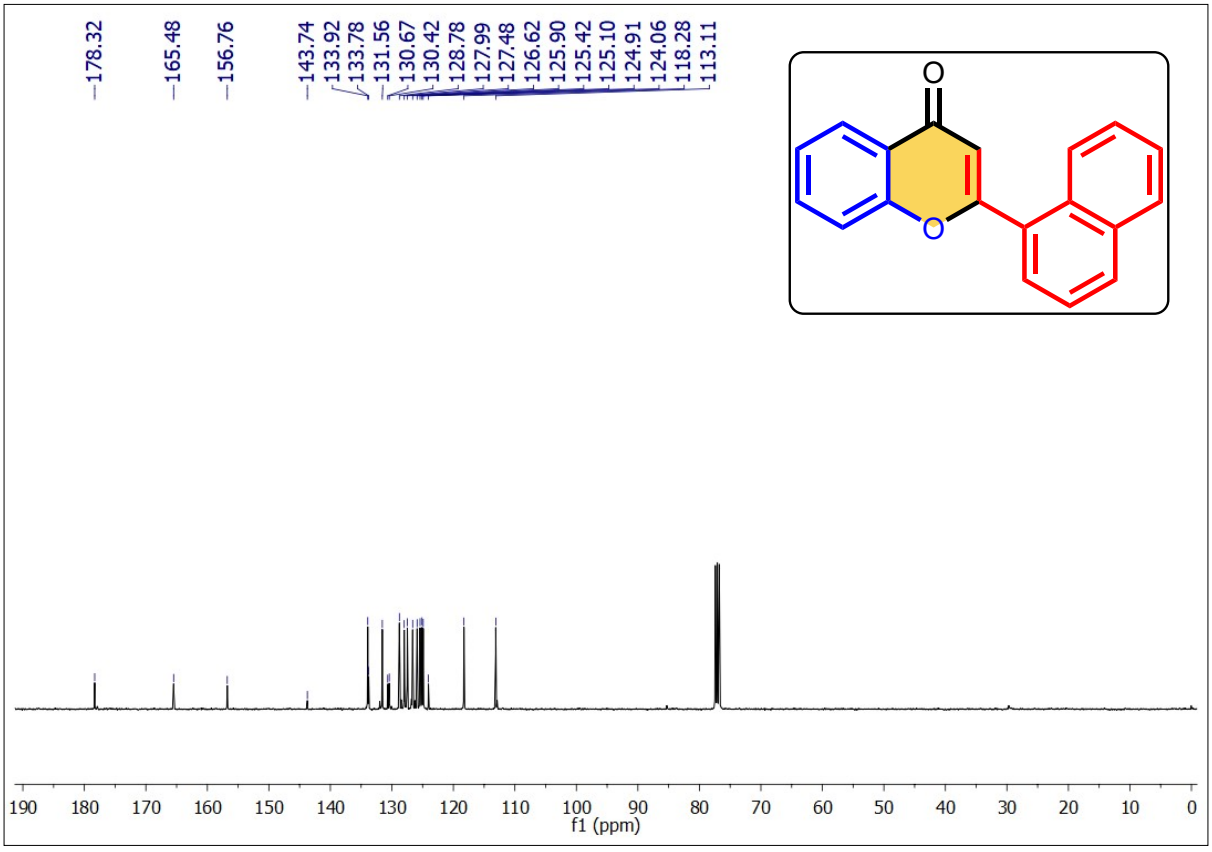
^{1}H and ^{13}C NMR spectra of 2-(Thiophen-2-yl)-4*H*-chromen-4-one (6h)



