Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Palladium-Catalyzed Selective C-C Bond Cleavage and Stereoselective Alkenylation between Cyclopropanol and 1,3-Diyne: One-Step Synthesis of Diverse Conjugated Enynes

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1. General Information:

Reactions were performed using borosil sealed tube vial under N_2 atmosphere. Column chromatography was done by using 230-400 mesh silica gel of Acme synthetic chemicals company. A gradient elution was performed by using distilled petroleum ether and ethyl acetate. TLC plates detected under UV light at 254 nm and vanillin. ^{1}H NMR, ^{13}C NMR, recorded on Bruker AV 400 and 700 MHz spectrometer using $CDCl_3$ as the deuterated solvent.[1] Multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, quint = quintet, sept = septet, m = multiplet, dd = doublet of doublet, dt = doublet of triplet, td = triplet of doublet, br = broad signal), integration, and coupling constants (*J*) in hertz (Hz). HRMS signal analysis was performed using micro TOF Q-II mass spectrometer. Reagents and starting materials were purchased from Sigma Aldrich, TCI, Avra, Spectrochem and other commercially available sources, used without further purification unless otherwise noted. Cyclopropanol was prepared according to the literature reported procedure.[2]

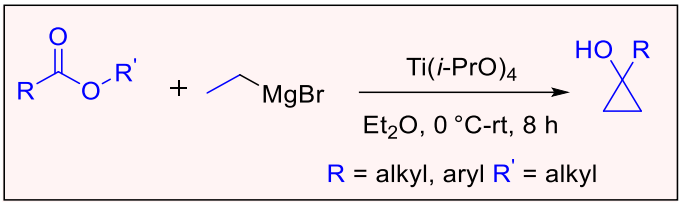
List of Abbreviation:

Et_2O (Diethyl ether), **EtOAc** (Ethyl acetate), **PCy_3** (Tricyclohexylphosphine), **TEMPO** ((2,2,6,6-Tetramethylpiperidin-1-yl)oxyl), **BHT** (Butylated hydroxytoluene), **TLC** (Thin layer chromatography).

2. Experimental details

2.1 General procedure for the synthesis of cyclopropanol

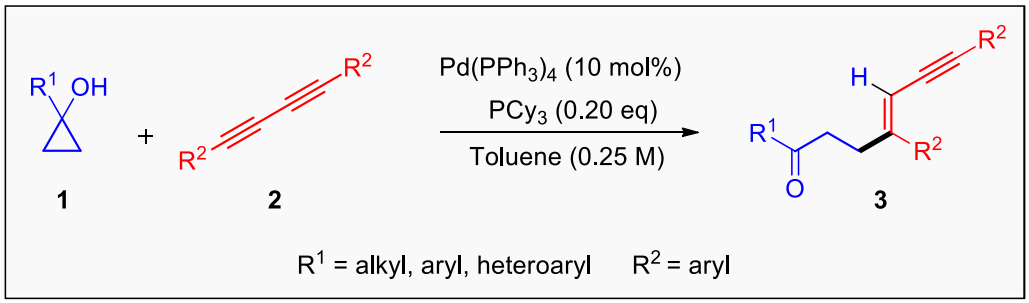
[General Procedure A]



Cyclopropanols were prepared according to a previously reported procedure.[2,3] To an oven-dried round bottom flask (100 mL) equipped with a magnetic stir bar, the ester (10 mmol) was dissolved in dry diethyl ether (30 mL). Ti(*i*-PrO)$_4$ (14.00 mmol, 1.40 equiv) was added to the solution and stirred for 2 min. Then ethylmagnesuim bromide (28.00 mmol, 28.mL, 1.0 mol/L in THF) was added dropwise to the solution at 0 °C. The solution generally turned dark green. After stirring at room temperature for 8 h, sulfuric acid solution (2.0 M, 20 mL) was added and stirred until all the solid dissolved to give a clear two-phase liquid. The liquid was separated and the aqueous solution was extracted with diethyl ether (3×30 mL). The organic layer was collected, washed with brine, and dried over anhydrous Na_2SO_4. The organic solution was filtered and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel (Hexane/EtOAc, 5:1) to provide the cyclopropanol product.

2.2 General procedure for titled transformation

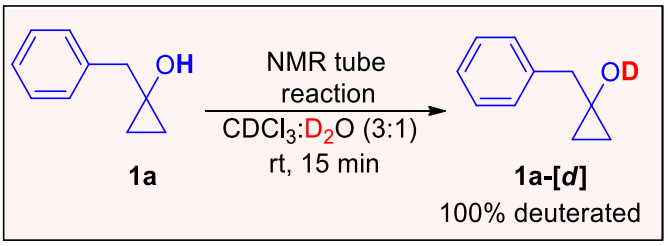
[General Procedure B]



A flame dried schlenk tube was charged with cyclopropanol **1** (0.20 mmol, 2.00 equiv), 1,3-diyne **2** (0.10 mmol, 1.00 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.00 mol %), PCy_3 (0.02 mmol, 20.00 mol %), and toluene (0.4 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel chromatography using hexane/ethyl acetate solvent system to afford the desired product **3**.

3. Mechanistic investigations:

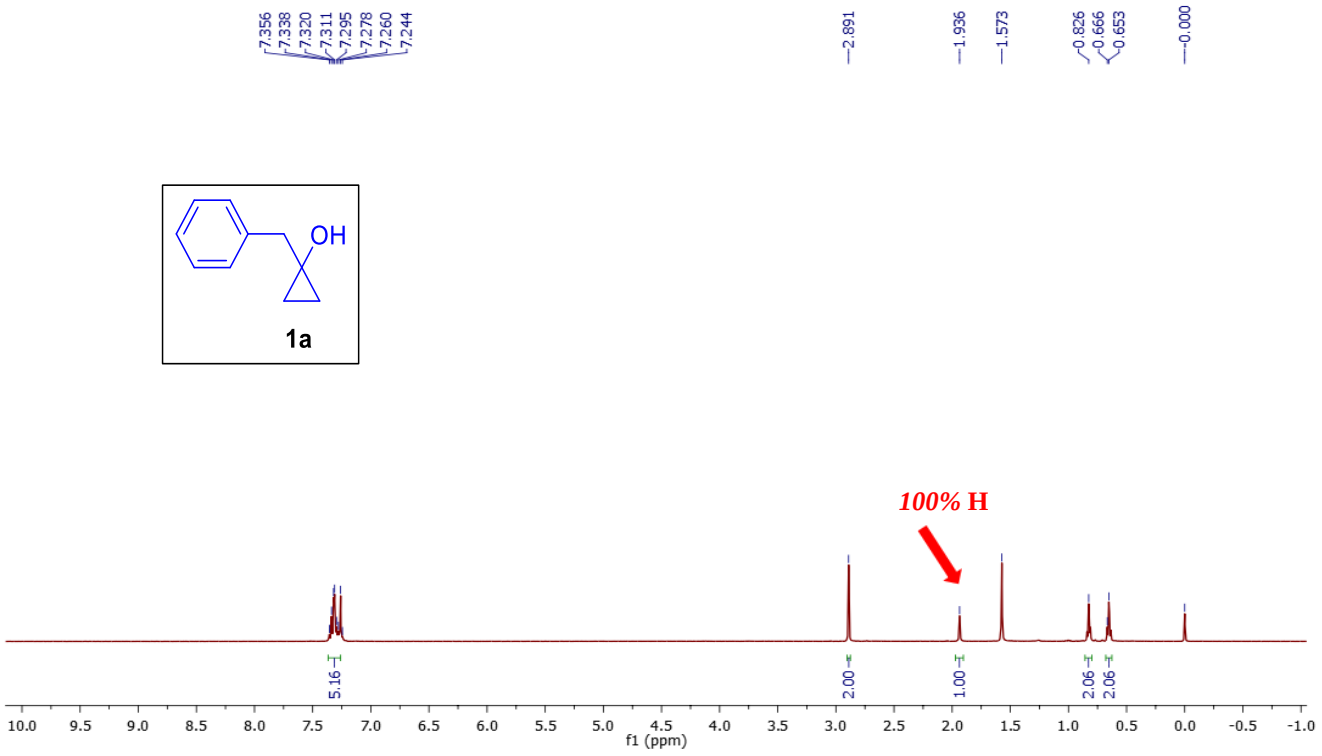
3.1 Preparation of deuterium-labeled cyclopropanol 1a-[*d*]



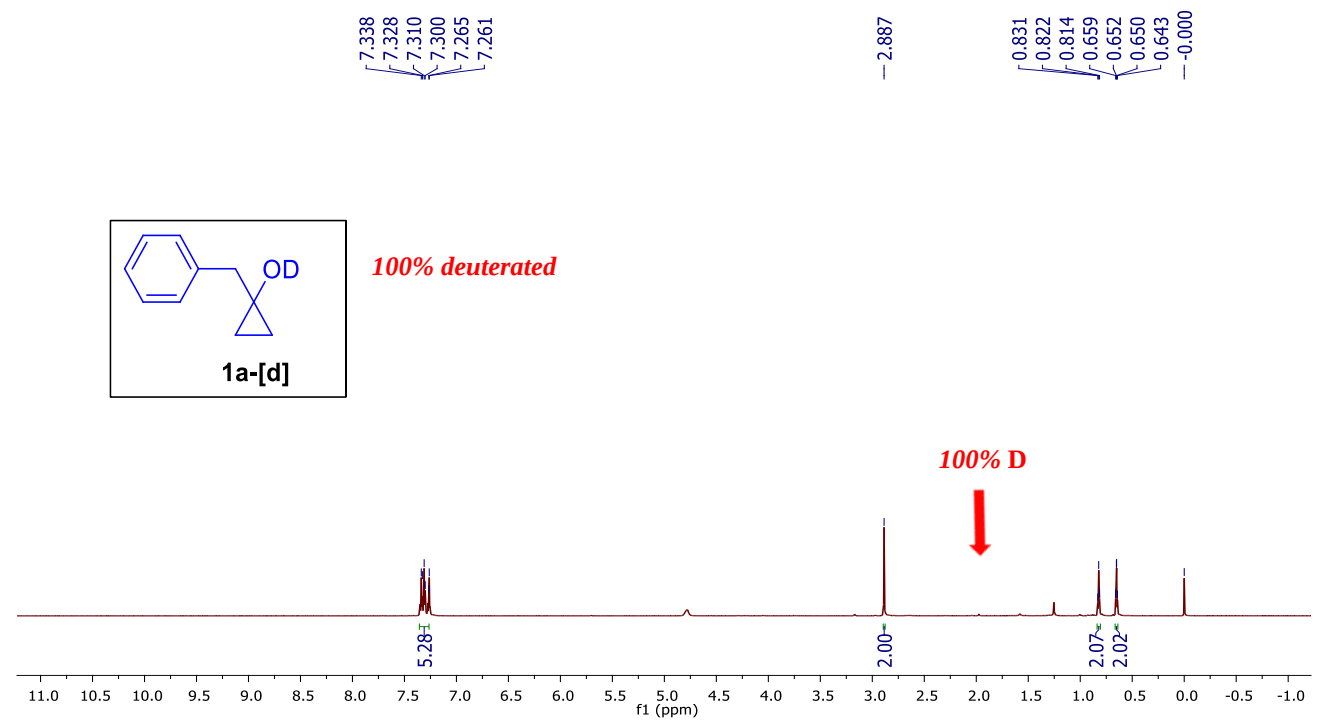
In a NMR tube (Norell® Standard Series™ 5 mm) cyclopropanol **1a** (50 mg, 0.33 mmol) was taken in $CDCl_3$:D_2O (3:1) mixture and the contents were sonicated for 5 min. NMR was recorded at different time intervals and at 10 min complete exchange (100%) was observed. So, we obtained 100% deuterated cyclopropanol **1a-[*d*]**.

NMR spectra of 1a and 1a-[*d*]

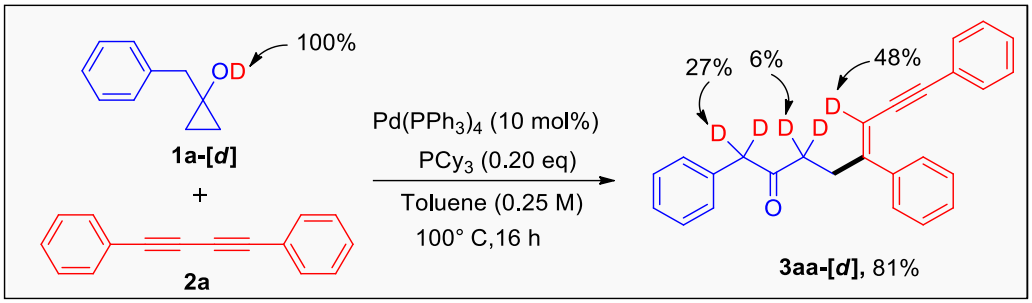
^{1}H NMR of 1a (400 MHz, $CDCl_3$)



^{1}H NMR of 1a-[*d*] (400 MHz, $CDCl_3$)



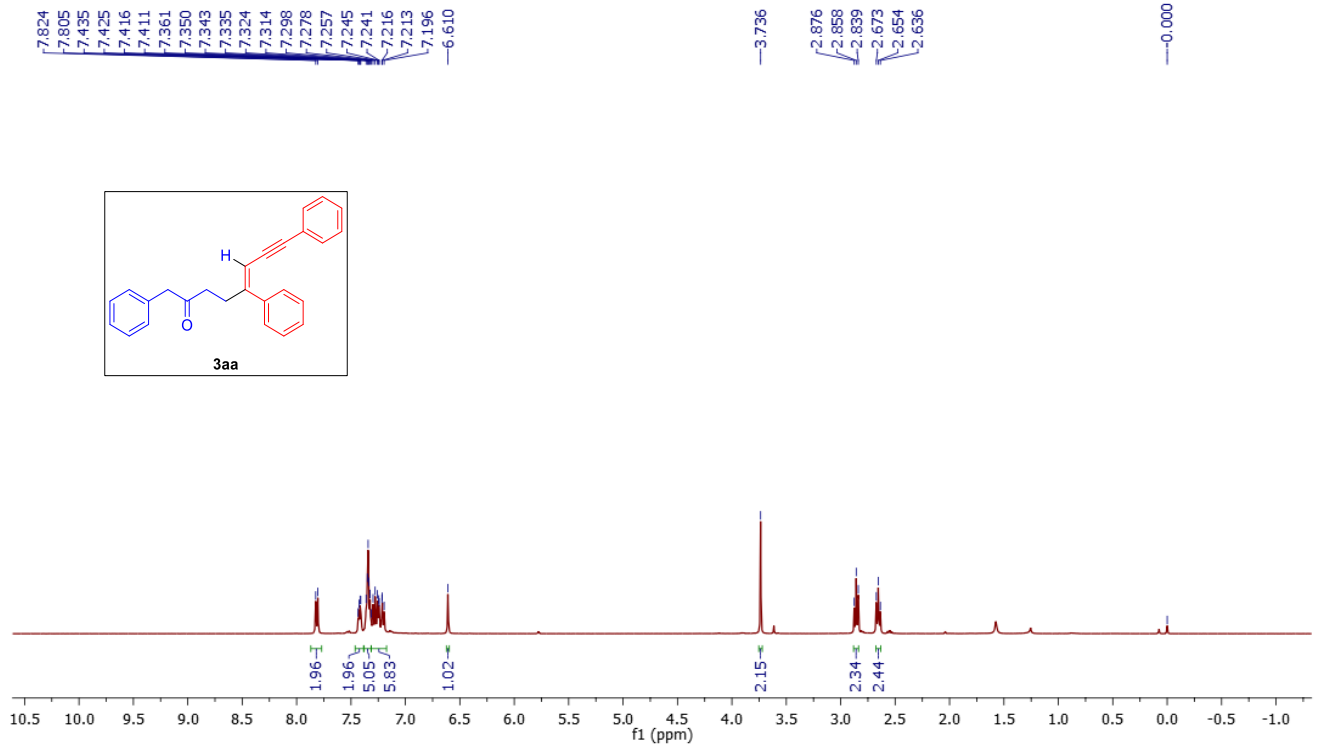
3.2 Deuterium-incorporation using deuterated cyclopropanol 1a-[*d*]



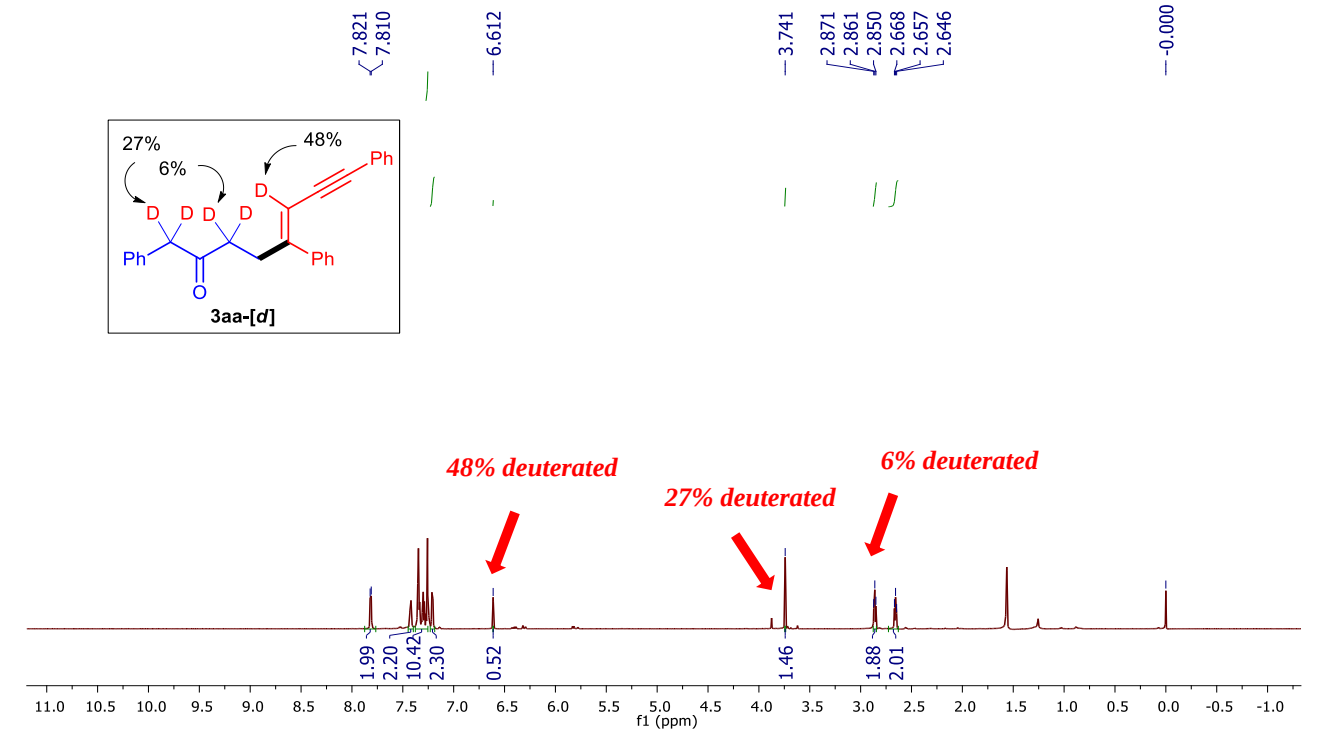
A flame dried schlenk tube was charged with cyclopropanols **1a-[*d*]** (0.20 mmol, 2.00 equiv), 1,3-diynes **2a** (0.10 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel chromatography using hexane/ethyl acetate solvent system to afford the desired product **3aa-[*d*]** in 81% yield.

NMR spectra of 3aa and 3aa-[*d*]

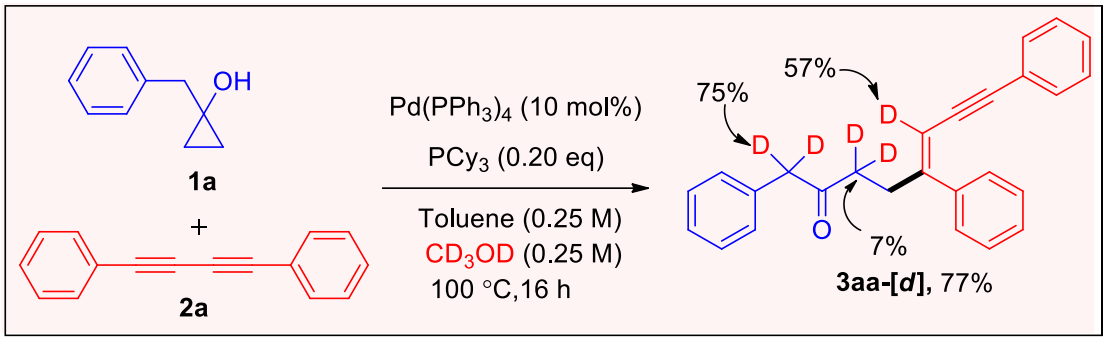
^{1}H NMR of 3aa (400 MHz, $CDCl_3$)



^{1}H NMR of 3aa-[*d*] (400 MHz, $CDCl_3$)



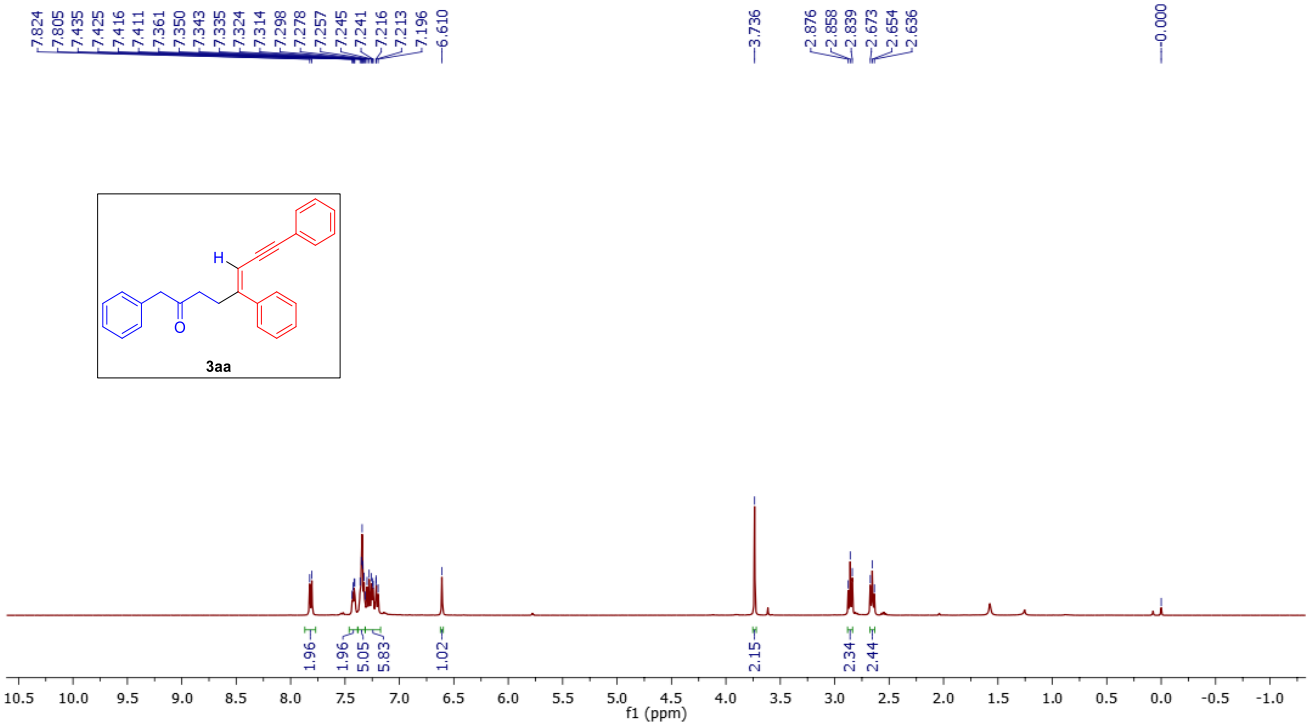
3.3 Deuterium-incorporation using deuterated solvent



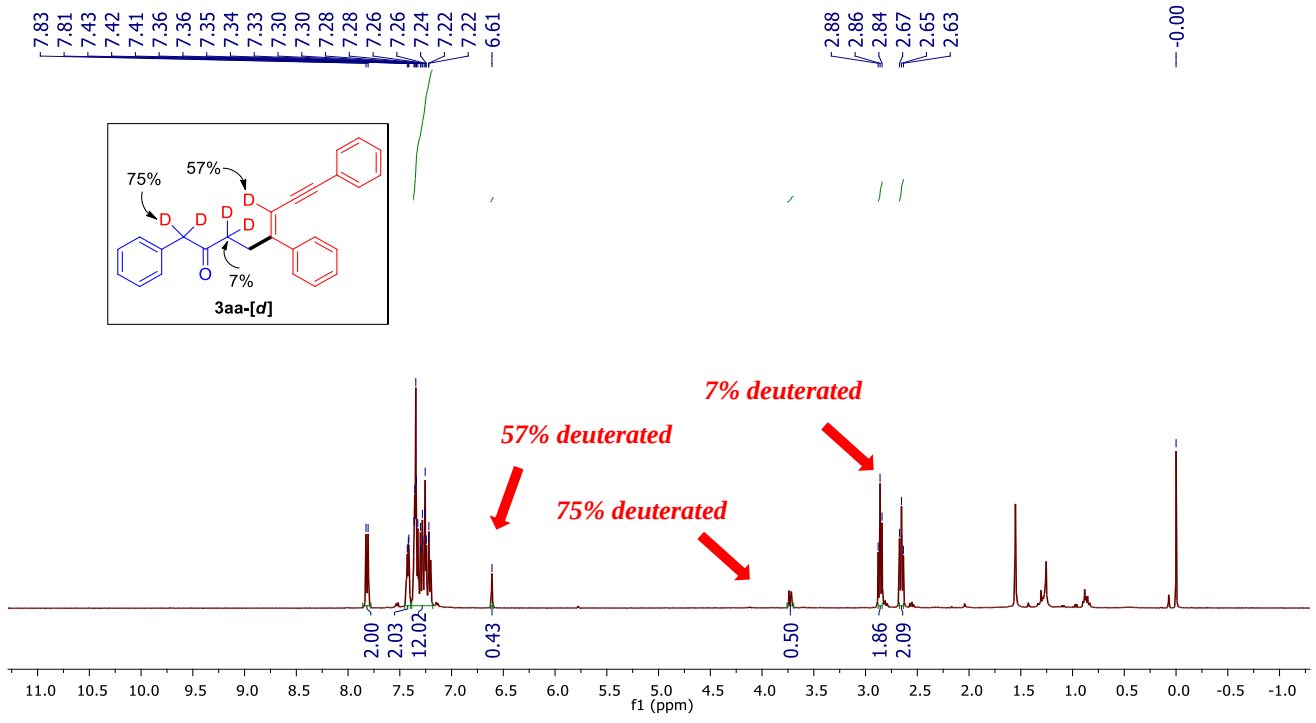
A flame dried schlenk tube was charged with cyclopropanols **1a** (0.20 mmol, 2.00 equiv), 1,3-diynes **2a** (0.10 mmol, 1.00 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M) and CD_3OD (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 ^oC in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel chromatography using hexane/ethyl acetate solvent system to afford the desired product **3aa'-[*d*]** in 77% yield with 57% and 75%, and 7% deuterium incorporation at the ethylenic, benzylic, and the carbonyl α-positions respectively.

NMR spectra of 3aa and 3aa-[*d*]

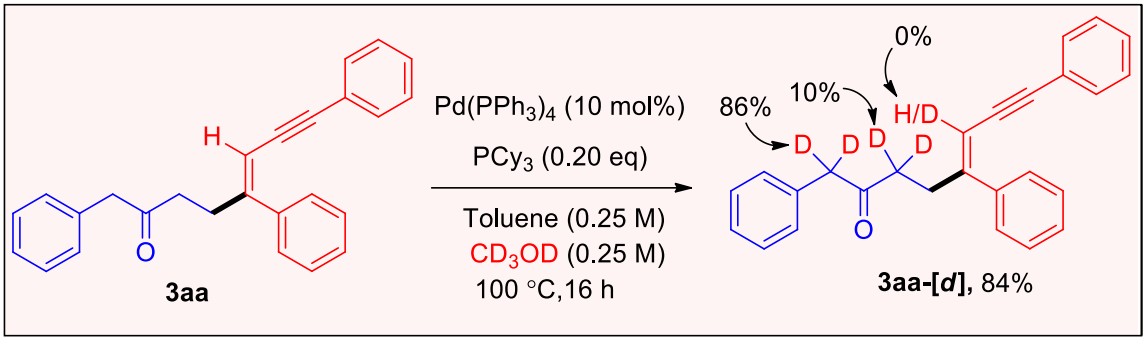
^{1}H NMR of 3aa (400 MHz, $CDCl_3$)



^{1}H NMR of 3aa-[*d*] (400 MHz, $CDCl_3$)



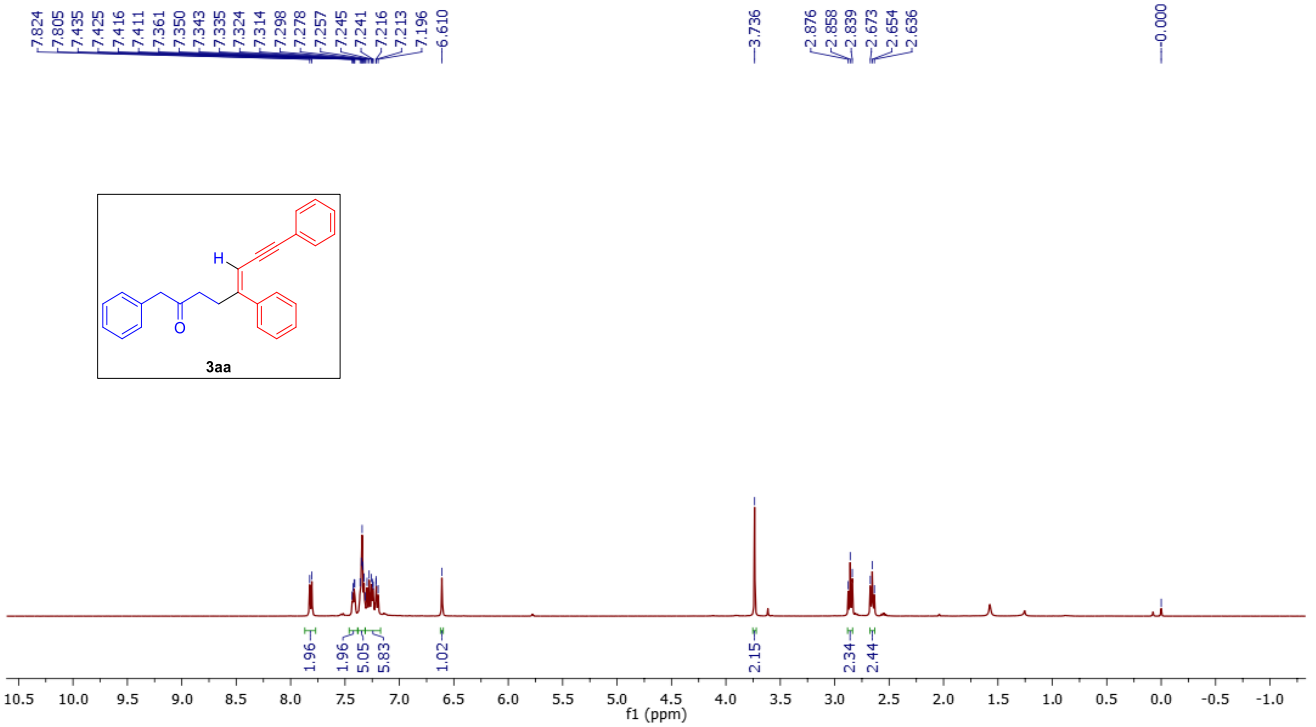
3.4 Deuterium-incorporation of 3aa using deuterated solvent



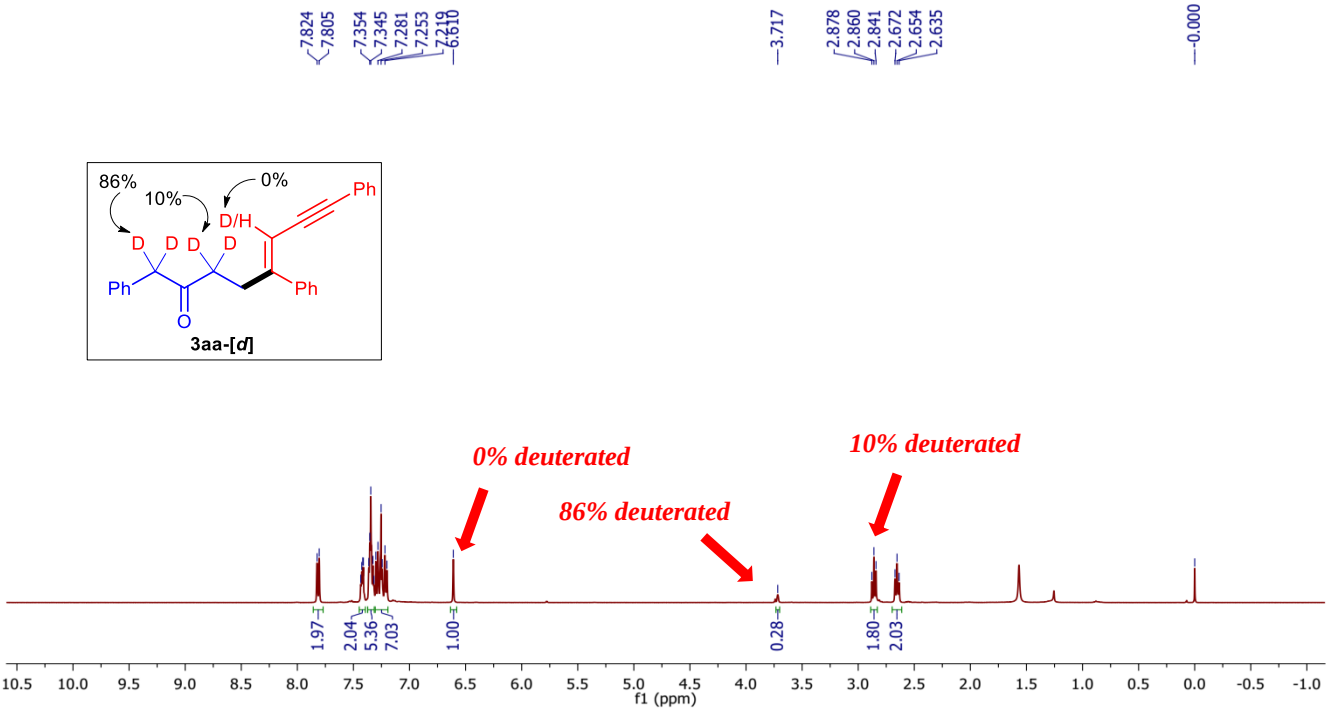
A flame dried schlenk tube was charged with alkenylated adduct **3aa** (0.10 mmol, 1.00 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M) and CD_3OD (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel chromatography using hexane/ethyl acetate solvent system to afford the desired product **3aa'-[*d*]** in 84% yield with no deuterium incorporation at the olefinic position while, 86% and 10% deuterium incorporation at the benzylic and the carbonyl α-positions respectively.

NMR spectra of 3aa and 3aa-[*d*]

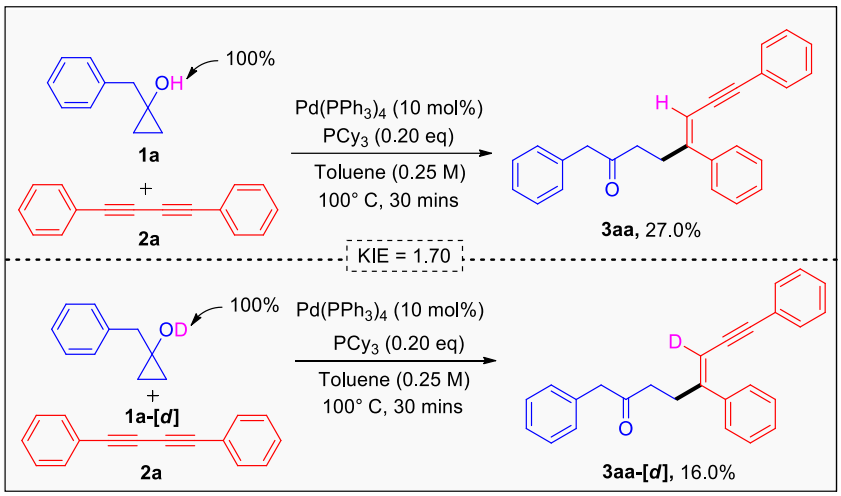
^{1}H NMR of 3aa (400 MHz, $CDCl_3$)



^{1}H NMR of 3aa-[*d*] (400 MHz, $CDCl_3$)



3.5 Kinetic isotope effect study:

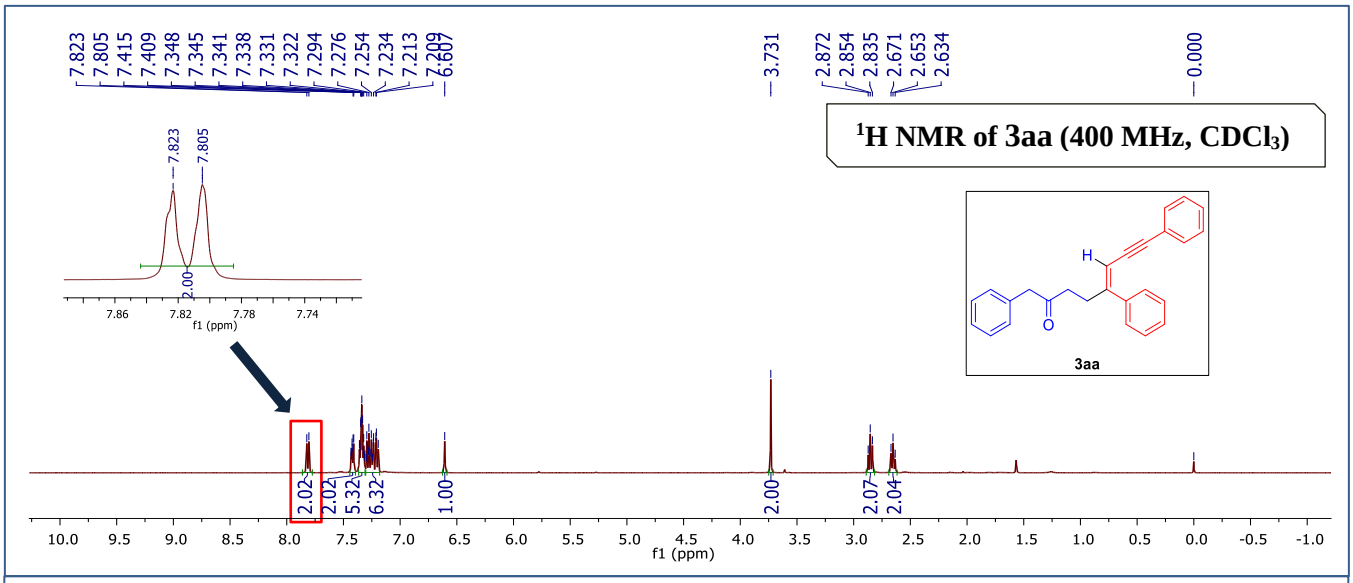


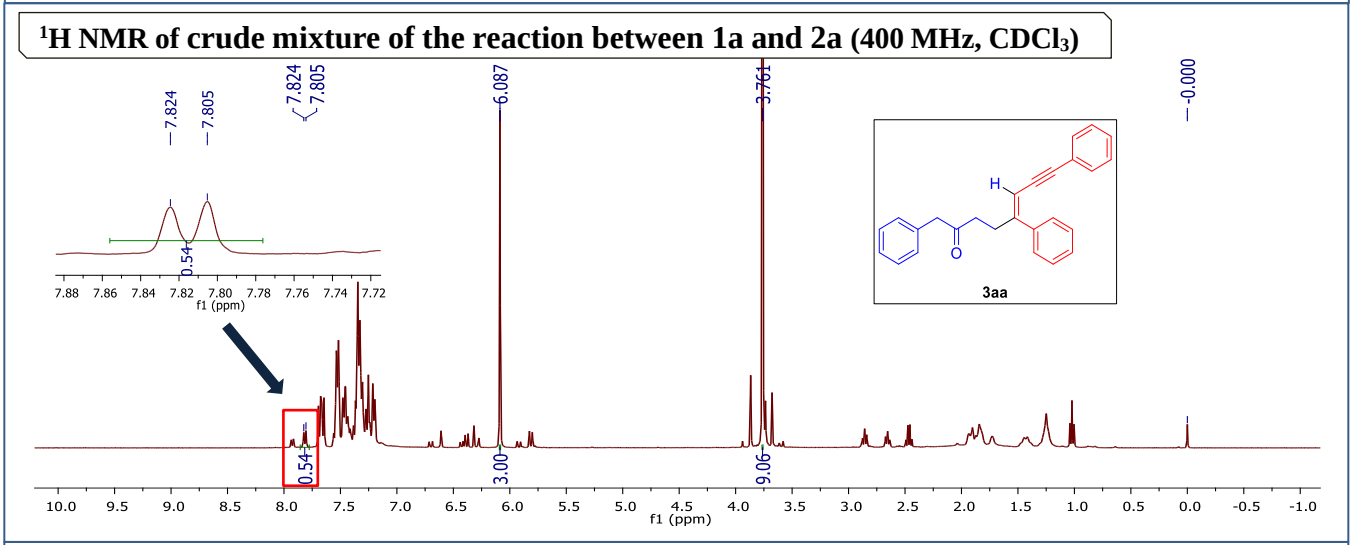
By following the general procedure, a parallel experiment was carried out using 100% protonated substrate (**1a)**. To a flame-dried 5.00 mL screw capped vial equipped with magnetic stir bar were charged [D]-**1a** (2.00 equiv), 1,4-diphenylbuta-1,3-diyne (**2a**, 1.00 equiv), $Pd(PPh_3)_4$ (10 mol %), PCy_3 (20.0 mol%), and toluene (0.25 mL). The reaction was carried out for 30 min at 100 °C in a pre-heated aluminum block. The product yield was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

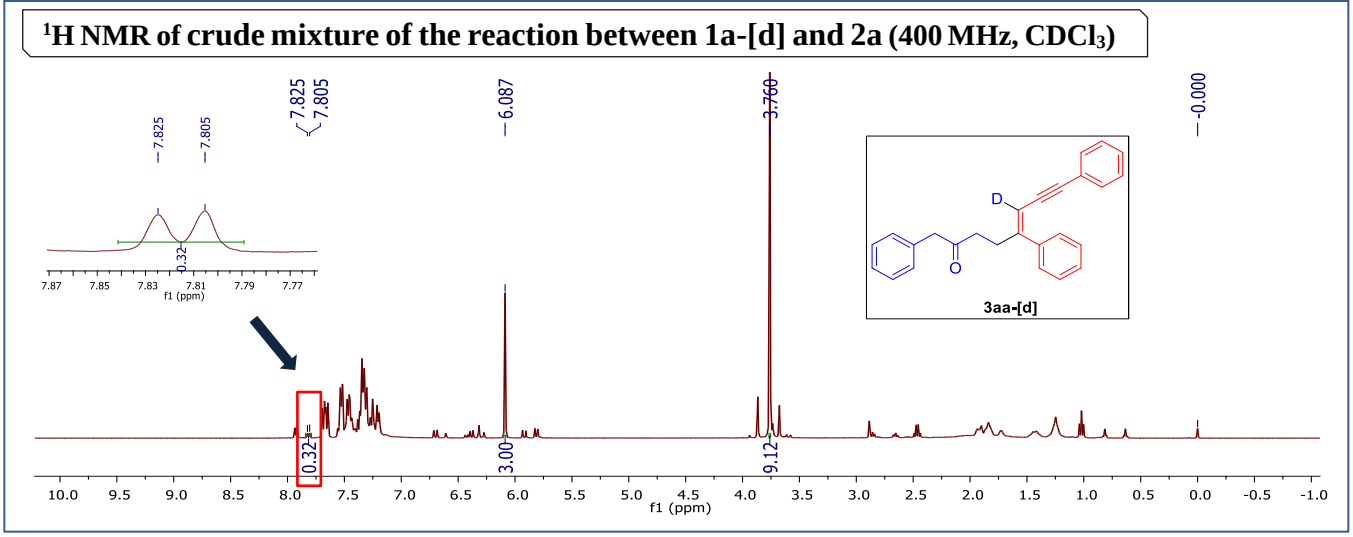
Similarly, by following the general procedure, a parallel experiment was carried out using 100% deuterated substrate ([D]-**1a)**. To a flame-dried 5.00 mL screw capped vial equipped with magnetic stir bar were charged [D]-**1a** (2.00 equiv), 1,4-diphenylbuta-1,3-diyne (**2a**, 1.00 equiv), $Pd(PPh_3)_4$ (10 mol %), PCy_3 (20.0 mol%), and toluene (0.25 mL). The reaction was carried out for 30 min at 100 °C in a pre-heated aluminum block. The product yield was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

The KIE value (1.70) was calculated from the obtained yields of the two products (**3aa** and **3aa-[*d*]**).