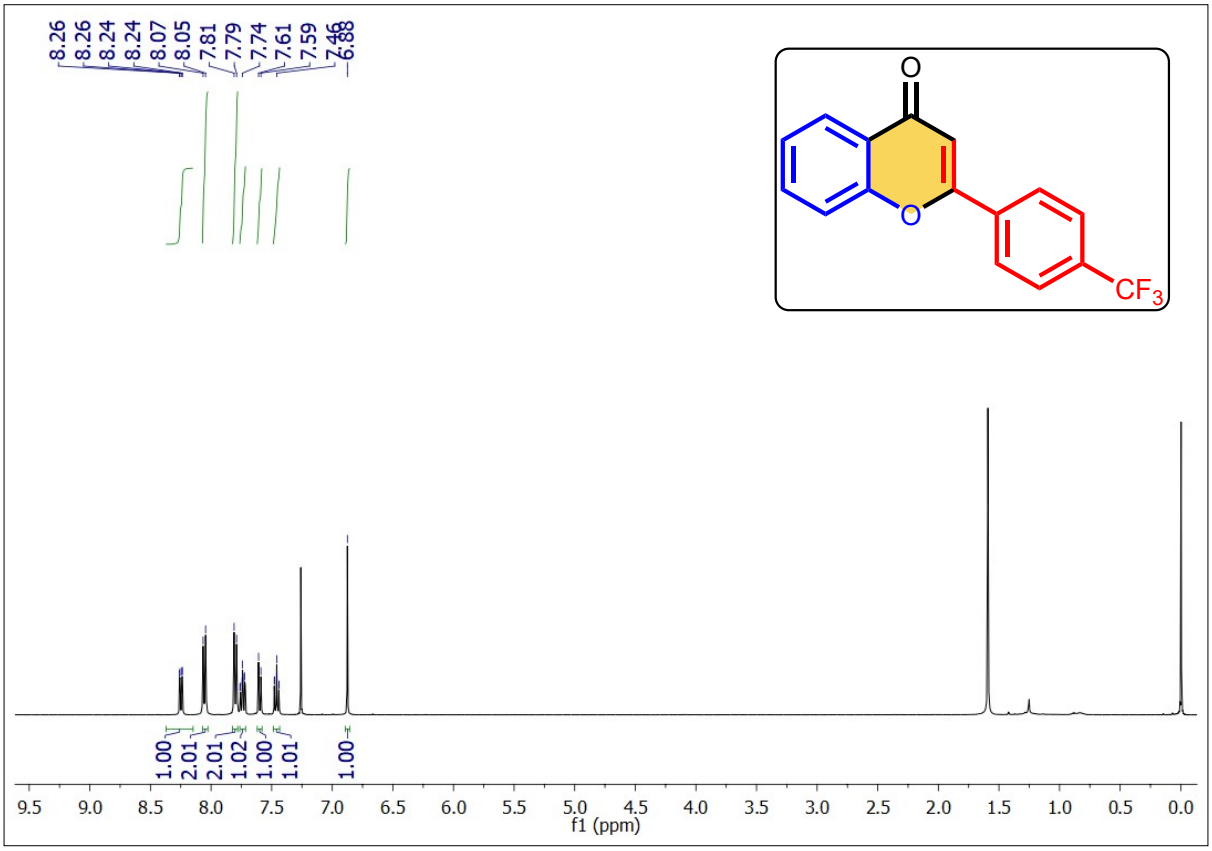


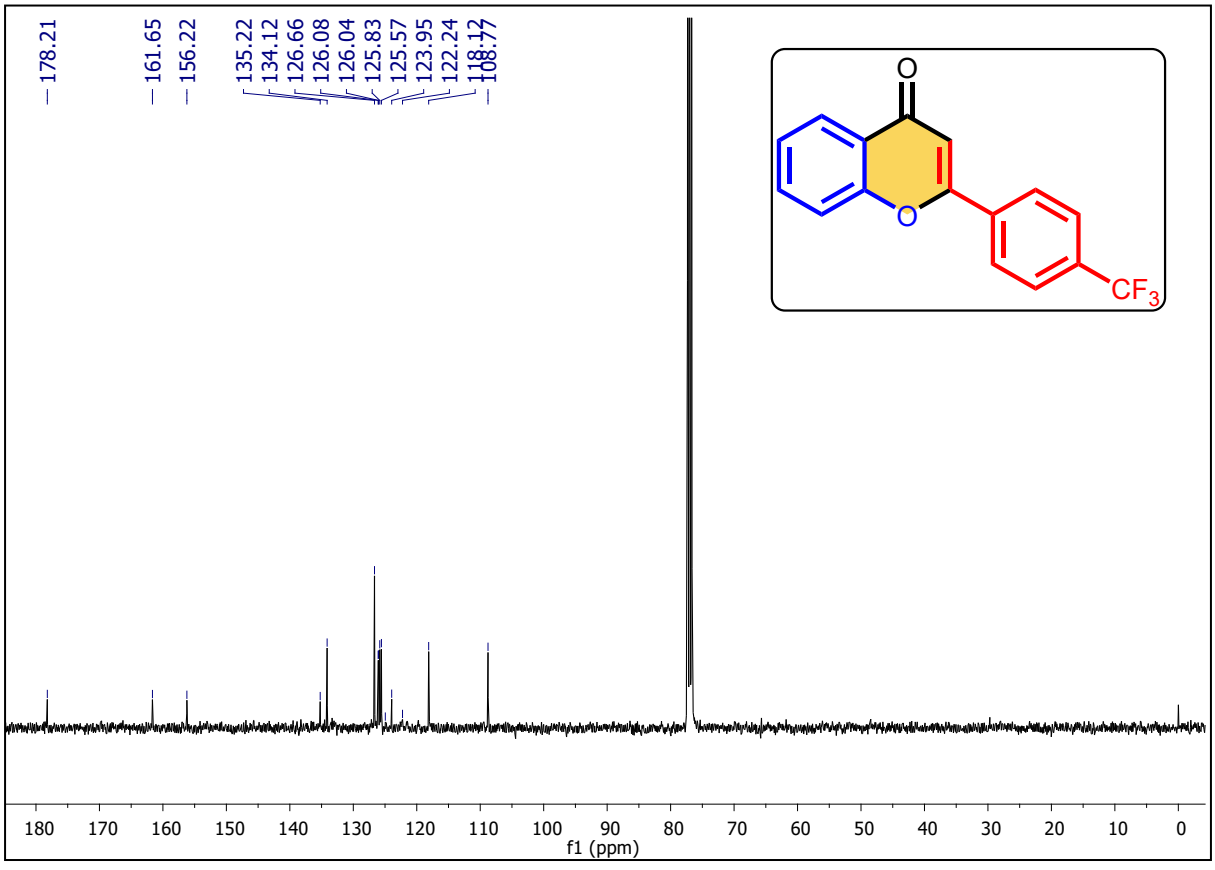
^{1}H and ^{13}C NMR spectra of 2-(Naphthalen-1-yl)-4*H*-chromen-4-one (6i)



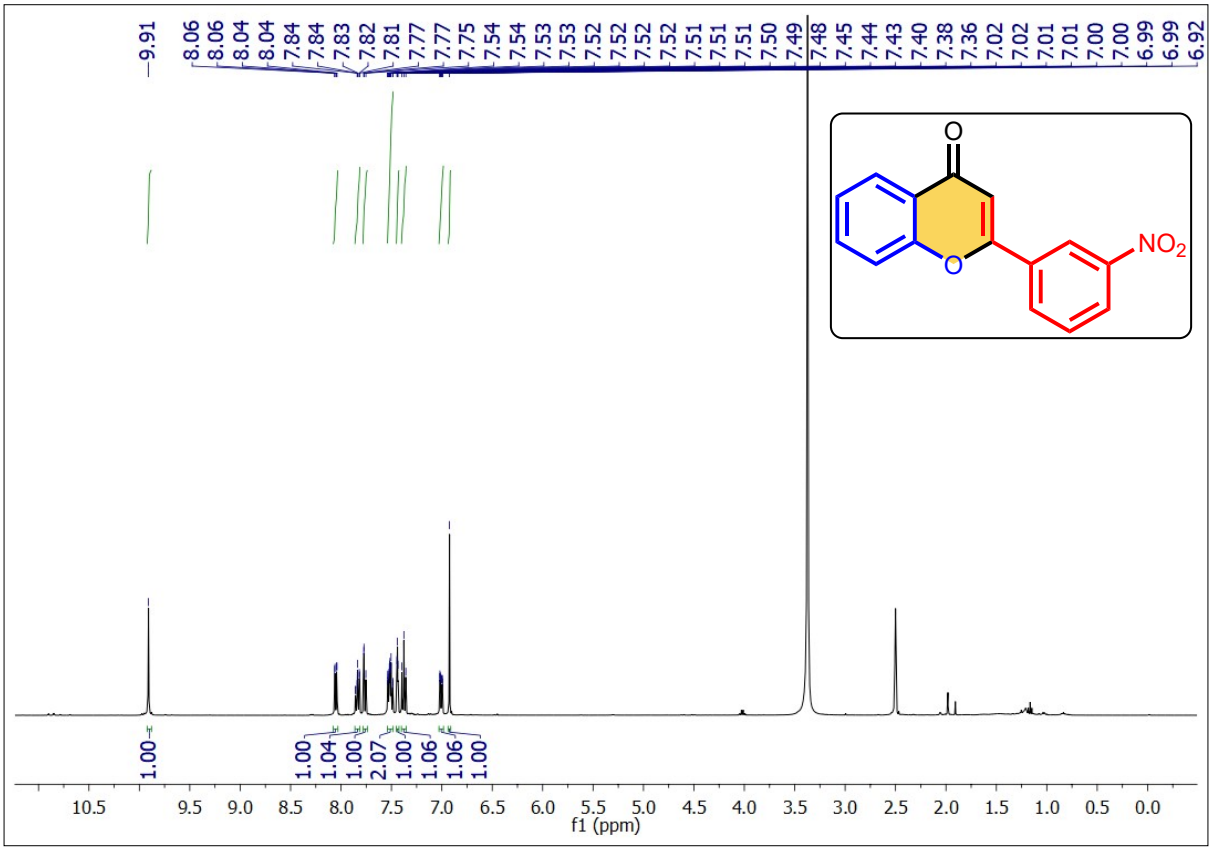


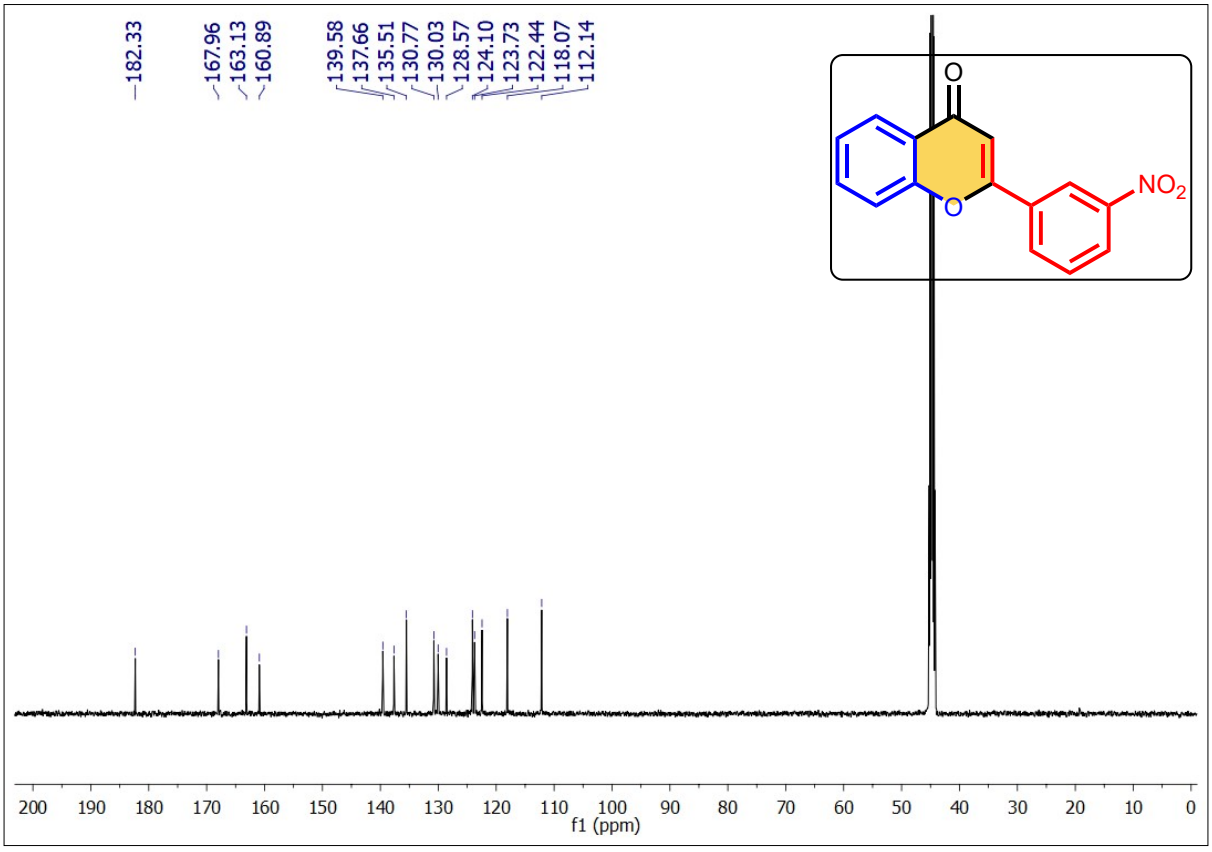
^{1}H and ^{13}C NMR spectra of 2-(4-(Trifluoromethyl)phenyl)-4*H*-chromen-4-one (6j)



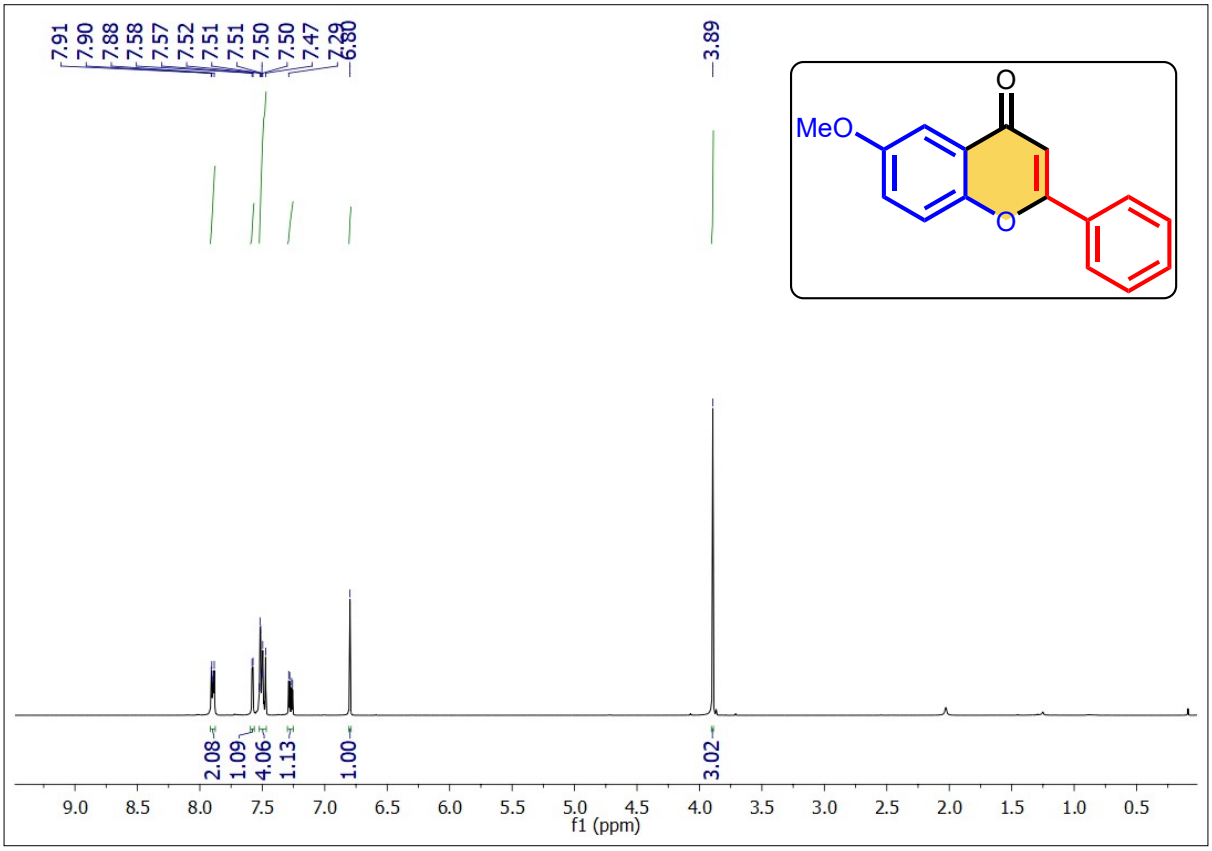


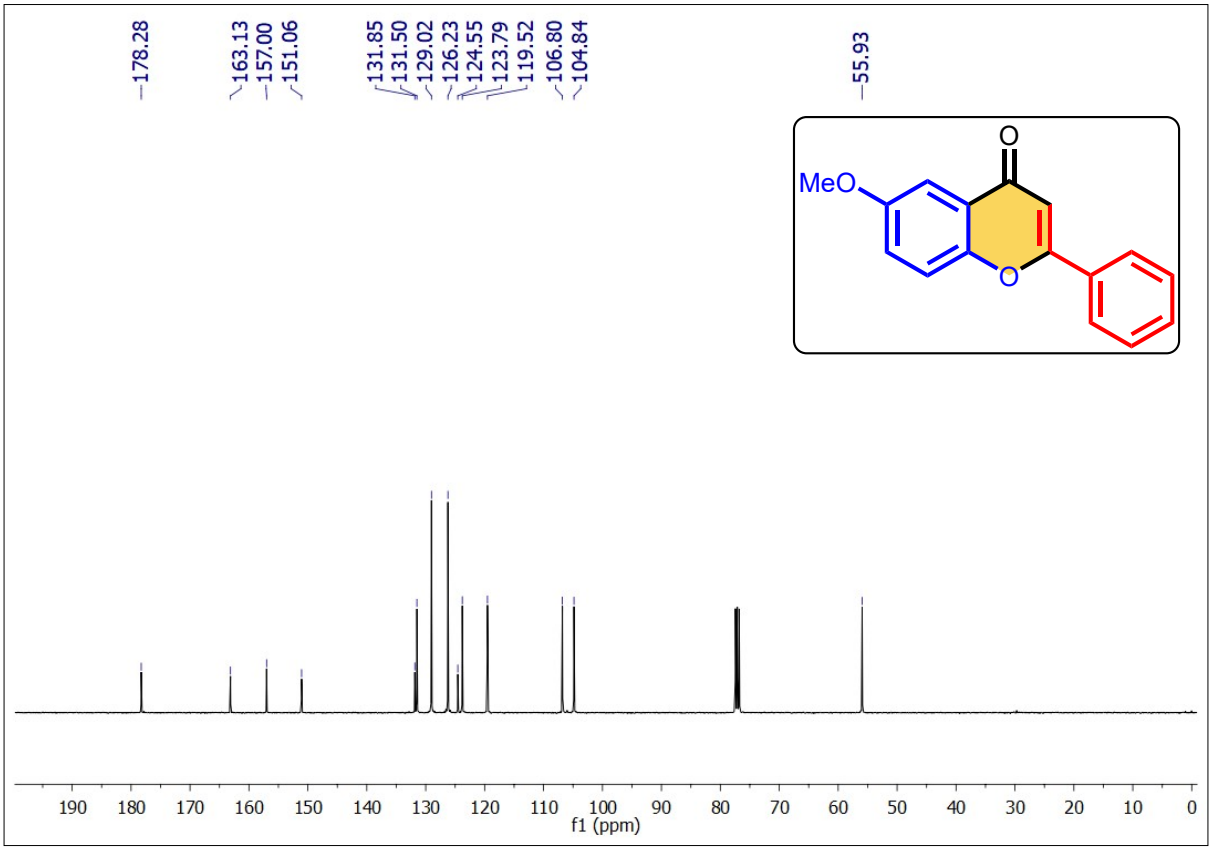
^{1}H and ^{13}C NMR spectra of 4-Nitrophenyl)-4*H*-chromen-4-one (6k)