NMR spectra of parallel intermolecular reaction between cyclopropanols (1a and 1a-[d])

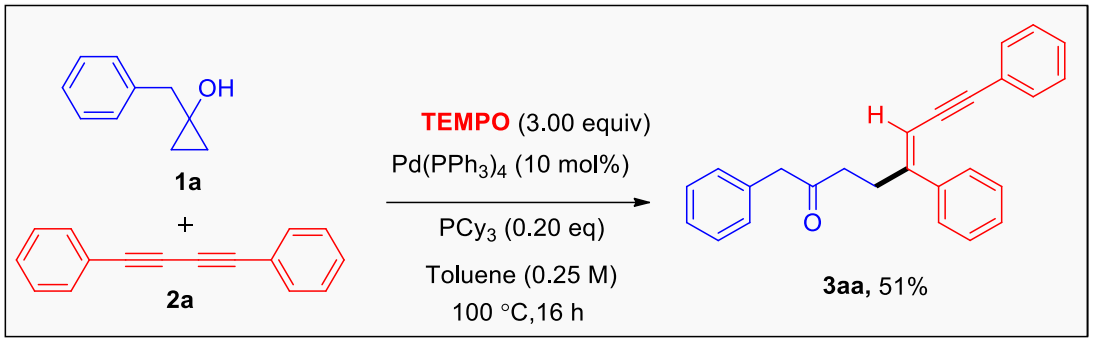






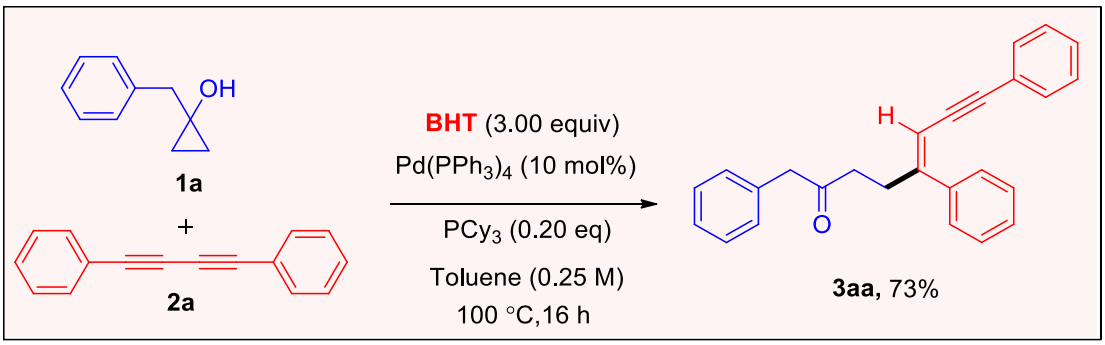
3.6 Palladium-catalyzed alkenylation of cyclopropanol in presence of radical scavengers

3.6.1 Alkenylation of cyclopropanol in presence of TEMPO



A flame dried schlenk tube was charged with cyclopropanol **1a** (0.20 mmol, 2.00 equiv), 1,3-diyne **2a** (0.10 mmol, 1.00 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), TEMPO (3 equiv) and toluene (0.4 mL 0.25M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel chromatography using hexane/ethyl acetate solvent system to afford the desired product **3aa** in 51% yield. No trapped intermediate is detected.

3.6.2 Alkenylation of cyclopropanol in presence of BHT

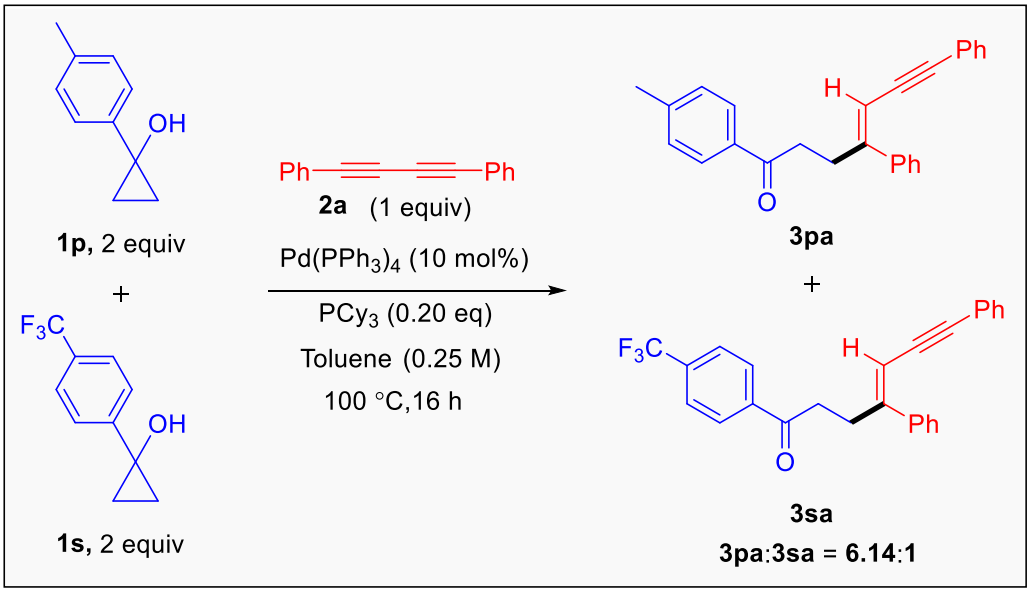


A flame dried schlenk tube was charged with cyclopropanol **1a** (0.2 mmol, 2.0 equiv), 1,3-diyne **2a** (0.10 mmol, 1.00 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), BHT (3 equiv) and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum

block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure, and the resulting crude was purified by silica gel chromatography using hexane/ethyl acetate solvent system to afford the desired product **3aa** in 73% yield. No trapped intermediate is detected.

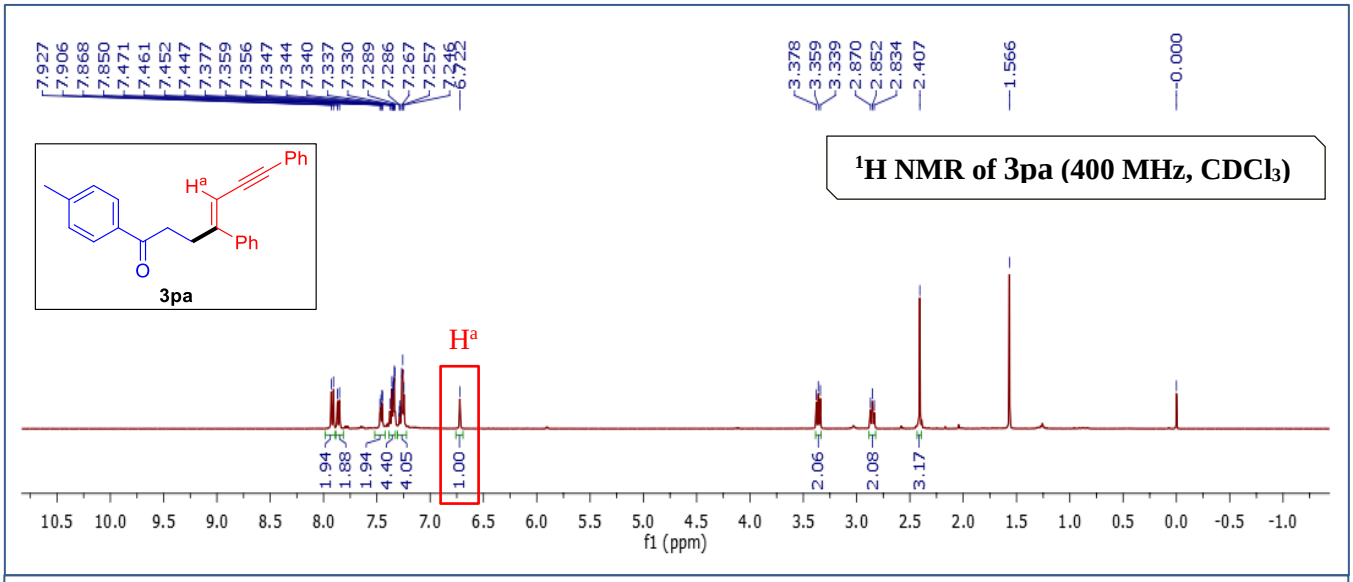
4. Competition experiments:

4.1.1 Intermolecular one pot competition reaction between two different cyclopropanols (1p and 1s)

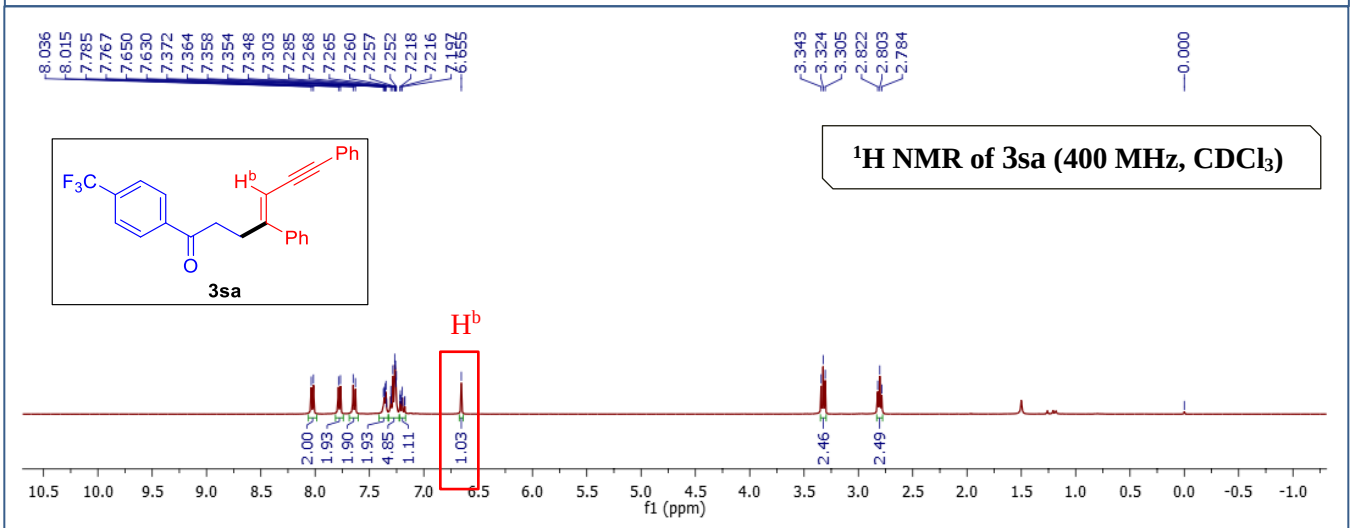


A flame dried schlenk tube was charged with different cyclopropanol **1p** (0.20 mmol, 2.00 equiv), **1s** (0.20 mmol, 2.00 equiv), 1,3-diynes **2a** (0.10 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The ratio of two products **3pa**:**3sa** (6.14:1) was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

NMR spectra of Intermolecular one pot competition reaction between two different cyclopropanols (1p and 1s)

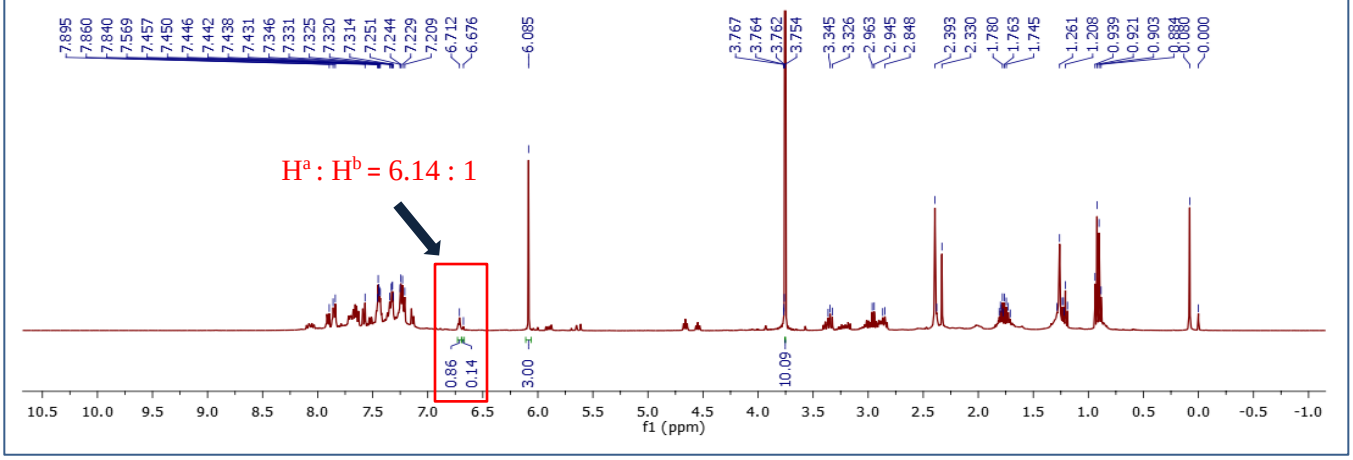


^{1}H NMR of 3pa (400 MHz, $CDCl_3$)

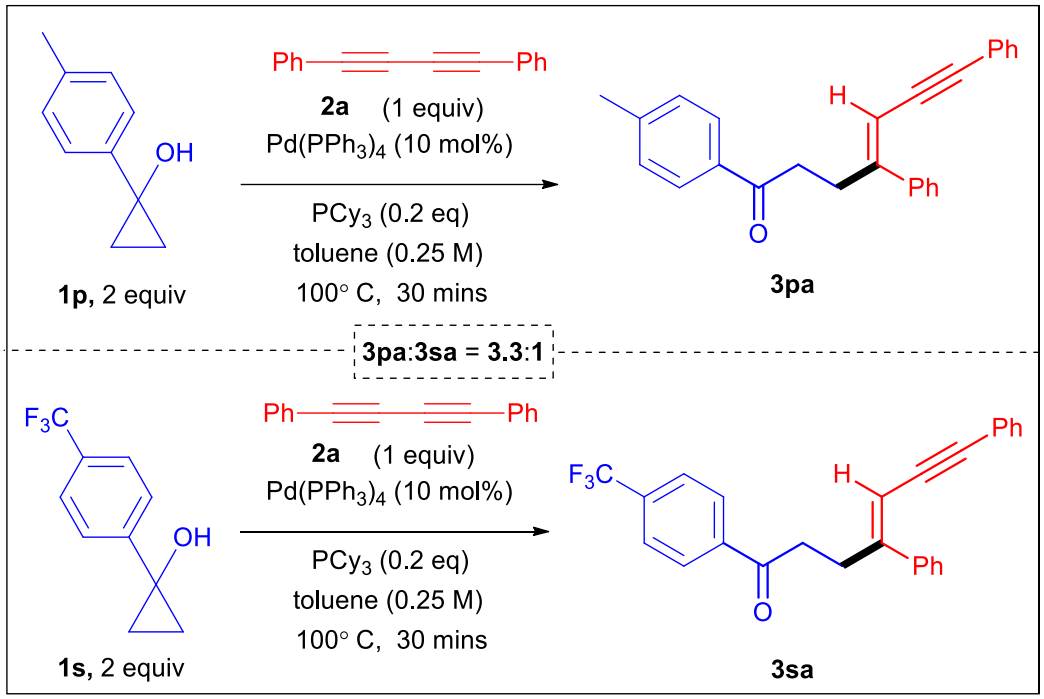


^{1}H NMR of 3sa (400 MHz, $CDCl_3$)

^{1}H NMR of crude mixture of the competition reaction between 2a, 1p and 1s (400 MHz, $CDCl_3$)



4.1.1 Intermolecular competition parallel reaction between two different cyclopropanols (1p and 1s)

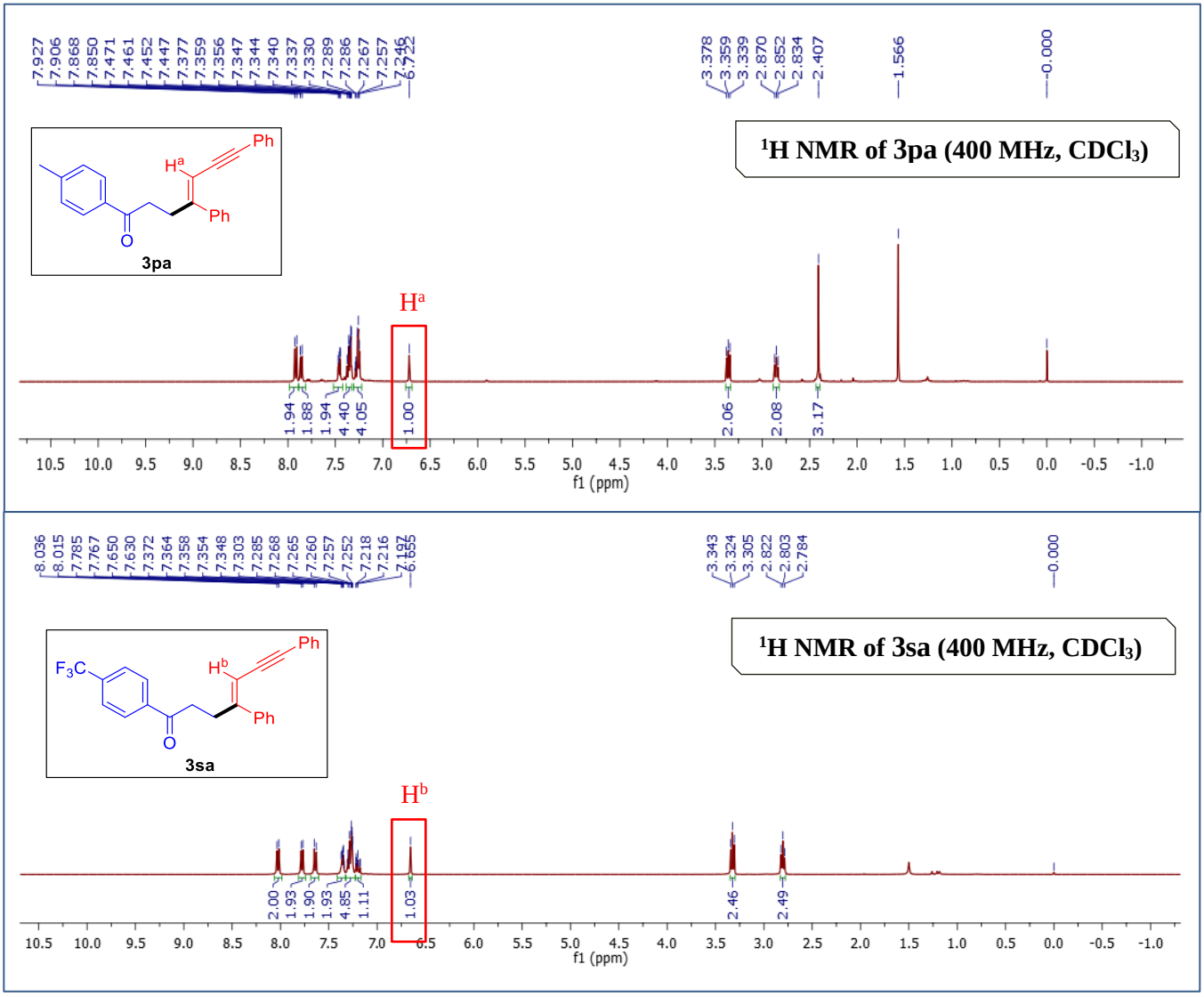


By following the general procedure, a parallel experiment was carried out. A flame dried schlenk tube was charged with cyclopropanol **1p** (0.20 mmol, 2.00 equiv), 1,3-diynes **2a** (0.10 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 15 min. After 15 min of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The yield of the product **3pa** was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

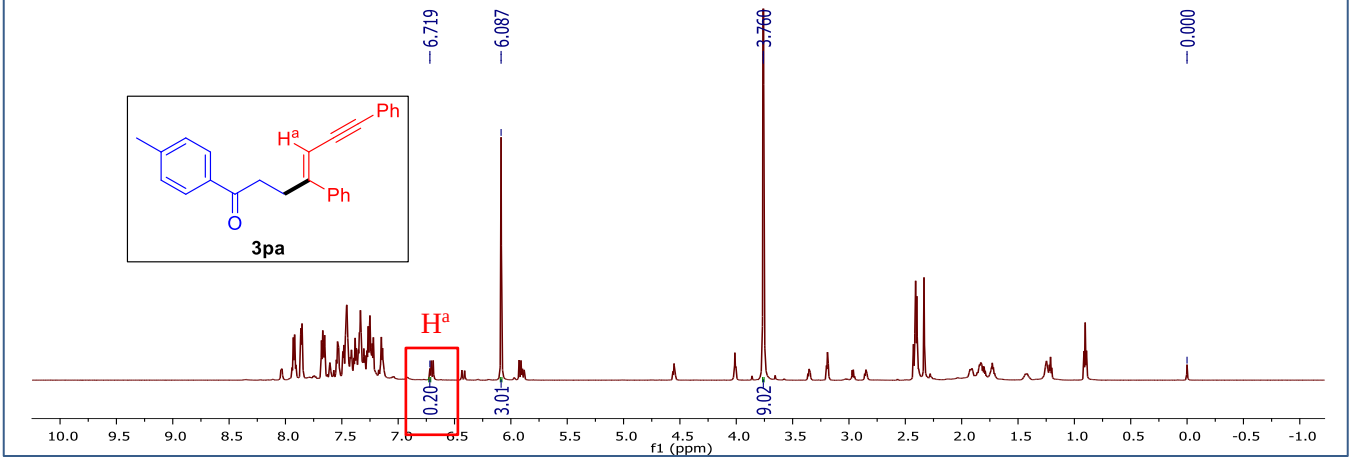
Similarly, by following the general procedure, a parallel experiment was carried out. A flame dried schlenk tube was charged with cyclopropanol **1s** (0.20 mmol, 2.00 equiv), 1,3-diynes **2a** (0.10 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 15 min. After 15 min of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5

mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The yield of the product **3sa** was calculated from the ^{1}H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

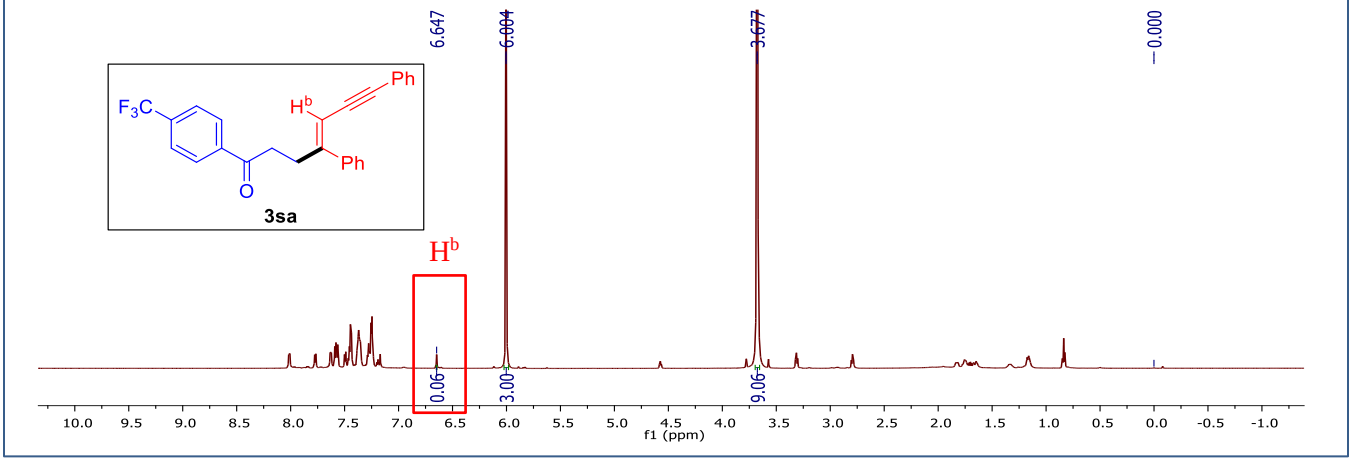
NMR spectra of intermolecular competition parallel reaction between two different cyclopropanols (1p and 1s) with diyne 2a



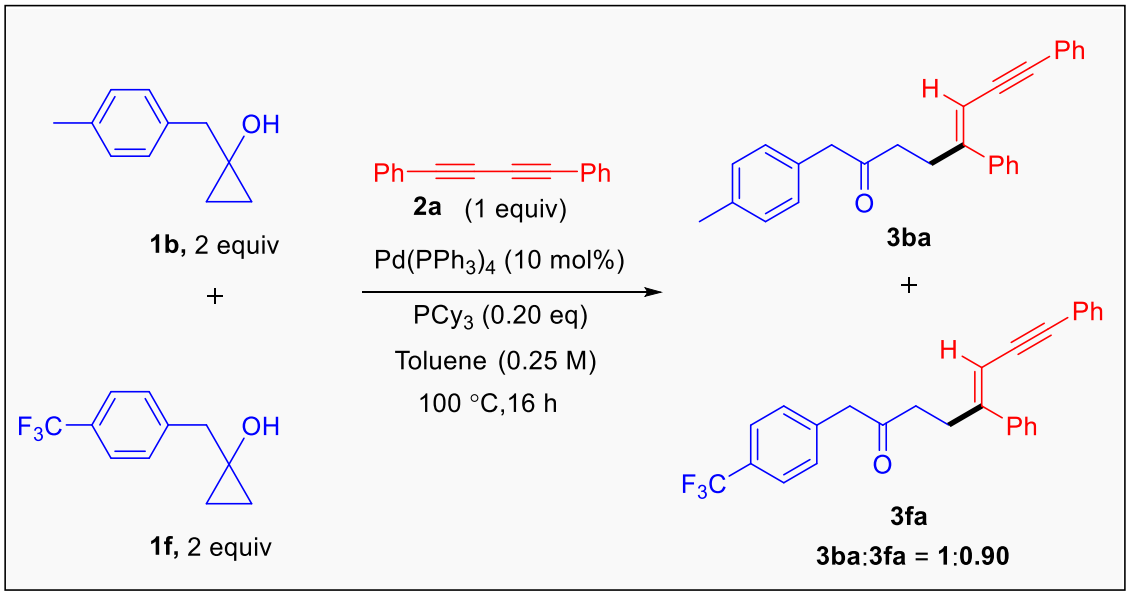
^{1}H NMR of crude mixture of the competition parallel reaction between 2a, 1p (700 MHz, $CDCl_3$)



^{1}H NMR of crude mixture of the competition parallel reaction between 2a, 1s (700 MHz, $CDCl_3$)

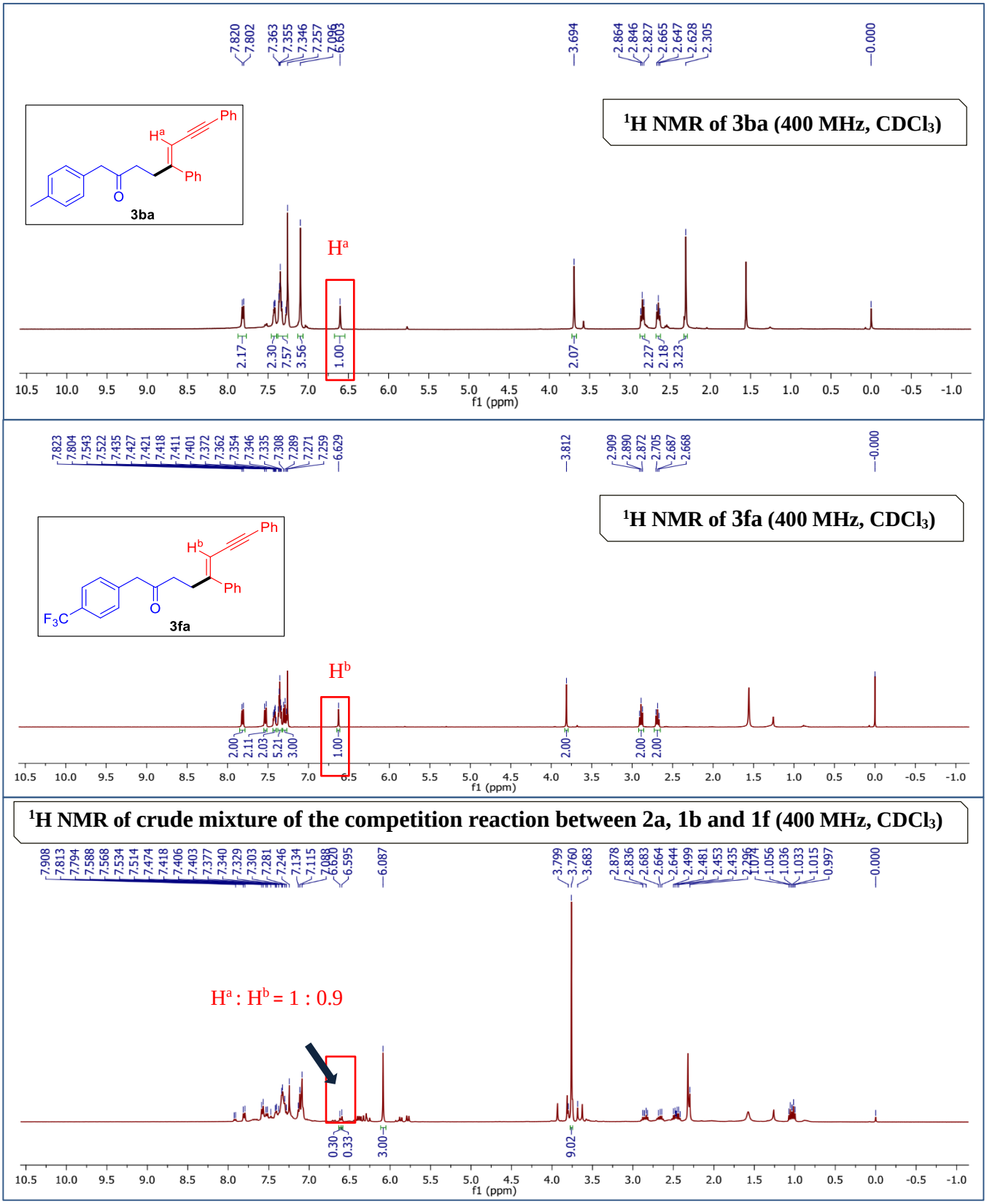


4.1.3 Intermolecular one pot competition reaction between two different cyclopropanols (1b and 1f)

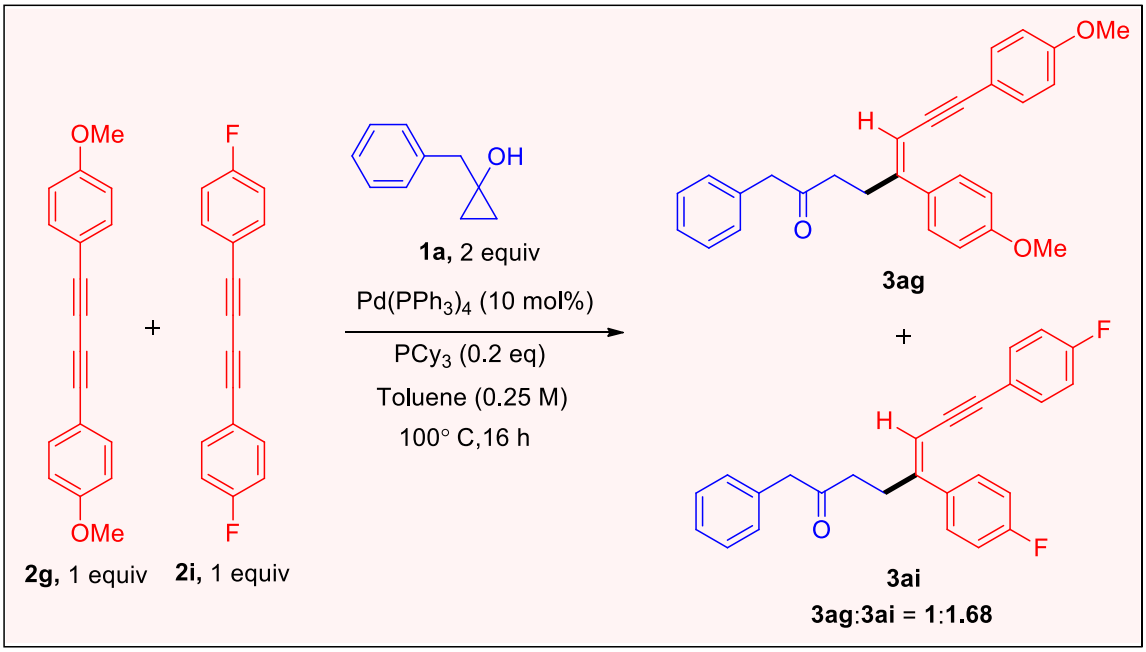


A flame dried schlenk tube was charged with different cyclopropanol **1b** (0.20 mmol, 2.00 equiv), **1f** (0.20 mmol, 2.00 equiv), 1,3-diynes **2a** (0.10 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The ratio of two products **3ba**:**3fa** (1:0.90) was calculated from the ^{1}H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

NMR spectra of Intermolecular competition reaction between two different cyclopropanols (1b and 1f)

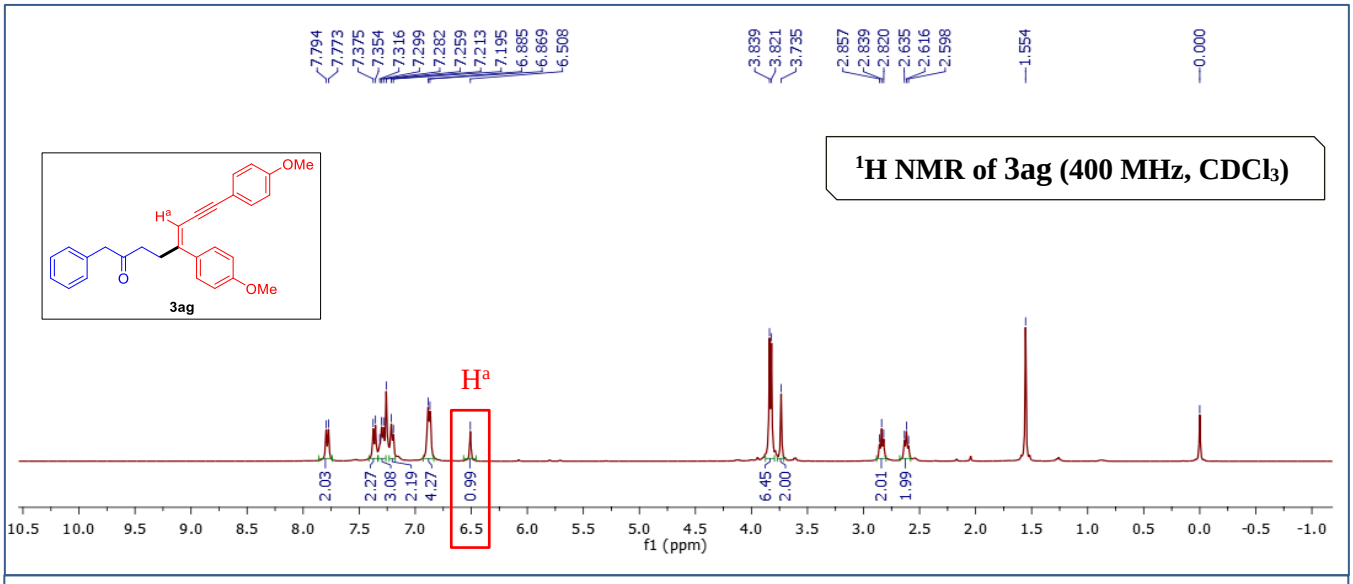


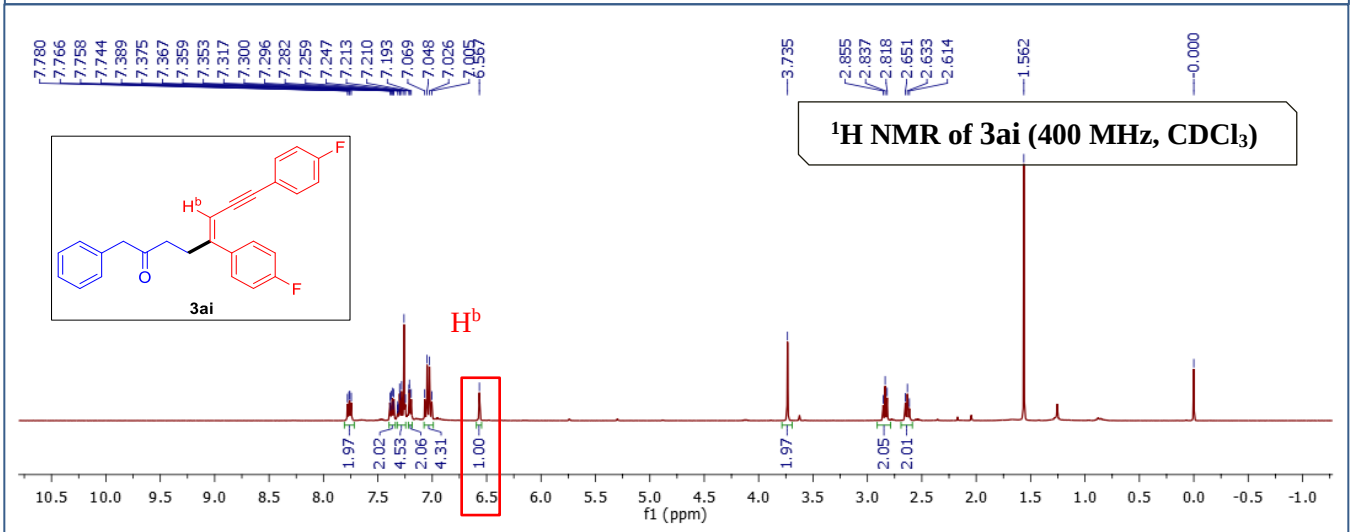
4.2.1 Intermolecular one pot competition reaction between two different diynes (2g and 2i) with cyclopropanol 1a

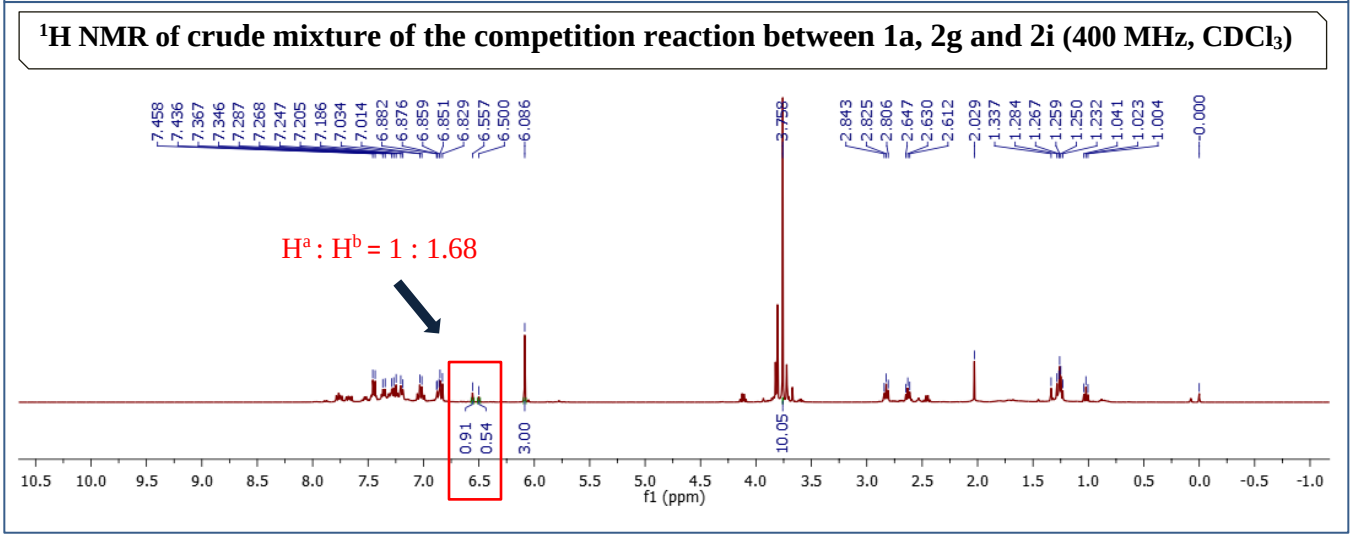


A flame dried schlenk tube was charged with cyclopropanol **1a** (0.20 mmol, 2.00 equiv), two different 1,3-diyne **2g** (0.10 mmol, 1.00 equiv), **2i** (0.10 mmol, 1.00 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The ratio of two products **3ag**:**3ai** (1:1.68) was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

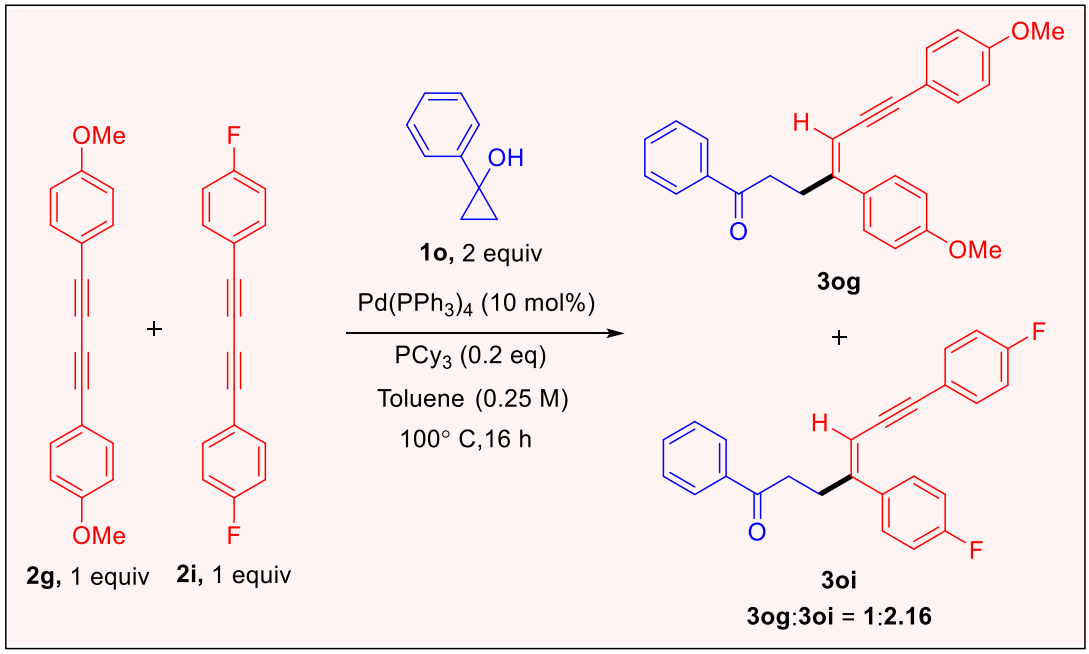
NMR spectra of Intermolecular competition reaction between two different diynes (2g and 2i) with cyclopropanol 1a





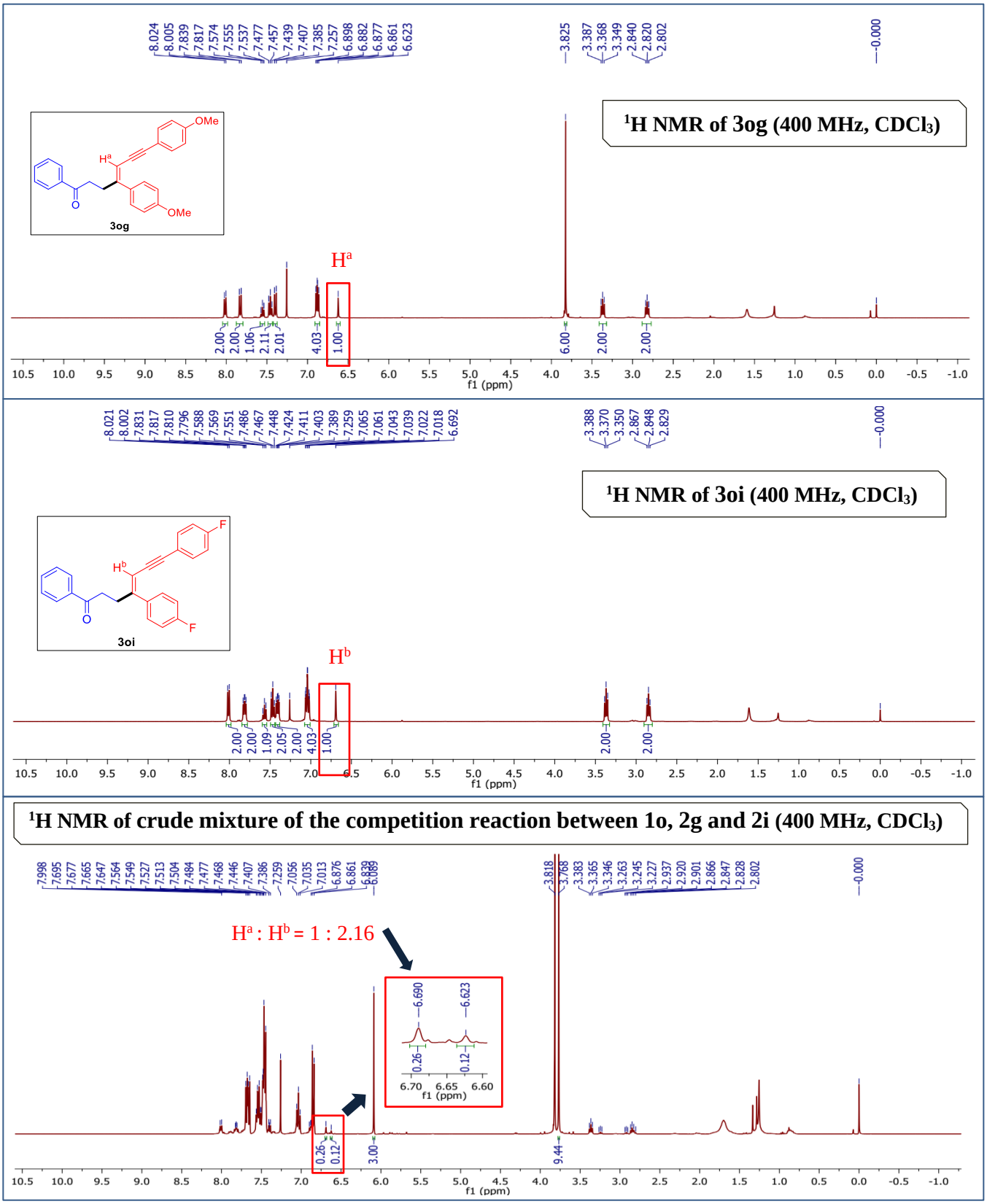


4.2.2 Intermolecular one pot competition reaction between two different diynes (2g and 2i) with cyclopropanol 1o

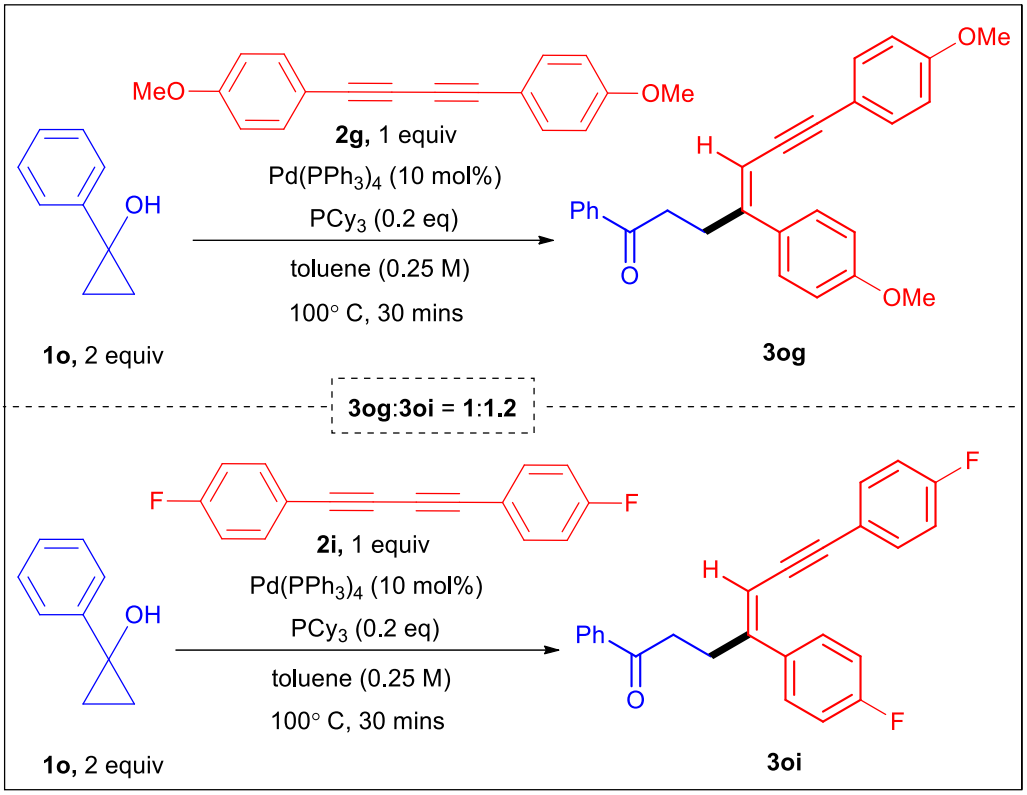


A flame dried schlenk tube was charged with cyclopropanol **1o** (0.20 mmol, 2.00 equiv), two different 1,3-diyne **2g** (0.10 mmol, 1.00 equiv), **2i** (0.10 mmol, 1.00 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 16 hours. The completion of the reaction was monitored by TLC. Upon completion of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The ratio of two products **3og**:**3oi** (1:2.16) was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