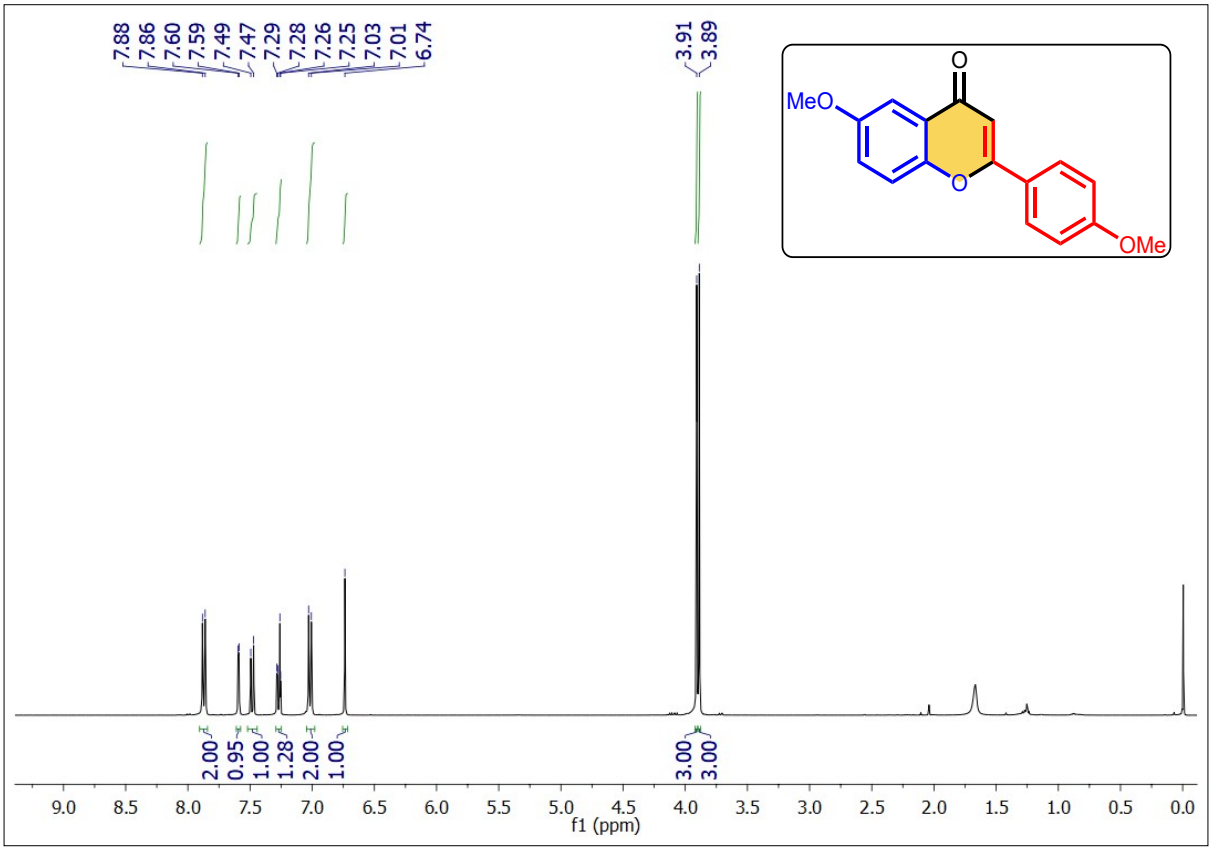


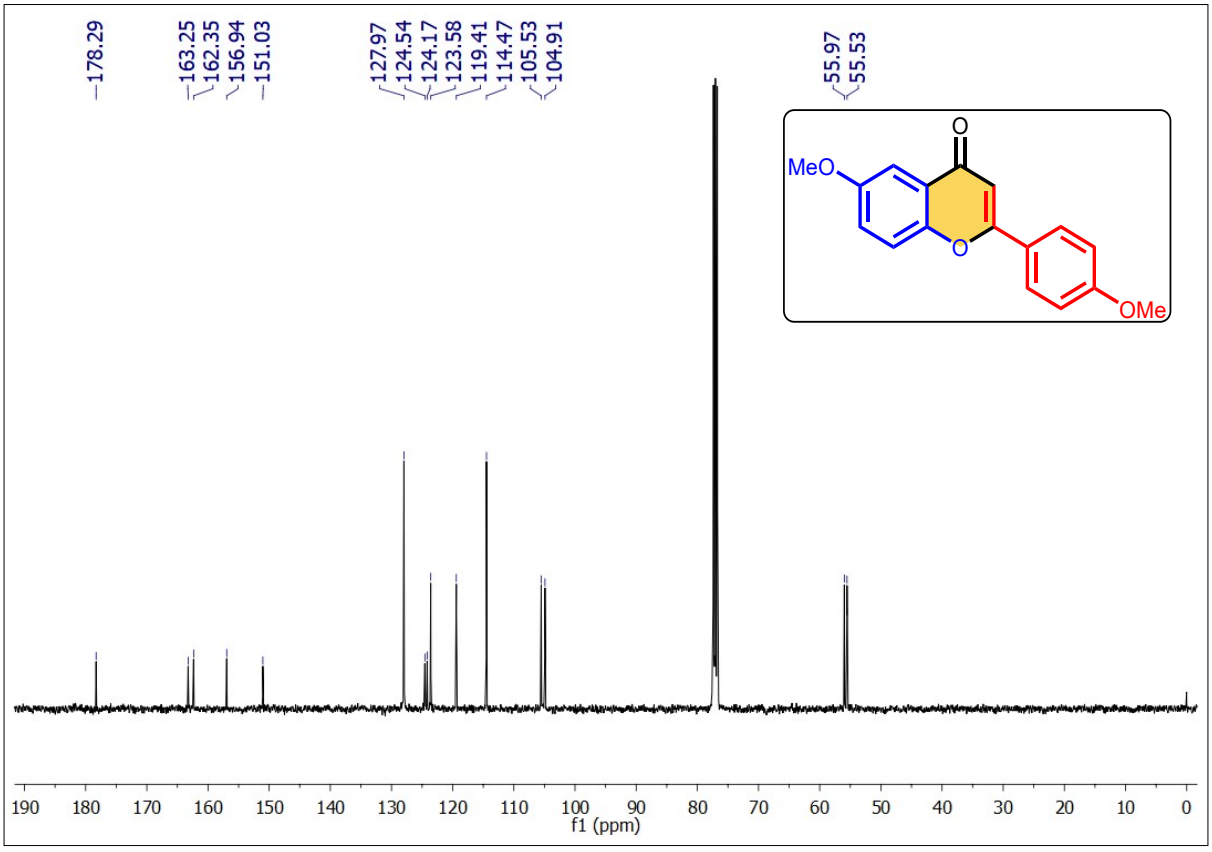
^{1}H and ^{13}C NMR spectra of 6-Methoxy-2-phenyl-4*H*-chromen-4-one (6l)



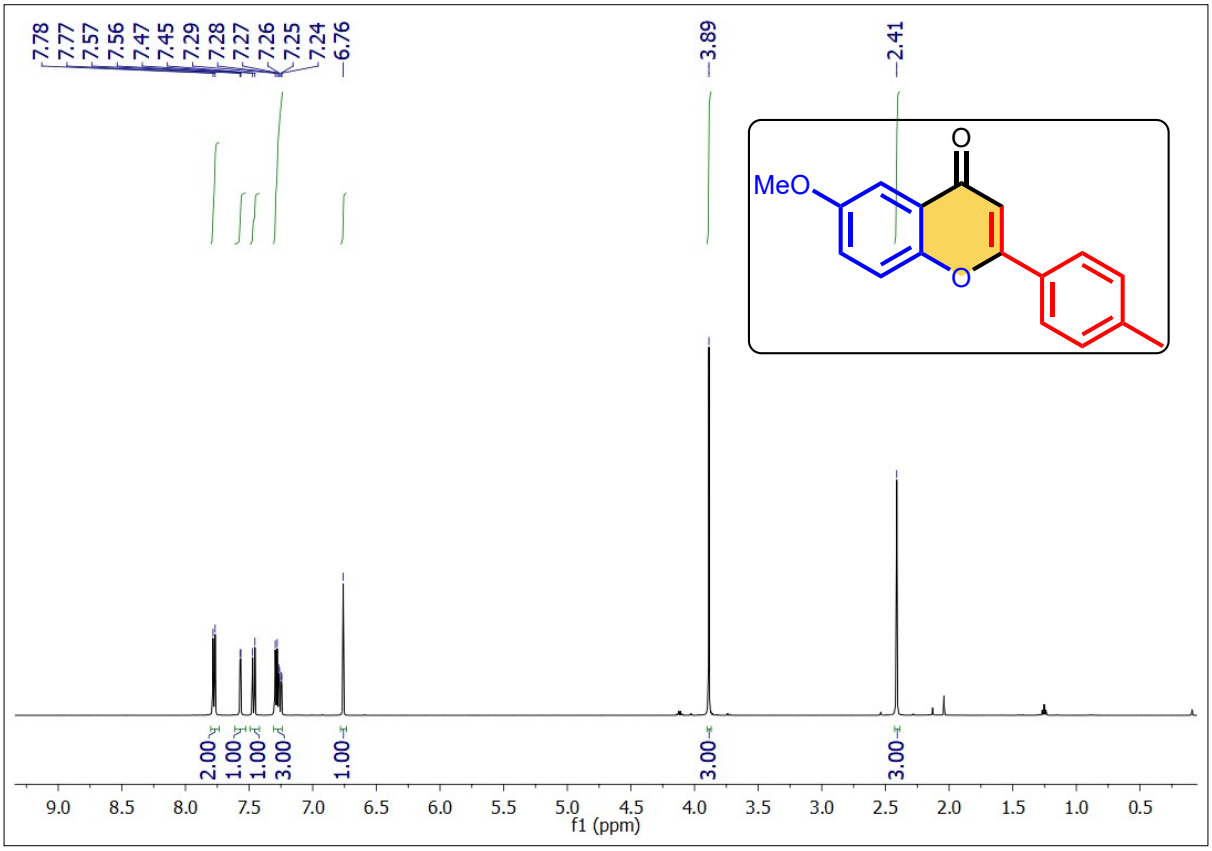


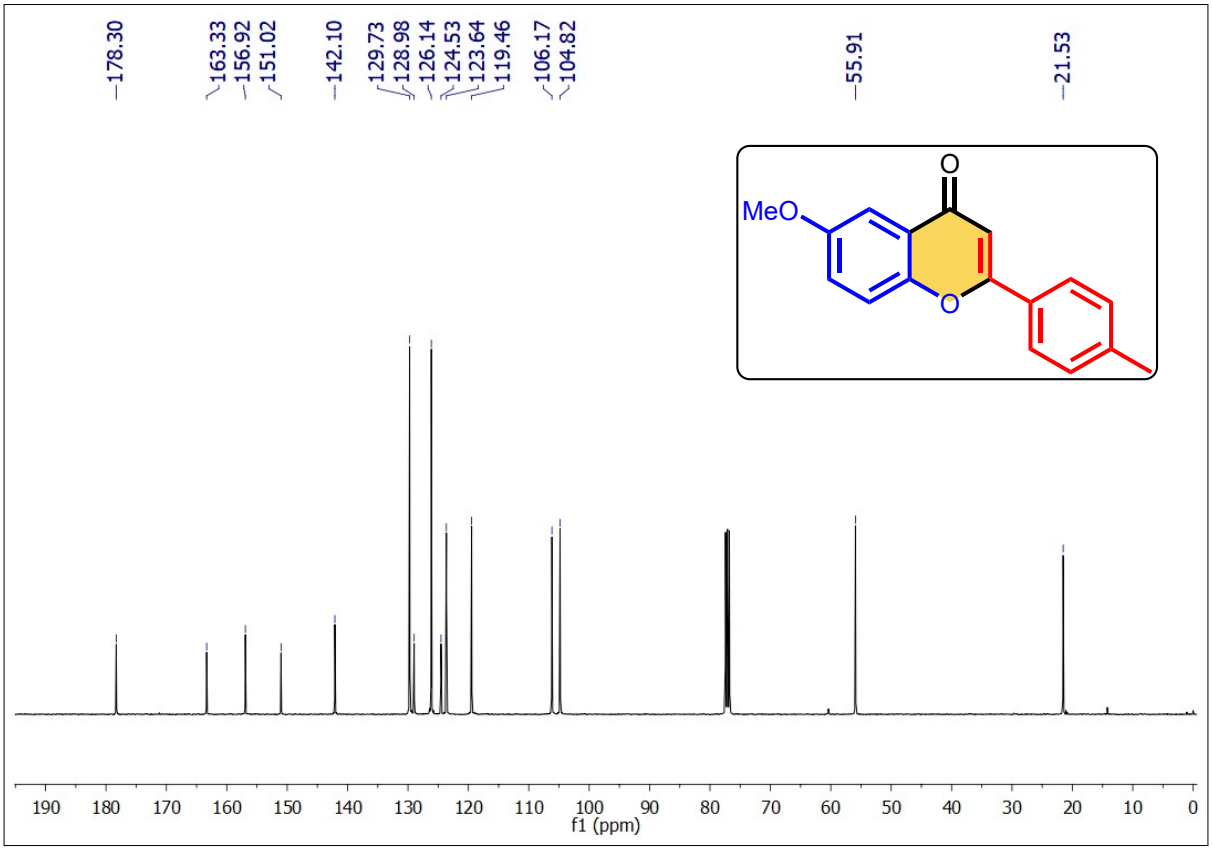
^{1}H and ^{13}C NMR spectra of 6-Methoxy-2-(4-methoxyphenyl)-4*H*-chromen-4-one (6m)