NMR spectra of Intermolecular one pot competition reaction between two different diynes (2g and 2i) with cyclopropanol 1o



4.2.3 Intermolecular parallel competition reaction between two different diynes (2g and 2i) with cyclopropanol 1o

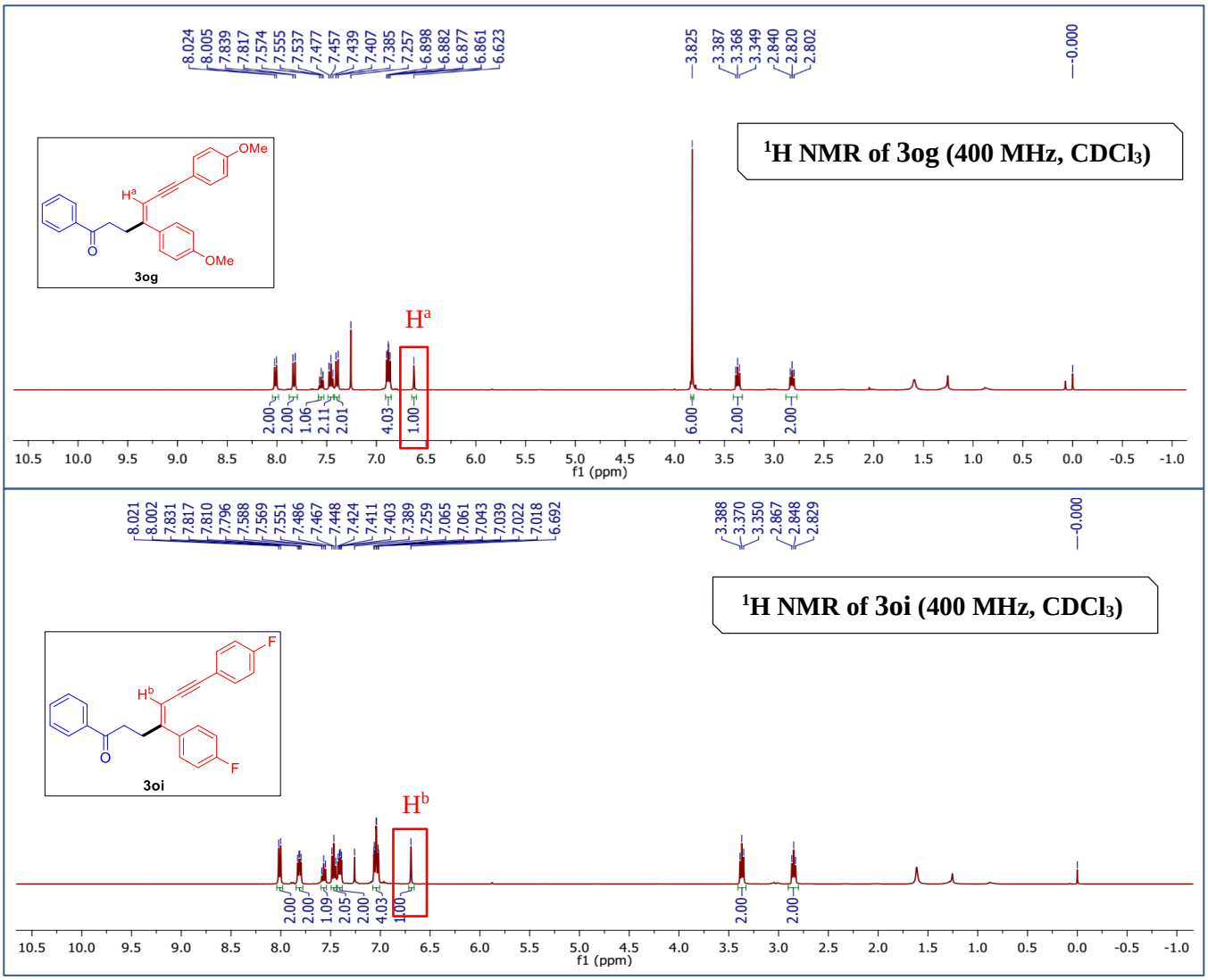


By following the general procedure, a parallel experiment was carried out. A flame dried schlenk tube was charged with cyclopropanol **1o** (0.20 mmol, 2.00 equiv), 1,3-diynes **2g** (0.10 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were then allowed to stir at 100 °C in a preheated aluminum block for 15 min. After 15 min of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The yield of the product **3og** was calculated from the ^1H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

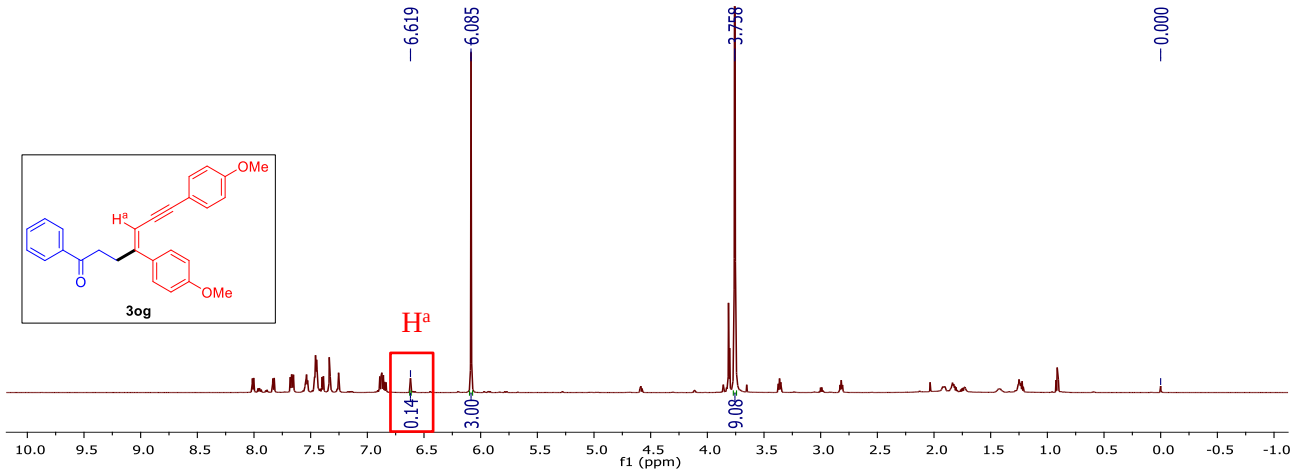
Similarly, by following the general procedure, a parallel experiment was carried out. A flame dried schlenk tube was charged with cyclopropanol **1o** (0.20 mmol, 2.00 equiv), 1,3-diynes **2i** (0.10 mmol, 1.0 equiv), $Pd(PPh_3)_4$ (0.01 mmol, 10.0 mol%), PCy_3 (0.02 mmol, 20.0 mol%), and toluene (0.40 mL 0.25 M). Then the Schlenk tube was thoroughly flushed with argon. The contents were

then allowed to stir at 100 °C in a preheated aluminum block for 15 min. After 15 min of the reaction, the tube was cooled down to room temperature, the reaction mixture was diluted with 5 mL of EtOAc and filtered with a plug Celite bed, followed by washing with 15 mL of EtOAc. The combined residue was concentrated under reduced pressure. The yield of the product **3oi** was calculated from the ^{1}H NMR analysis of the crude using 1,3,5-trimethoxy benzene as internal standard (see the following spectra).

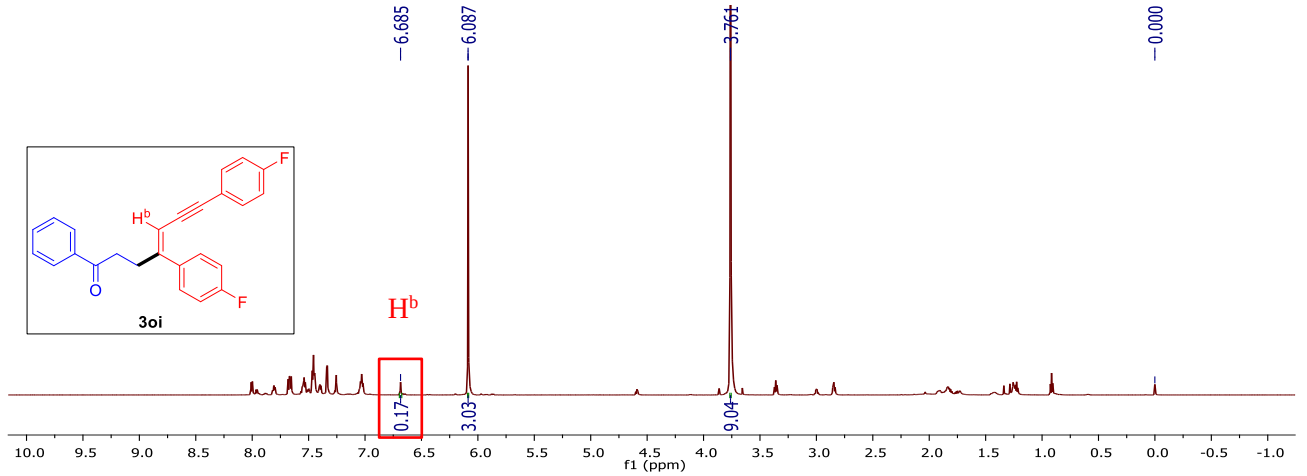
NMR spectra of Intermolecular parallel competition reaction between two different diynes (2g and 2i) with cyclopropanol 1o



^{1}H NMR of crude mixture of the competition parallel reaction between 1o, 2i (700 MHz, $CDCl_3$)

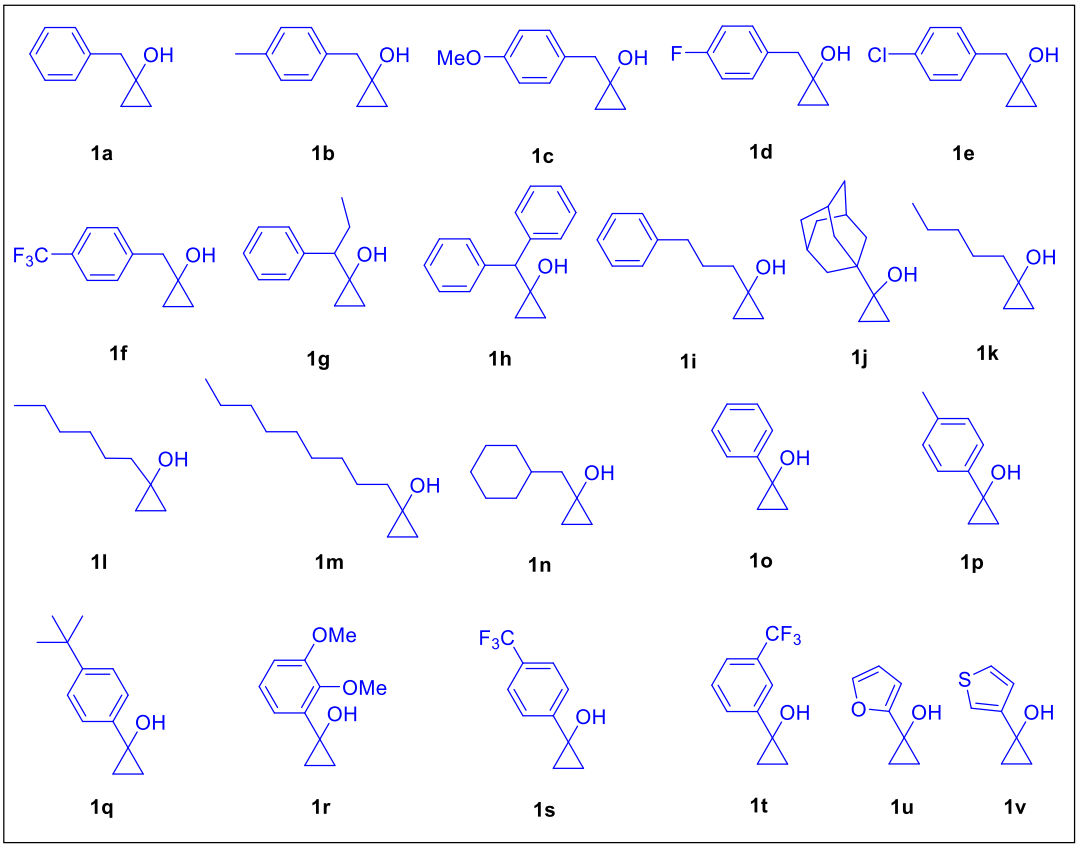


^{1}H NMR of crude mixture of the competition parallel reaction between 1o, 2g (700 MHz, $CDCl_3$)



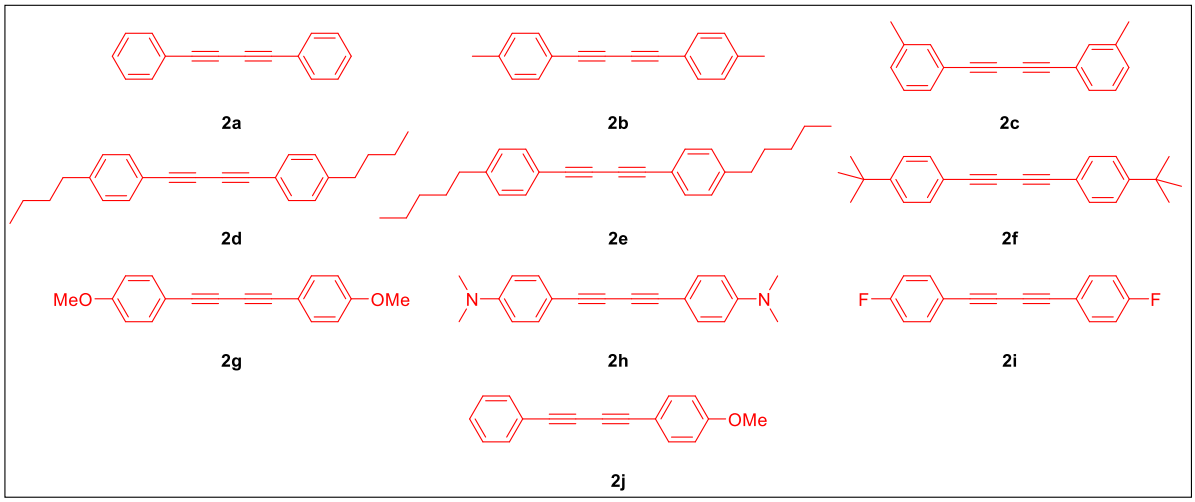
5. Experimental characterization data for the starting materials and products

Cyclopropanols used in this study:



Cyclopropanols **1a-1u** were synthesized according to the previously reported procedure[2, 3] (general procedure A), and spectroscopic data were identical to those.

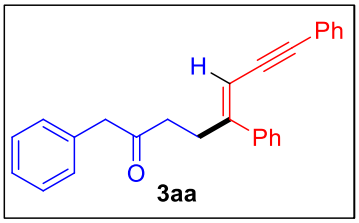
1,3-Diynes used in this study:



1,3-Diynes **2a-2j** were synthesized according to the reported literature procedure[4] and spectroscopic data were identical to those.

5.1 Experimental characterization data for the alkynylated adducts:

(*Z*)-1,5,8-triphenyloct-5-en-7-yn-2-one (3aa)



3aa was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3aa** (60 mg) in 86% yield.

Physical State: colorless gel.

R_f-value: 0.45 (10% EtOAc/hexane).

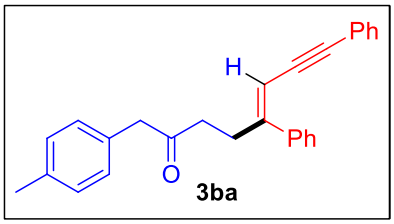
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 7.6 Hz, 2H), 7.43-7.41 (m, 2H), 7.36-7.31 (m, 5H), 7.29-7.19 (m, 6H), 6.61 (s, 1H), 3.73 (s, 2H), 2.85 (t, J = 7.2 Hz, 2H), 2.65 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.7, 136.8, 135.5, 134.4, 131.8, 129.8, 129.0, 128.8, 128.7, 128.7, 128.5, 128.2, 127.3, 123.5, 120.6, 96.5, 89.1, 50.8, 41.2, 33.6.

IR (KBr, cm^{-1}**):** 3087, 3062, 3030, 2957, 2859, 2199, 1716, 1652, 1598.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{22}NaO$: 373.1563; Found 373.1544.

(*Z*)-5,8-diphenyl-1-(p-tolyl)oct-5-en-7-yn-2-one (3ba)



3ba was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ba** (57 mg) in 78% yield**.**

Physical State: colorless gel.

R_f-value: 0.45 (10% EtOAc/hexane).

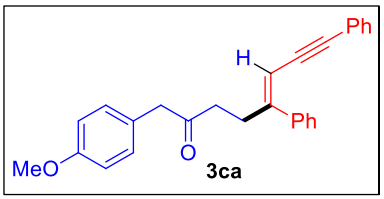
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 7.2 Hz, 2H), 7.41 (t, J = 3.6 Hz, 2H), 7.36-7.25 (m, 7H), 7.09 (s, 3H), 6.60 (s, 1H), 3.69 (s, 2H), 2.84 (t, J = 7.2 Hz, 2H), 2.64 (t, J = 7.2 Hz, 2H), 2.30 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 208.0, 136.9, 136.8, 135.5, 131.8, 131.4, 129.8, 129.6, 129.5, 128.8, 128.7, 128.5, 128.4, 123.6, 120.7, 96.5, 89.1, 50.4, 41.0, 33.6, 21.4.

IR (KBr, cm^{-1}**):** 3080, 3052, 2951, 2920, 2897, 2860, 2194, 1717, 1683, 1674, 1652, 1595.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{24}NaO$: 387.1719; Found 387.1743.

(*Z*)-1-(4-methoxyphenyl)-5,8-diphenyloct-5-en-7-yn-2-one (3ca)



3ca

3ca was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ca** (62 mg) in 82% yield.

Physical State: pale yellow gel

R_f-value: 0.40 (10% EtOAc/hexane).

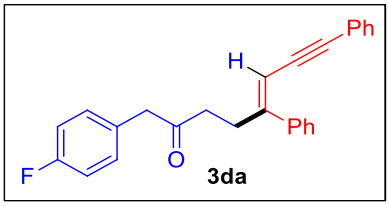
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, J = 7.6 Hz, 2H), 7.35-7.32 (m, 2H), 7.28-7.24 (m, 5H), 7.17 (t, J = 7.2 Hz, 1H), 7.03 (d, J = 8.8 Hz, 2H), 6.74 (d, J = 8.4 Hz, 2H), 6.52 (s, 1H), 3.67 (s, 3H), 3.58 (s, 2H), 2.76 (t, J = 7.2 Hz, 2H), 2.56 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 208.1, 158.9, 136.8, 135.5, 131.8, 130.7, 128.79, 128.75, 128.74, 128.5, 128.2, 126.5, 123.5, 120.6, 114.5, 96.5, 89.1, 55.5, 49.9, 40.9, 33.6.

IR (KBr, cm^{-1}**):** 3060, 3036, 2959, 2841, 2199, 1715, 1682, 1601, 1589.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{24}NaO_2$: 403.1669; Found 403.1666.

(*Z*)-1-(4-fluorophenyl)-5,8-diphenyloct-5-en-7-yn-2-one (3da)



3da

3da was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3da** (57 mg) in 77% yield.

Physical State: colorless gel.

R_f-value: 0.40 (10% EtOAc/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J = 7.2 Hz, 2H), 7.43-7.41 (m, 2H), 7.36-7.32 (m, 5H), 7.26 (t, J = 7.6 Hz, 1H), 7.16-7.12 (m, 2H), 6.96 (t, J = 8.8 Hz, 2H), 6.61 (s, 1H), 3.70 (s, 2H), 2.85 (t, J = 7.2 Hz, 2H), 2.66 (t, J = 7.2 Hz, 2H).

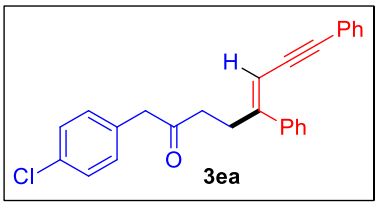
^{13}C NMR (100 MHz, $CDCl_3$): δ 207.4, 162.3 (d, $J_{C\text{-}F}$ = 244.0 Hz), 136.7, 135.6, 131.7, 131.3 (d, $J_{C\text{-}F}$ = 8.0 Hz), 130.1 (d, $J_{C\text{-}F}$ = 4.0 Hz), 128.84, 128.80, 128.7, 128.5, 128.3, 123.5, 120.5, 115.8 (d, $J_{C\text{-}F}$ = 21.0 Hz), 96.6, 89.0, 49.7, 41.2, 33.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ -115.7.

IR (KBr, cm^{-1}**):** 3088, 3055, 2959, 2925, 2853, 2191, 1717, 1683, 1675, 1652, 1575, 1222, 1158.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{21}FNaO$: 391.1469; Found 391.1478.

(*Z*)-1-(4-chlorophenyl)-5,8-diphenyloct-5-en-7-yn-2-one (3ea)



3ea was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ea** (48 mg) in 63% yield.

Physical State: colorless gel.

R_f-value: 0.50 (10% EtOAc/hexane).

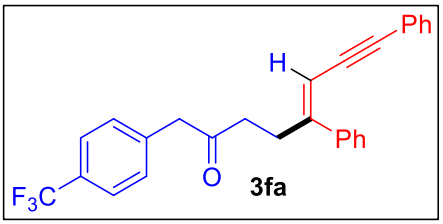
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 7.2 Hz, 2H), 7.43-7.40 (m, 2H), 7.37-7.33 (m, 5H), 7.28-7.23 (m, 3H), 7.1 (d, J = 8.4 Hz, 2H), 6.61 (s, 1H), 3.70 (s, 2H), 2.85 (t, J = 7.2 Hz, 2H), 2.66 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.1, 136.7, 135.7, 133.3, 132.8, 131.8, 131.1, 129.6, 129.1, 128.85, 128.81, 128.5, 128.3, 123.5, 120.4, 96.6, 89.0, 49.9, 41.3, 33.5.

IR (KBr, cm^{-1}**):** 3083, 3059, 3026, 2964, 2902, 2191, 1714, 1683, 1674, 1652, 1596, 1558, 755.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{21}ClNaO$: 407.1173; Found 407.1198.

(*Z*)-5,8-diphenyl-1-(4-(trifluoromethyl)phenyl)oct-5-en-7-yn-2-one (3fa)



3fa was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3fa** (51 mg) in 61% yield.

Physical State: colorless solid.

R_f-value: 0.50 (10% EtOAc/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 7.6 Hz, 2H), 7.53 (d, J = 8.4 Hz, 2H), 7.43-7.40 (m, 2H), 7.37-7.33 (m, 5H), 7.28 (t, J = 7.6 Hz, 3H), 6.62 (s, 1H), 3.81 (s, 2H), 2.89 (t, J = 7.6 Hz, 2H), 2.68 (t, J = 7.6 Hz, 2H).

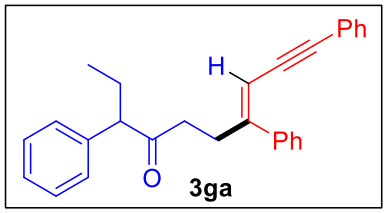
^{13}C NMR (100 MHz, $CDCl_3$): δ 206.6, 138.3, 136.7, 135.8, 131.7, 130.2, 128.9, 128.8, 128.5, 128.4, 128.3, 125.9 (q, $J_{C\text{-}F}$ = 3.0 Hz), 123.4, 123.1 (q, $J_{C\text{-}F}$ = 272.3 Hz), 120.3, 96.6, 89.0, 50.3, 41.5.

^{19}F NMR (376 MHz, $CDCl_3$): δ -62.60.

IR (KBr, cm^{-1}**):** 3062, 3024, 2959, 2925, 2853, 2196, 1717, 1618, 1598.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{21}NaO$: 441.1437; Found 441.1437.

(*Z*)-3,7,10-triphenyldec-7-en-9-yn-4-one (3ga)



3ga was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ga** (69 mg) in 91% yield.

Physical State: colorless gel.

R_f-value: 0.55 (10% EtOAc/hexane).

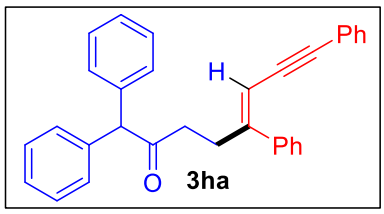
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 7.6 Hz, 2H), 7.39-7.20 (m, 13H), 6.55 (s, 1H), 3.5 (t, J = 7.2 Hz, 1H), 2.78-2.74 (m, 2H), 2.67-2.60 (m, 1H), 2.57-2.50 (m, 1H), 2.11-2.04 (m, 1H), 1.76-1.69 (m, 1H), 0.81 (t, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 209.9, 139.2, 136.8, 135.4, 131.8, 131.6, 129.1, 128.78, 128.71, 128.4, 128.2, 128.1, 127.4, 123.6, 120.7, 96.4, 89.1, 61.4, 41.1, 33.7, 25.4, 12.4.

IR (KBr, cm^{-1}**):** 3082, 3060, 3026, 2963, 2874, 2199, 1716, 1683, 1668, 1652, 1598.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{28}H_{26}NaO$: 401.1876; Found 401.1903.

(*Z*)-1,1,5,8-tetraphenyloct-5-en-7-yn-2-one (3ha)



3ha was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ha** (43 mg) in 50% yield.

Physical State: colorless gel.

R_f-value: 0.55 (10% EtOAc/hexane).

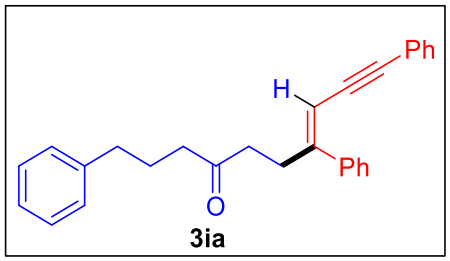
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, J = 8.4 Hz, 2H), 7.36-7.31 (m, 7H), 7.30-7.25 (m, 5H), 7.24-7.20 (m, 6H), 6.61 (s, 1H), 5.17 (s, 1H), 2.95 (t, J = 7.2 Hz, 2H), 2.69 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 208.0, 138.6, 136.8, 135.7, 131.8, 129.3, 129.2, 129.07, 129.03, 128.8, 128.78, 128.74, 128.71, 128.5, 128.4, 128.2, 127.5, 123.5, 120.5, 96.6, 89.1, 64.9, 41.9, 33.9.

IR (KBr, cm^{-1}**):** 3085, 2360, 3026, 2959, 2855, 2193, 1716, 1653, 1597, 1659, 1494.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{32}H_{26}ONa$: 449.1876; Found 449.1848.

(*Z*)-1,7,10-triphenyldec-7-en-9-yn-4-one (3ia)



3ia was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ia** (56 mg) in 74% yield.

Physical State: colorless gel.

R_f-value: 0.50 (10% EtOAc/hexane).

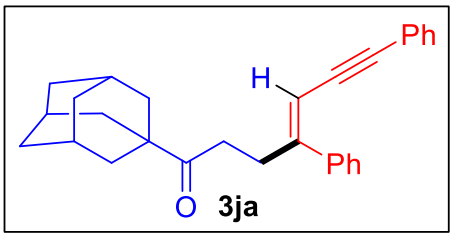
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, J = 7.6 Hz, 2H), 7.46-7.43 (m, 2H), 7.36-7.32 (m, 5H), 7.27-7.22 (m, 3H), 7.18-7.12 (m, 3H), 6.64 (s, 1H), 2.77 (t, J = 7.6 Hz, 2H), 2.66 (t, J = 7.6 Hz, 2H), 2.60 (t, J = 7.2 Hz, 2H), 2.46 (t, J = 7.2 Hz, 2H), 1.92 (quintet, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 210.1, 141.9, 136.8, 135.5, 131.8, 128.8, 128.78, 128.77, 128.6, 128.5, 128.2, 126.2, 123.5, 120.8, 96.5, 89.2, 42.6, 42.0, 35.4, 33.5, 25.5.

IR (KBr, cm^{-1}**):** 3082, 3060, 3024, 2926, 2856, 2194, 1712, 1672, 1596, 1570, 1489.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{27}O$: 379.2056; Found 379.2043.

(*Z*)-1-((3r,5r,7r)-adamantan-1-yl)-4,7-diphenylhept-4-en-6-yn-1-one (3ja)



3ja was prepared according to general procedure B. The acrude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ja** (51 mg) in 64% yield.

Physical State: colorless gel.

R_f-value: 0.60 (10% EtOAc/hexane).

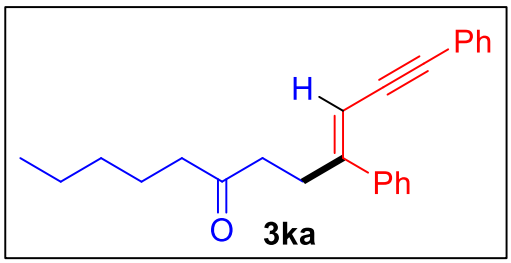
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, J = 7.6 Hz, 2H), 7.48-7.46 (m, 2H), 7.34 (t, J = 8.0 Hz, 4H), 7.25 (t, J = 8.4 Hz, 2H), 6.65 (s, 1H), 2.85 (t, J = 7.6 Hz, 2H), 2.64 (t, J = 7.6 Hz, 2H), 2.03 (s, 3H), 1.84 (br, 6H), 1.71 (q, J = 2.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 215.0, 136.9, 135.4, 131.8, 128.8, 128.79, 128.72, 128.5, 128.1, 123.7, 121.3, 96.3, 89.4, 46.7, 38.5, 36.9, 35.6, 33.6, 28.3.

IR (KBr, cm^{-1}**):** 3055, 3031, 2906, 2850, 2196, 1698, 1596, 1490, 1446.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{29}H_{31}O$: 395.2369; Found 395.2358.

(*Z*)-9,12-diphenyldodec-9-en-11-yn-6-one (3ka)



3ka was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ka** (42 mg) in 64% yield.

Physical State: colorless gel.

R_f-value: 0.70 (10% EtOAc/hexane).

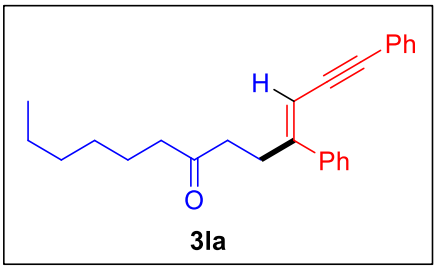
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, J = 7.2 Hz, 2H), 7.46 (dd, J = 7.6, 4.4 Hz, 2H), 7.37-7.33 (m, 4H), 7.28-7.24 (m, 2H), 6.66 (s, 1H), 2.80 (t, J = 7.2 Hz, 2H), 2.68 (t, J = 7.2 Hz, 2H), 2.45 (t, J = 7.6 Hz, 2H), 1.62-1.57 (m, 3H), 1.30-1.25 (m, 4H), 0.86 (t, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 210.7, 136.8, 135.5, 131.8, 131.6, 128.8, 128.7, 128.5, 128.2, 123.6, 120.9, 96.5, 89.2, 43.5, 41.9, 33.6, 31.7, 23.8, 22.8, 14.2.

IR (KBr, cm^{-1}**):** 3083, 3061, 3021, 2956, 2928, 2856, 2198, 1713, 1633, 1596, 1517, 1489.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{24}H_{26}NaO$: 353.1876; Found 353.1851.

(*Z*)-1,4-diphenyltridec-3-en-1-yn-7-one (3la)



3la was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3la** (49 mg) in 71% yield.

Physical State: colorless gel.

R_f-value: 0.65 (10% EtOAc/hexane).

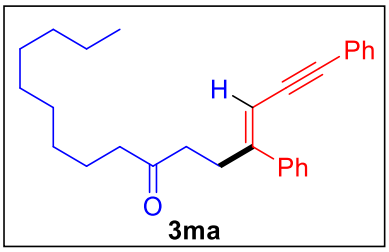
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, J = 7.6 Hz, 2H), 7.47 (dd, J = 7.6, 4.4 Hz, 2H), 7.37-7.33 (m, 5H), 7.26 (d, J = 2.4 Hz, 1H), 6.65 (s, 1H), 2.80 (t, J = 7.2 Hz, 2H), 2.68 (t, J = 7.2 Hz, 2H), 2.45 (t, J = 7.2 Hz, 2H), 1.58 (quintet, J = 7.2 Hz, 2H), 1.25 (br, 6H), 0.85 (t, J = 6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 210.8, 136.8, 135.5, 132.2, 131.8, 128.8, 128.7, 128.5, 128.2, 123.6, 120.9, 96.5, 89.2, 43.5, 41.9, 33.6, 31.9, 29.2, 24.1, 22.8, 14.3.

IR (KBr, cm^{-1}**):** 3060, 3026, 2956, 2928, 2859, 2203, 1732, 1698, 1667, 1651, 1633, 1489.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{25}H_{28}ONa$: 367.2032; Found 367.2018.

(*Z*)-1,4-diphenylhexadec-3-en-1-yn-7-one (3ma)



3ma

3ma was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ma** (52 mg) in 67% yield.

Physical State: colorless gel.

R_f-value: 0.75 (10% EtOAc/hexane).

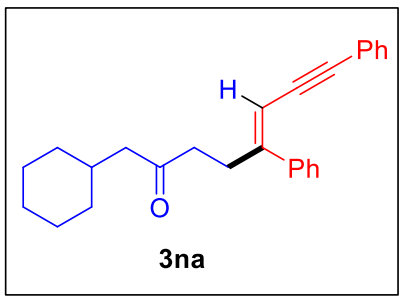
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (d, J = 7.6 Hz, 2H), 7.46 (dd, J = 7.6, 4.4 Hz, 2H), 7.36-7.32 (m, 5H), 7.27-7.23 (m, 1H), 6.65 (s, 1H), 2.79 (t, J = 7.2 Hz, 2H), 2.67 (t, J = 8.0 Hz, 2H), 2.44 (t, J = 7.6 Hz, 2H), 1.58 (t, J = 7.2 Hz, 2H), 1.30-1.24 (m 12H), 0.87 (t, J = 6.4 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 209.5, 135.9, 134.5, 130.8, 127.8, 127.7, 127.5, 127.3, 127.2, 122.7, 120.0, 95.5, 88.3, 42.5, 40.9, 32.6, 31.2, 28.7, 28.63, 28.60, 23.2, 21.9, 13.4.

IR (KBr, cm^{-1}**):** 3083, 3058, 3023, 2954, 2924, 2853, 2194, 1716, 1698, 1683, 1667, 1597, 1455.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{28}H_{34}ONa$: 409.2502; Found 409.2495.

(*Z*)-1-cyclohexyl-5,8-diphenyloct-5-en-7-yn-2-one (3na)



3na

3na was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3na** (57 mg) in 80% yield.

Physical State: colorless gel.

R_f-value: 0.60 (10% EtOAc/hexane).

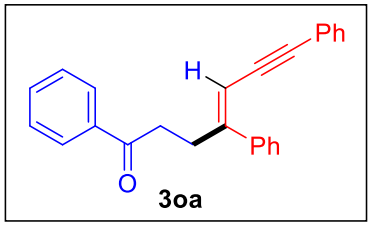
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, J = 7.6 Hz, 2H), 7.52-7.50 (m, 2H), 7.40-7.37 (m, 5H), 2.29 (t, J = 7.2 Hz, 1H), 6.69 (s, 1H), 2.82 (t, J = 7.2 Hz, 2H), 2.71 (t, J = 7.2 Hz, 2H), 2.36 (d, J = 6.8 Hz, 2H), 1.92-1.86 (m, 1H), 1.71-1.68 (m, 5H), 1.33-1.24 (m, 3H), 1.0-0.9 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 210.3, 136.8, 135.5, 131.8, 128.79, 128.76, 128.5, 128.3, 128.1, 123.6, 120.9, 96.4, 89.2, 51.2, 42.6, 34.3, 33.58, 33.54, 26.5, 26.4.

IR (KBr, cm^{-1}**):** 3060, 3026, 2923, 2851, 2196, 1713, 1676, 1597, 1489, 1448, 1375, 1282.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{28}NaO$: 379.2032; Found 379.2025.

(*Z*)-1,4,7-triphenylhept-4-en-6-yn-1-one (3oa)



3oa was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3oa** (48 mg) in 72% yield.

Physical State: colorless gel.

R_f-value: 0.45 (10% EtOAc/hexane).

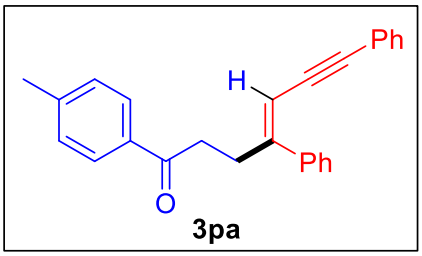
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 8.0 Hz, 2H), 7.86 (d, J = 7.6 Hz, 2H), 7.55 (t, J = 7.2 Hz, 1H), 7.47-7.44 (m, 4H), 7.37-7.32 (m, 5H), 7.26 (t, J = 7.6 Hz, 1H), 6.72 (s, 1H), 3.38 (t, J = 7.6 Hz, 2H), 2.85 (t, J = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 199.6, 137.2, 136.8, 135.6, 133.4, 131.8, 128.9, 128.8, 128.7, 128.5, 128.4, 128.2, 123.6, 121.0, 96.6, 89.3, 38.2, 34.0.

IR (KBr, cm^{-1}**):** 3081, 3059, 3024, 2925, 2851, 2194, 1732, 1686, 1673, 1651, 1596, 1580.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{25}H_{20}NaO$: 359.1406; Found 359.1397.

(*Z*)-4,7-diphenyl-1-(m-tolyl)hept-4-en-6-yn-1-one (3pa)



3pa was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3pa** (36 mg) in 52% yield.

Physical State: colorless gel.

R_f-value: 0.45 (10% EtOAc/hexane).

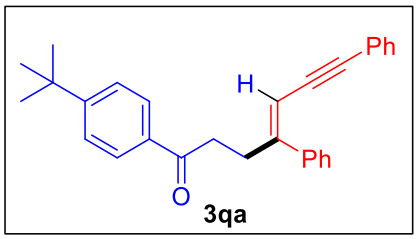
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, J = 8.4 Hz, 2H), 7.86 (d, J = 7.2 Hz, 2H), 7.46 (dd, J = 7.6, 4.0 Hz, 2H), 7.37-7.33 (m, 4H), 7.28-7.24 (m, 4H), 6.72 (s, 1H), 3.35 (t, J = 7.6 Hz, 2H), 2.85 (t, J = 7.6 Hz, 2H), 2.40 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 199.3, 144.1, 136.9, 135.6, 134.8, 131.8, 129.6, 128.8, 128.7, 128.58, 128.55, 128.2, 123.6, 121.1, 96.6, 89.4, 38.1, 34.1, 21.9.

IR (KBr, cm^{-1}**):** 3080, 3059, 3033, 2959, 2923, 2852, 2191, 1717, 1699, 1683, 1652, 1575.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{23}O$: 351.1743; Found 351.1731.

(*Z*)-1-(3-(tert-butyl)phenyl)-4,7-diphenylhept-4-en-6-yn-1-one (3qa)



3qa was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3qa** (45 mg) in 58% yield.

Physical State: colorless gel.

R_f-value: 0.68 (10% EtOAc/hexane).

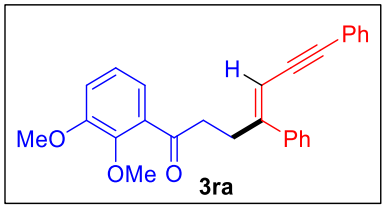
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, J = 8.8 Hz, 2H), 7.86 (d, J = 7.2 Hz, 2H), 7.48-7.44 (m, 4H), 7.37-7.32 (m, 5H), 7.26 (t, J = 7.6 Hz, 1H), 6.72 (s, 1H), 3.36 (t, J = 7.2 Hz, 2H), 2.85 (t, J = 7.2 Hz, 2H), 1.33 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 199.3, 157.2, 136.9, 135.6, 134.7, 131.8, 131.6, 128.8, 128.7, 128.5, 128.4, 128.2, 125.8, 123.6, 121.1, 96.6, 89.4, 38.1, 35.4, 34.1, 31.4.

IR (KBr, cm^{-1}**):** 3078, 3059, 3022, 2962, 2933, 2867, 2194, 1717, 1683, 1652, 1569, 1158.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{28}NaO$: 415.2032; Found 415.2049.

(*Z*)-1-(2,3-dimethoxyphenyl)-4,7-diphenylhept-4-en-6-yn-1-one (3ra)



3ra was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ra** (61 mg) in 77% yield.

Physical State: colorless gel**.**

R_f-value: 0.60 (20% EtOAc/hexane).

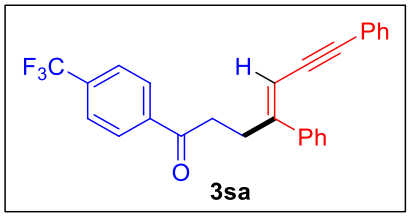
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, J = 7.6 Hz, 2H), 7.45 (dd, J = 8.0, 4.4 Hz, 2H), 7.37-7.31 (m, 5H), 7.27-7.25 (m, 1H), 7.18 (dd, J = 7.6, 2.0 Hz, 1H), 7.07 (t, J = 8.0 Hz, 1H), 7.03 (dd, J = 8.0, 1.6 Hz, 1H), 6.69 (s, 1H), 3.90 (s, 3H), 3.88 (s, 3H), 3.38 (t, J = 7.6 Hz, 2H), 2.82 (t, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 202.5, 153.3, 148.5, 137.0, 135.4, 134.3, 131.8, 128.8, 128.7, 128.6, 128.5, 128.1, 124.4, 123.7, 121.2, 121.1, 115.9, 96.4, 89.4, 61.8, 56.3, 42.8, 34.0.

IR (KBr, cm^{-1}**):** 3057, 3013, 2935, 2835, 2194, 1679, 1580, 1474, 1428, 1355, 1309, 1264, 1180.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{24}NaO_3$: 419.1618; Found 419.1625.

(*Z*)-4,7-diphenyl-1-(4-(trifluoromethyl)phenyl)hept-4-en-6-yn-1-one (3sa)



3sa

3sa was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3sa** (49 mg) in 60% yield.

Physical State: colorless gel.

R_f-value: 0.60 (10% EtOAc/hexane).

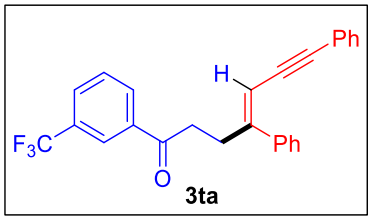
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 7.2 Hz, 2H), 7.64 (d, J = 8.0 Hz, 2H), 7.37-7.34 (m, 2H), 7.30-7.25 (m, 5H), 7.21-7.17 (m, 1H), 6.65 (s, 1H), 3.32 (t, J = 7.6 Hz, 2H), 2.80 (t, J = 7.6 Hz, 2H).

^{13}C NMR (176 MHz, $CDCl_3$): δ 198.7, 139.9, 136.7, 135.9, 134.7 (q, $J_{C\text{-}F}$ = 33.4 Hz), 131.80, 128.89, 128.85, 128.81, 128.78, 128.6, 128.3, 126.05 (q, $J_{C\text{-}F}$ = 3.5 Hz), 123.9 (q, $J_{C\text{-}F}$ = 272.8 Hz), 123.5, 120.5, 96.8, 89.1, 38.4, 33.8. **^{19}F NMR (376 MHz, $CDCl_3$):** δ -63.0.