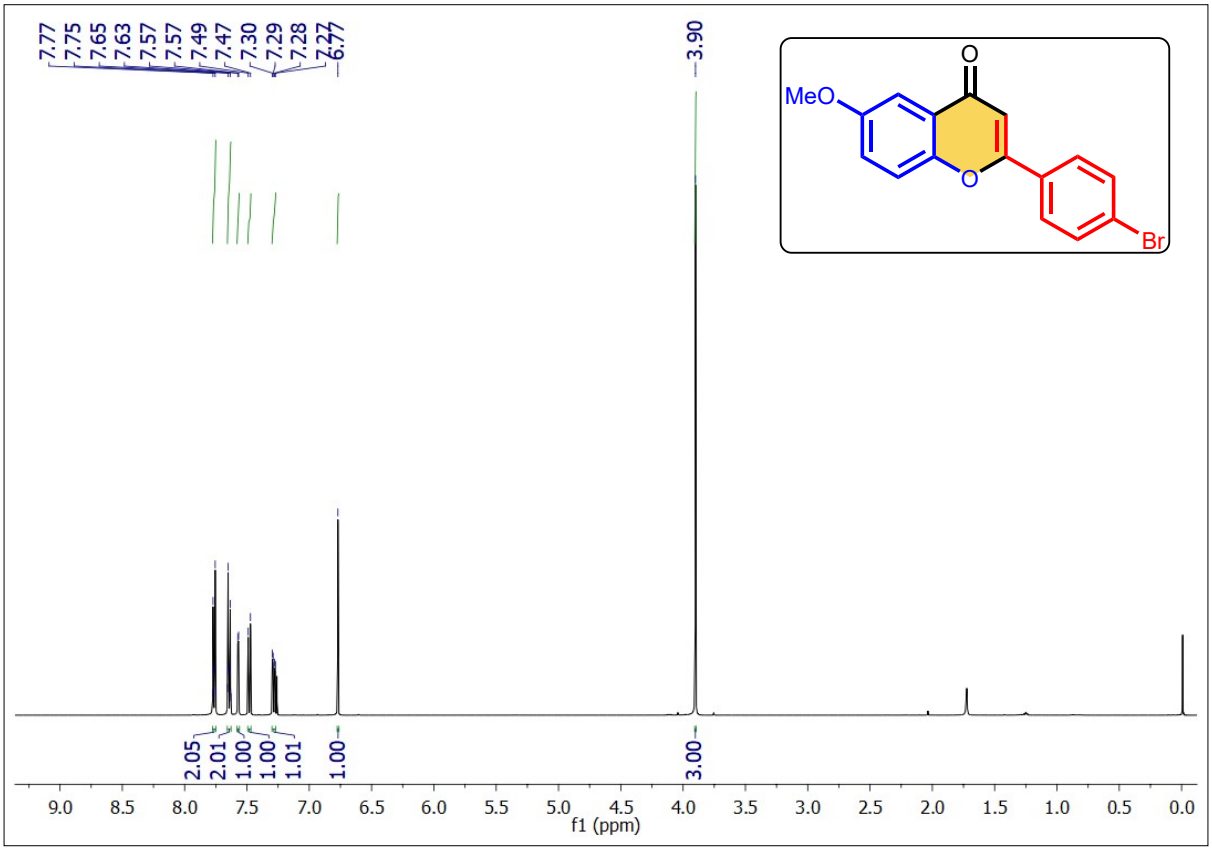


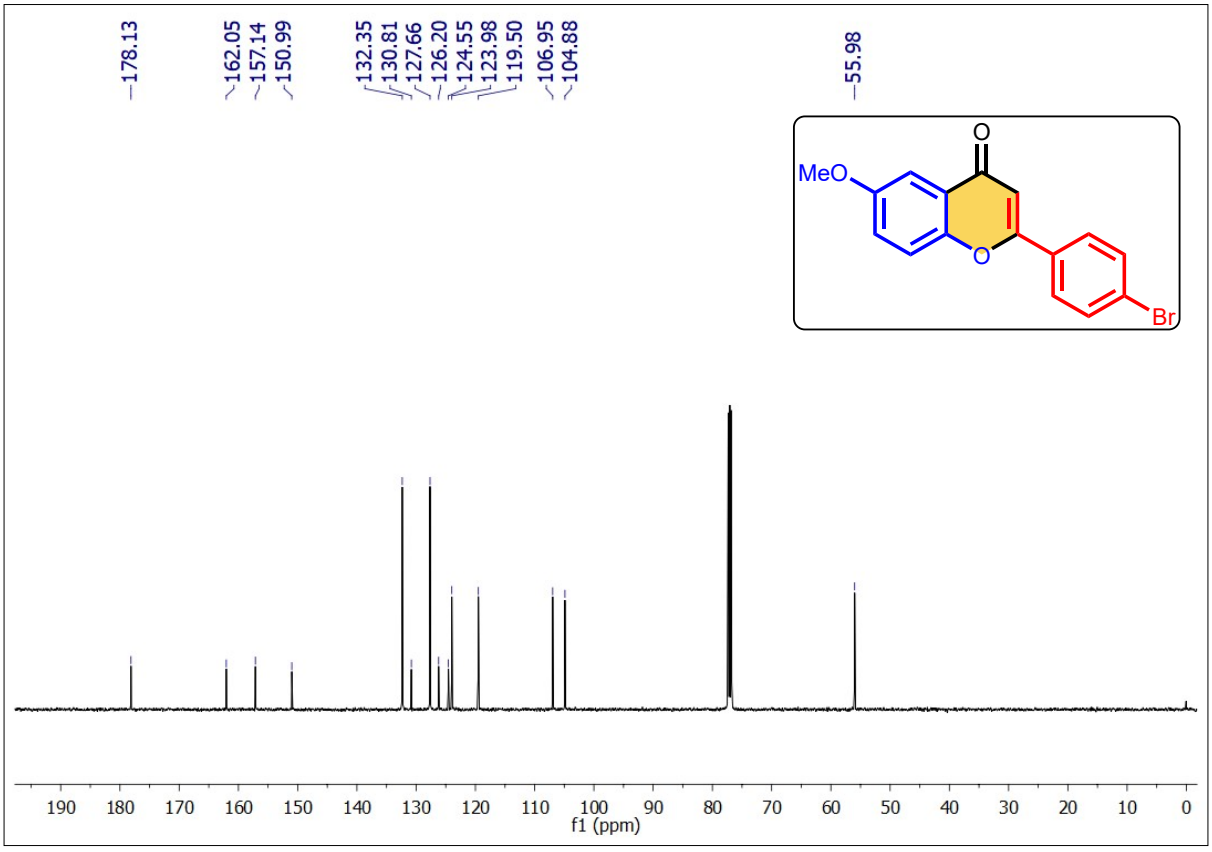
^{1}H and ^{13}C NMR spectra of 6-Methoxy-2-(p-tolyl)-4*H*-chromen-4-one (6n)



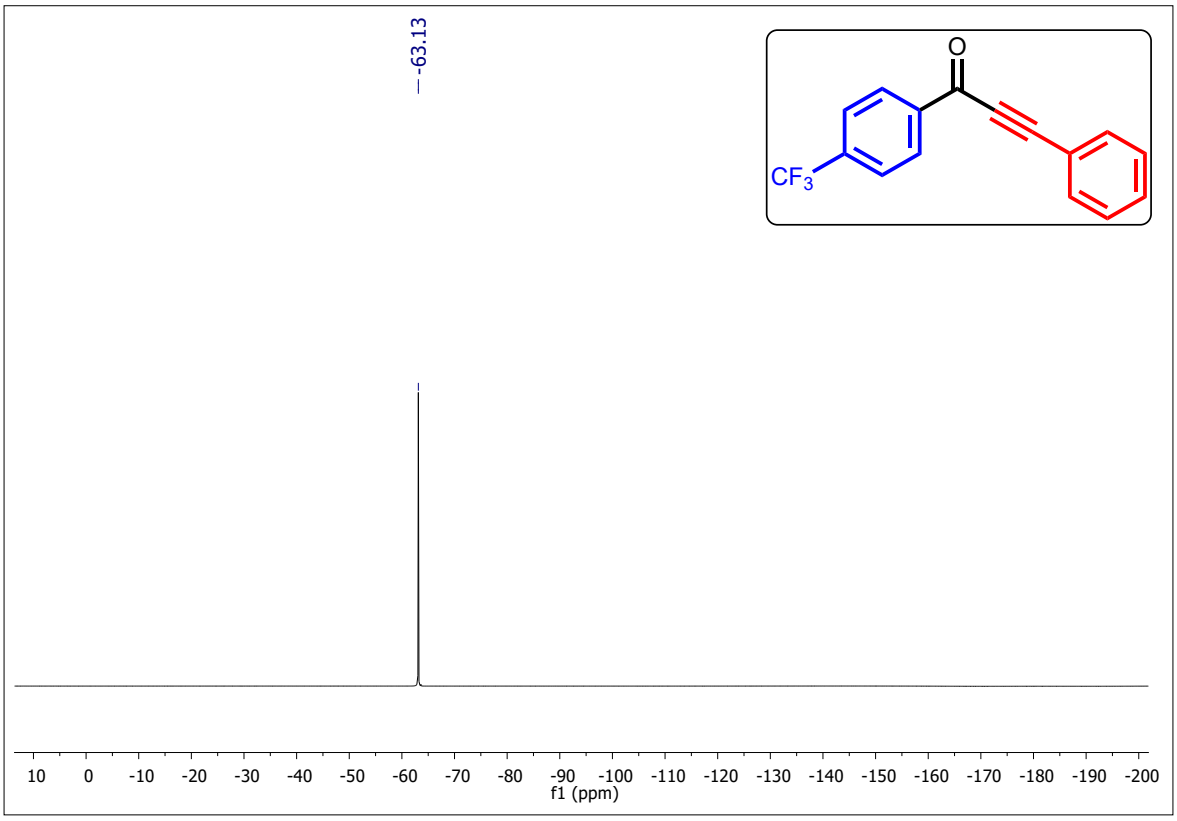


^{1}H and ^{13}C NMR spectra of 6-Bromo-2-(*p*-tolyl)-4*H*-chromen-4-one (6o)

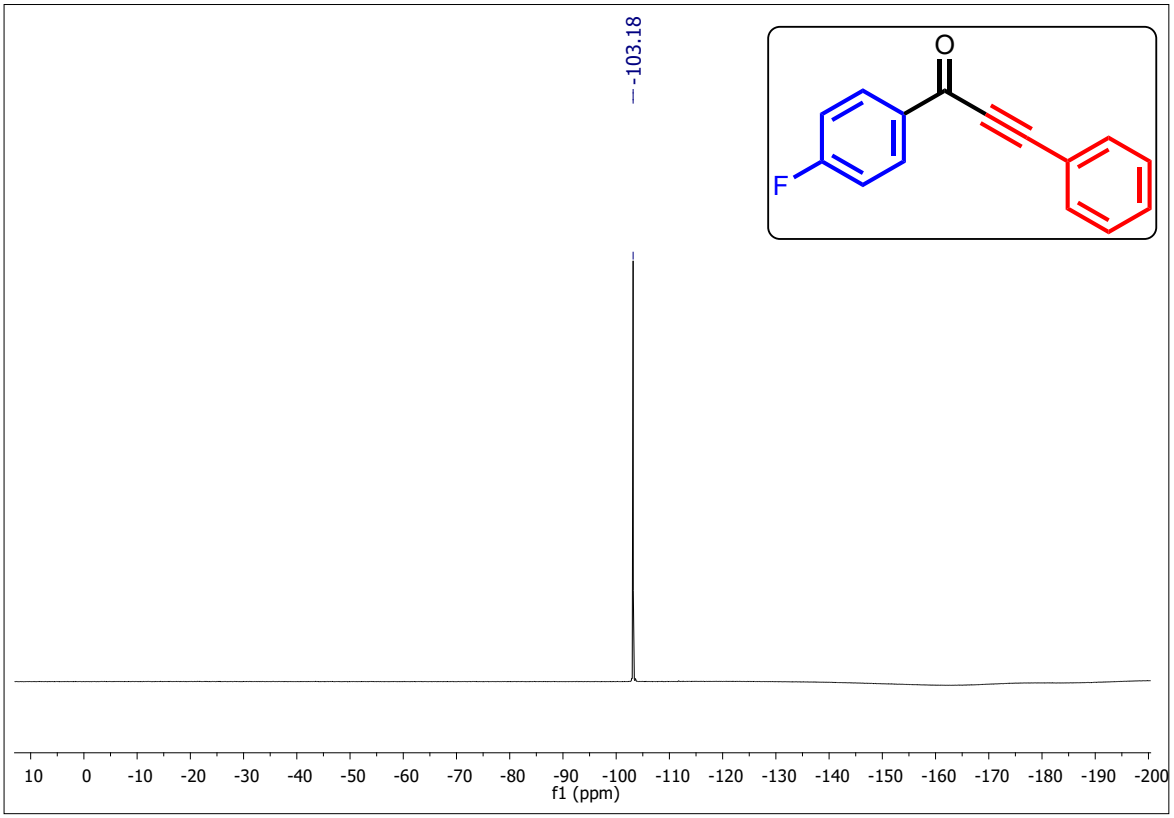




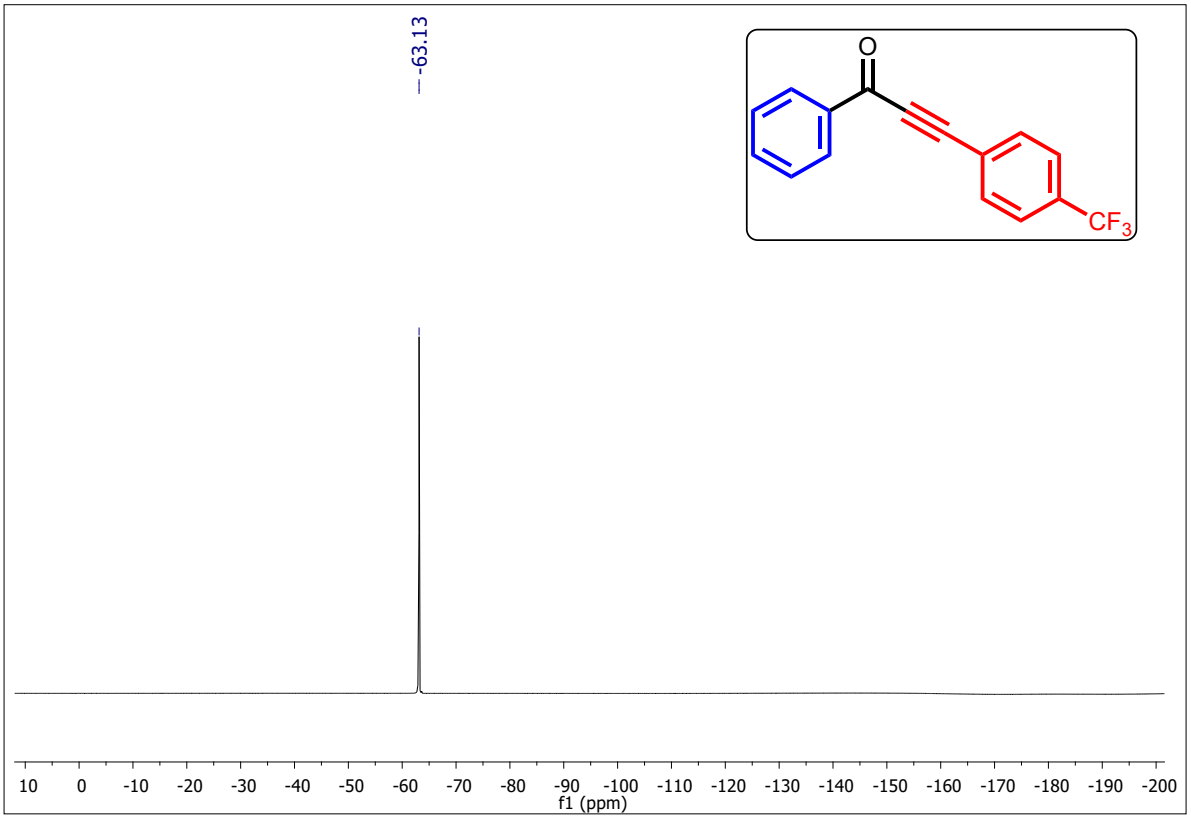
^{19}F NMR spectra of 3-Phenyl-1-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (3g)



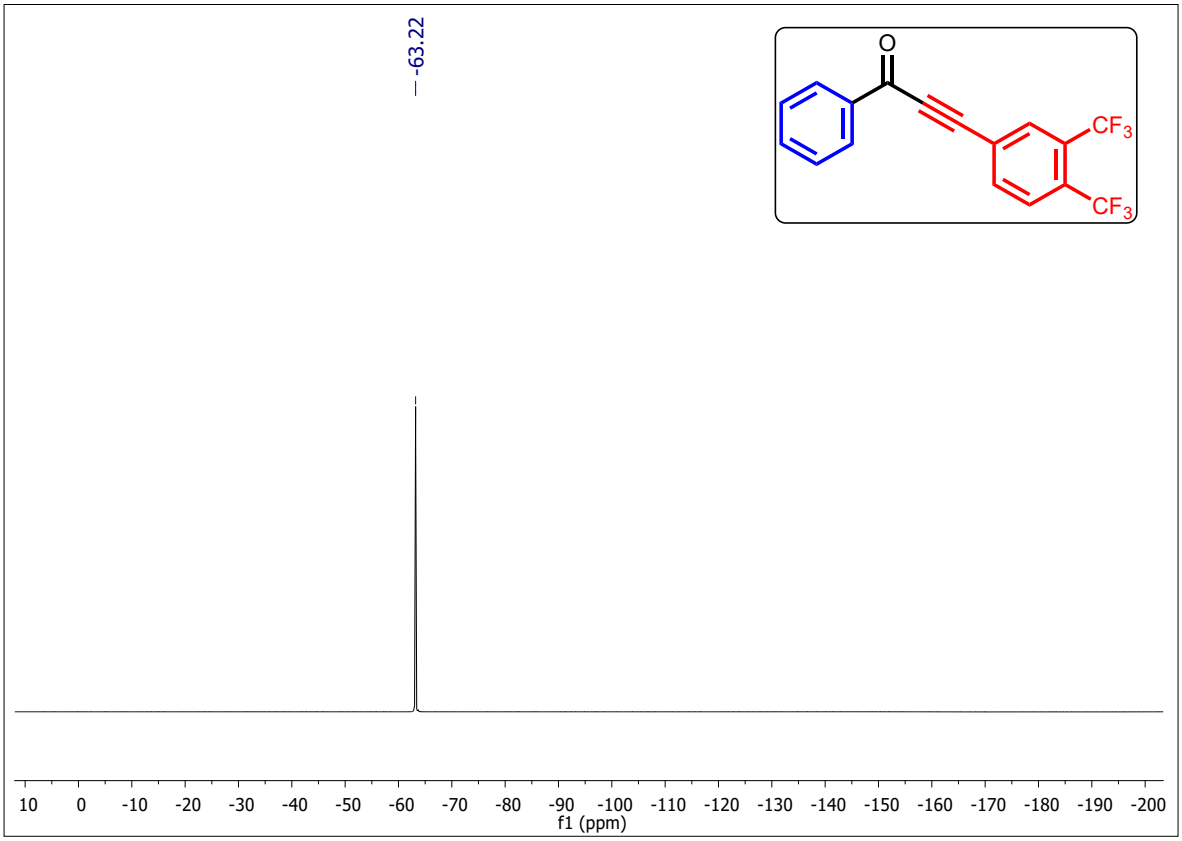
^{19}F NMR spectra of 1-(4-Fluorophenyl)-3-phenylprop-2-yn-1-one (3l)