IR (KBr, cm^{-1}**):** 3081, 3060, 3022, 2955, 2926, 2854, 2194, 1717, 1694, 1675, 1652, 1575, 1202.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{19}F_3NaO$: 427.1280; Found 427.1307.

(*Z*)-4,7-diphenyl-1-(3-(trifluoromethyl)phenyl)hept-4-en-6-yn-1-one (3ta)



3ta

3ta was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ta** (55 mg) in 68% yield.

Physical State: colorless gel. **R_f -value:** 0.58 (10% EtOAc/hexane).

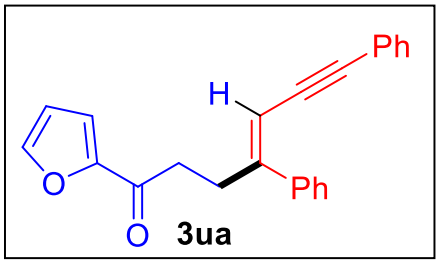
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.26 (s, 1H), 8.18 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 7.2 Hz, 2H), 7.81 (d, J = 7.6 Hz, 1H), 7.59 (t, J = 8.0 Hz, 1H), 7.45-7.43 (m, 2H), 7.38-7.33 (m, 5H), 7.27 (t, J = 7.2 Hz, 1H), 6.73 (s, 1H), 3.40 (t, J = 7.2 Hz, 2H), 2.88 (t, J = 7.2 Hz, 2H).

^{13}C NMR (176 MHz, $CDCl_3$): δ 198.3, 137.7, 136.7, 135.9, 131.8, 131.6 (q, $J_{C\text{-}F}$ = 33.4 Hz), 131.5, 129.8 (q, $J_{C\text{-}F}$ = 3.5 Hz), 129.6, 128.87, 128.85, 128.80, 128.5, 128.3, 125.3 (q, $J_{C\text{-}F}$ = 5.2 Hz), 124.0 (q, $J_{C\text{-}F}$ = 272.8 Hz), 123.4, 120.5, 96.8, 89.1, 38.2, 33.9. **^{19}F NMR (376 MHz, $CDCl_3$):** δ -62.7.

IR (KBr, cm^{-1}**):** 3060, 3028, 2964, 2925, 2855, 2195, 1691, 1609, 1490, 1440, 1270, 1169, 1128.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{19}F_3NaO$: 427.1280; Found 427.1282.

(*Z*)-1-(furan-2-yl)-4,7-diphenylhept-4-en-6-yn-1-one (3ua)



3ua was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ua** (40 mg) in 62% yield.

Physical State: colorless gel.

R_f-value: 0.40 (10% EtOAc/hexane).

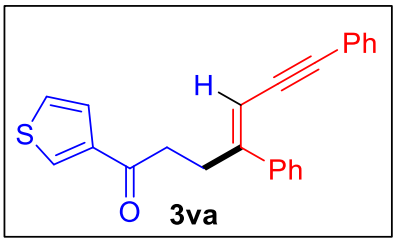
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (d, J = 7.6 Hz, 2H), 7.47 (dd, J = 7.2, 4.0 Hz, 2H), 7.37-7.33 (m, 4H), 7.28-7.22 (m, 4H), 6.70 (s, 1H), 6.52 (dd, J = 3.6, 1.6 Hz, 1H), 3.23 (t, J = 7.6 Hz, 2H), 2.84 (t, J = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 188.8, 146.7, 136.8, 135.7, 132.5, 132.4, 131.8, 128.8, 128.7, 128.5, 128.2, 123.6, 120.7, 117.5, 112.5, 96.6, 89.2, 37.9, 33.8.

IR (KBr, cm^{-1}**):** 3057, 3028, 2927, 2853, 2195, 1717, 1673, 1598, 1567, 1466, 1356, 1267, 1159.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{19}O_2$: 327.1380; Found 327.13.

(*Z*)-4,7-diphenyl-1-(thiophen-3-yl)hept-4-en-6-yn-1-one (3va)



3va was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3va** (57 mg) in 83% yield.

Physical State: colorless gel.

R_f-value: 0.40 (10% EtOAc/hexane).

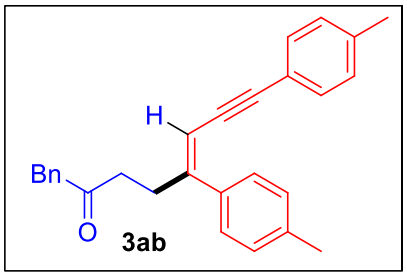
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.10 (dd, J = 2.8, 1.2 Hz, 1H), 7.85 (d, J = 7.6 Hz, 2H), 7.59 (dd, J = 5.2, 1.2 Hz, 2H), 7.45 (dd, J = 7.6, 4.0 Hz, 1H), 7.37-7.25 (m, 7H), 6.71 (s, 1H), 3.28 (t, J = 7.2 Hz, 2H), 2.84 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 194.0, 142.6, 136.8, 135.7, 132.3, 131.8, 128.8, 128.7, 128.5, 128.2, 127.3, 126.7, 123.6, 120.8, 96.6, 89.3, 39.4, 34.0.

IR (KBr, cm^{-1}**):** 3104, 3087, 3059, 2961, 2897, 2194, 1717, 1674, 1635, 1595, 1539,753, 691.

HRMS (ESI) m/z: calcd for $[M+Na]^+$ $C_{23}H_{18}NaOS$: 365.0971; found 365.1001.

(*Z*)-1-phenyl-5,8-di-*p*-tolyloct-5-en-7-yn-2-one (3ab)



3ab was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ab** (66 mg) in 87% yield.

Physical State: colorless gel

R_f-value: 0.42 (10% EtOAc/hexane).

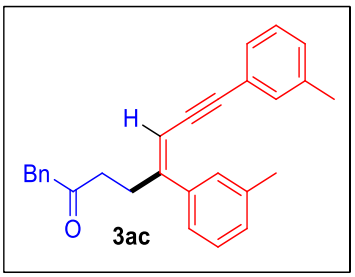
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, J = 8.4 Hz, 2H), 7.32-7.23 (m, 5H), 7.20-7.18 (m, 2H), 7.14 (dd, J = 8.0, 1.6 Hz, 4H), 6.54 (s, 1H), 3.72 (s, 2H), 2.84 (t, J = 7.2 Hz, 2H), 2.62 (t, J = 7.2 Hz, 2H), 2.36 (s, 3H), 2.34 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.8, 138.8, 138.0, 135.1, 134.5, 134.1, 131.6, 129.8, 129.5, 129.2, 129.0, 128.7, 127.3, 120.6, 119.7, 96.7, 88.7, 50.8, 41.3, 33.6, 21.8, 21.6.

IR (KBr, cm^{-1}**):** 3084, 3058, 3027, 2954, 2919, 2863, 2191, 1713, 1606, 1507.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{28}H_{26}NaO$: 401.1876; Found 401.1872.

(*Z*)-1-phenyl-5,8-di-*m*-tolyloct-5-en-7-yn-2-one (3ac)



3ac was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ac** (59 mg) in 78% yield.

Physical State: colorless gel.

R_f-value: 0.48 (10% EtOAc/hexane).

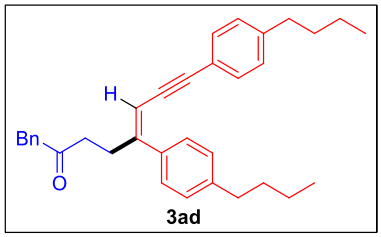
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (s, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.31-7.19 (m, 9H), 7.15-7.12 (m, 1H), 7.07 (d, J = 7.6 Hz, 1H), 6.57 (s, 1H), 3.73 (s, 2H), 2.84 (t, J = 7.2 Hz, 2H), 2.63 (t, J = 7.2 Hz, 2H), 2.35 (s, 3H), 2.35 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.8, 138.4, 137.9, 136.7, 135.8, 134.5, 132.3, 129.8, 129.6, 129.4, 129.05, 129.01, 128.8, 128.6, 128.4, 127.3, 126.0, 123.4, 120.4, 96.8, 89.0, 50.8, 41.2, 33.6, 21.8, 21.5.

IR (KBr, cm^{-1}**):** 3085, 3028, 2952, 2859, 2187, 1715, 1599, 1578.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{28}H_{27}O$: 379.2056; Found 379.2049.

(*Z*)-5,8-bis(4-butylphenyl)-1-phenyloct-5-en-7-yn-2-one (3ad)



3ad

3ad was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ad** (67 mg) in 72% yield.

Physical State: colorless gel.

R_f-value: 0.55 (10% EtOAc/hexane).

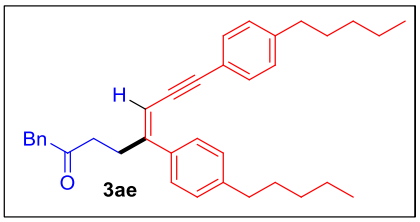
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.29-7.23 (m, 3H), 7.21-7.14 (m, 6H), 6.55 (s, 1H), 3.72 (s, 2H), 2.84 (t, J = 7.2 Hz, 2H), 2.64-2.58 (m, 6H), 1.62-1.57 (m, 4H), 1.39-1.32 (m, 4H), 0.92 (q, J = 7.2 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.9, 143.9, 143.1, 135.1, 134.5, 134.3, 131.7, 129.8, 129.0, 128.8, 128.7, 128.6, 127.3, 120.8, 119.6, 96.8, 88.7, 50.8, 50.1, 41.3, 35.9, 35.8, 33.8, 33.76, 33.72, 22.68, 22.64, 14.2.

IR (KBr, cm^{-1}**):** 3084, 3059, 3026, 2955, 2928, 2874, 2192, 1716, 1683, 1675, 1604, 1558.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{34}H_{38}NaO$: 485.2815; Found 485.2775.

(*Z*)-5,8-bis(4-pentylphenyl)-1-phenyloct-5-en-7-yn-2-one (3ae)



3ae

3ae was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ae** (61 mg) in 62% yield.

Physical State: colorless gel.

R_f-value: 0.55 (10% EtOAc/hexane).

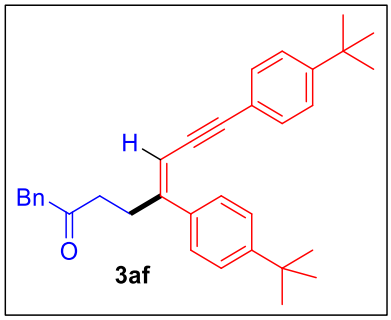
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 7.6 Hz, 2H), 7.29 (d, J = 7.2 Hz, 2H), 7.24-7.19 (m, 3H), 7.17-7.14 (m, 4H), 6.55 (s, 1H), 3.73 (s, 2H), 2.84 (t, J = 7.6 Hz, 2H), 2.64-2.57 (m, 6H), 1.64-1.59 (m, 4H), 1.32 (br, 8H), 0.89 (q, J = 6.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.9, 143.9, 143.2, 135.1, 134.5, 134.3, 131.7, 129.8, 129.0, 128.8, 128.7, 128.6, 127.3, 120.8, 119.6, 96.8, 88.7, 50.8, 41.3, 36.2, 36.1, 33.7, 31.8, 31.7, 31.39, 31.32, 22.8, 21.0, 14.3.

IR (KBr, cm^{-1}**):** 3027, 2956, 2926, 2856, 2193, 1713, 1673, 1606, 1506.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{36}H_{43}O$: 491.3308; Found 491.3288.

(*Z*)-5,8-bis(4-(tert-butyl)phenyl)-1-phenyloct-5-en-7-yn-2-one (3af)



3af was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3af** (56 mg) in 61% yield.

Physical State: colorless gel.

R_f-value: 0.52 (10% EtOAc/hexane).

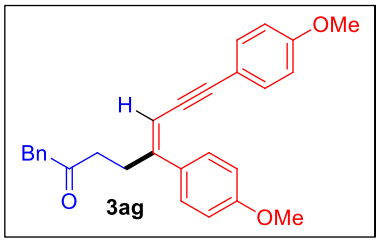
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 8.4 Hz, 2H), 7.31-7.27 (m, 6H), 7.22 (d, J = 7.6 Hz, 2H), 7.18 (d, J = 5.6 Hz, 1H), 7.13 (d, J = 7.2 Hz, 2H), 6.49 (s, 1H), 3.66 (s, 2H), 2.77 (t, J = 7.2 Hz, 2H), 2.56 (t, J = 7.2 Hz, 2H), 1.26 (s, 9H), 1.25 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.9, 152.0, 151.3, 135.0, 134.5, 134.1, 131.5, 129.8, 129.0, 128.5, 127.3, 125.7, 125.4, 120.7, 119.8, 96.8, 88.7, 50.8, 41.4, 35.1, 35.0, 33.7, 31.6, 31.5.

IR (KBr, cm^{-1}**):** 3097, 3034, 2963, 2911, 2893, 2872, 2196, 1714, 1683, 1652, 1634, 1575.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{34}H_{38}NaO$: 485.2815; Found 485.2781.

(*Z*)-5,8-bis(4-methoxyphenyl)-1-phenyloct-5-en-7-yn-2-one (3ag)



3ag was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ag** (63 mg) in 77% yield.

Physical State: colorless gel.

R_f-value: 0.50 (20% EtOAc/hexane).

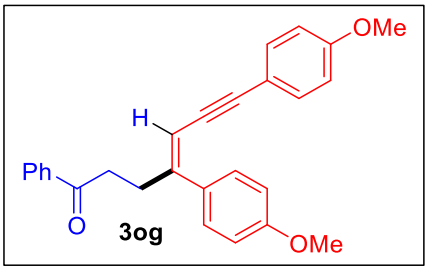
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 7.31-7.25 (m, 3H), 7.20 (d, J = 7.2 Hz, 2H), 6.87 (d, J = 6.4 Hz, 4H), 6.50 (s, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.73 (s, 2H), 2.83 (t, J = 7.2 Hz, 2H), 2.61 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 208.0, 160.0, 159.5, 134.5, 134.3, 133.2, 130.1, 129.89, 129.83, 129.0, 127.3, 118.4, 115.9, 114.4, 113.9, 96.3, 88.2, 55.7, 55.6, 50.8, 41.4, 33.6.

IR (KBr, cm^{-1}**):** 3081, 3061, 3029, 2956, 2932, 2836, 2189, 1716, 1682, 1604, 1568, 1505, 1246, 1176, 1030.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{28}H_{26}NaO_3$: 433.1774; Found 433.1759.

(*Z*)-4,7-bis(4-methoxyphenyl)-1-phenylhept-4-en-6-yn-1-one (3og)



3og was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3og** (59 mg) in 74% yield.

Physical State: yellow gel.

R_f-value: 0.50 (20% EtOAc/hexane).

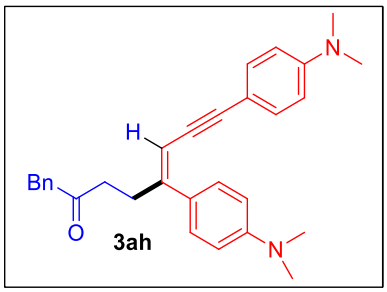
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 7.6 Hz, 2H), 7.82 (d, J = 8.8 Hz, 2H), 7.55 (t, J = 7.6 Hz, 1H), 7.45 (t, J = 8.0 Hz, 2H), 7.39 (d, J = 8.5 Hz, 2H), 6.89-6.86 (m, 4H), 6.62 (s, 1H), 3.82 (s, 6H), 3.36 (t, J = 7.6 Hz, 2H), 2.82 (t, J = 8.0 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 199.9, 160.0, 159.5, 137.3, 134.3, 133.3, 133.2, 130.1, 129.9, 128.9, 128.4, 118.7, 115.9, 114.4, 113.9, 96.40, 88.44, 55.68, 55.63, 38.4, 34.1.

IR (KBr, cm^{-1}**):** 3061, 3003, 2931, 2836, 2189, 1680, 1606, 1569, 1505, 1248, 1174, 1030.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{24}NaO_3$: 419.1618; Found 419.1600.

(*Z*)-5,8-bis(4-(dimethylamino)phenyl)-1-phenyloct-5-en-7-yn-2-one (3ah)



3ah was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ah** (57 mg) in 65% yield.

Physical State: colorless gel.

R_f-value: 0.35 (10% EtOAc/hexane).

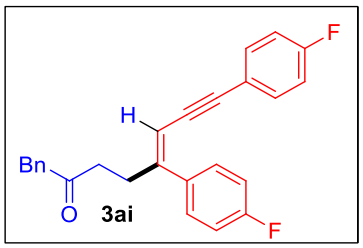
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, J = 9.2 Hz, 2H), 7.34-7.19 (m, 7H), 6.69-6.66 (m, 4H), 6.42 (s, 1H), 3.73 (s, 2H), 3.00 (s, 6H), 2.97 (s, 6H), 2.84 (t, J = 7.2 Hz, 2H), 2.59 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 208.4, 150.3, 150.2, 135.8, 134.6, 133.9, 132.8, 130.3, 129.86, 129.84, 129.0, 127.2, 116.2, 112.2, 112.1, 97.4, 88.2, 50.8, 41.7, 40.7, 40.6, 33.9.

IR (KBr, cm^{-1}**):** 3038, 2920, 2852, 2808, 2179, 1710, 1640, 1606, 1579, 1447, 1358, 1264, 1188.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{30}H_{33}N_2O$: 437.2587; Found 437.2601.

(*Z*)-5,8-bis(4-fluorophenyl)-1-phenyloct-5-en-7-yn-2-one (3ai)



3ai was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3ai** (48 mg) in 62% yield.

Physical State: colorless gel. **R_f -value:** 0.40 (10% EtOAc/hexane).

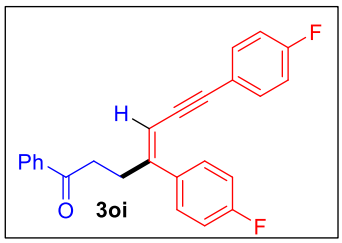
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (dd, J = 8.8, 5.6 Hz, 2H), 7.38-7.35 (m, 2H), 7.32-7.24 (m, 3H), 7.21-7.19 (m, 2H), 7.03 (q, J = 8.4 Hz, 4H), 6.56 (s, 1H), 3.73 (s, 2H), 2.83 (t, J = 7.2 Hz, 2H), 2.63 (t, J = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 207.6, 164.0 (d, $J_{C\text{-}F}$ = 47.0 Hz), 161.5 (d, $J_{C\text{-}F}$ = 44.0 Hz), 134.4, 133.6 (d, $J_{C\text{-}F}$ = 9.0 Hz), 133.4 (d, $J_{C\text{-}F}$ = 9.0 Hz), 132.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.4 (d, $J_{C\text{-}F}$ = 8.0 Hz), 130.2 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.7, 129.1, 120.2 (d, $J_{C\text{-}F}$ = 2.0 Hz), 119.5 (d, $J_{C\text{-}F}$ = 4.0 Hz), 116.1 (d, $J_{C\text{-}F}$ = 22.0 Hz), 115.4 (d, $J_{C\text{-}F}$ = 22.0 Hz), 95.3, 88.5, 50.8, 41.1, 33.3. **^{19}F NMR (376 MHz, $CDCl_3$):** δ -110.2, -112.9.

IR (KBr, cm^{-1}**):** 2960, 2924, 2848, 2197, 1716, 1699, 1683, 1652, 1599, 1157.

HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{21}F_2O$: 387.1555; Found 387.1543.

(*Z*)-4,7-bis(4-fluorophenyl)-1-phenylhept-4-en-6-yn-1-one (3oi)



3oi was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3oi** (70 mg) in 94% yield.

Physical State: yellow gel. **R_f -value:** 0.40 (10% EtOAc/hexane).

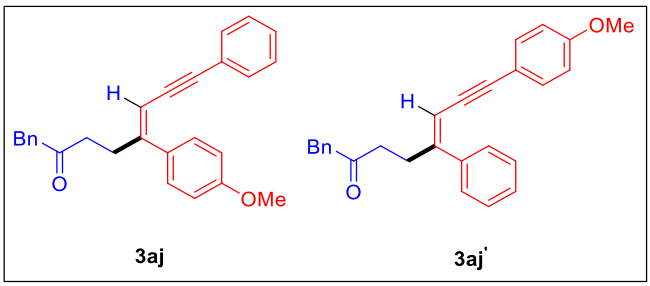
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, J = 7.6 Hz, 2H), 8.83-8.79 (m, 2H), 7.56 (t, J = 7.6 Hz, 1H), 7.46 (t, J = 7.6 Hz, 2H), 7.42-7.41 (m, 2H), 7.04 (td, J = 8.8, 1.6 Hz, 4H), 6.69 (s, 1H), 3.37 (t, J = 7.2 Hz, 2H), 2.84 (t, J = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 199.5, 163.9 (d, $J_{C\text{-}F}$ = 44.0 Hz), 161.5 (d, $J_{C\text{-}F}$ = 42.0 Hz), 137.2, 134.5, 133.6 (d, $J_{C\text{-}F}$ = 4.0 Hz), 133.4, 133.0 (d, $J_{C\text{-}F}$ = 4.0 Hz), 130.4 (d, $J_{C\text{-}F}$ = 8.0 Hz), 128.9, 128.4, 120.5 (d, $J_{C\text{-}F}$ = 2.0 Hz), 119.5 (d, $J_{C\text{-}F}$ = 4.0 Hz), 116.1 (d, $J_{C\text{-}F}$ = 22.0 Hz), 115.4 (d, $J_{C\text{-}F}$ = 21.0 Hz), 99.4, 88.7, 38.0, 33.8. **^{19}F NMR (376 MHz, $CDCl_3$):** δ -110.35, -113.05.

IR (KBr, cm^{-1}**):** 3063, 2925, 2924, 2853, 2198, 1736, 1681, 1598, 1504, 1448, 1229, 1110.

HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{25}H_{18}F_2NaO$: 395.1223; Found 395.1225.

(*Z*)-8-(4-methoxyphenyl)-1,5-diphenyloct-5-en-7-yn-2-one (3aj) and (*Z*)-5-(4-methoxyphenyl)-1,8-diphenyloct-5-en-7-yn-2-one (3aj') (1:1)



(3aj+3aj') was prepared according to general procedure B. The crude reaction mixture was purified by column chromatography using silica gel (230-400 mesh) giving **3aj** (58 mg) in 76% yield.

Physical State: yellow gel,

R_f-value: 0.40 (10% EtOAc/hexane).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, J = 7.7 Hz, 2H), 7.79 (d, J = 8.4 Hz, 2H), 7.43 (d, J = 7.7 Hz, 2H), 7.36-7.32 (m, 7H), 7.30-7.28 (m, 4H), 7.25-7.24 (m, 4H), 7.20 (d, J = 7.7 Hz, 4H), 6.88 (d, J = 9.1 Hz, 4H), 6.56 (s, 1H), 6.54 (s, 1H), 3.83 (s, 3H), 3.81 (s, 3H), 3.75 (s, 4H), 2.86-2.83 (m, 4H), 2.65-2.61 (m, 4H).

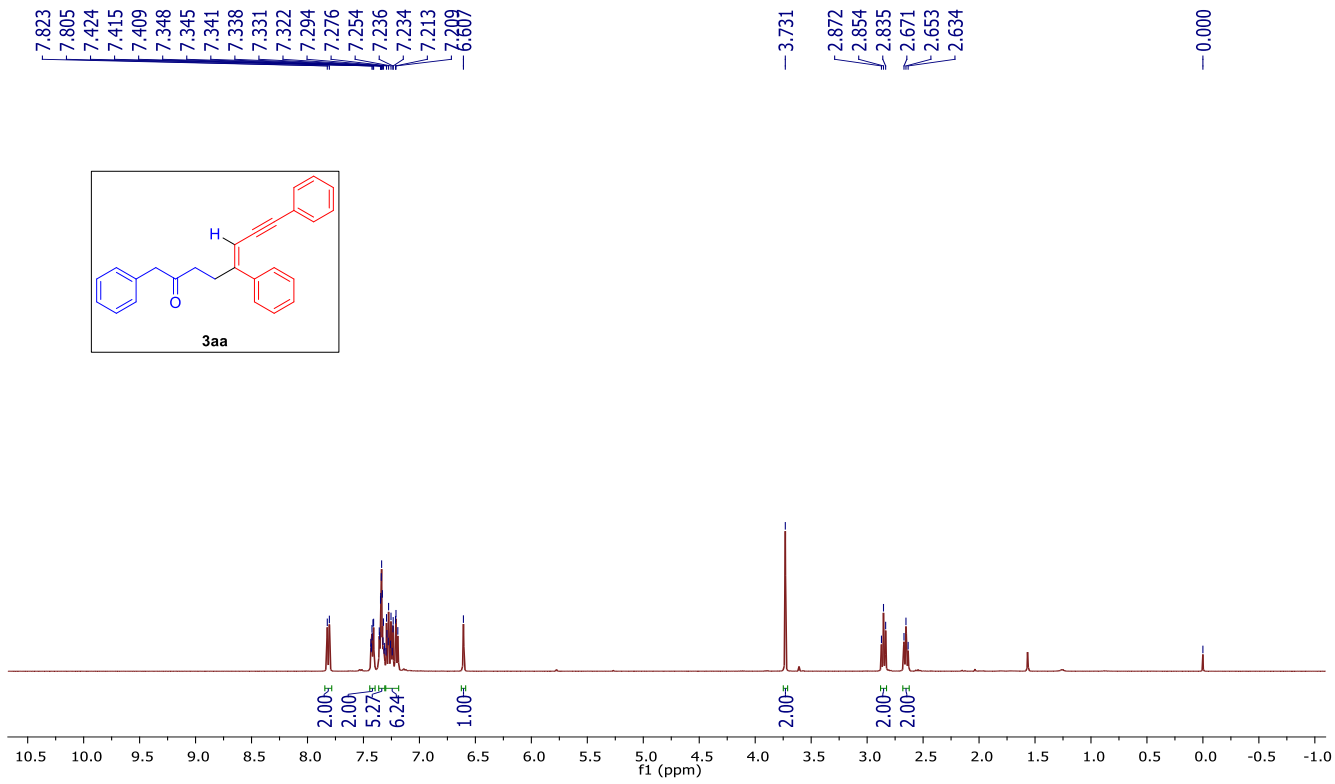
^{13}C NMR (100 MHz, $CDCl_3$): δ 207.9, 207.8, 160.1, 159.6, 136.9, 135.1, 134.7, 134.5, 133.3, 131.7, 130.1, 129.8, 129.7, 129.0, 128.75, 128.73, 128.6, 128.4, 128.0, 127.3, 123.7, 120.9, 118.0, 115.7, 114.4, 113.9, 96.7, 96.2, 89.4, 87.9, 55.67, 55.61, 50.82, 50.81, 41.35, 41.30, 33.6, 33.5.

IR (KBr, cm^{-1}**):** 3056, 3031, 2956, 2928, 2840, 2191, 1712, 1602, 1505, 1448, 1356, 1253, 1176, 1080.

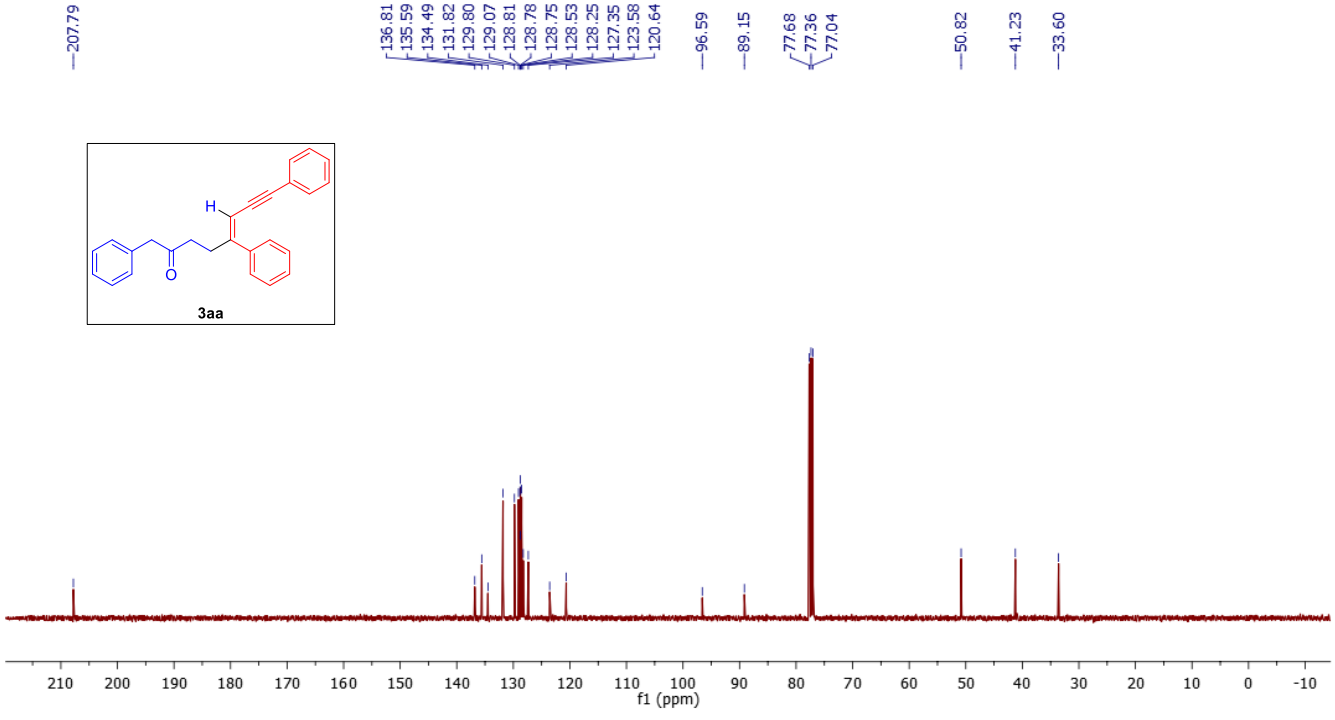
HRMS (ESI) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{24}NaO_2$: 403.1669; Found 403.1663.

6. Copies of NMR spectra of the products:

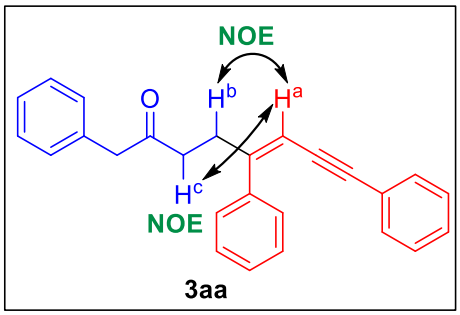
^{1}H NMR of 3aa (400 MHz, $CDCl_3$)

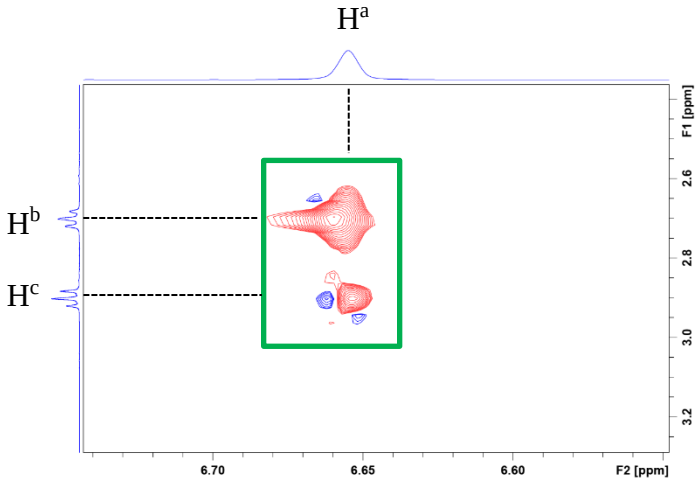


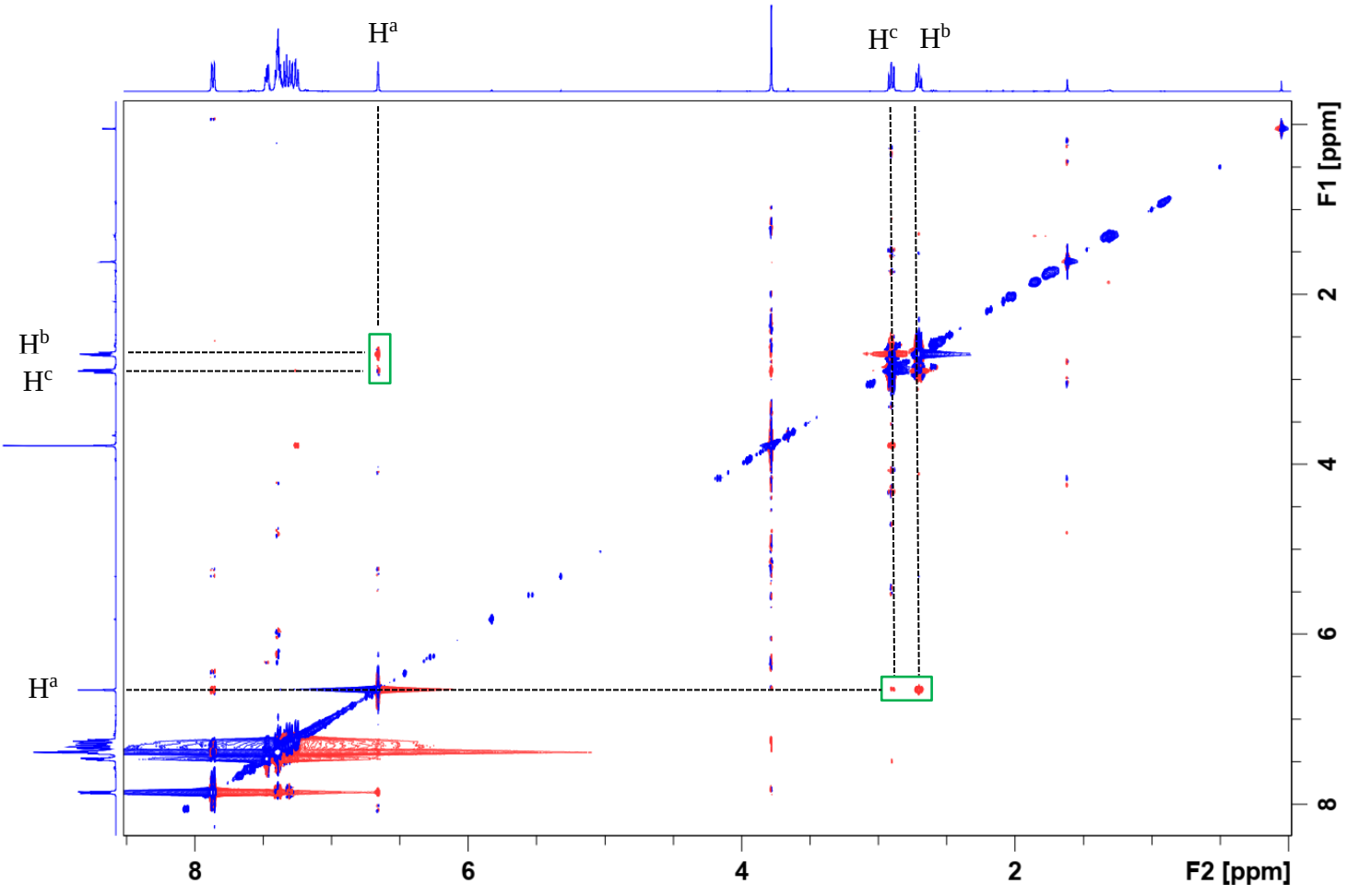
^{13}C NMR of 3aa (100 MHz, $CDCl_3$)



2D-NOE of 3aa

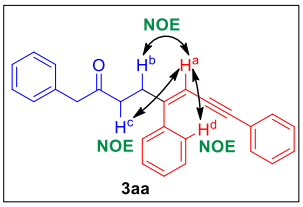

NOE
O
H^b
H^a
H^c
NOE
3aa


H^a
H^b
H^c
F1 [ppm]
2.6
2.8
3.0
3.2
6.70
6.65
6.60
F2 [ppm]


H^a
H^c
H^b
H^b
H^c
H^a
F1 [ppm]
2
4
6
8
8
6
4
2
F2 [ppm]

1D-NOE of 3aa

Irradiated at H_a



H^a H^b

mixing time 0 sec

6.647

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)

H^d H^a H^c H^b

mixing time 0.25 sec

7.857 7.847 6.646 2.894 2.692

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)

H^d H^a H^c H^b

mixing time 0.50 sec

7.857 7.847 6.647 2.894 2.692

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)

H^d H^a H^c H^b

mixing time 0.80 sec

7.858 7.847 6.647 2.894 2.693

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)

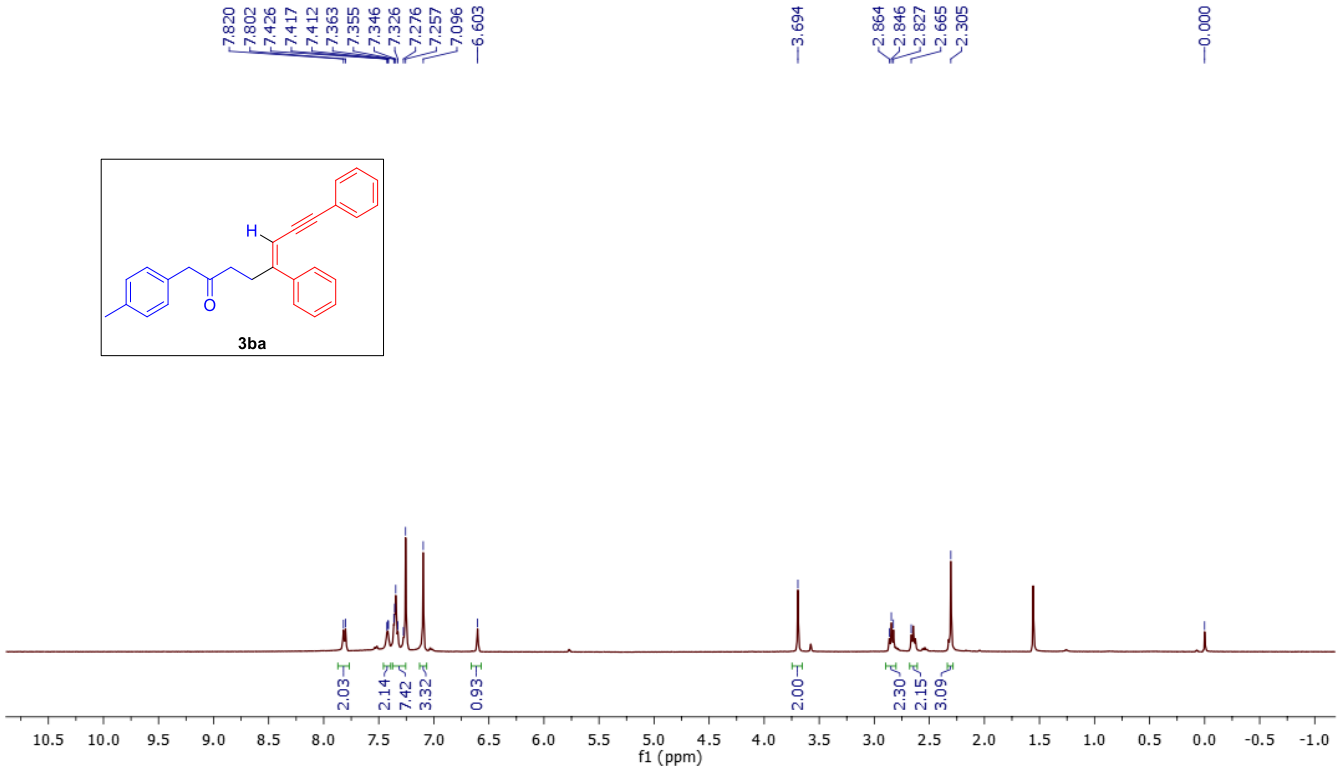
H^d H^a H^c H^b

mixing time 1.00 sec

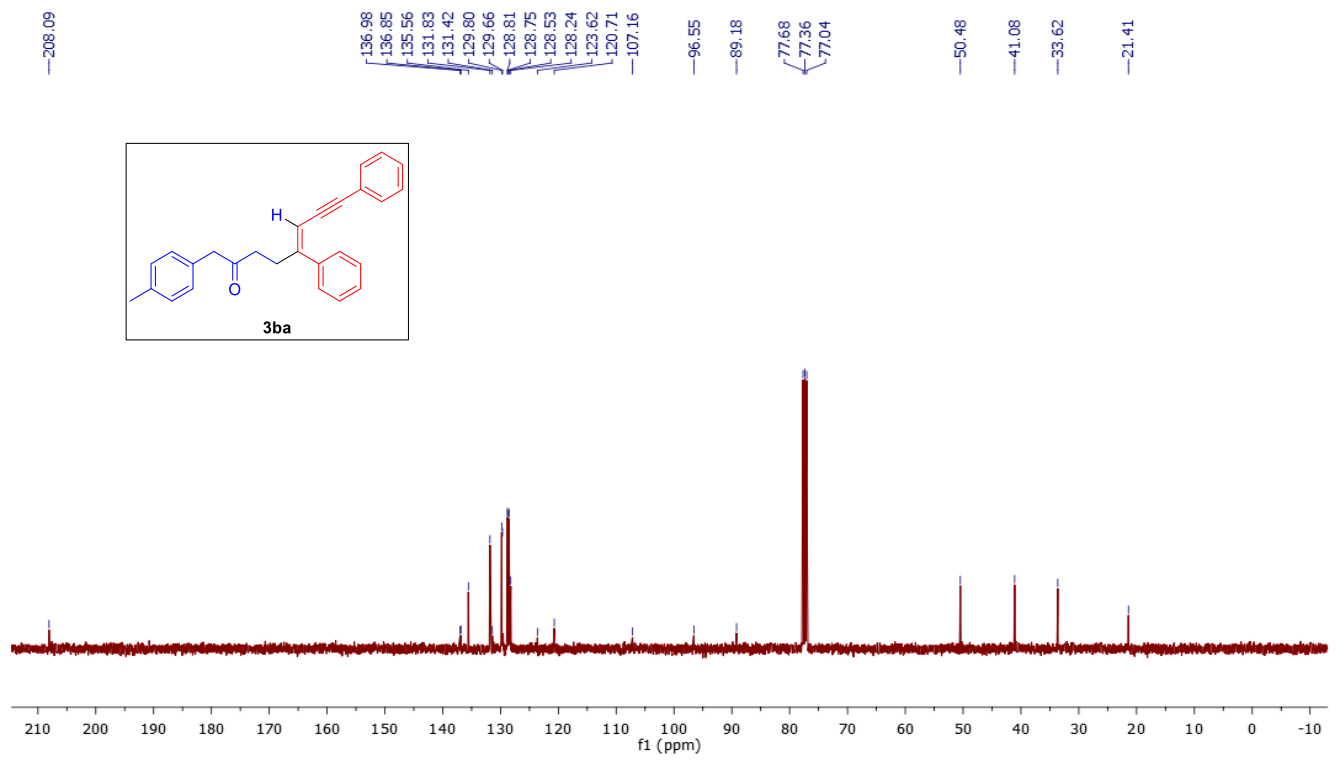
7.858 7.847 6.647 2.895 2.693

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)

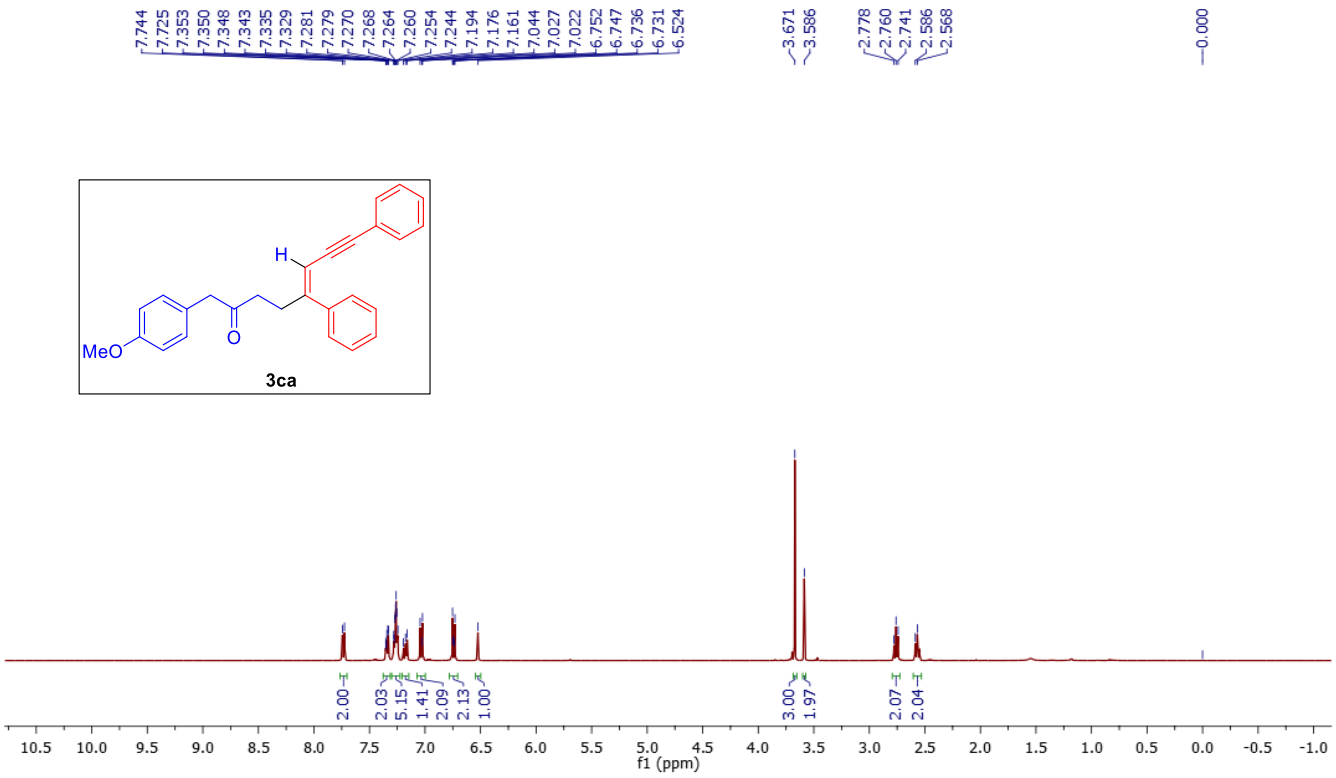
^{1}H NMR of 3ba (400 MHz, $CDCl_3$)



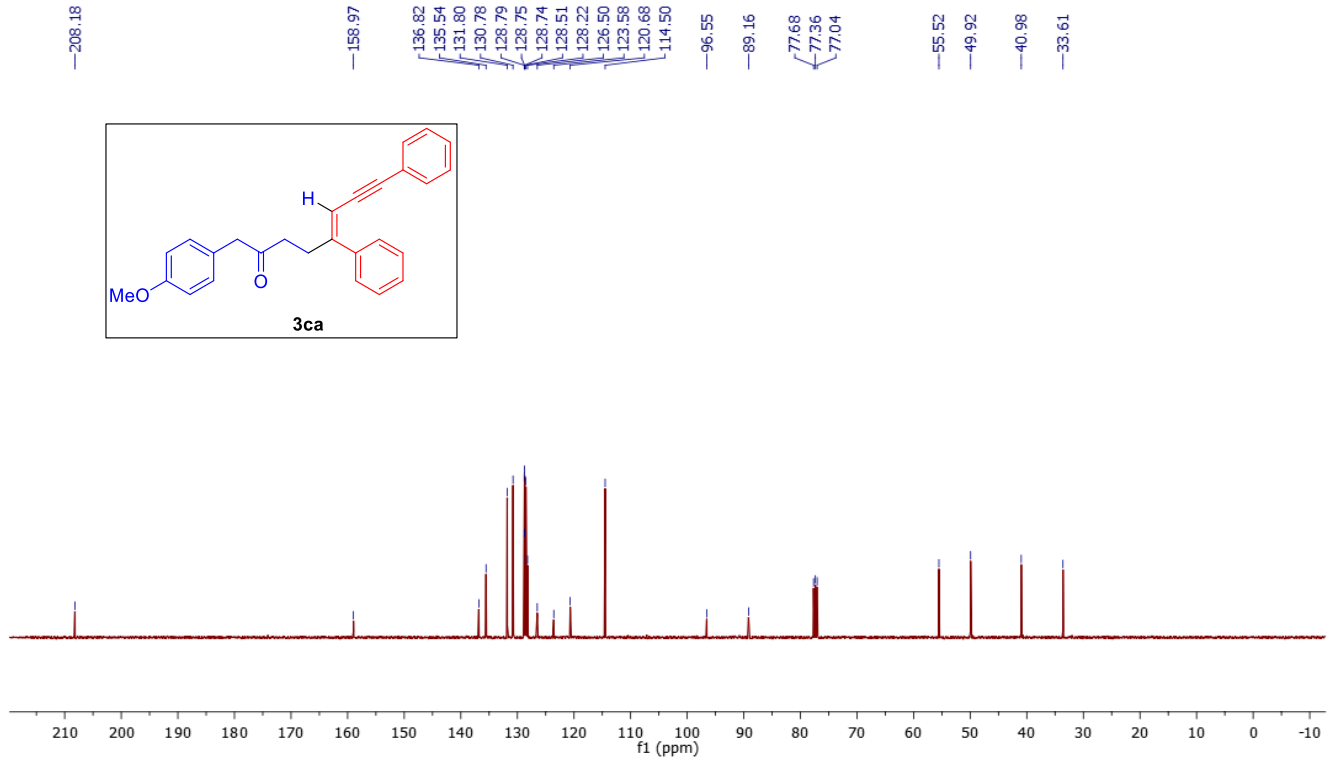
^{13}C NMR of 3ba (100 MHz, $CDCl_3$)



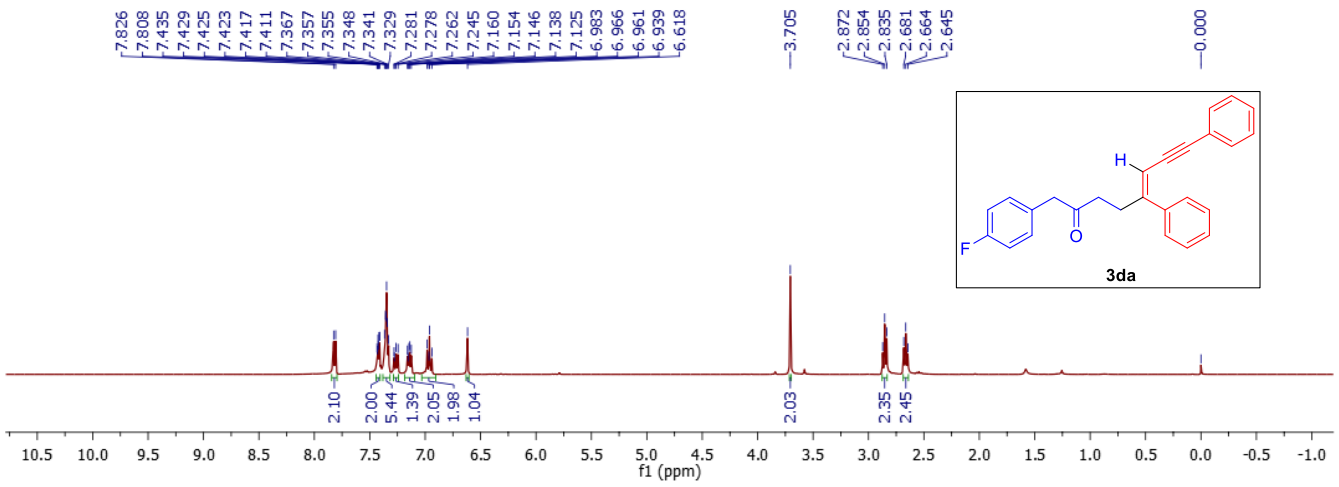
^{1}H NMR of 3ca (400 MHz, $CDCl_3$)



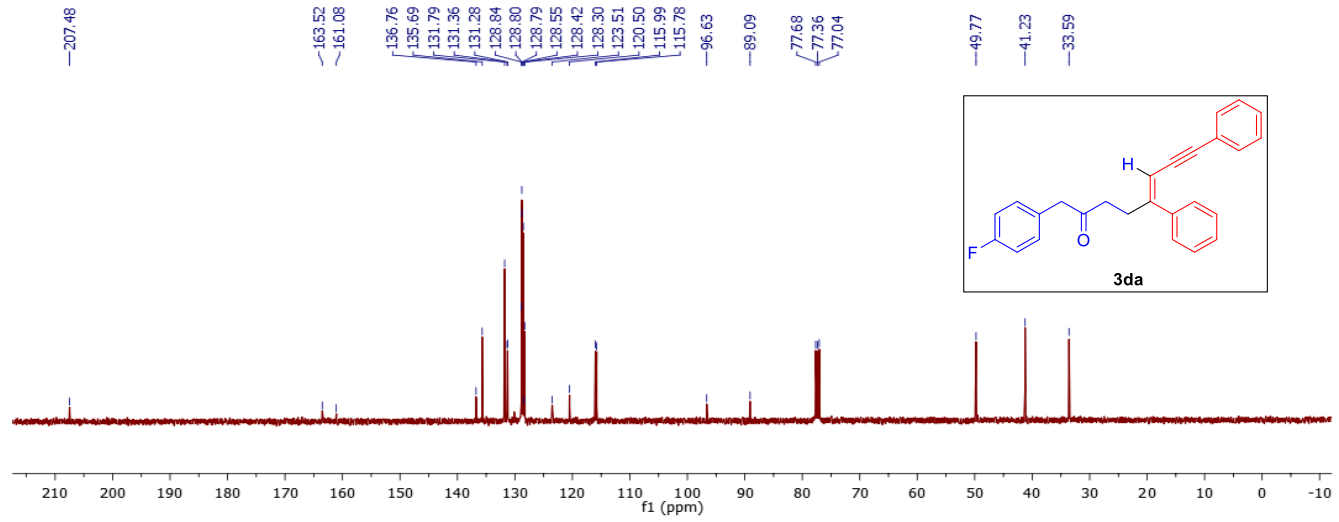
^{13}C NMR of 3ca (100 MHz, $CDCl_3$)



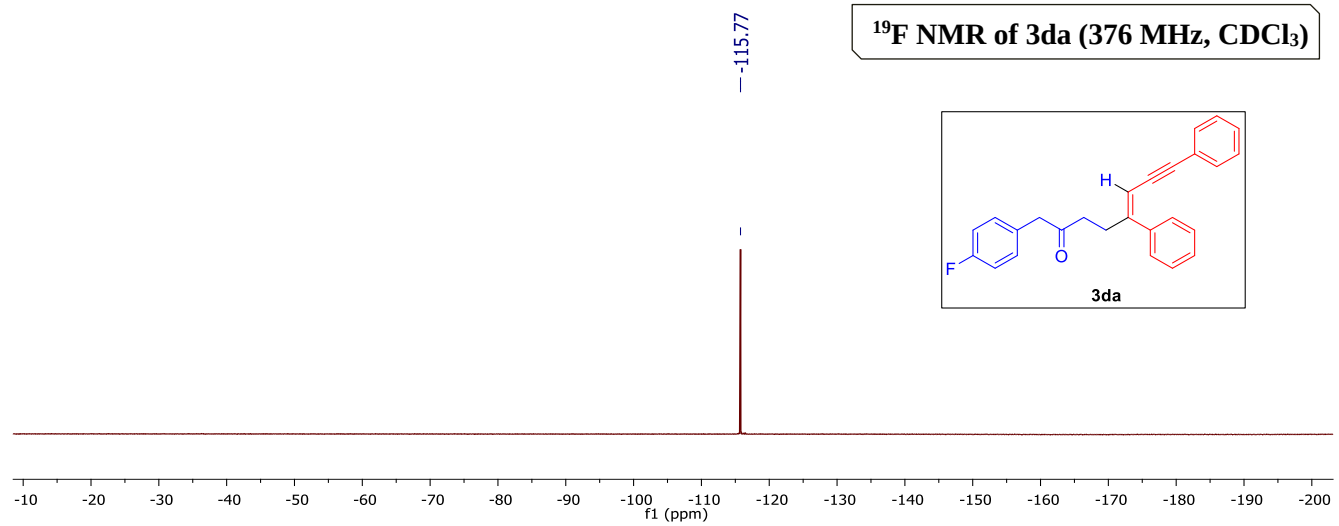
^{1}H NMR of 3da (400 MHz, $CDCl_3$)



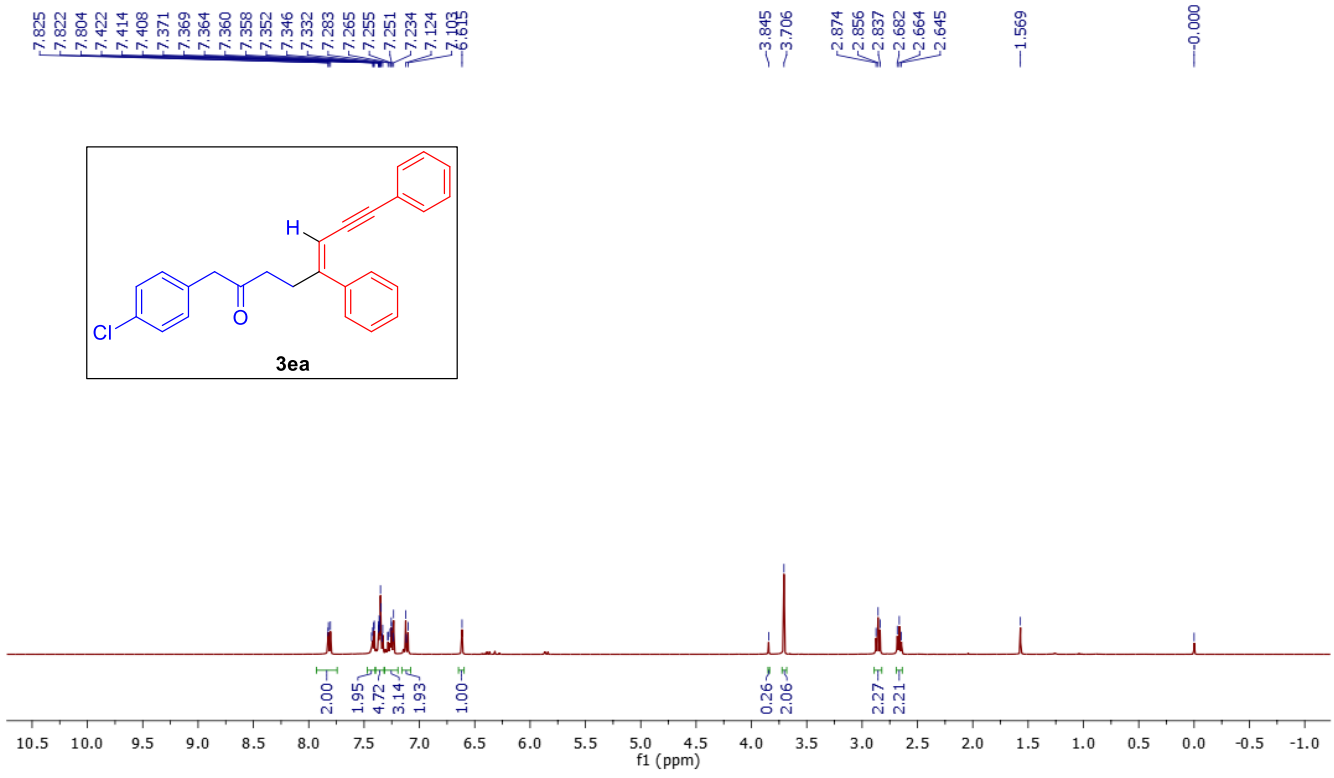
^{13}C NMR of 3da (100 MHz, $CDCl_3$)



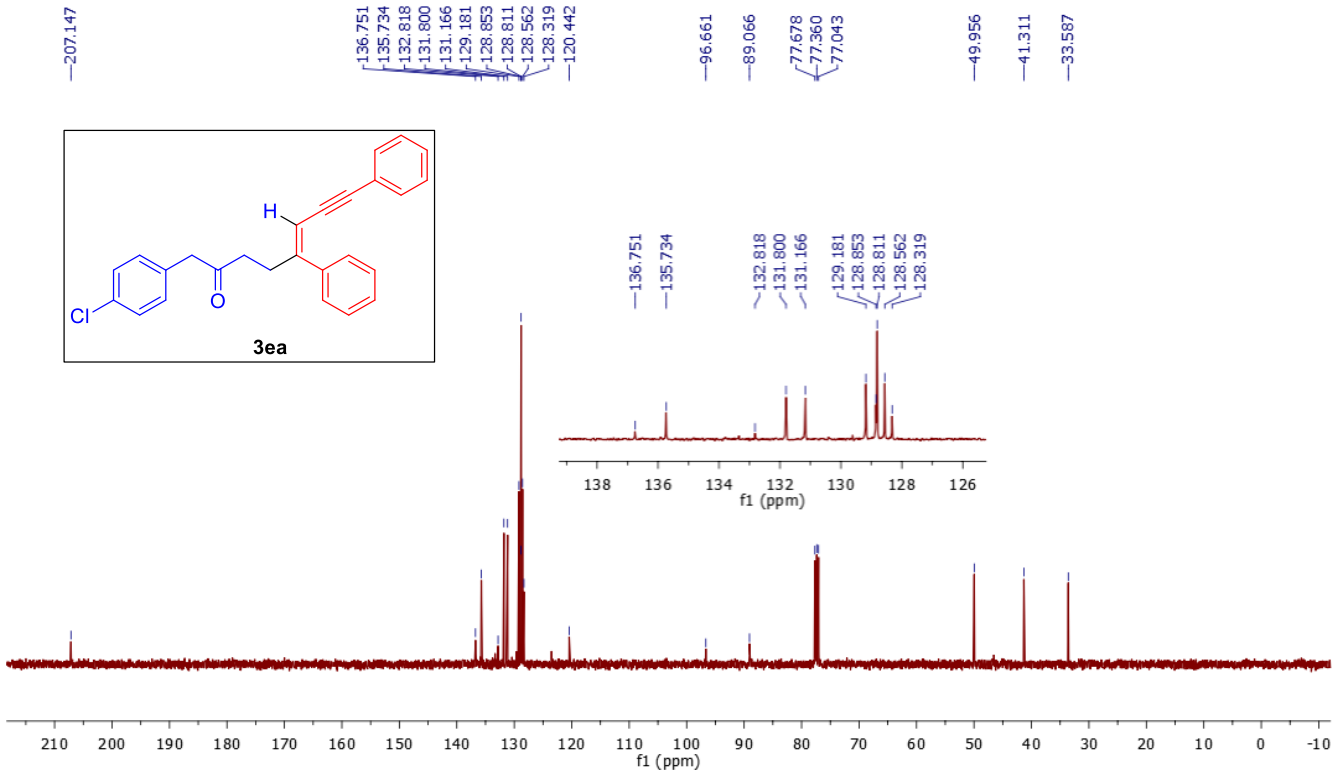
^{19}F NMR of 3da (376 MHz, $CDCl_3$)



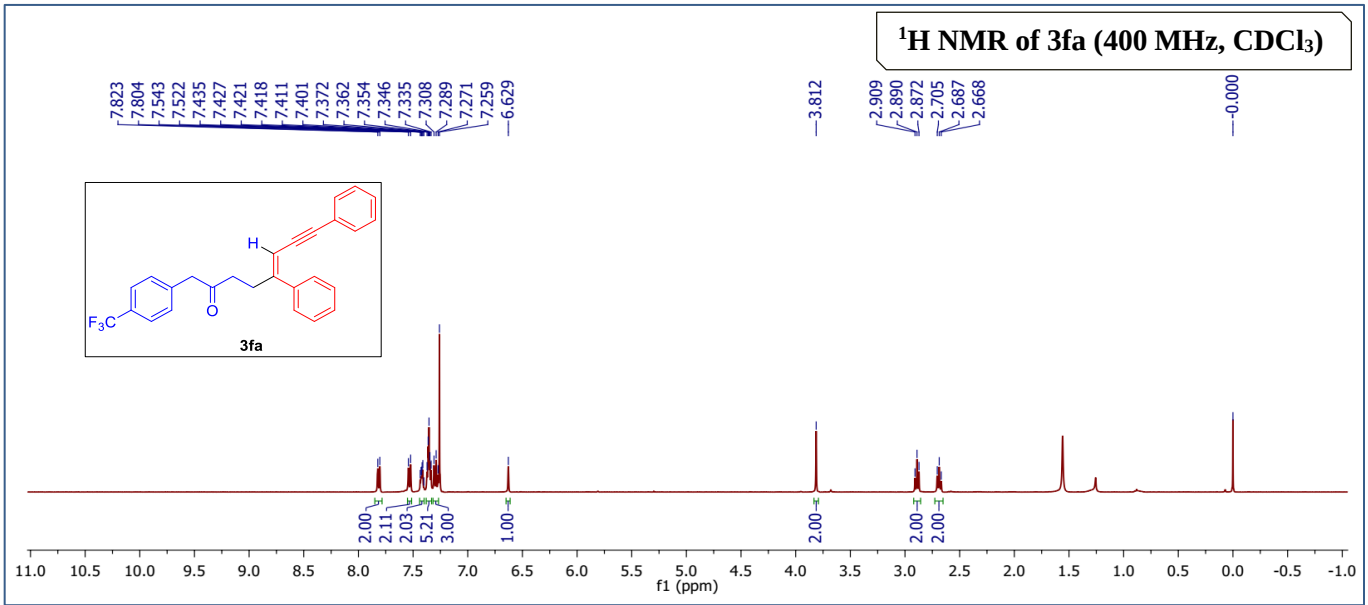
^{1}H NMR of 3ea (400 MHz, $CDCl_3$)



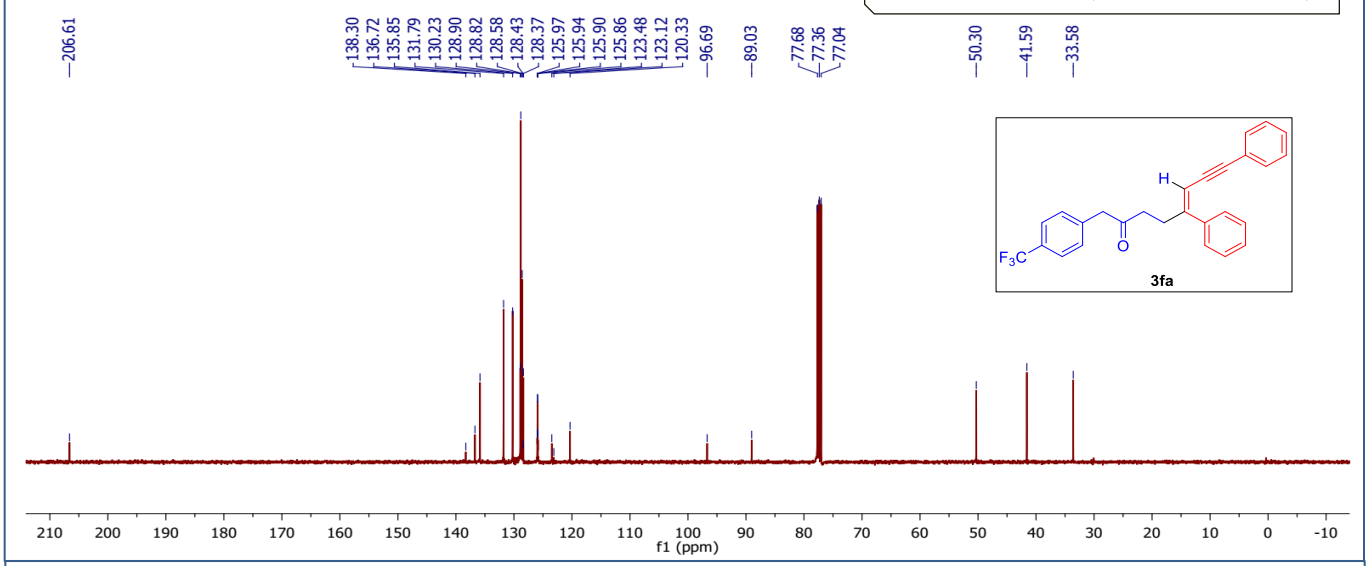
^{13}C NMR of 3ea (100 MHz, $CDCl_3$)



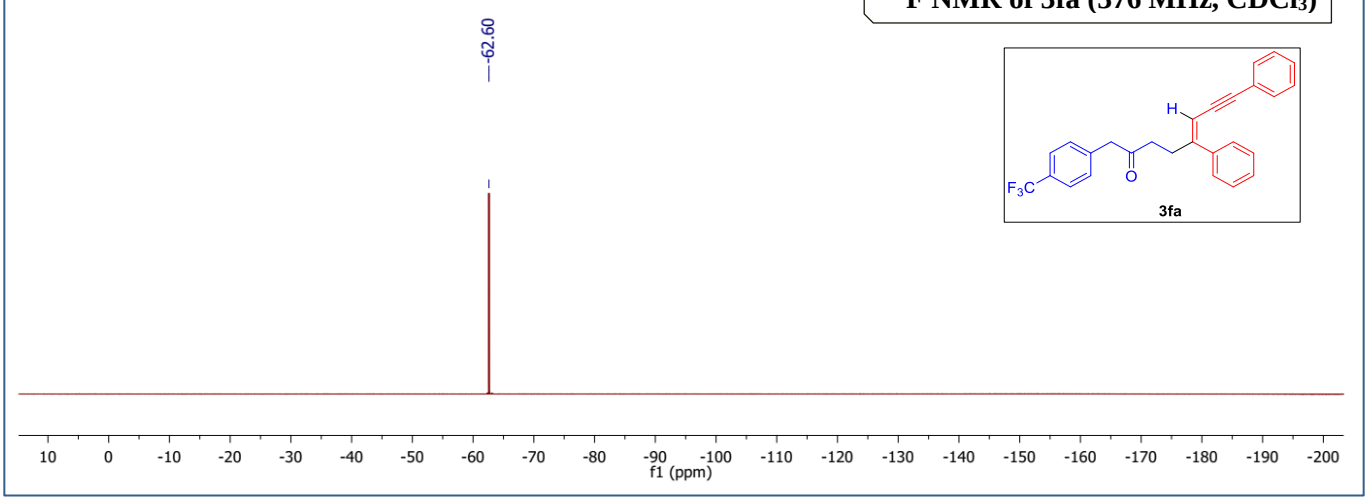
^{1}H NMR of 3fa (400 MHz, $CDCl_3$)



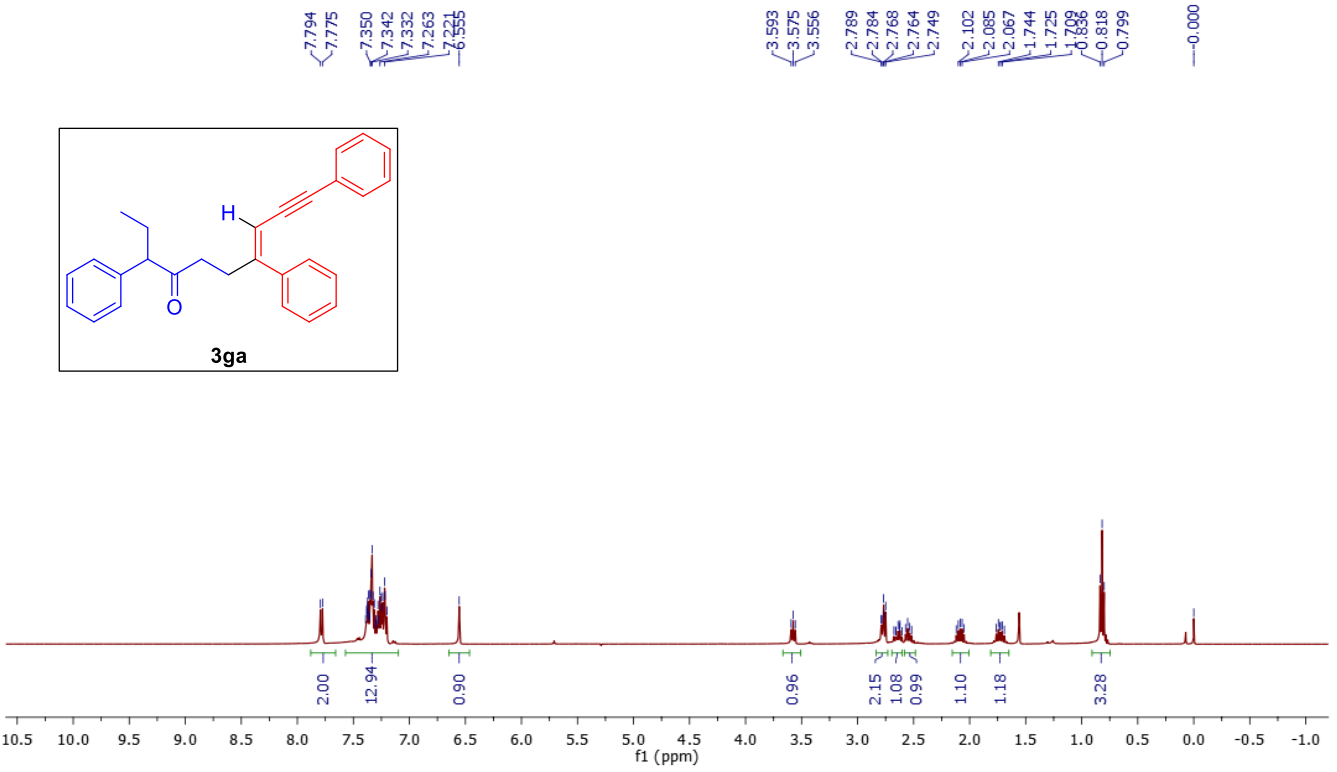
^{13}C NMR of 3fa (100 MHz, $CDCl_3$)



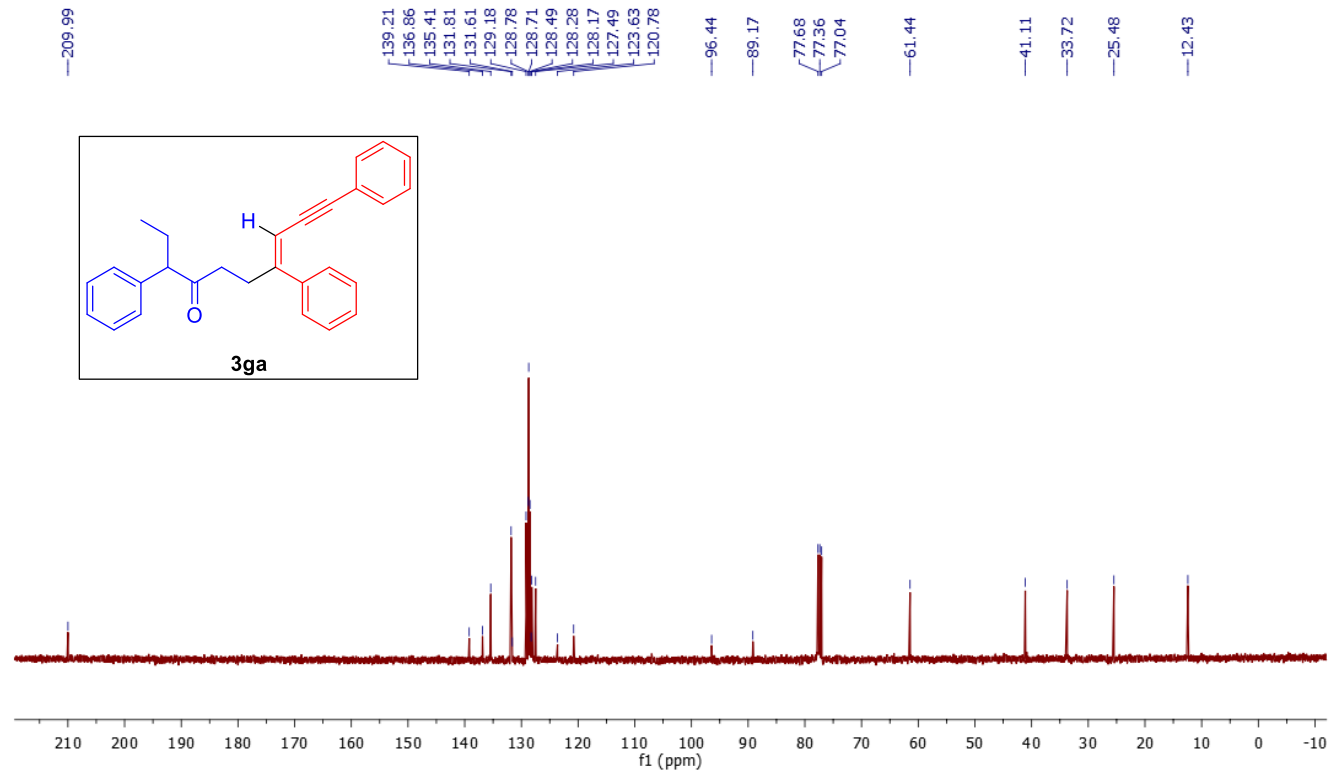
^{19}F NMR of 3fa (376 MHz, $CDCl_3$)



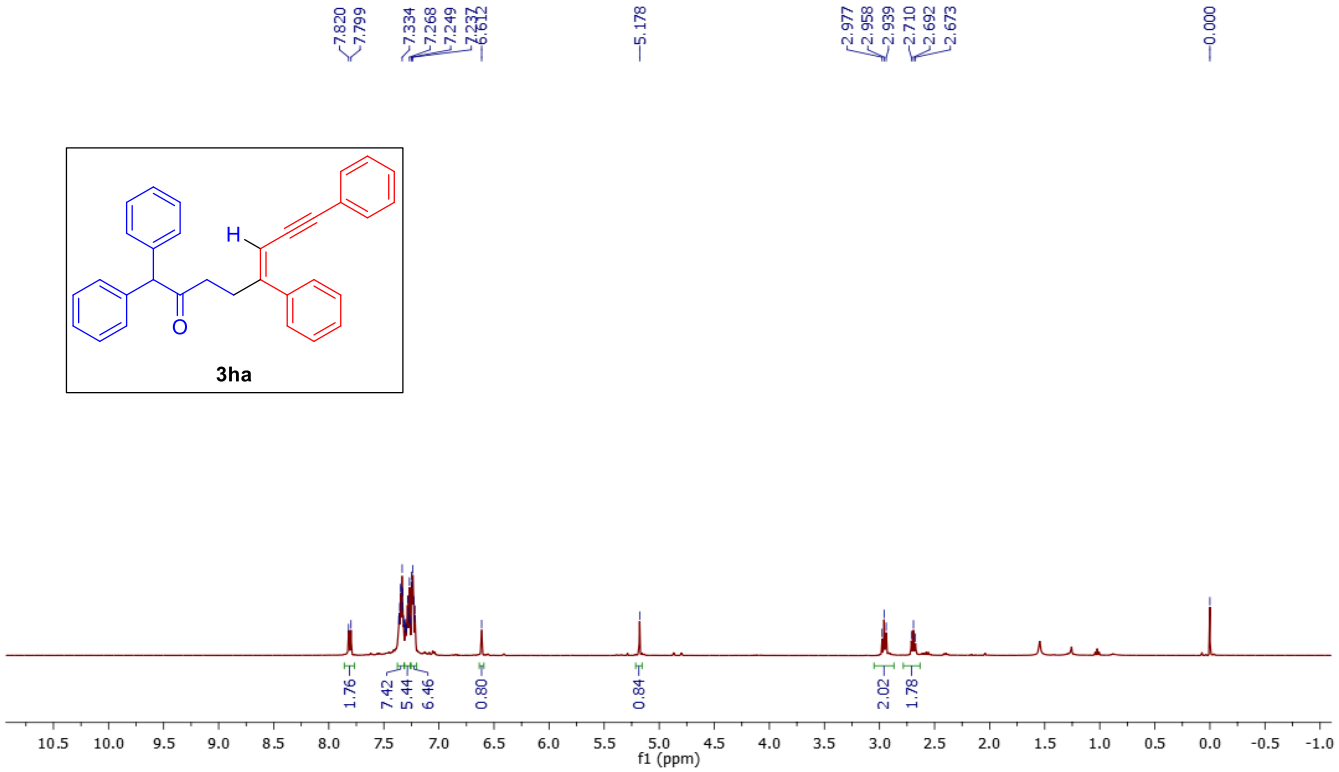
^{1}H NMR of 3ga (400 MHz, $CDCl_3$)



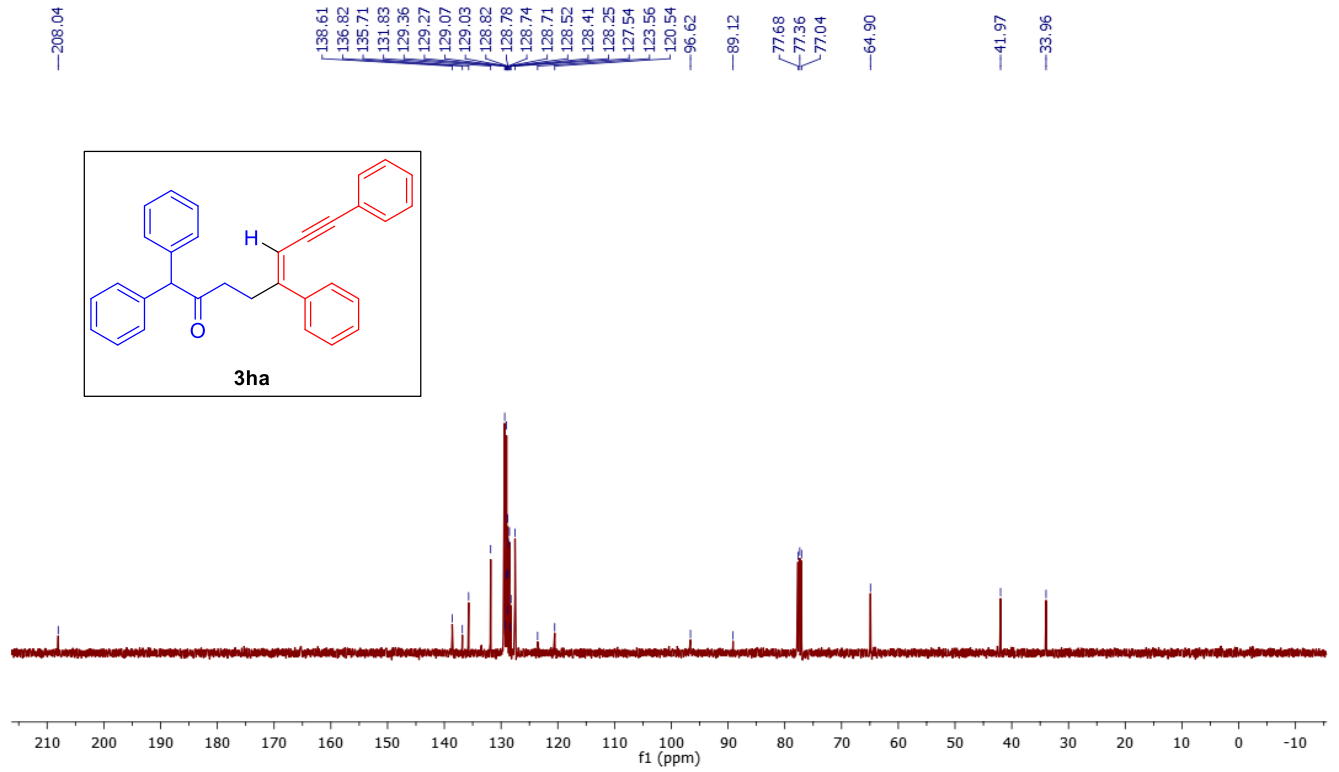
^{13}C NMR of 3ga (100 MHz, $CDCl_3$)



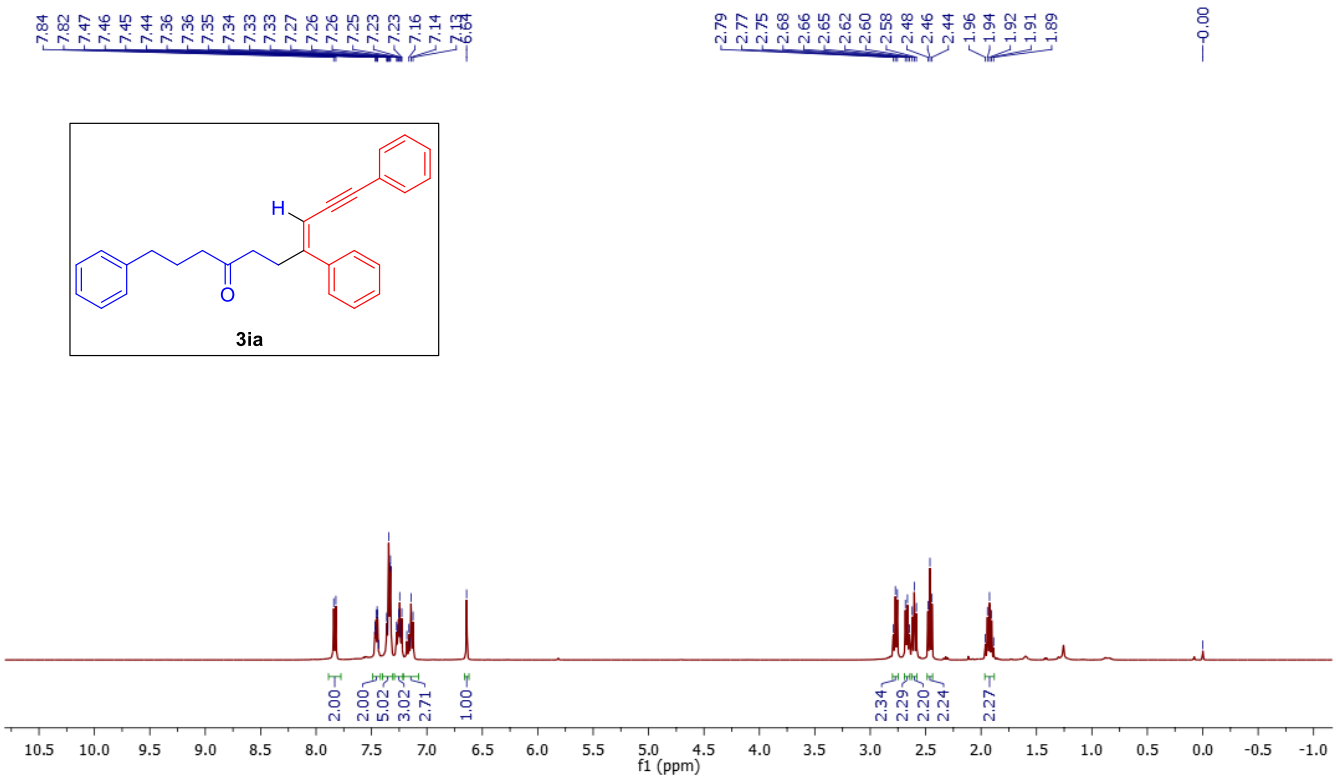
^{1}H NMR of 3ha (400 MHz, $CDCl_3$)



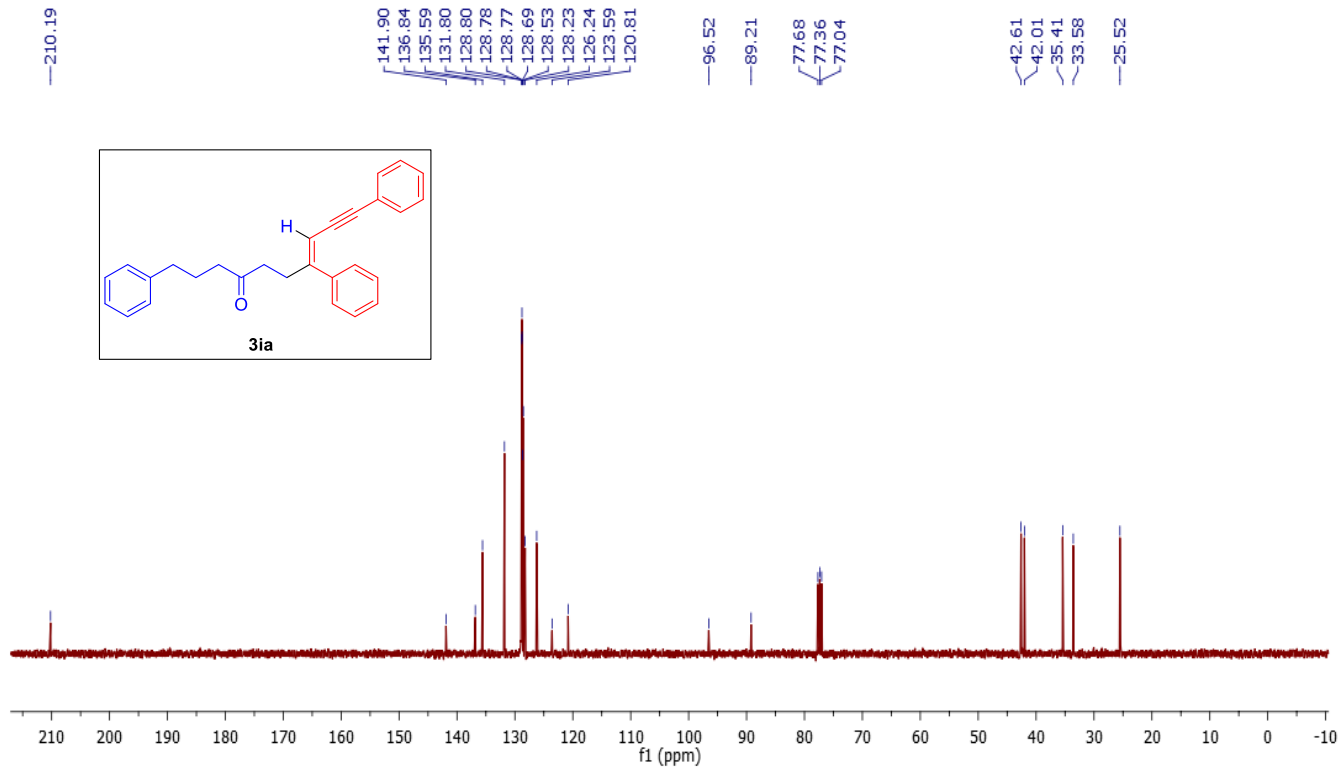
^{13}C NMR of 3ha (100 MHz, $CDCl_3$)



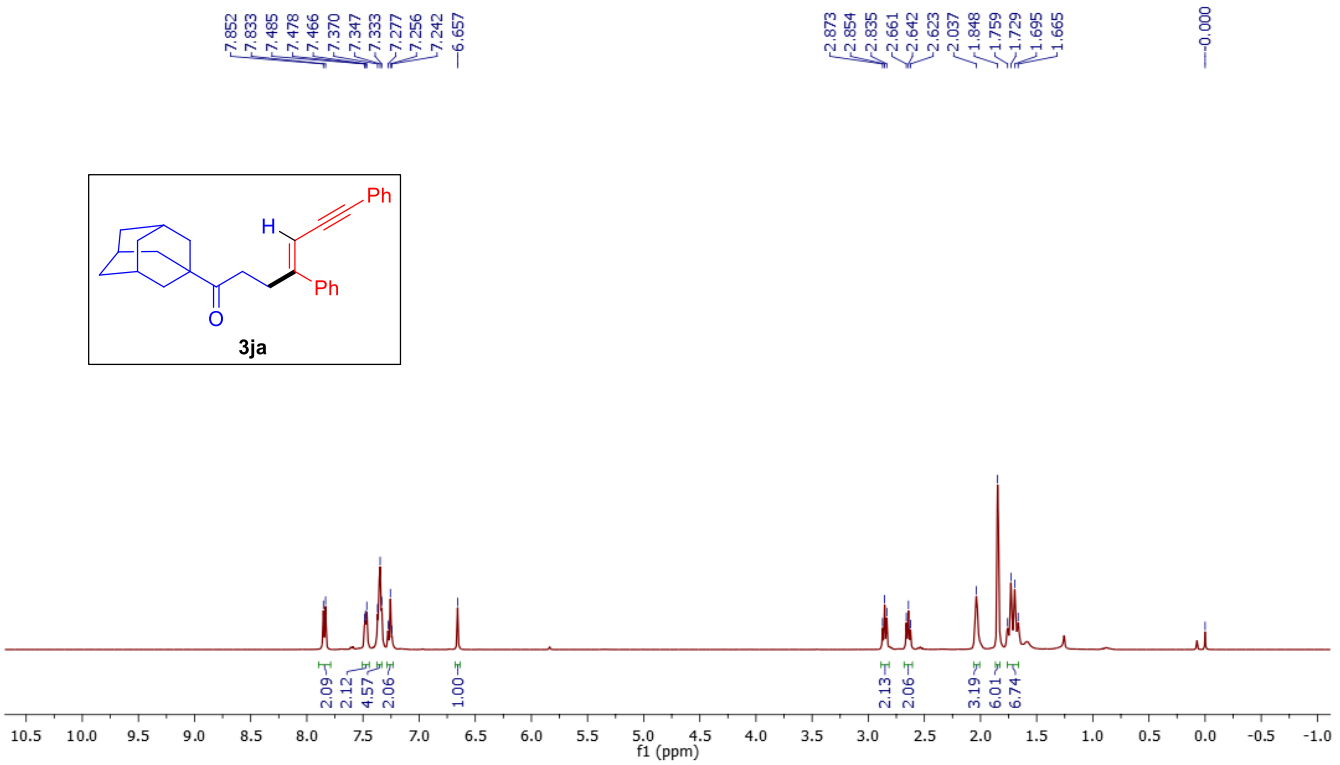
^{1}H NMR of 3ia (400 MHz, $CDCl_3$)