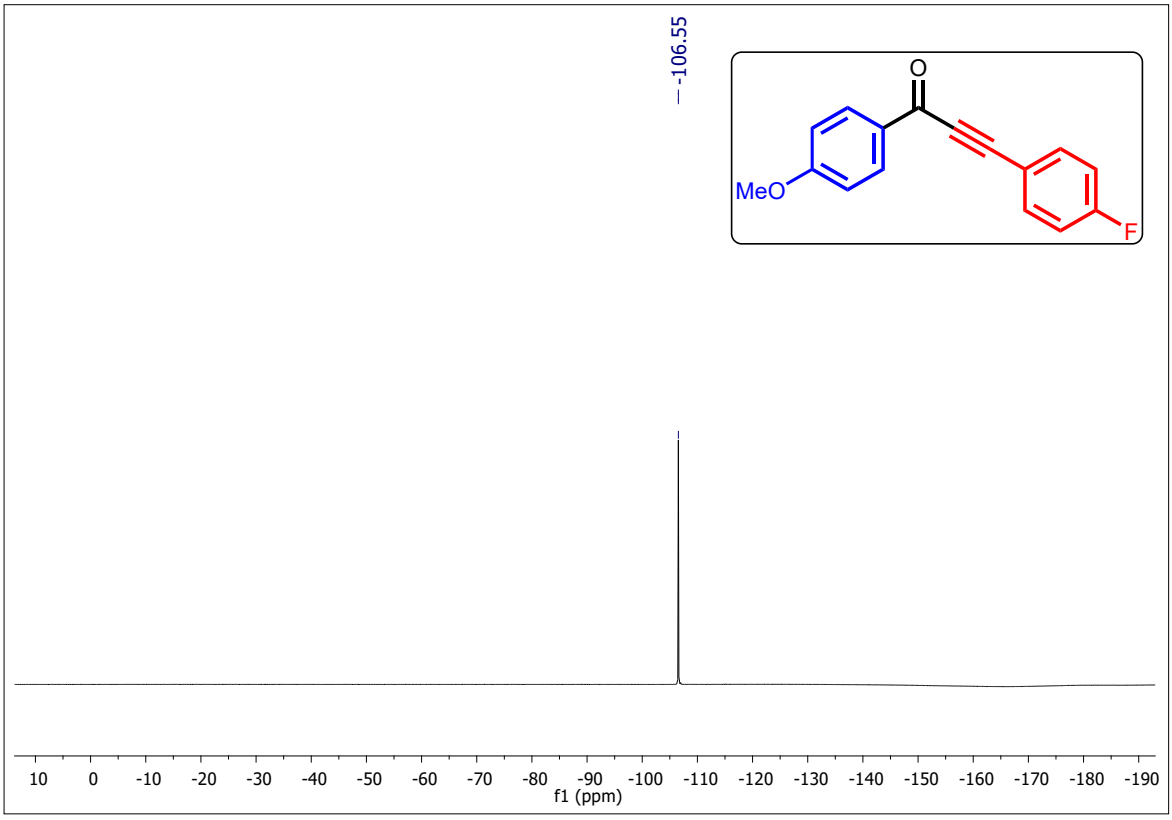
^{19}F NMR spectra of 1-Phenyl-3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-one (3t)



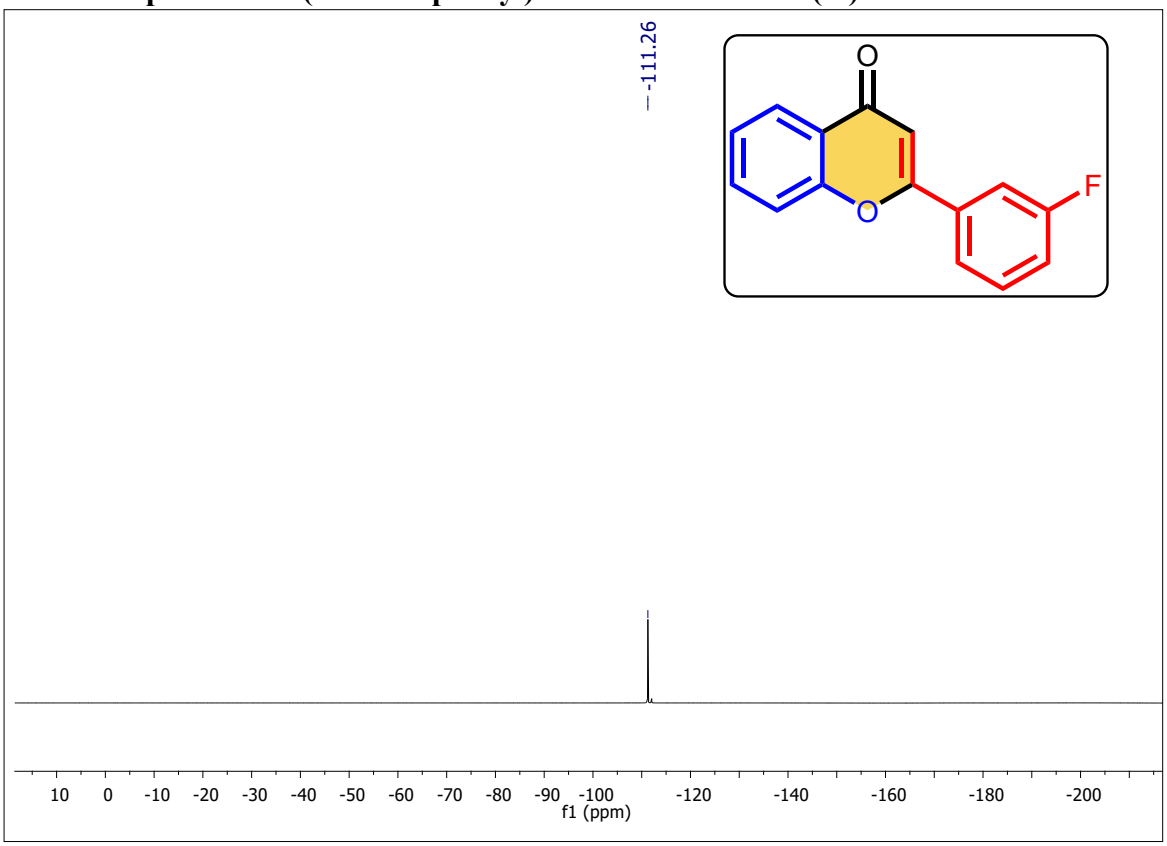
^{19}F NMR spectra of 3-(3,4-Bis(trifluoromethyl)phenyl)-1-phenylprop-2-yn-1-one (3u)



^{19}F NMR spectra of 3-(4-fluorophenyl)-1-(4-methoxyphenyl)prop-2-yn-1-one (3w)



^{19}F NMR spectra of 2-(3-Fluorophenyl)-4*H*-chromen-4-one (6f)



^{19}F NMR spectra of 2-(4-(Trifluoromethyl)phenyl)-4*H*-chromen-4-one (6j)