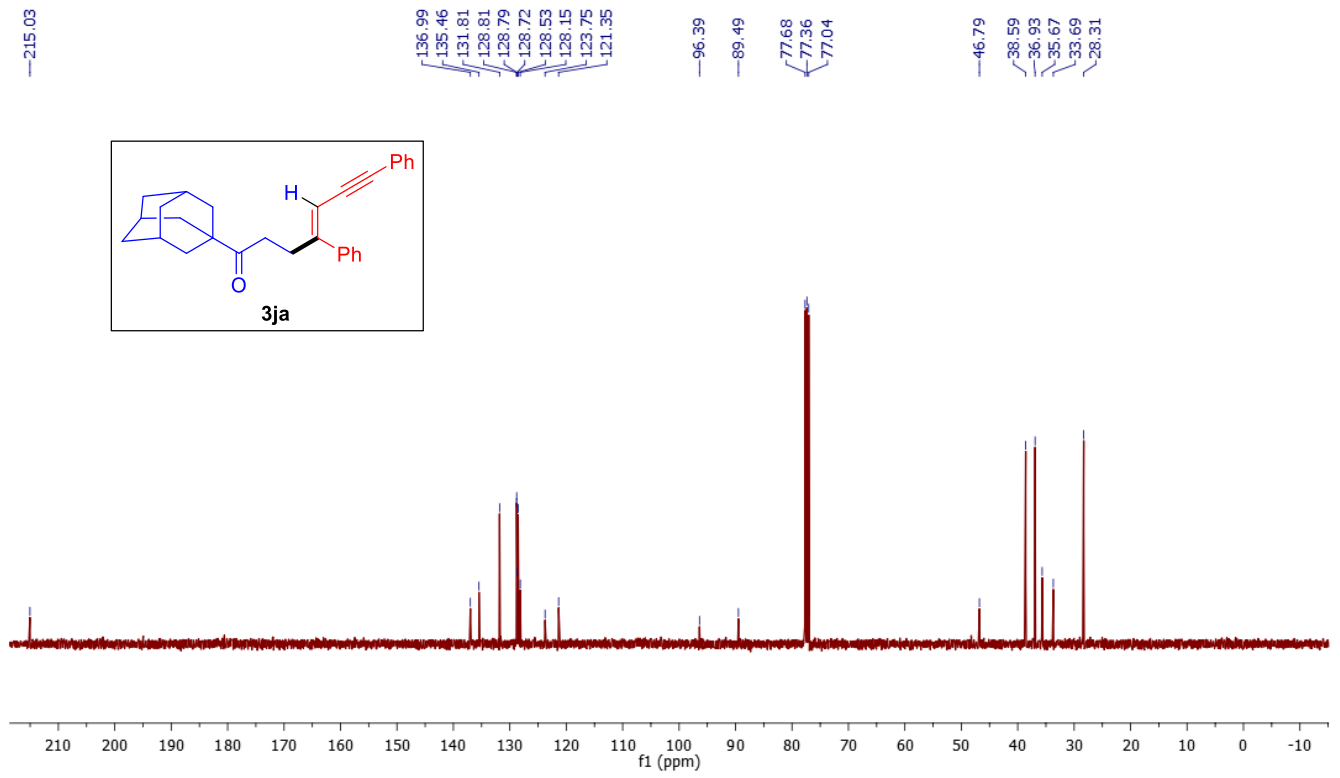
^{13}C NMR of 3ia (100 MHz, $CDCl_3$)



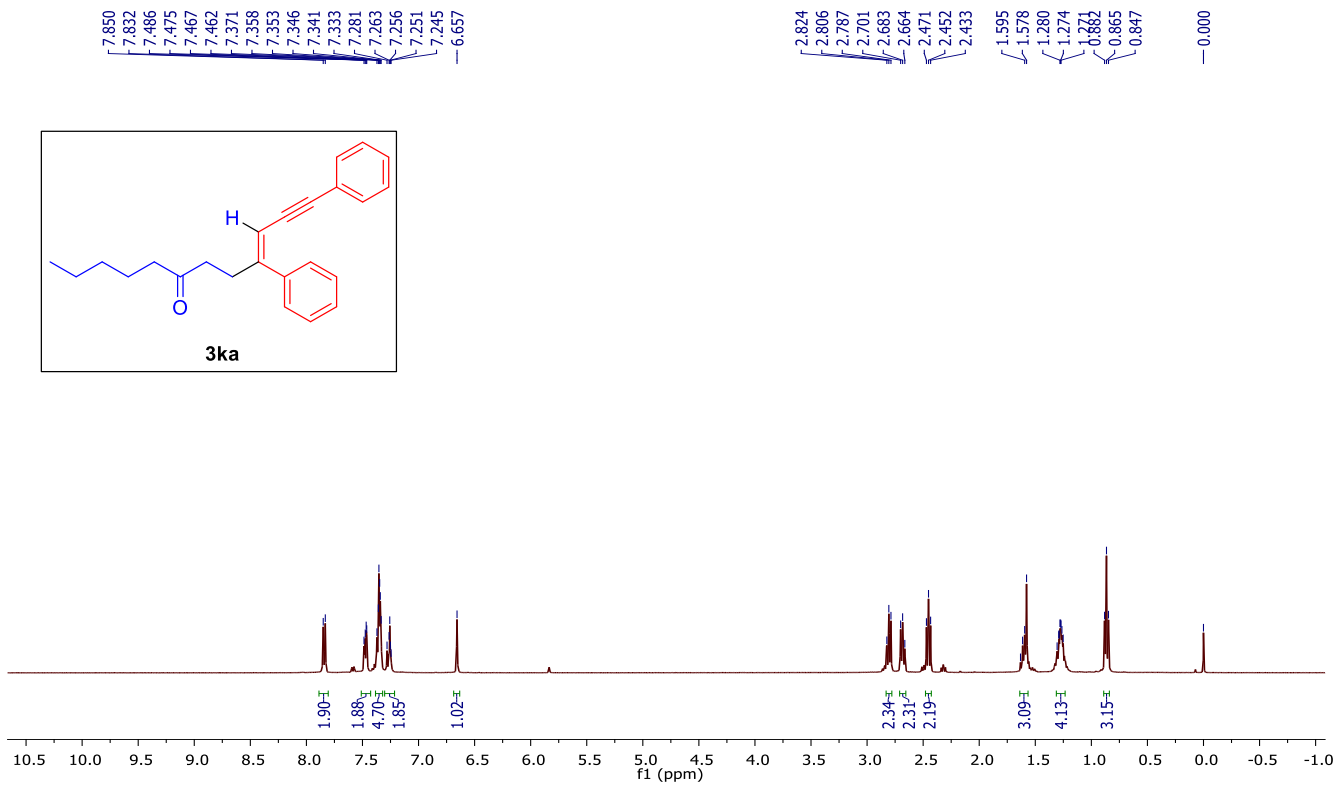
^{1}H NMR of 3ja (400 MHz, $CDCl_3$)



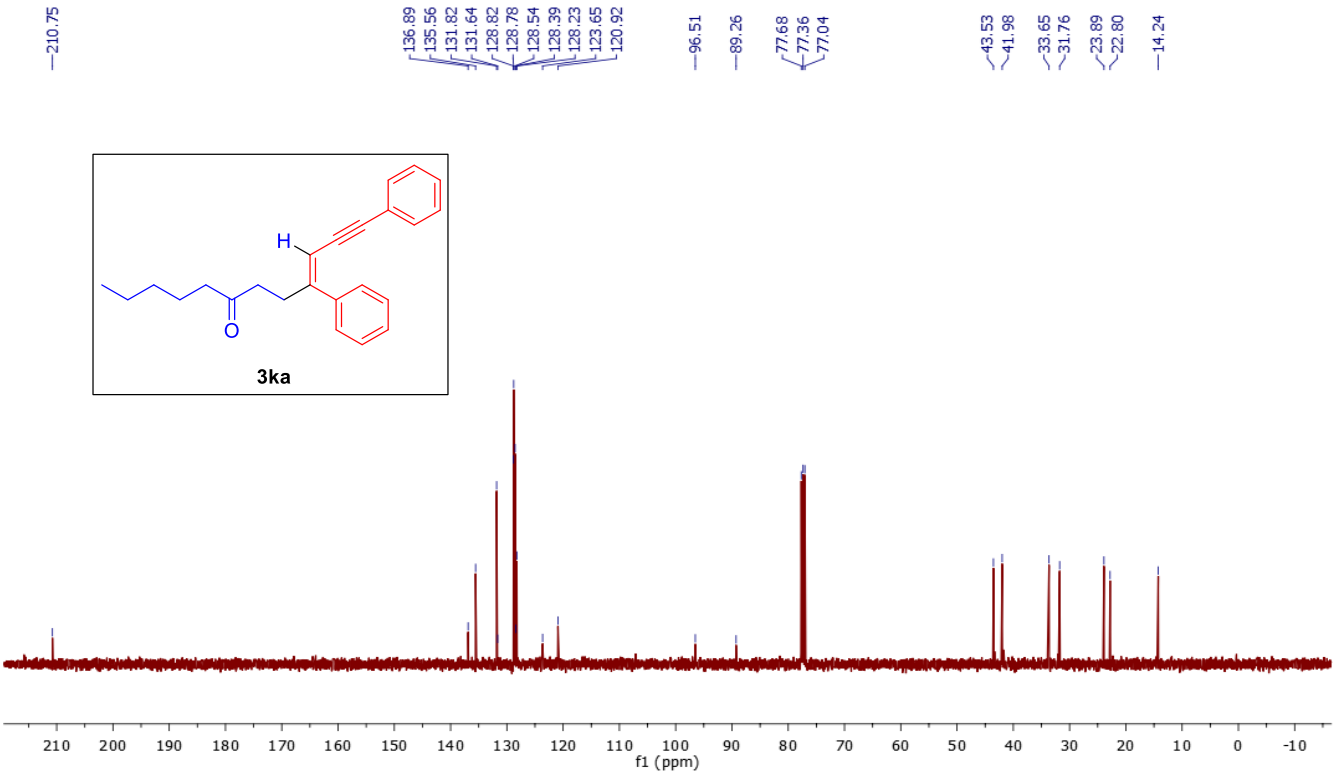
^{13}C NMR of 3ja (100 MHz, $CDCl_3$)



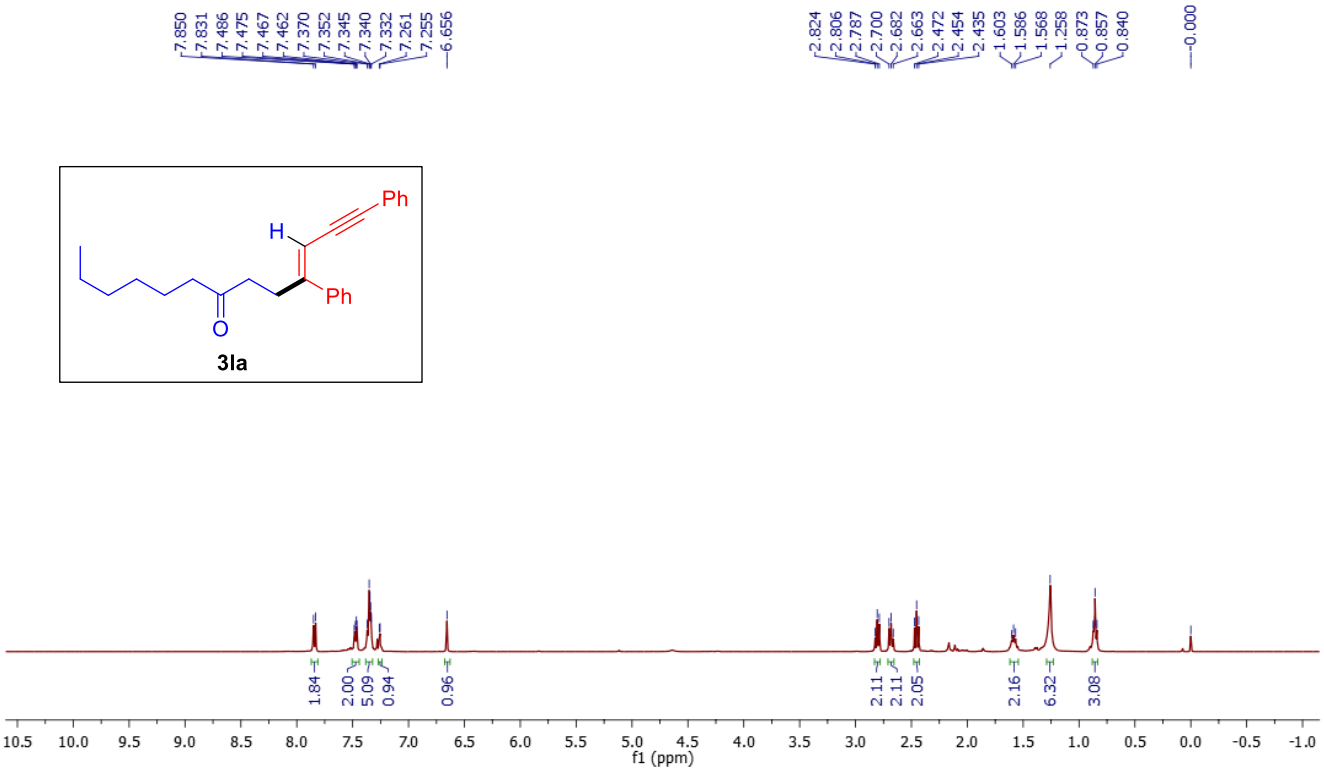
^{1}H NMR of 3ka (400 MHz, $CDCl_3$)



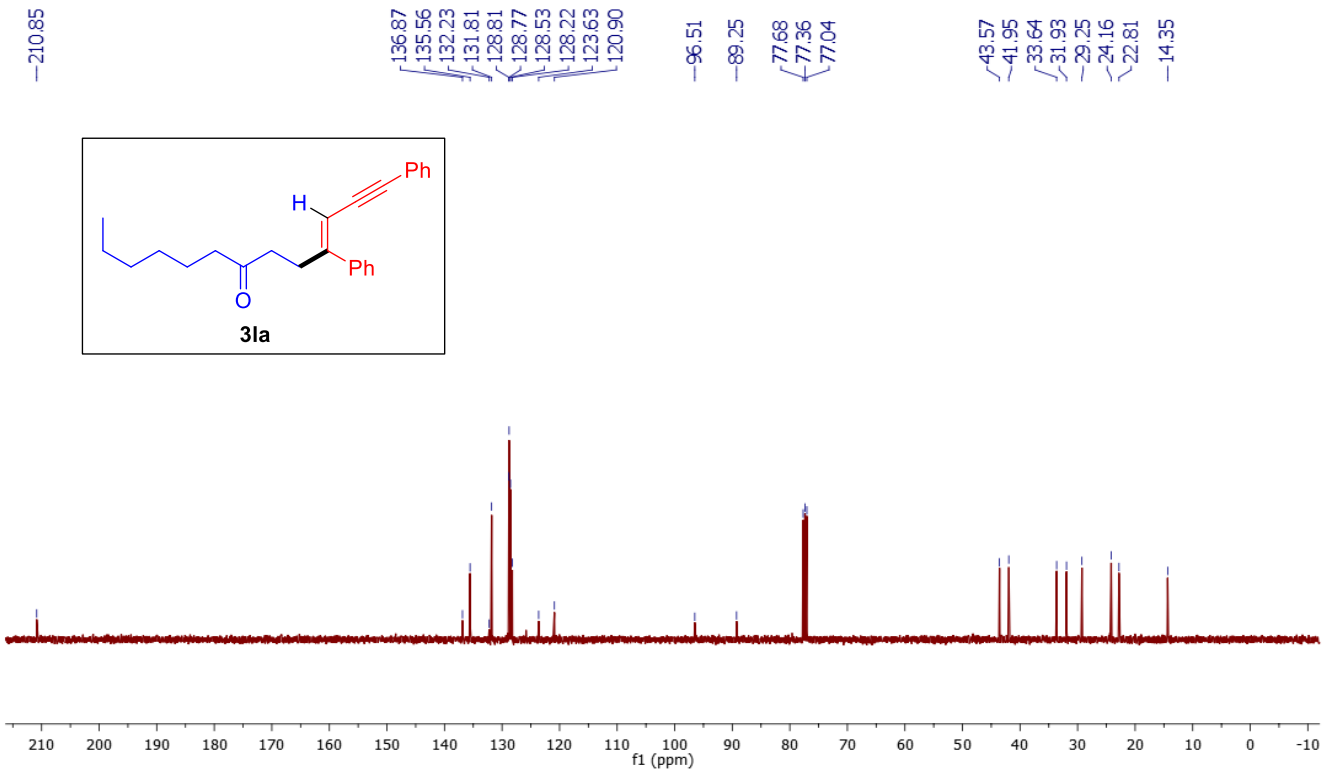
^{13}C NMR of 3ka (100 MHz, $CDCl_3$)



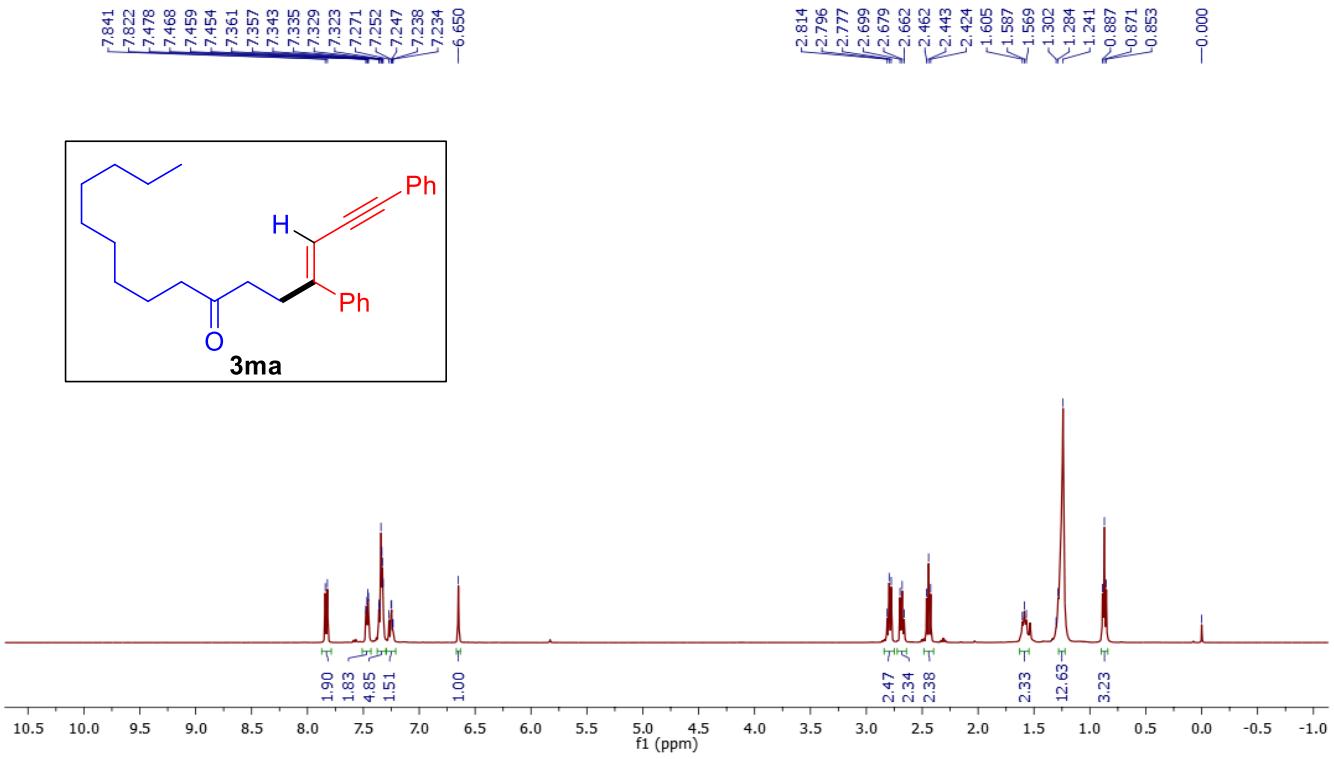
^{1}H NMR of 3la (400 MHz, $CDCl_3$)



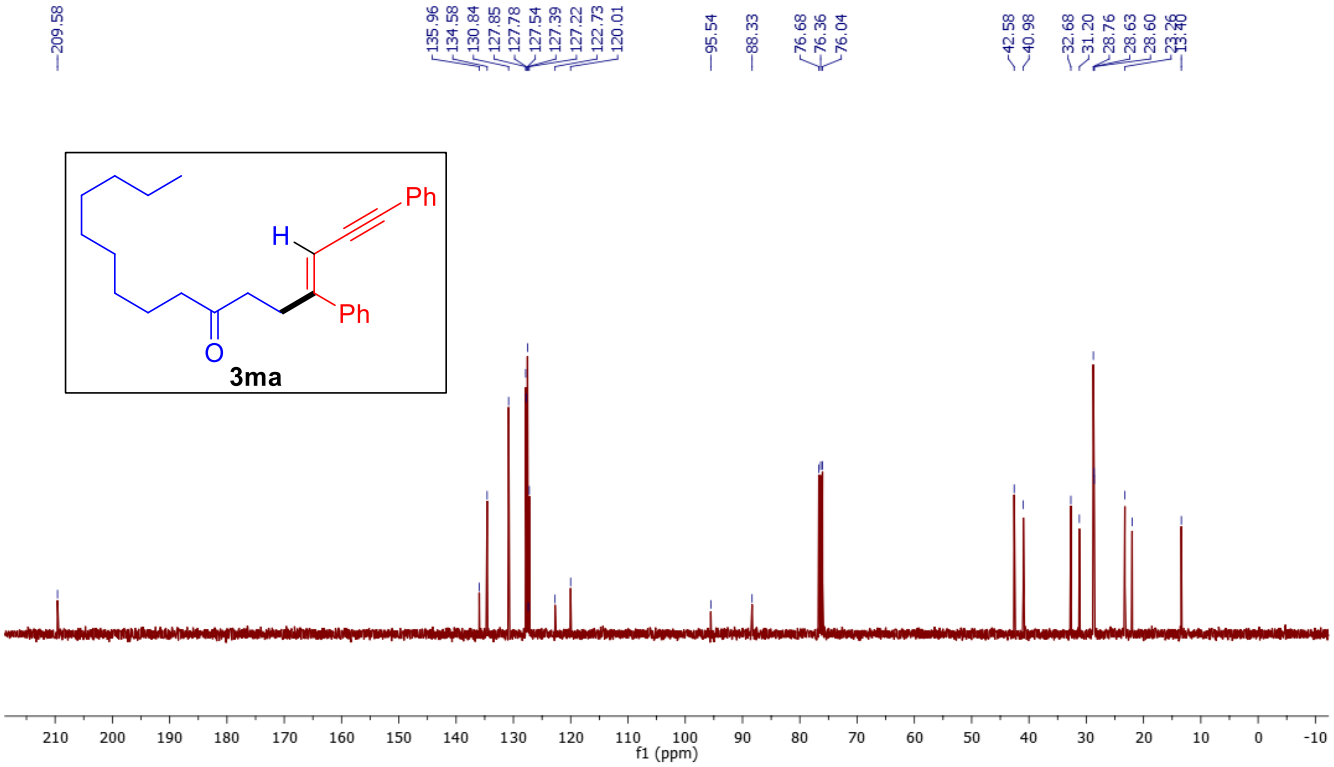
^{13}C NMR of 3la (100 MHz, $CDCl_3$)



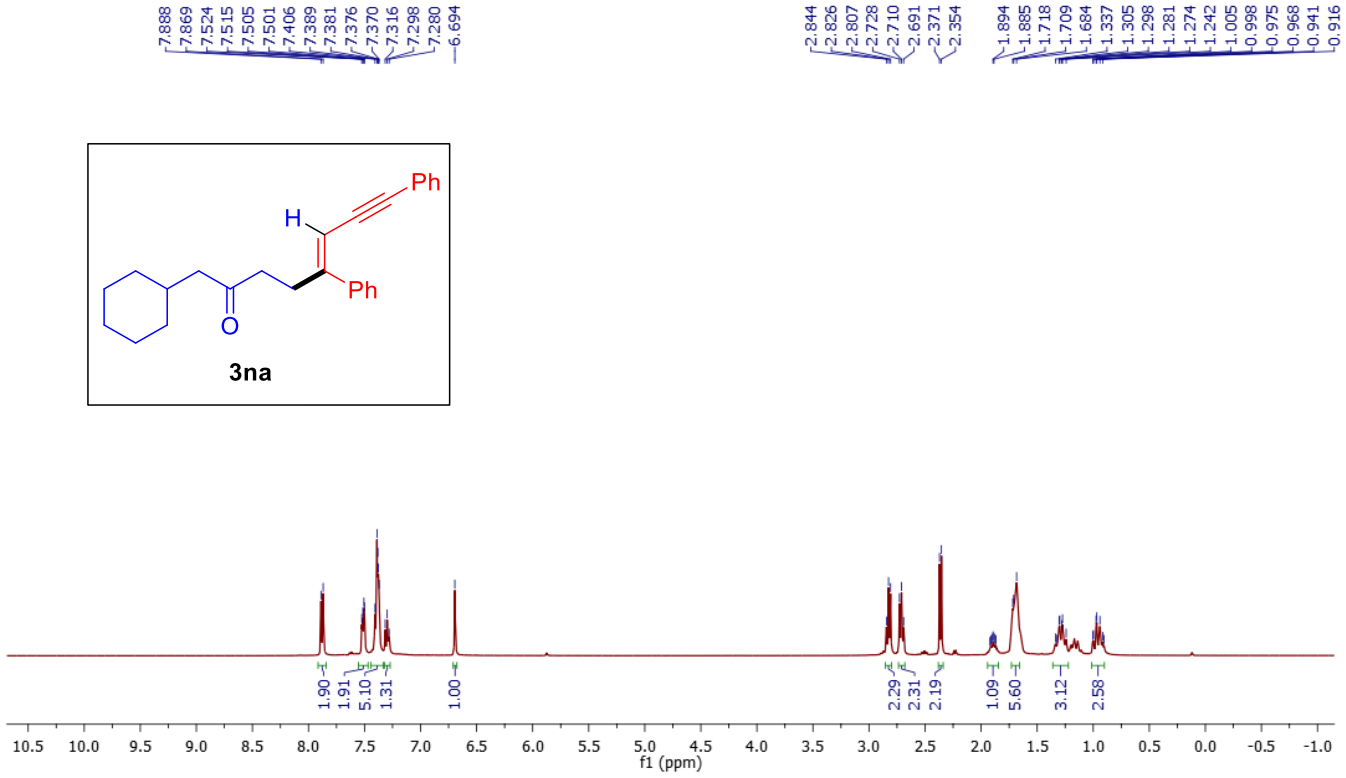
^{1}H NMR of 3ma (400 MHz, $CDCl_3$)



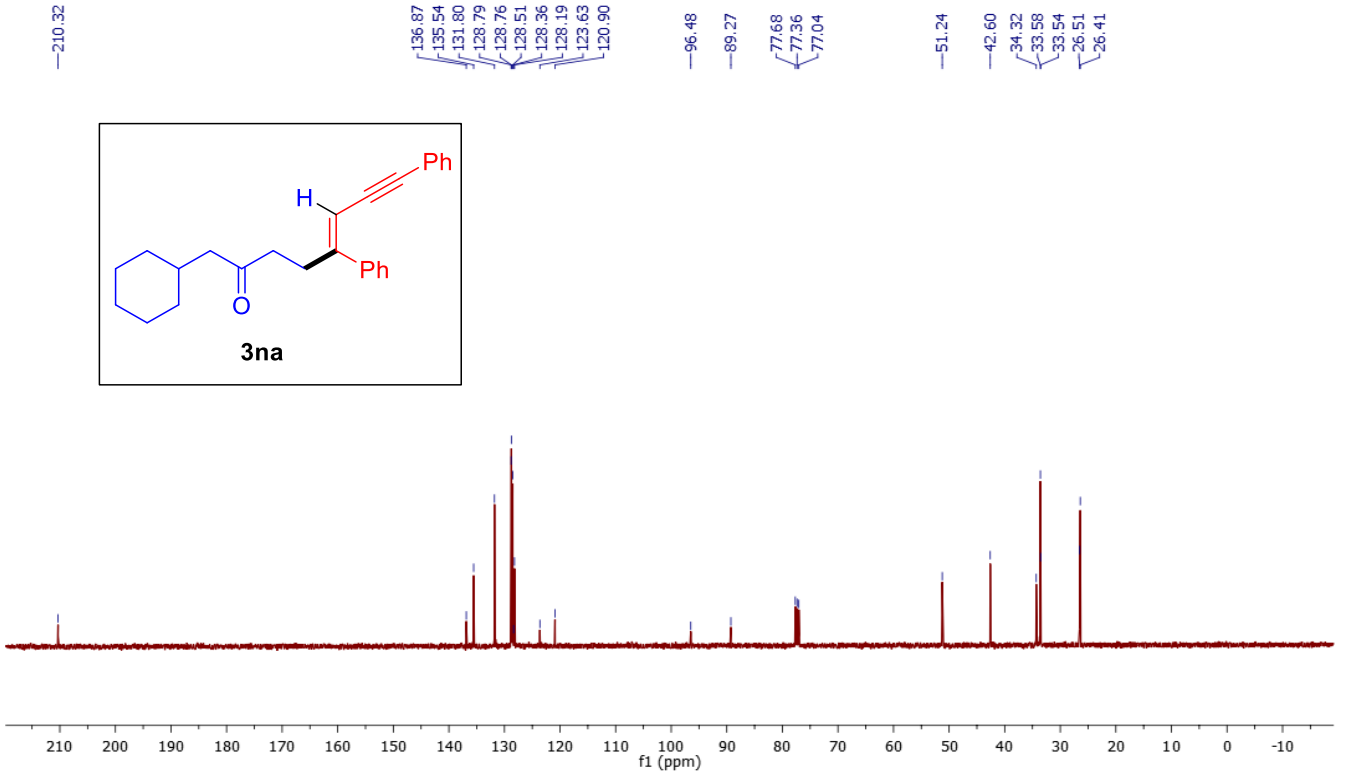
^{13}C NMR of 3ma (100 MHz, $CDCl_3$)



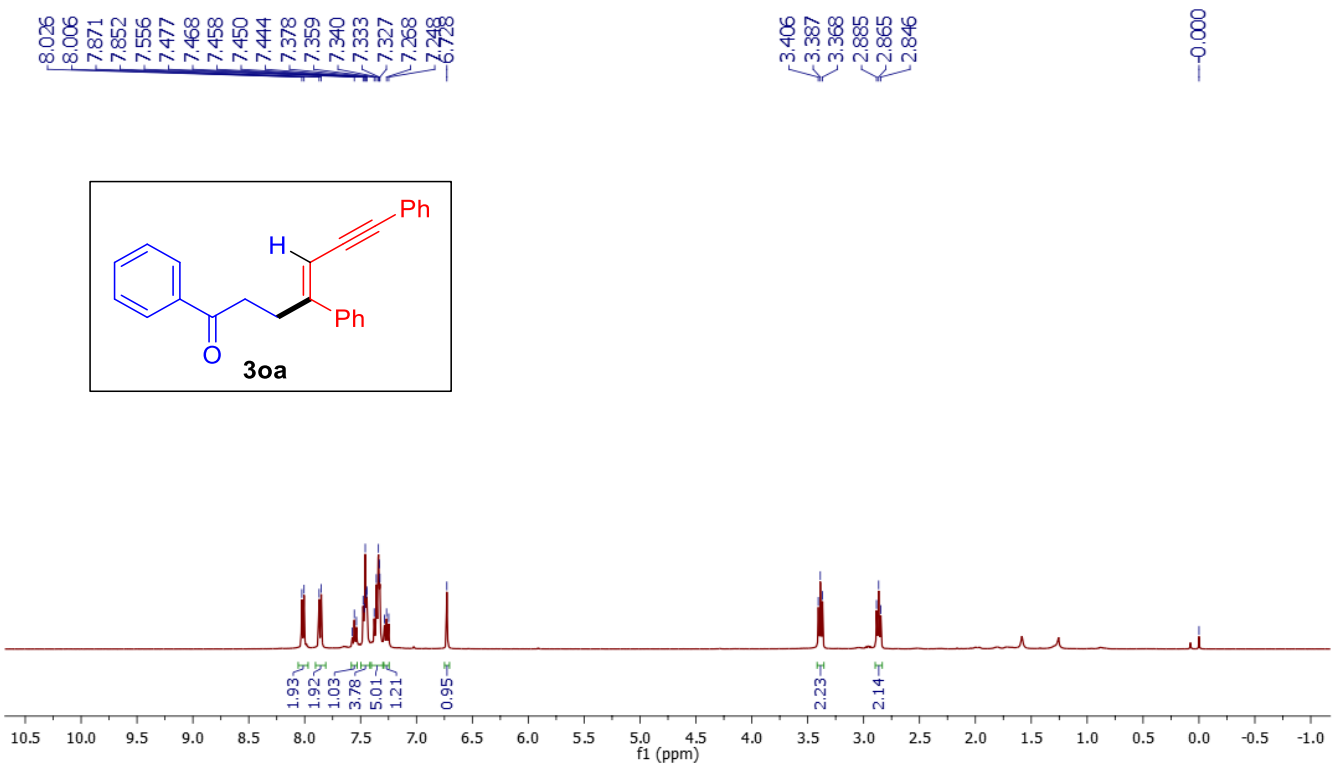
^{1}H NMR of 3na (400 MHz, $CDCl_3$)



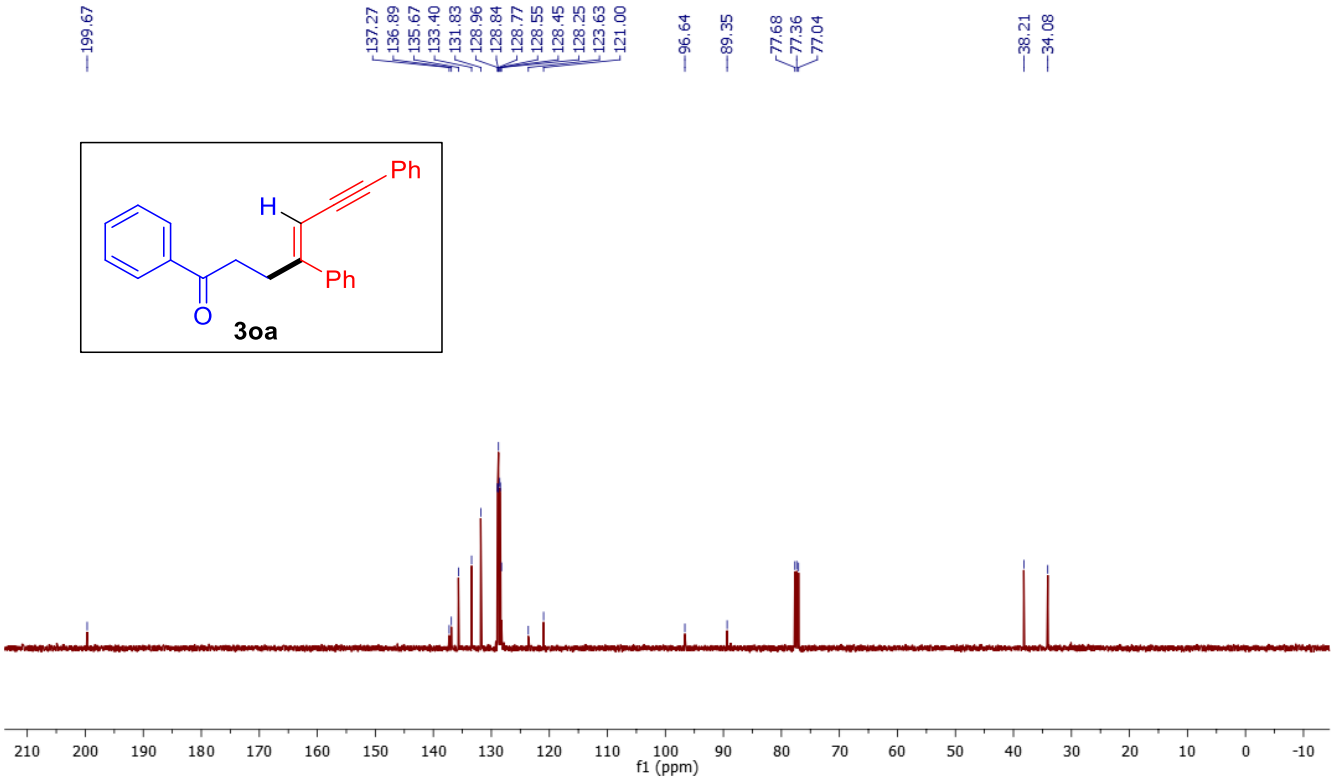
^{13}C NMR of 3na (100 MHz, $CDCl_3$)



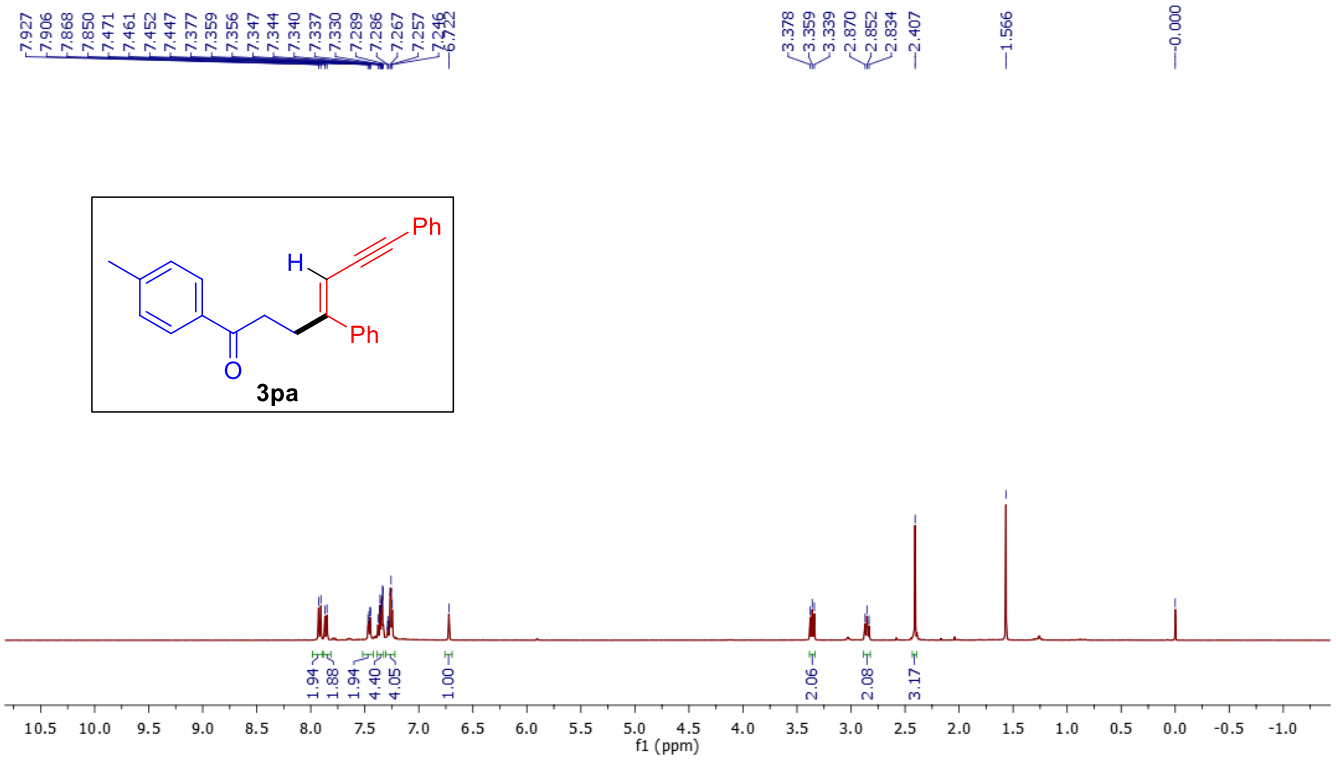
^{1}H NMR of 3oa (400 MHz, $CDCl_3$)



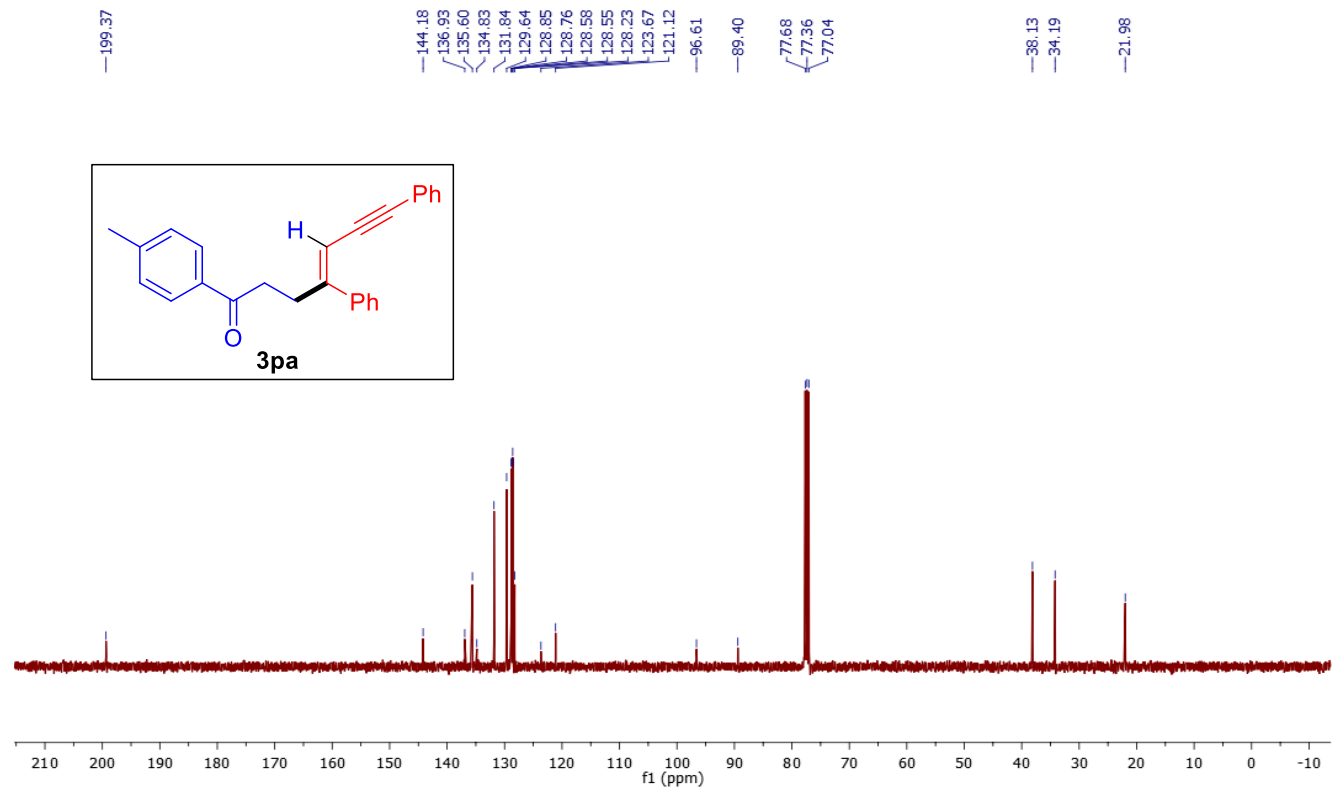
^{13}C NMR of 3oa (100 MHz, $CDCl_3$)



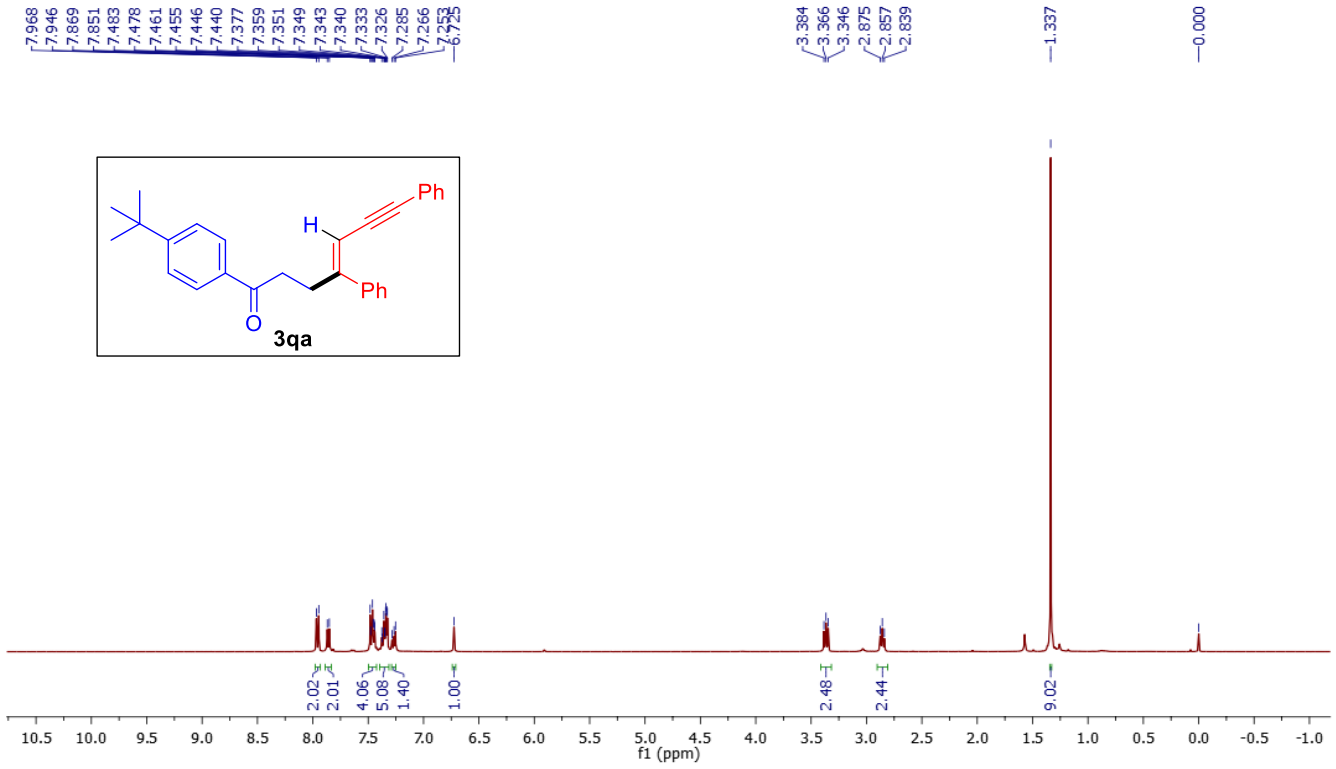
^{1}H NMR of 3pa (400 MHz, $CDCl_3$)



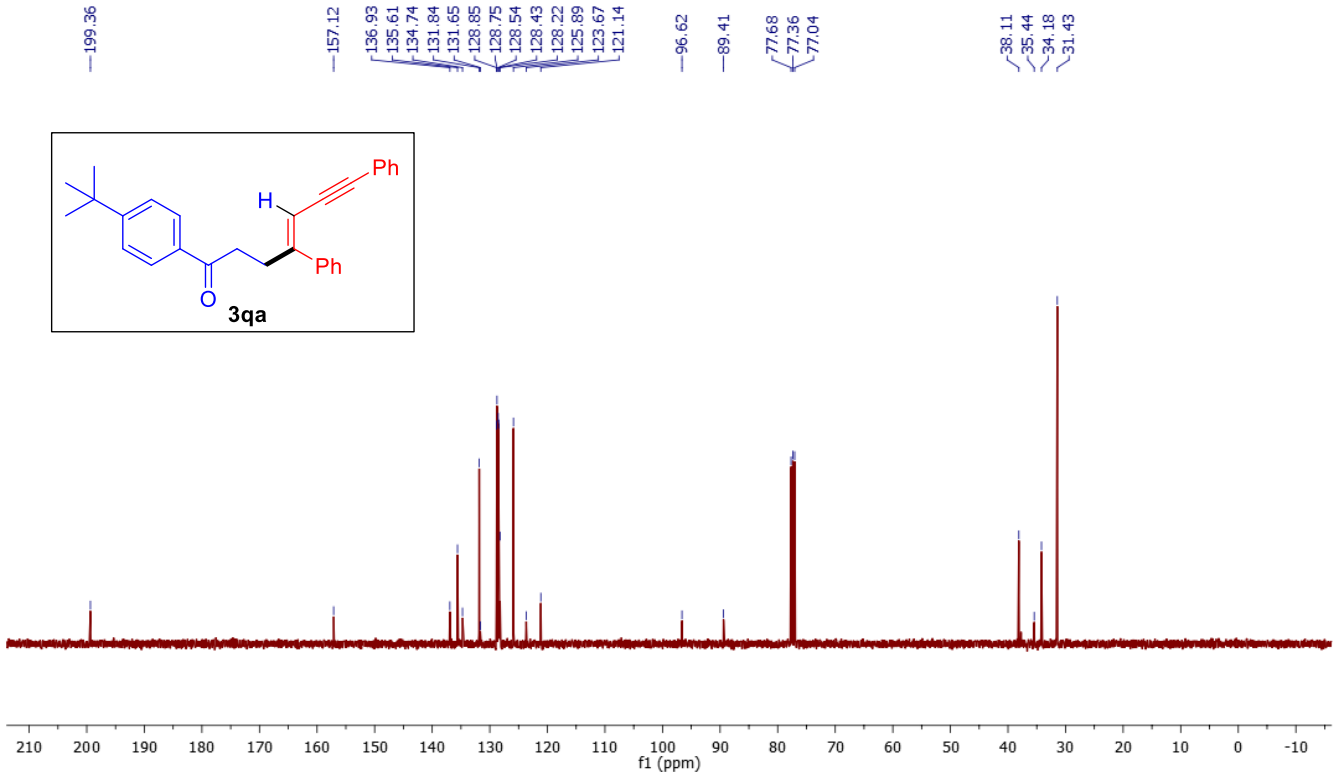
^{13}C NMR of 3pa (100 MHz, $CDCl_3$)



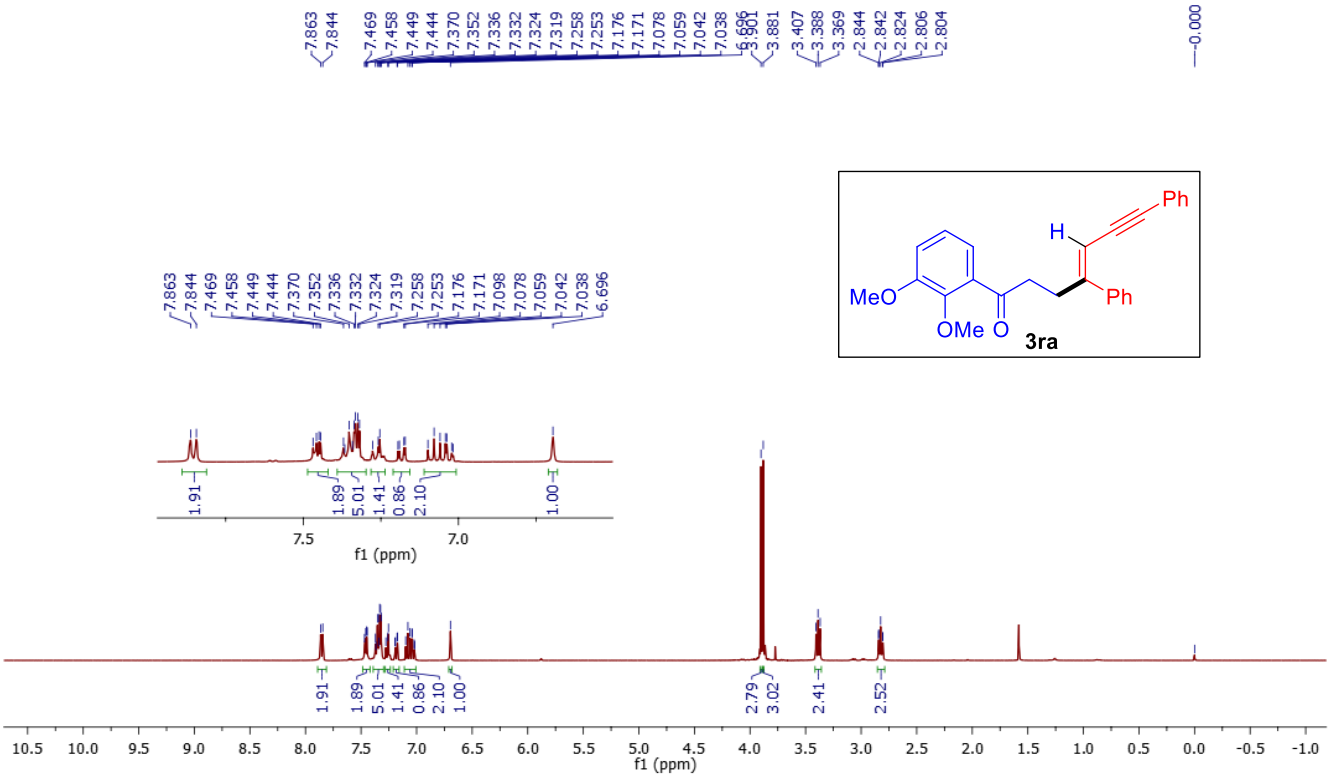
^{1}H NMR of 3qa (400 MHz, $CDCl_3$)



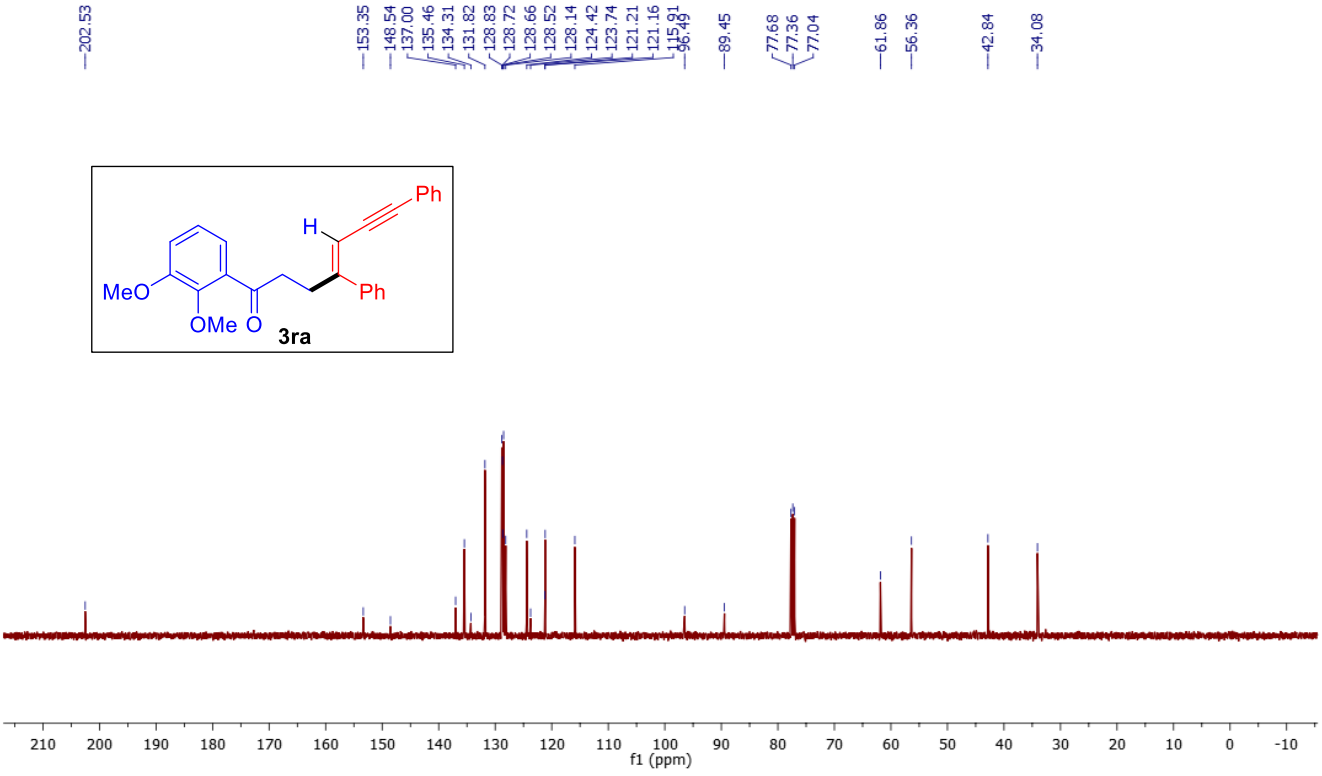
^{13}C NMR of 3qa (100 MHz, $CDCl_3$)

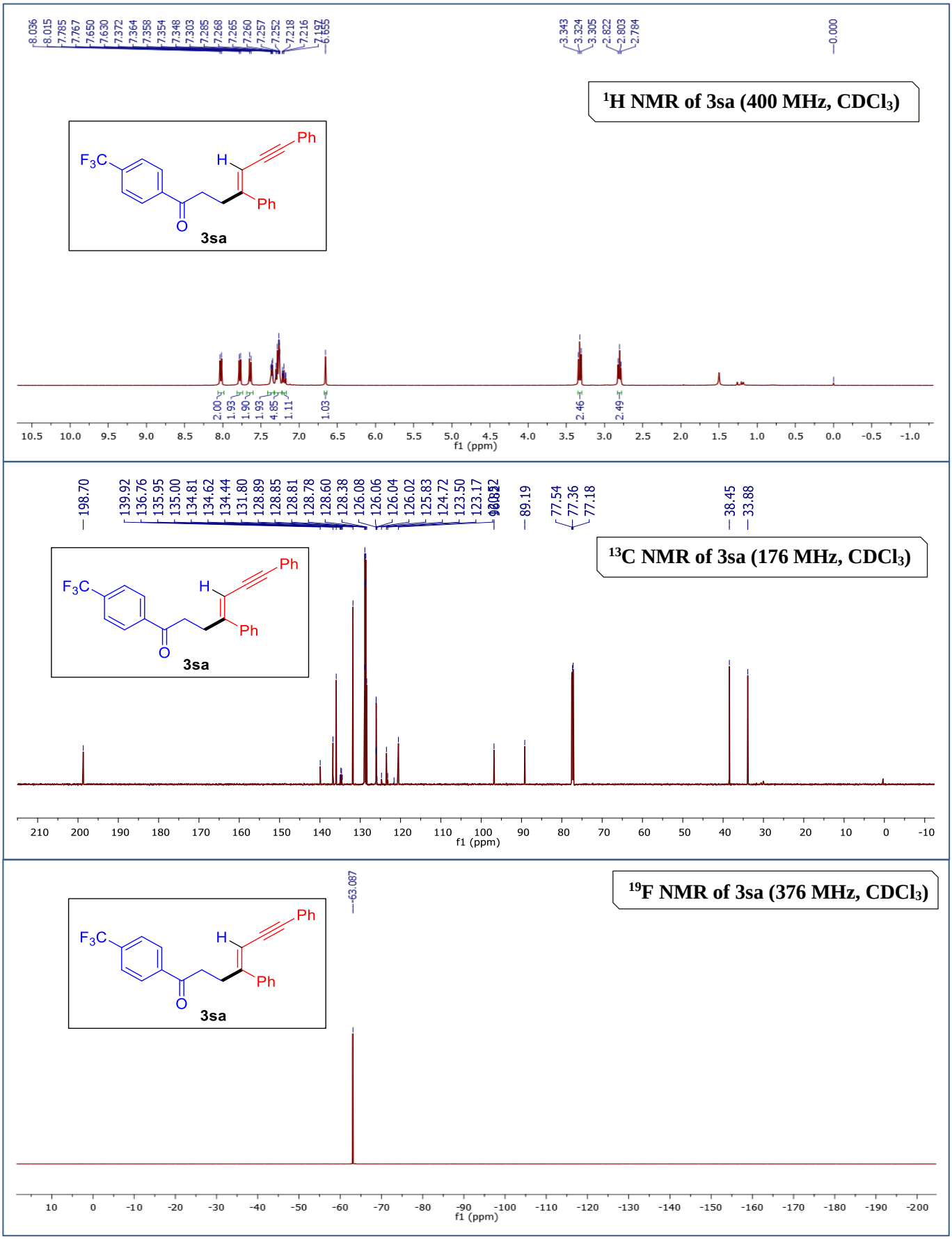


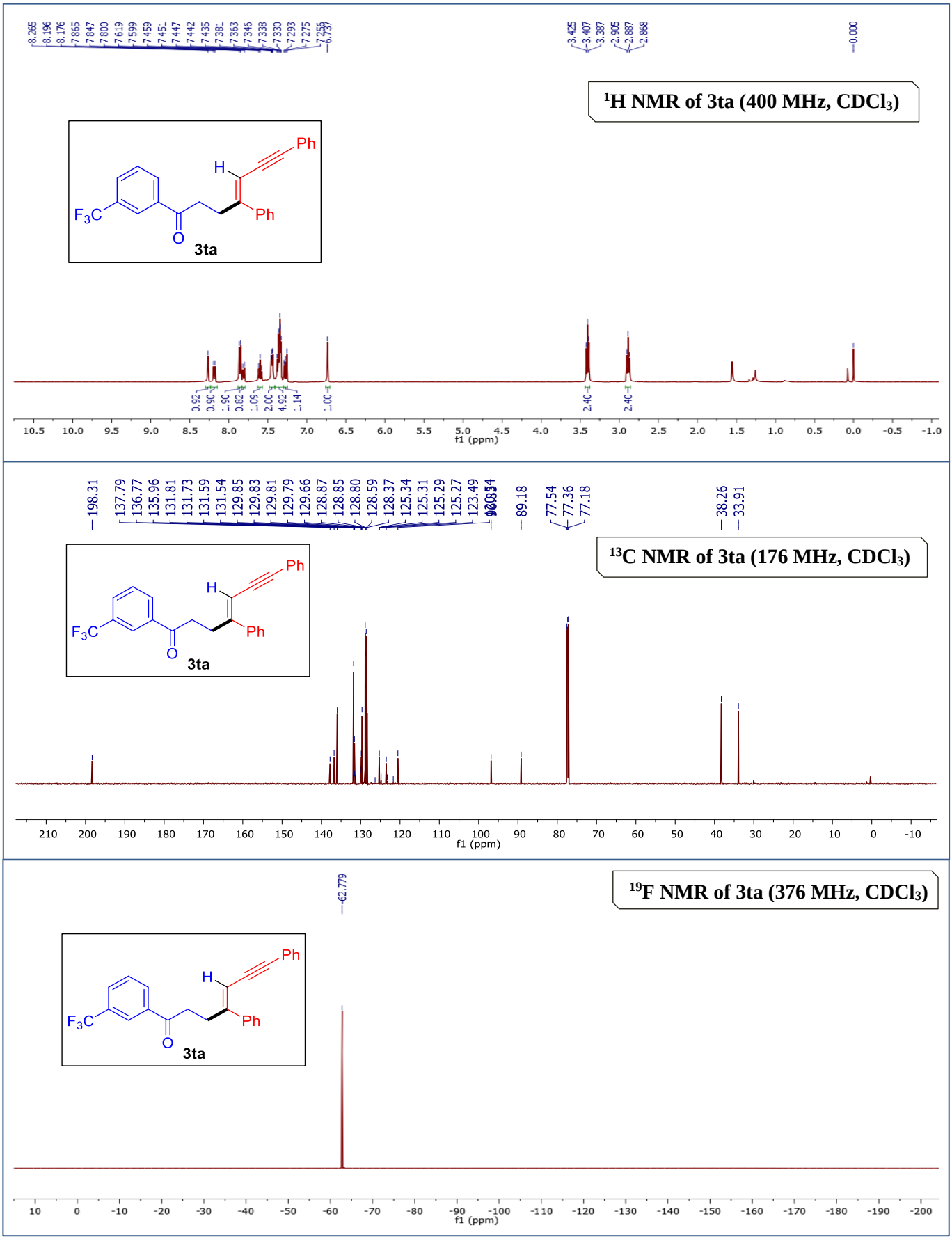
^{1}H NMR of 3ra (400 MHz, $CDCl_3$)



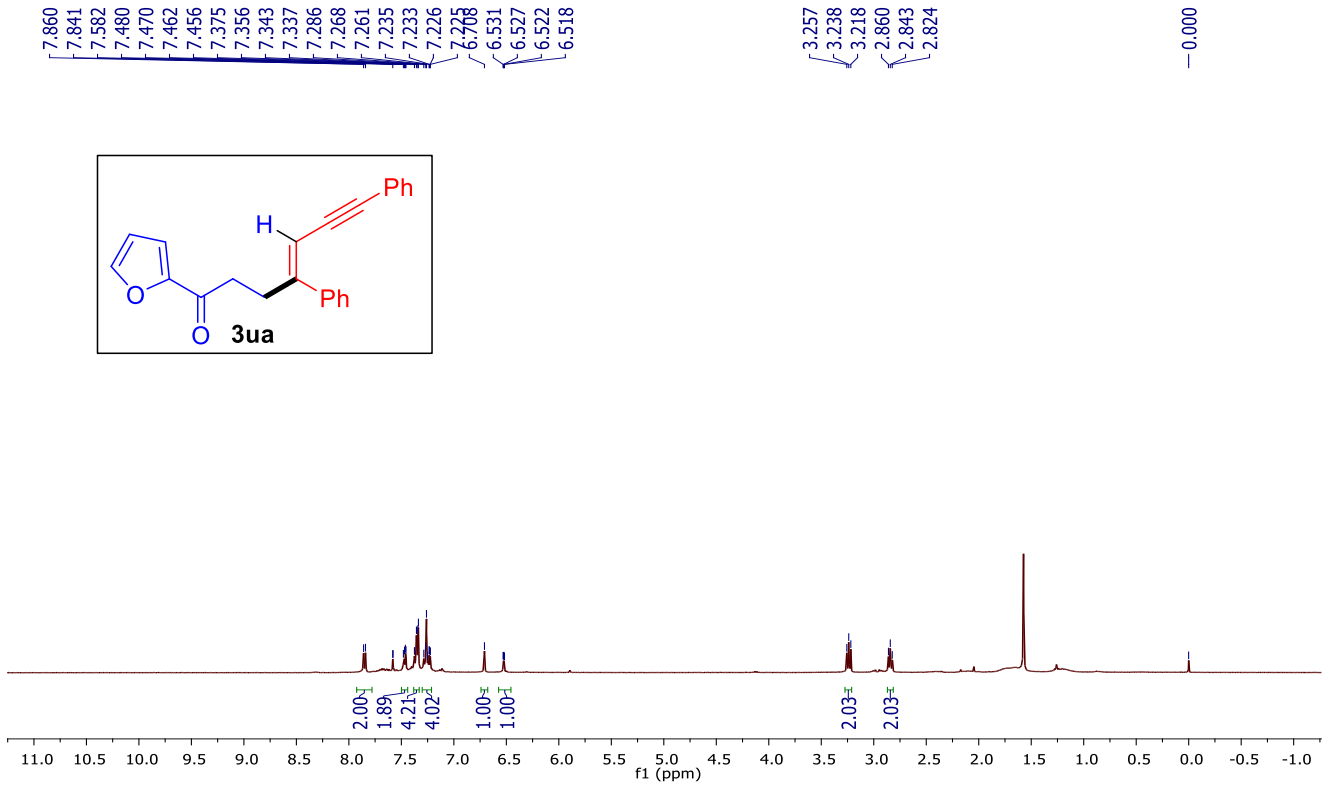
^{13}C NMR of 3ra (100 MHz, $CDCl_3$)



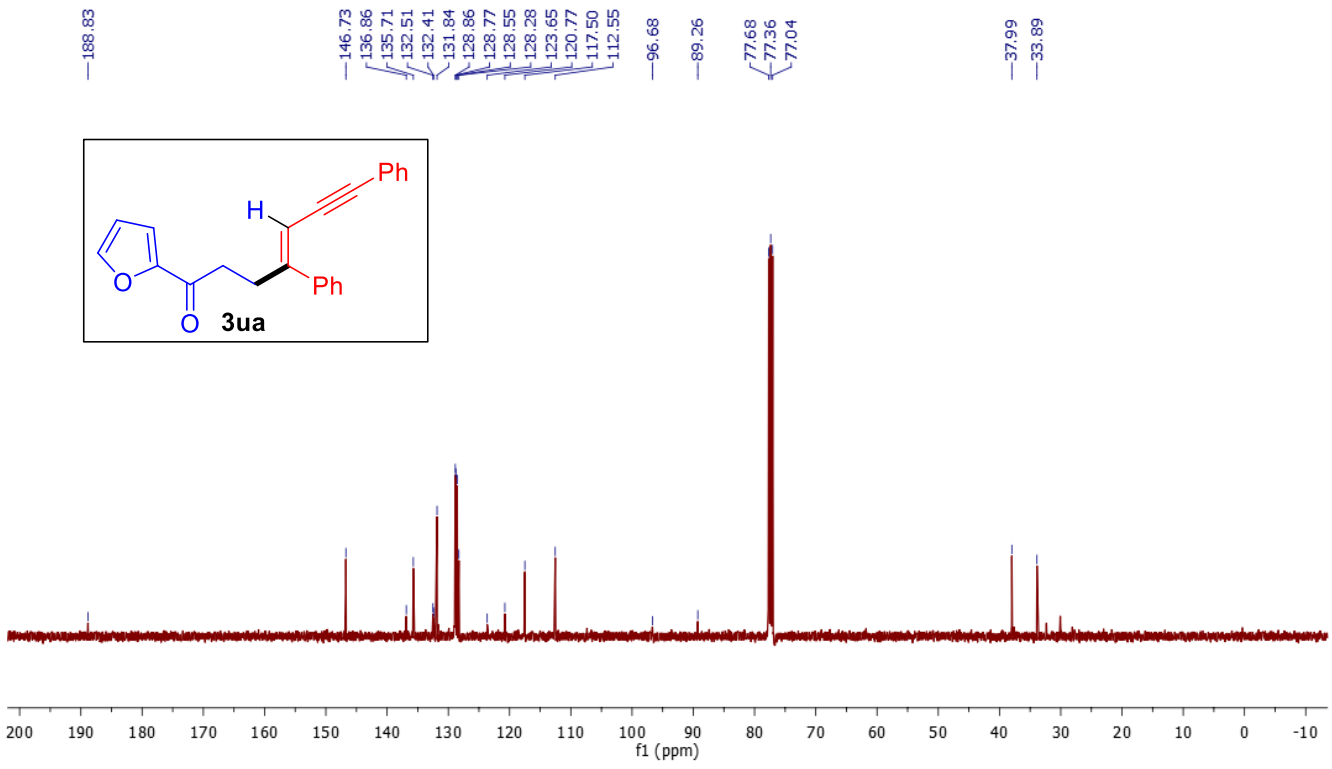

8.036
8.015
7.785
7.767
7.650
7.630
7.372
7.364
7.358
7.354
7.348
7.303
7.285
7.268
7.265
7.260
7.257
7.252
7.218
7.216
7.197
6.655
3.343
3.324
3.305
2.822
2.803
2.784
0.000
1H NMR of 3sa (400 MHz, CDCl3)
F3C
Ph
H
Ph
O
3sa
2.00
1.93
1.90
1.93
4.85
1.11
1.03
2.46
2.49
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
198.70
139.92
136.76
135.95
135.00
134.81
134.62
134.44
131.80
128.89
128.85
128.81
128.78
128.60
128.38
126.08
126.06
126.04
126.02
125.83
124.72
123.50
123.17
89.19
77.54
77.36
77.18
38.45
33.88
13C NMR of 3sa (176 MHz, CDCl3)
F3C
Ph
H
Ph
O
3sa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
-63.087
19F NMR of 3sa (376 MHz, CDCl3)
F3C
Ph
H
Ph
O
3sa
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)


^{1}H NMR of 3ta (400 MHz, CDCl$_3$)
^{13}C NMR of 3ta (176 MHz, CDCl$_3$)
^{19}F NMR of 3ta (376 MHz, CDCl$_3$)
3ta
f1 (ppm)

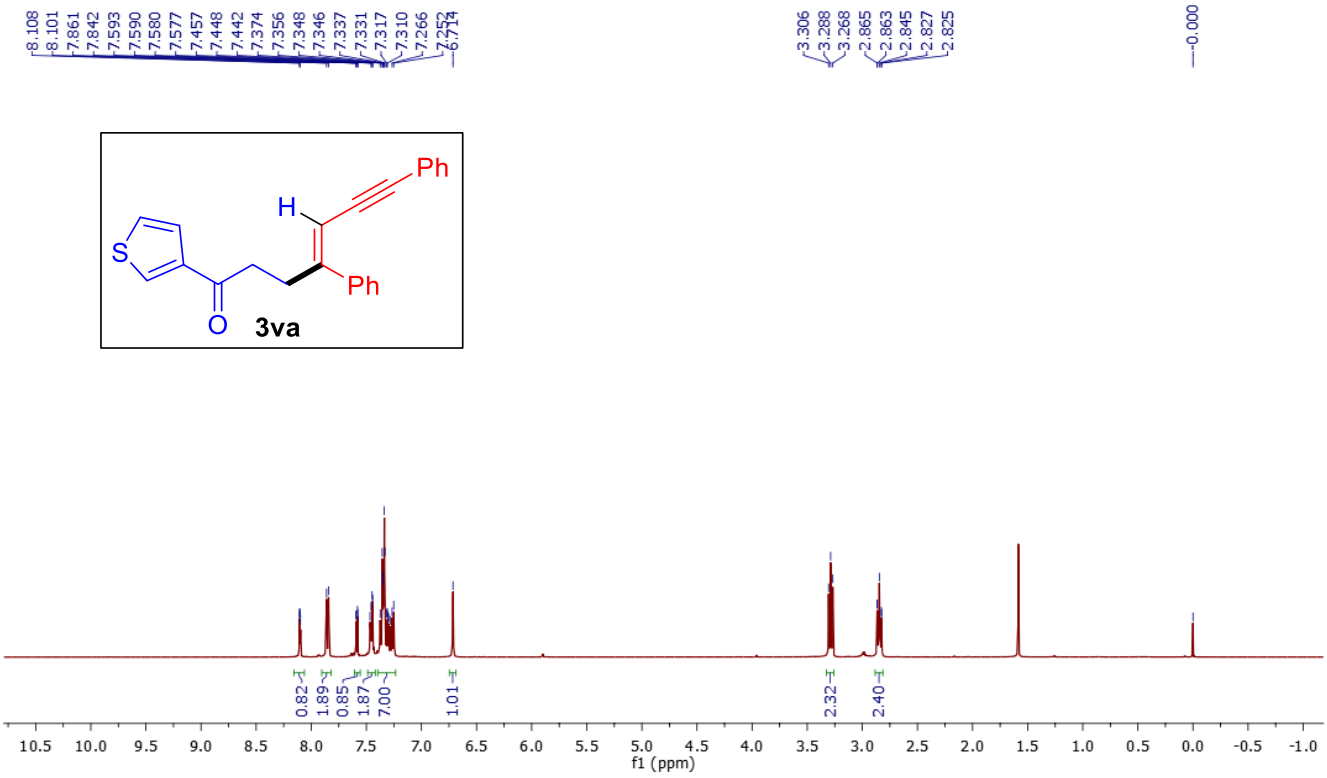
^{1}H NMR of 3ua (400 MHz, $CDCl_3$)



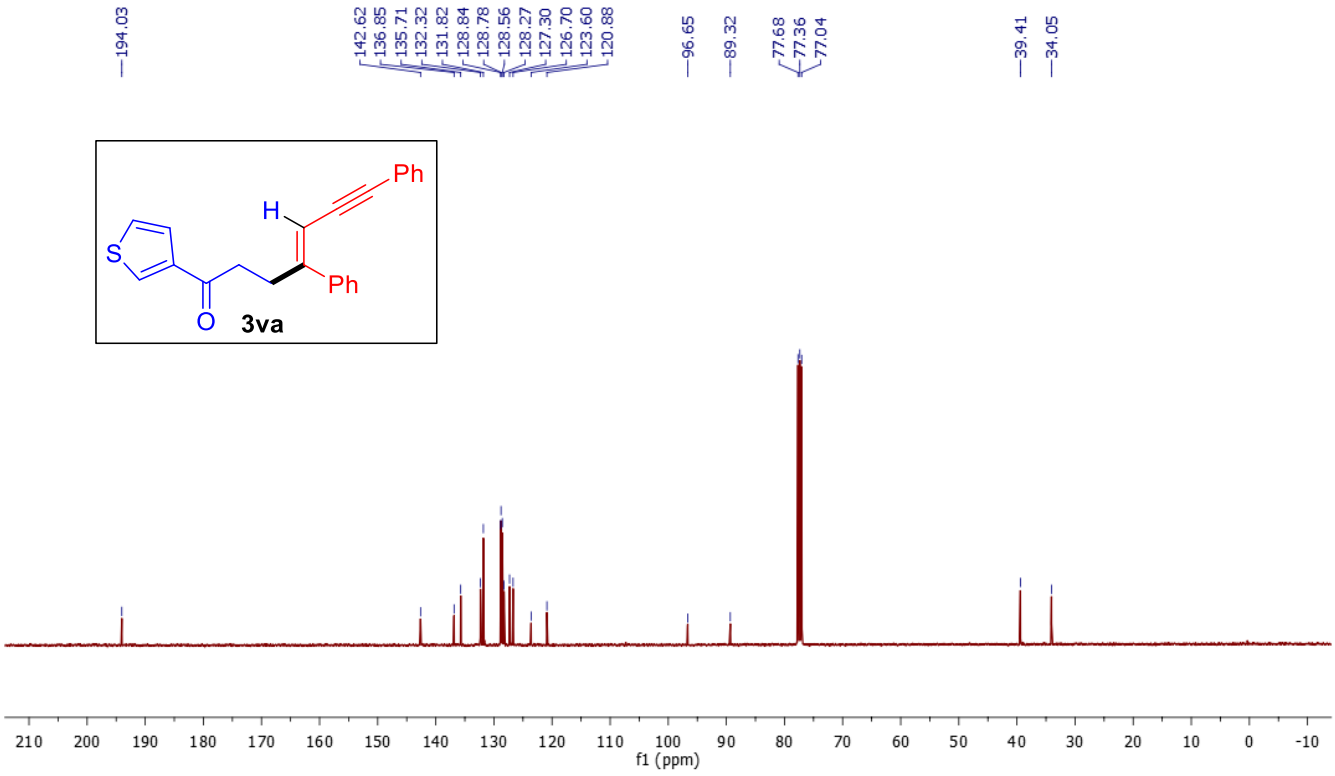
^{13}C NMR of 3ua (100 MHz, $CDCl_3$)



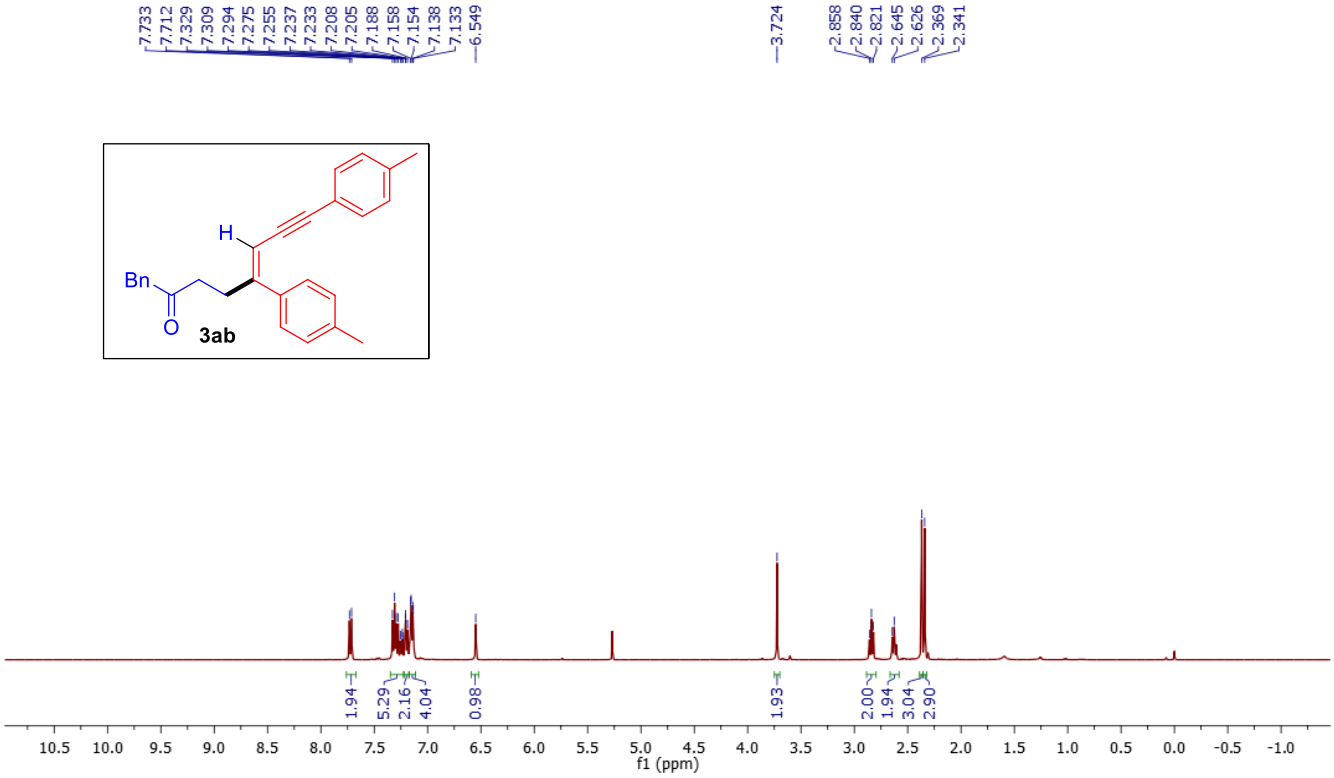
^{1}H NMR of 3va (400 MHz, $CDCl_3$)



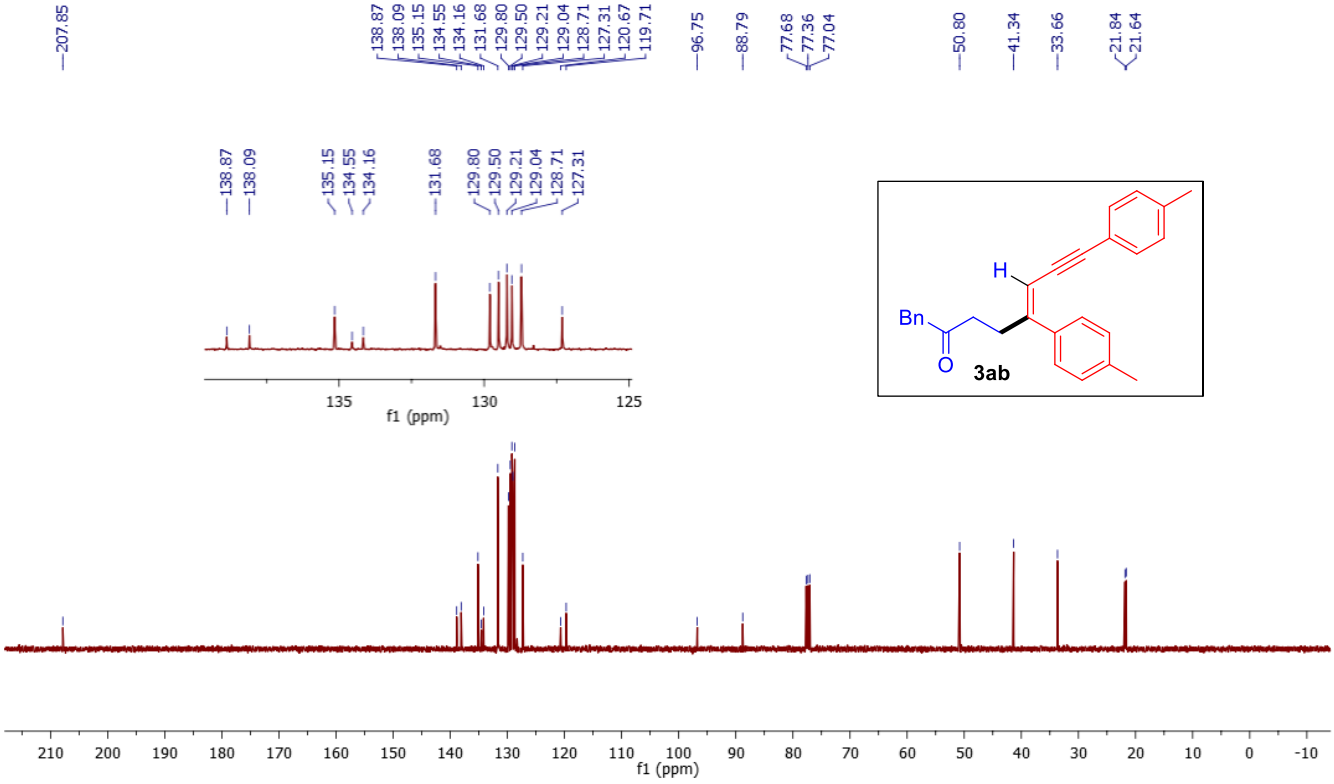
^{13}C NMR of 3va (100 MHz, $CDCl_3$)



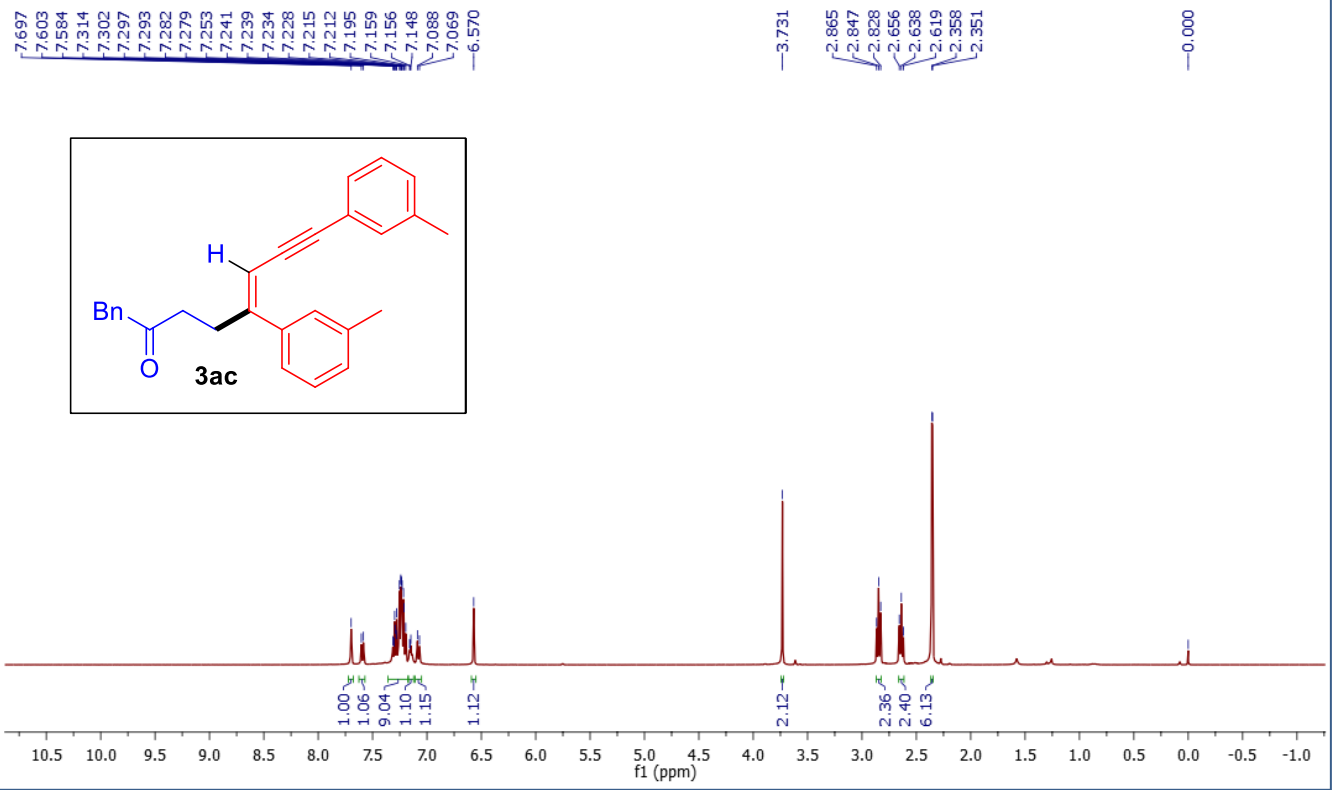
^{1}H NMR of 3ab (400 MHz, $CDCl_3$)



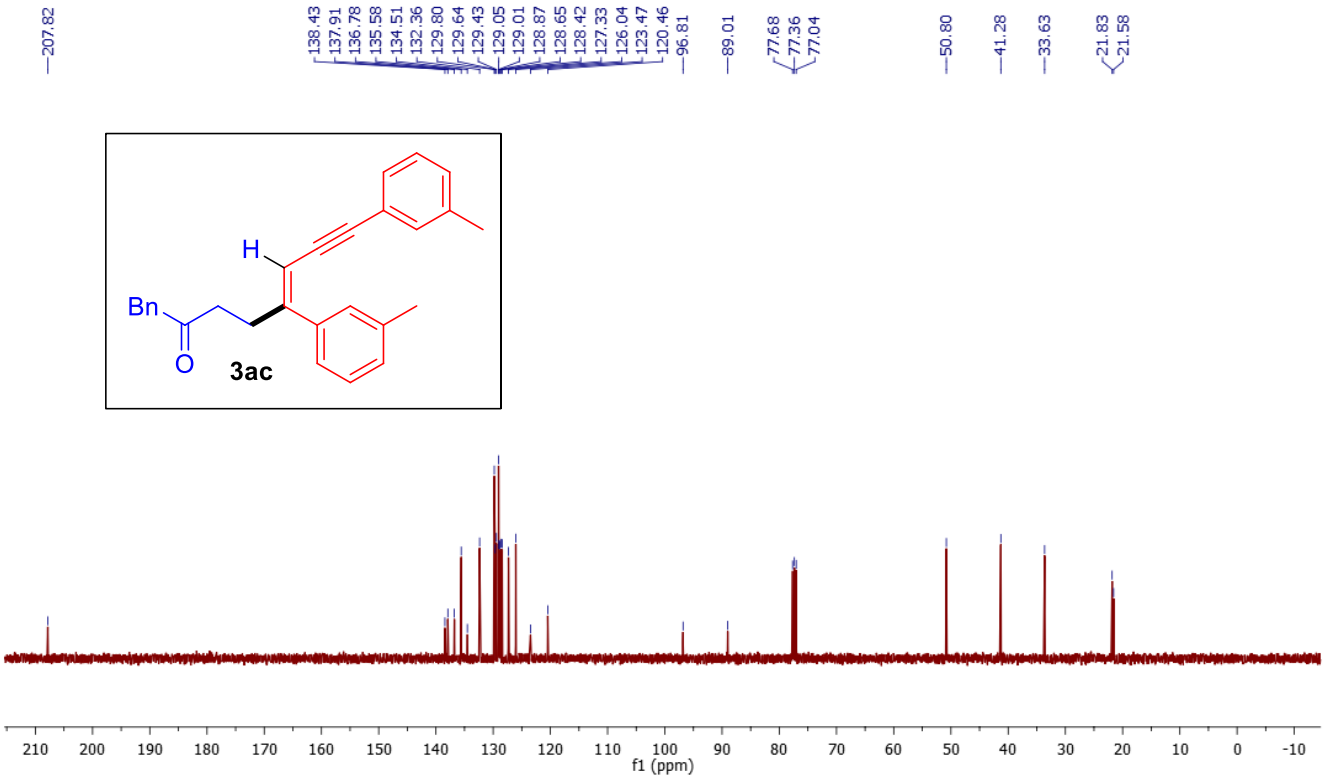
^{13}C NMR of 3ab (100 MHz, $CDCl_3$)



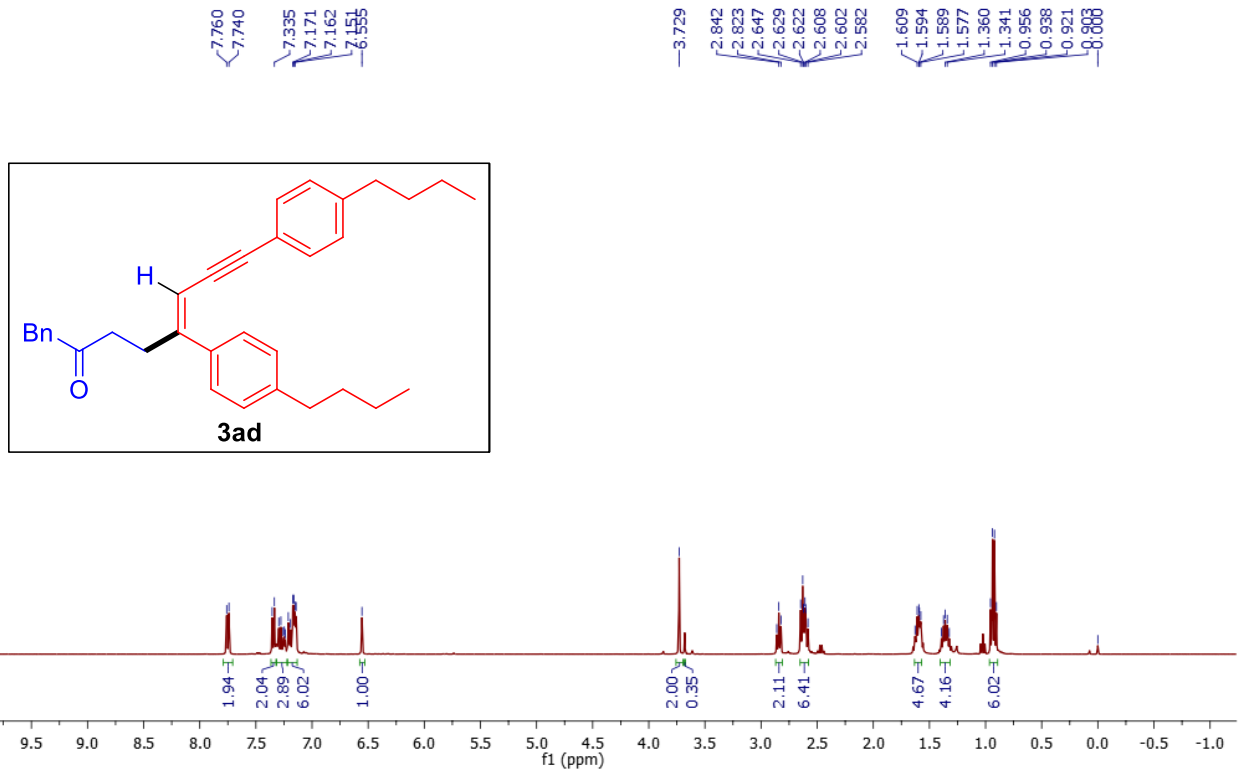
^{1}H NMR of 3ac (400 MHz, $CDCl_3$)



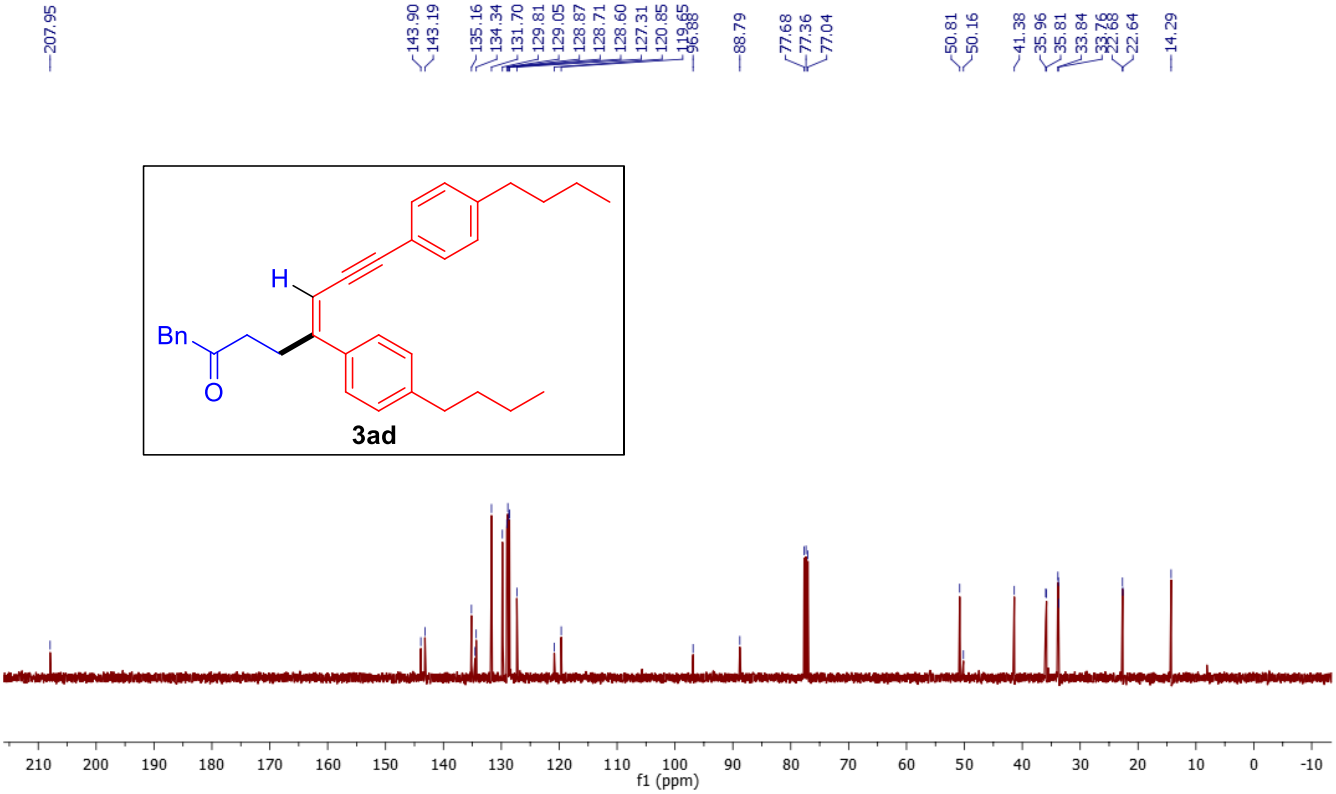
^{13}C NMR of 3ac (100 MHz, $CDCl_3$)



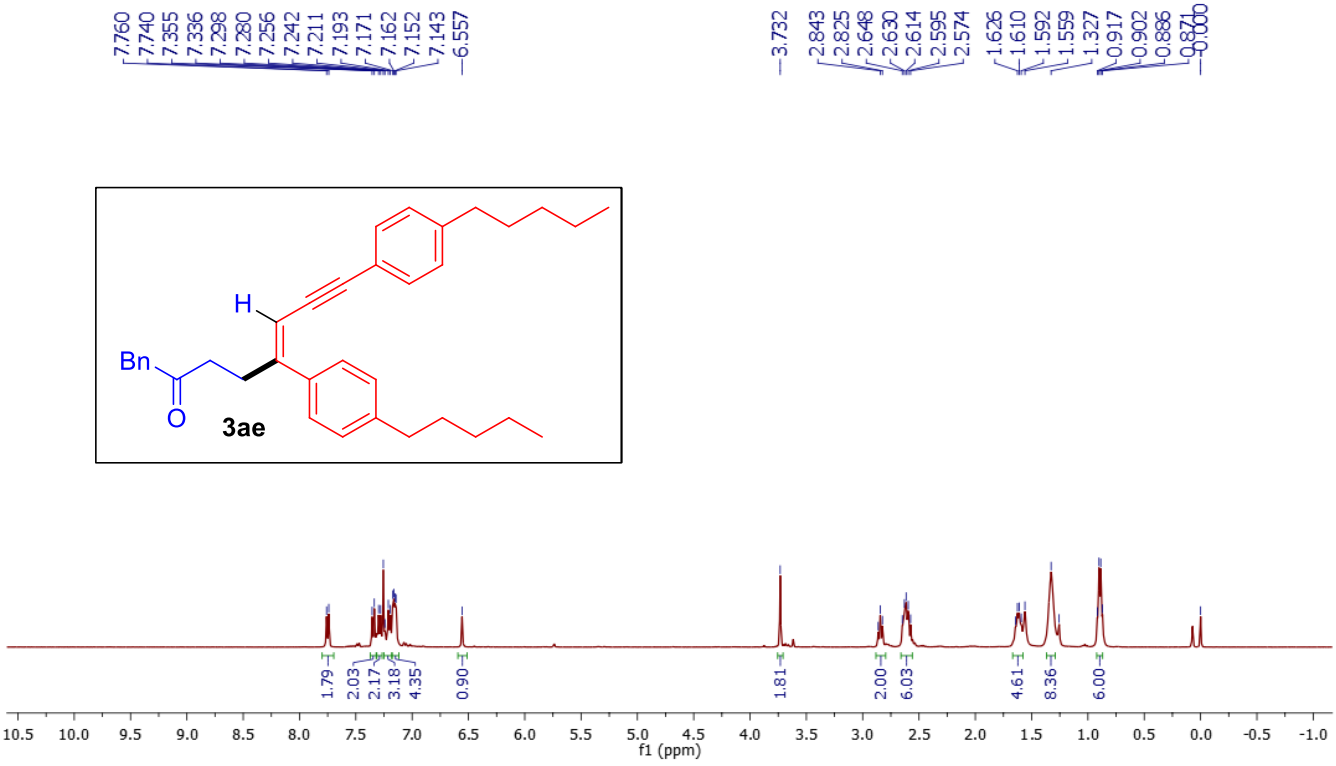
^{1}H NMR of 3ad (400 MHz, $CDCl_3$)



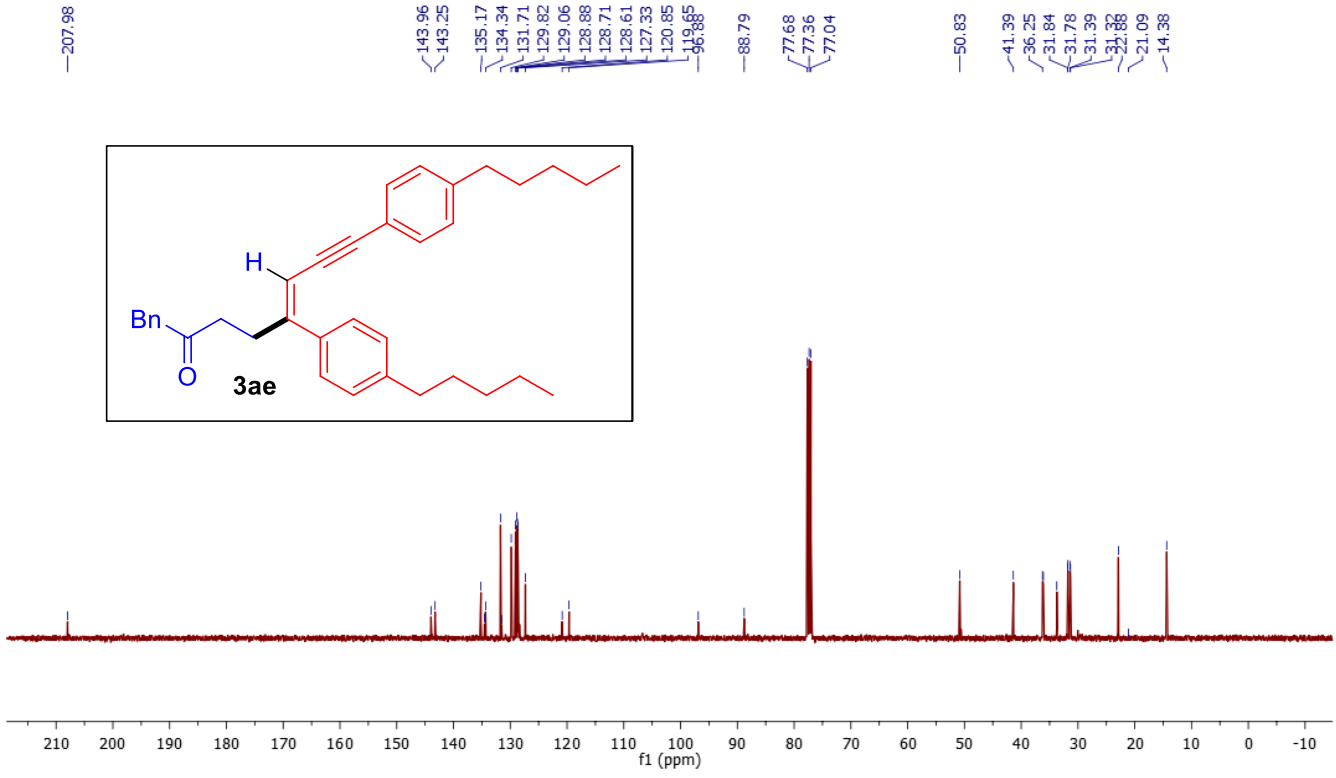
^{13}C NMR of 3ad (100 MHz, $CDCl_3$)



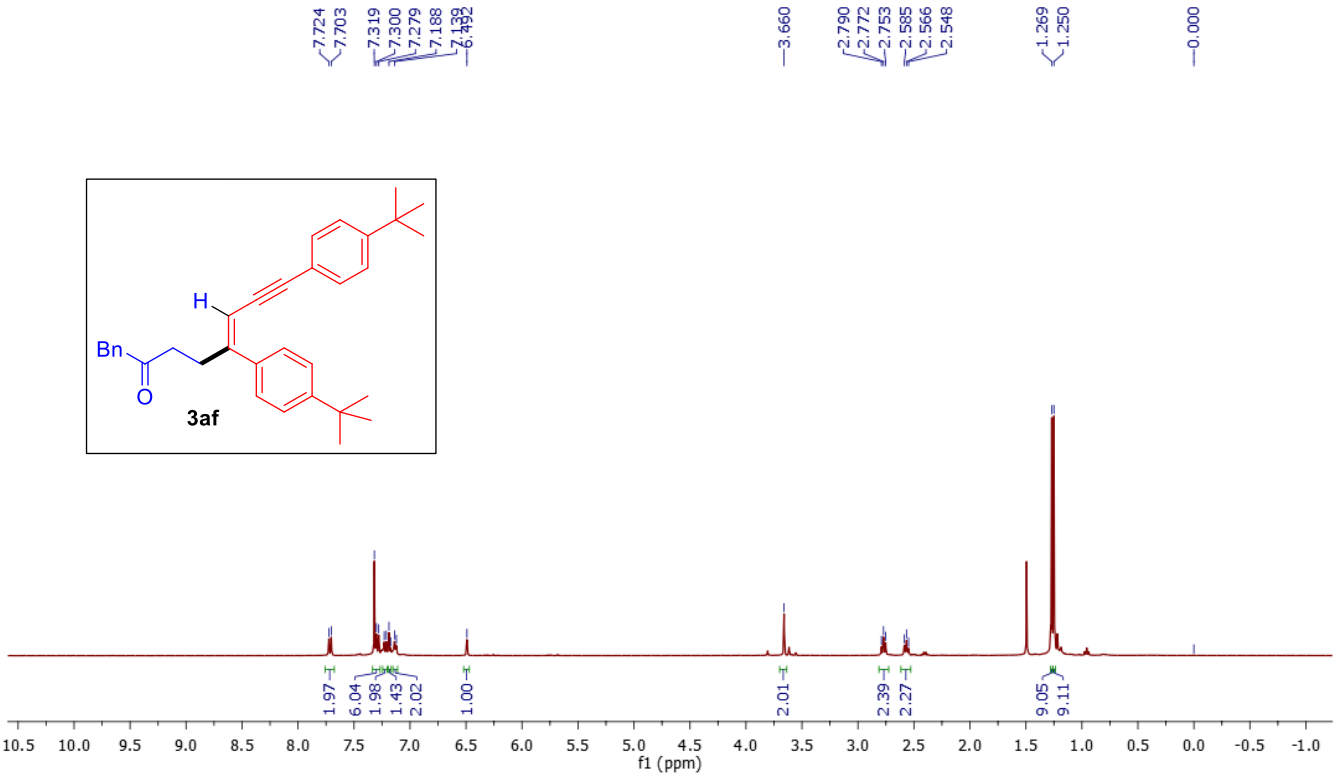
^{1}H NMR of 3ae (400 MHz, $CDCl_3$)



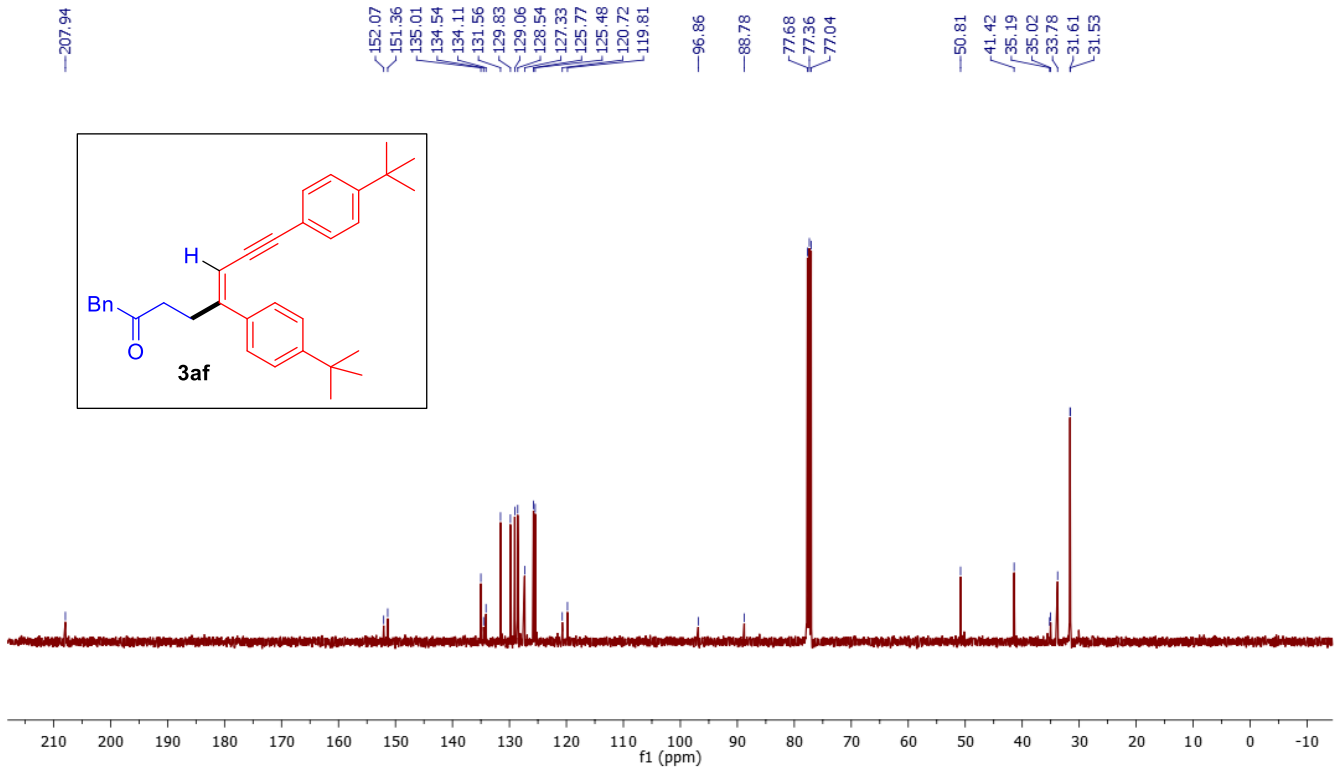
^{13}C NMR of 3ae (100 MHz, $CDCl_3$)



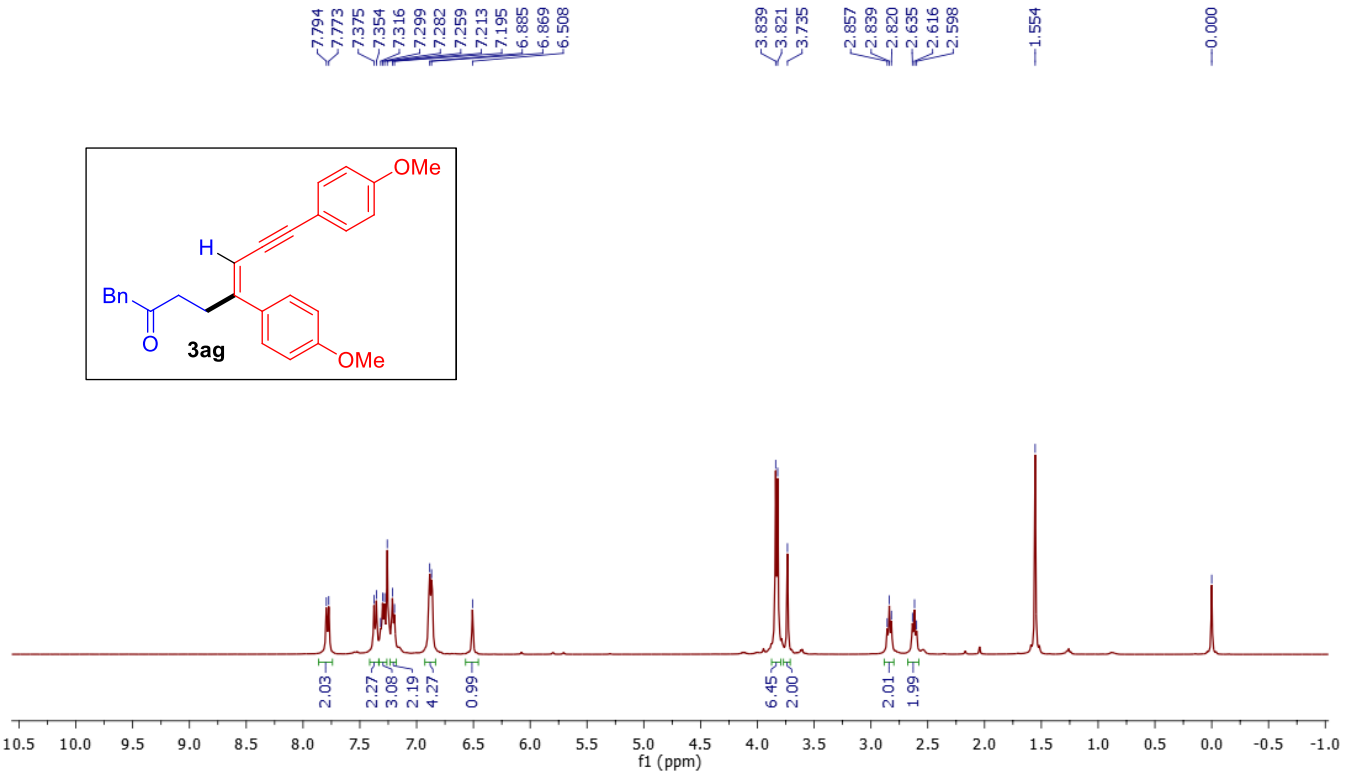
^{1}H NMR of 3af (400 MHz, $CDCl_3$)



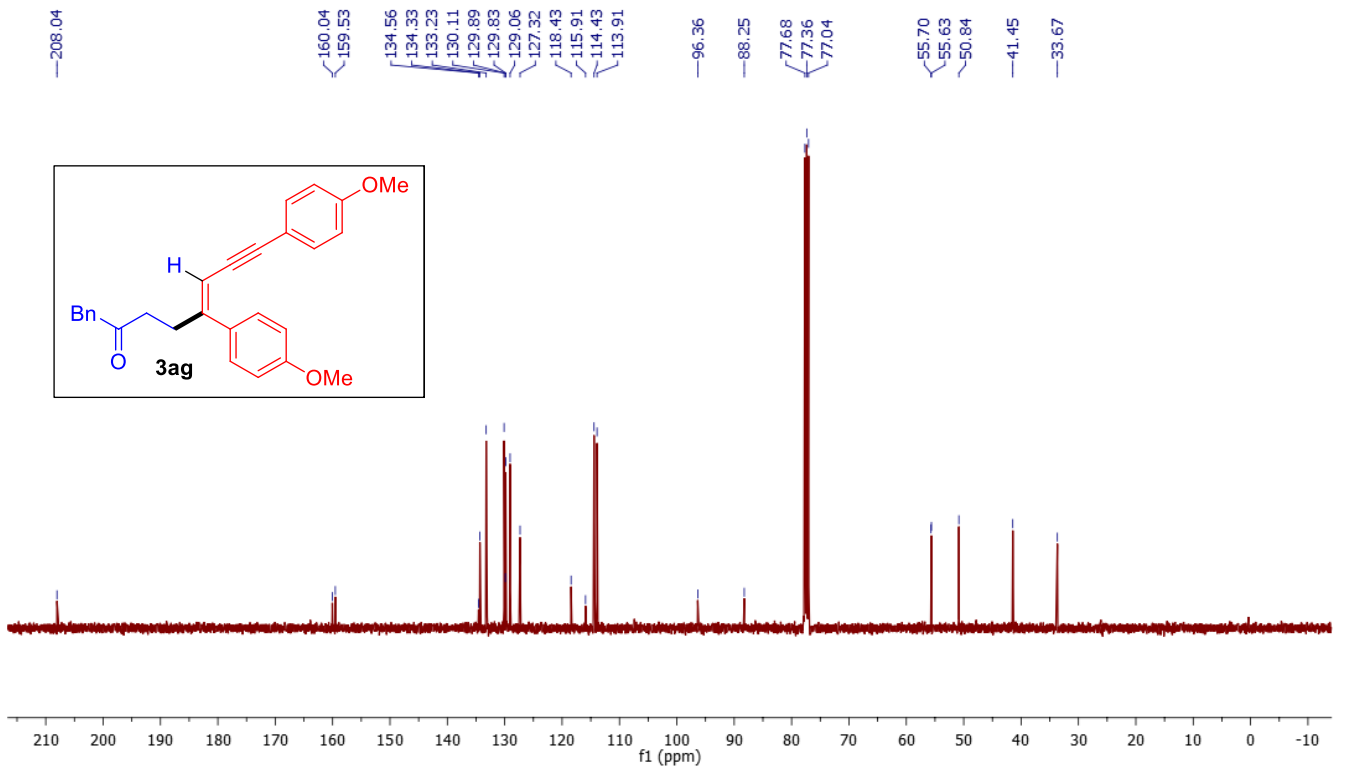
^{13}C NMR of 3af (100 MHz, $CDCl_3$)



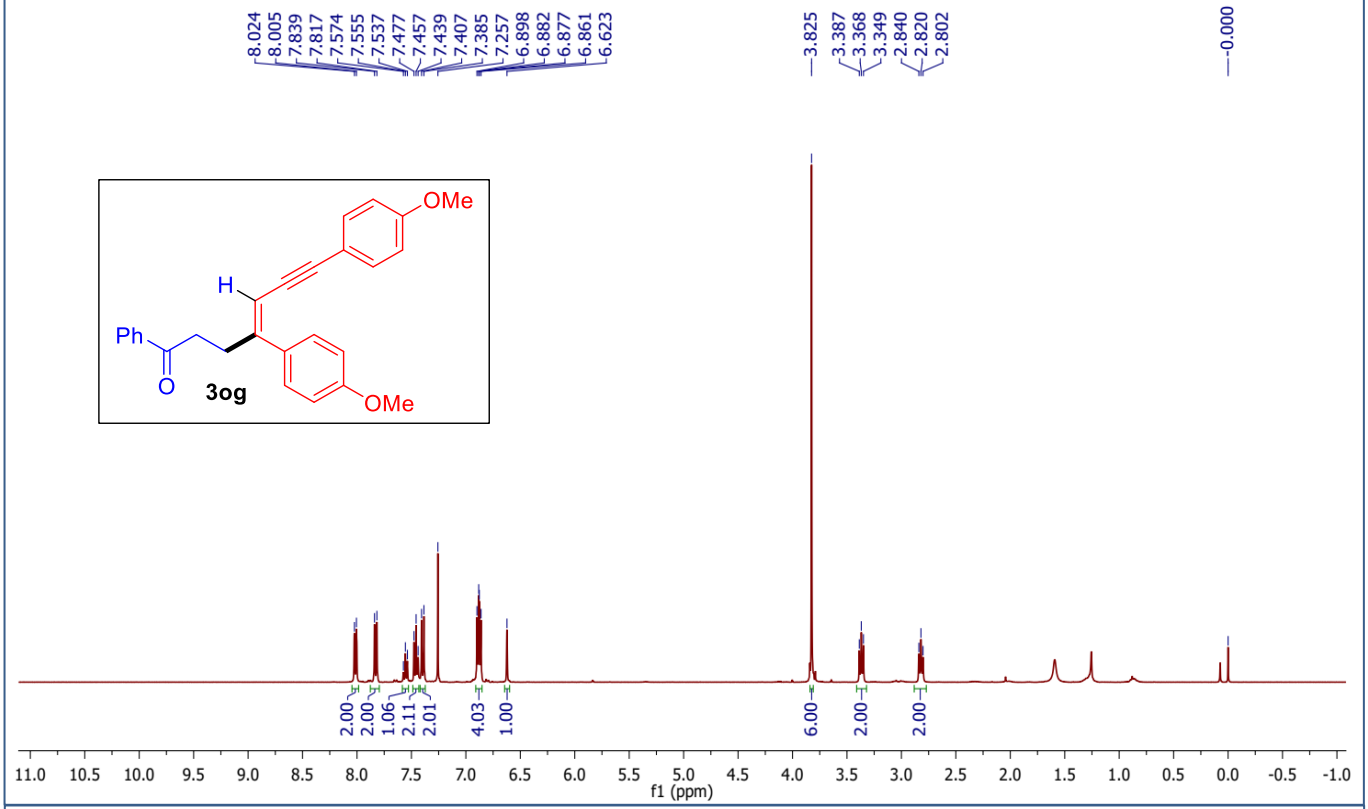
^{1}H NMR of 3ag (400 MHz, $CDCl_3$)



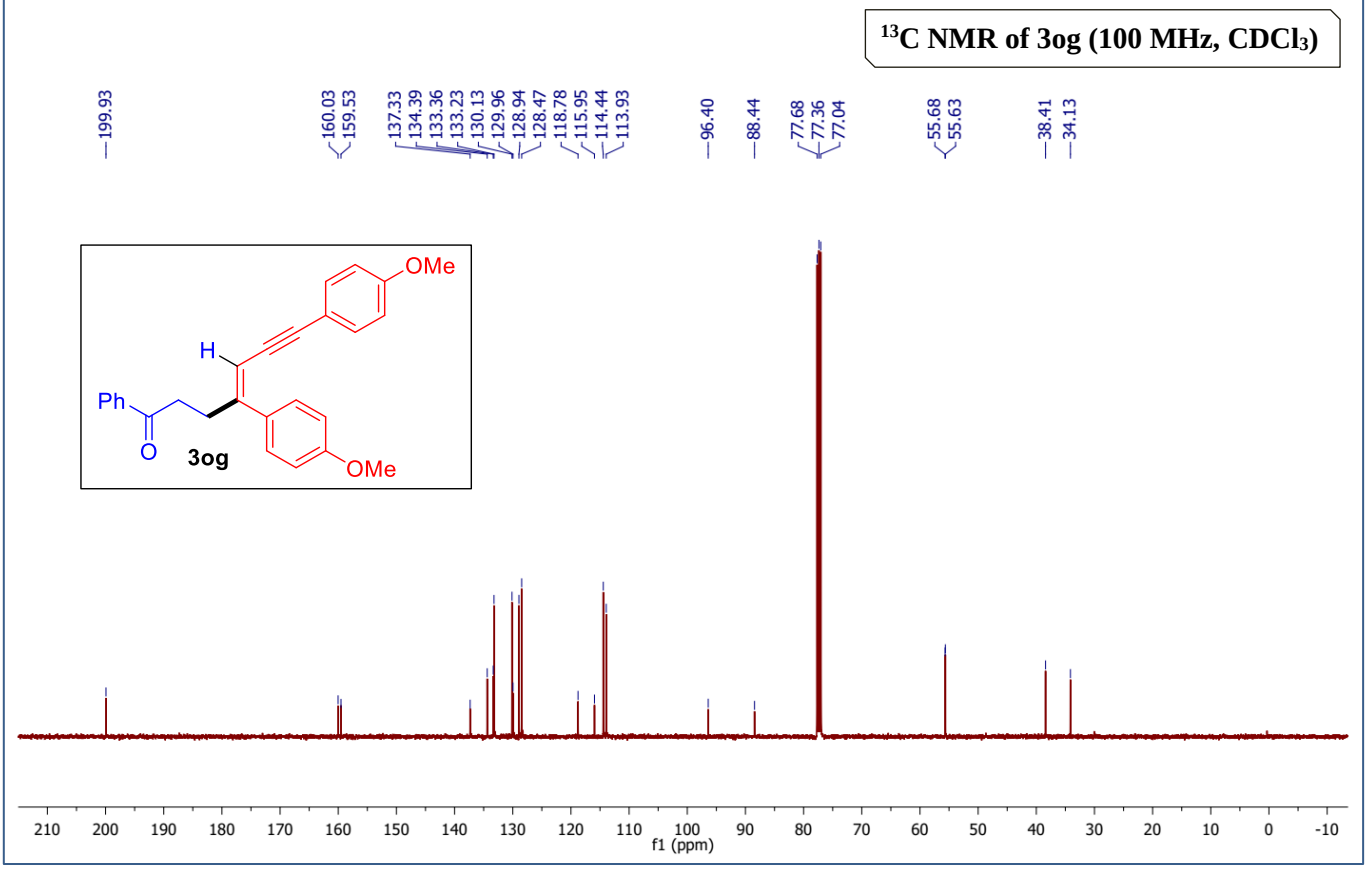
^{13}C NMR of 3ag (100 MHz, $CDCl_3$)



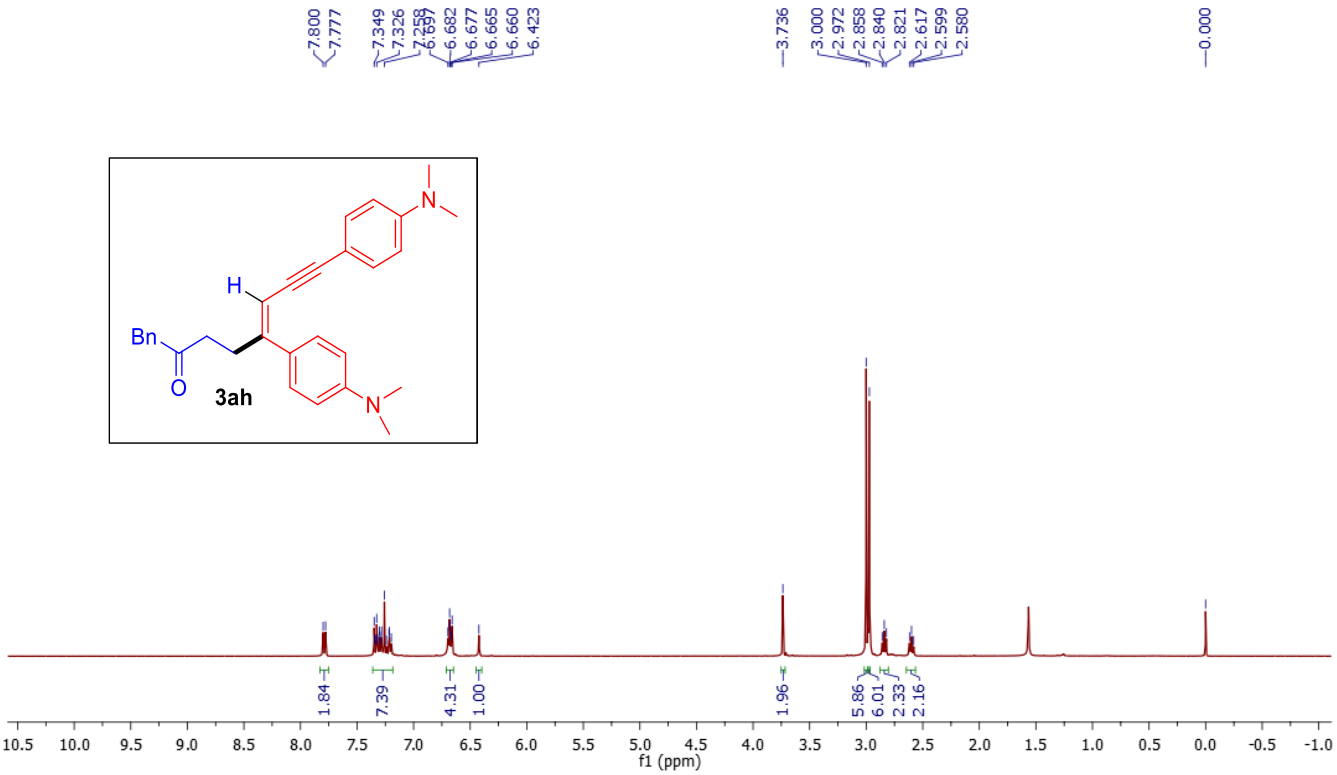
^{1}H NMR of 3og (400 MHz, $CDCl_3$)



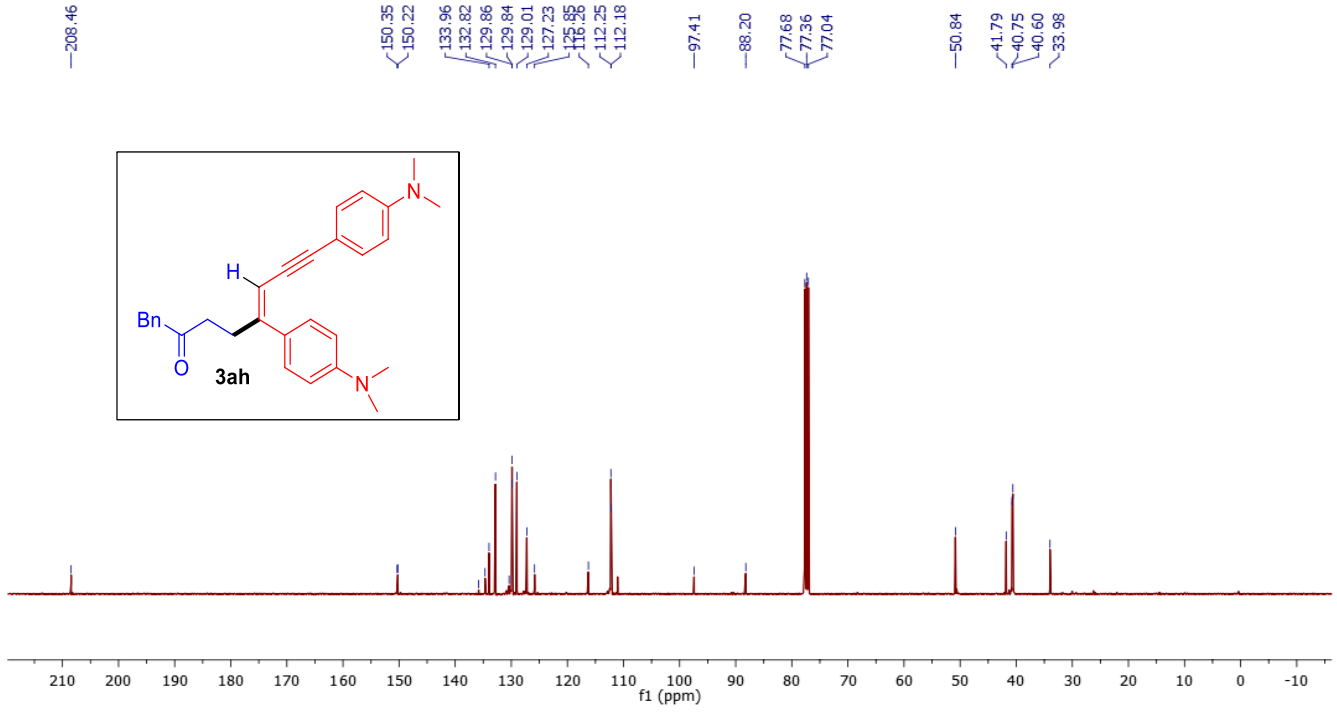
^{13}C NMR of 3og (100 MHz, $CDCl_3$)



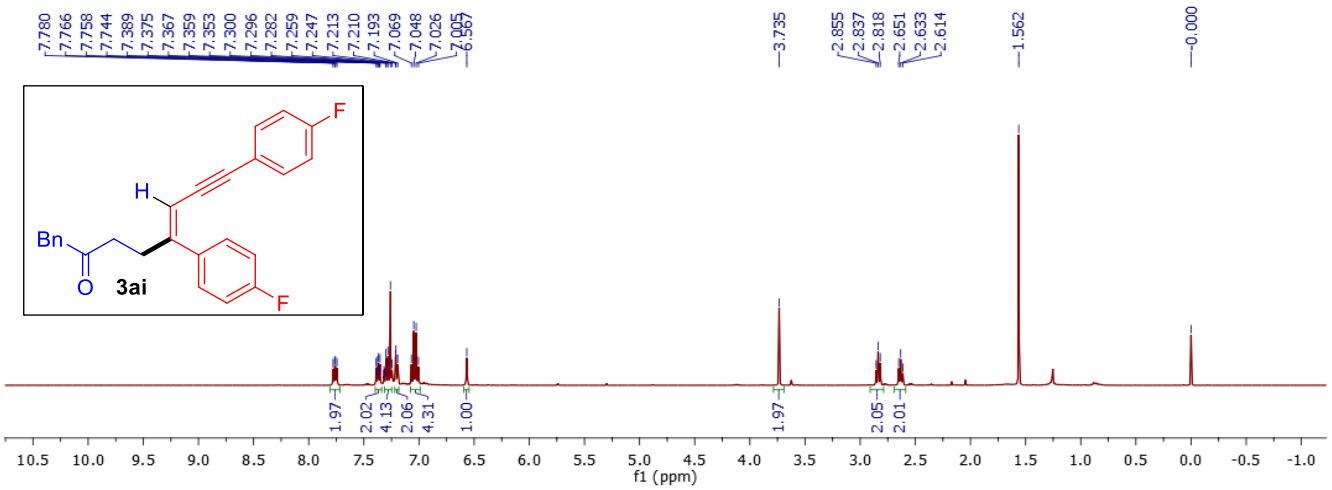
^{1}H NMR of 3ah (400 MHz, $CDCl_3$)



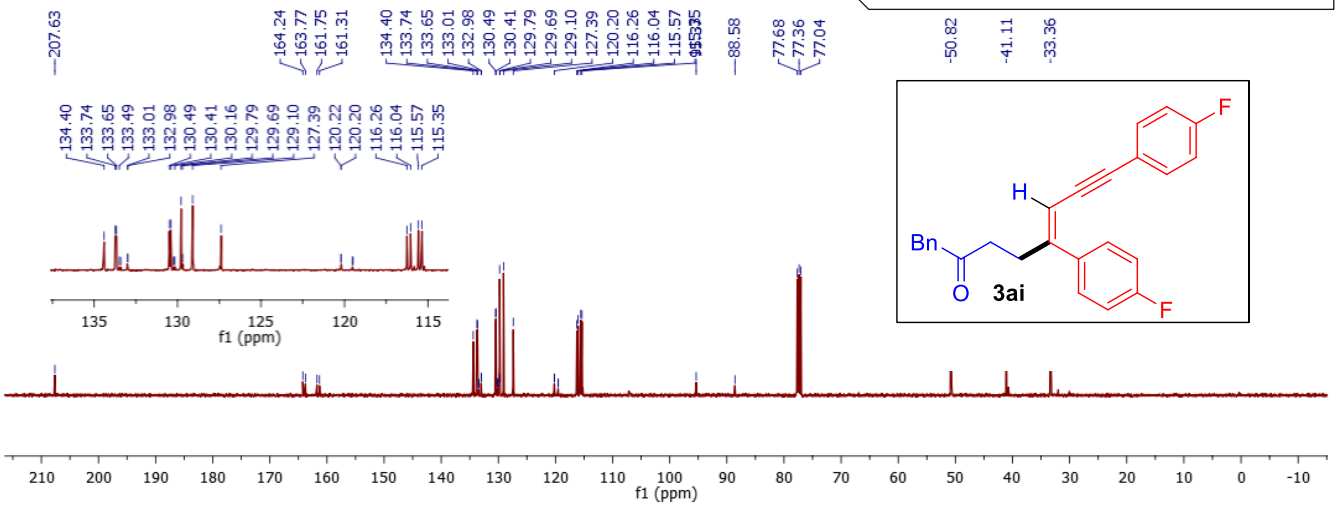
^{13}C NMR of 3ah (100 MHz, $CDCl_3$)



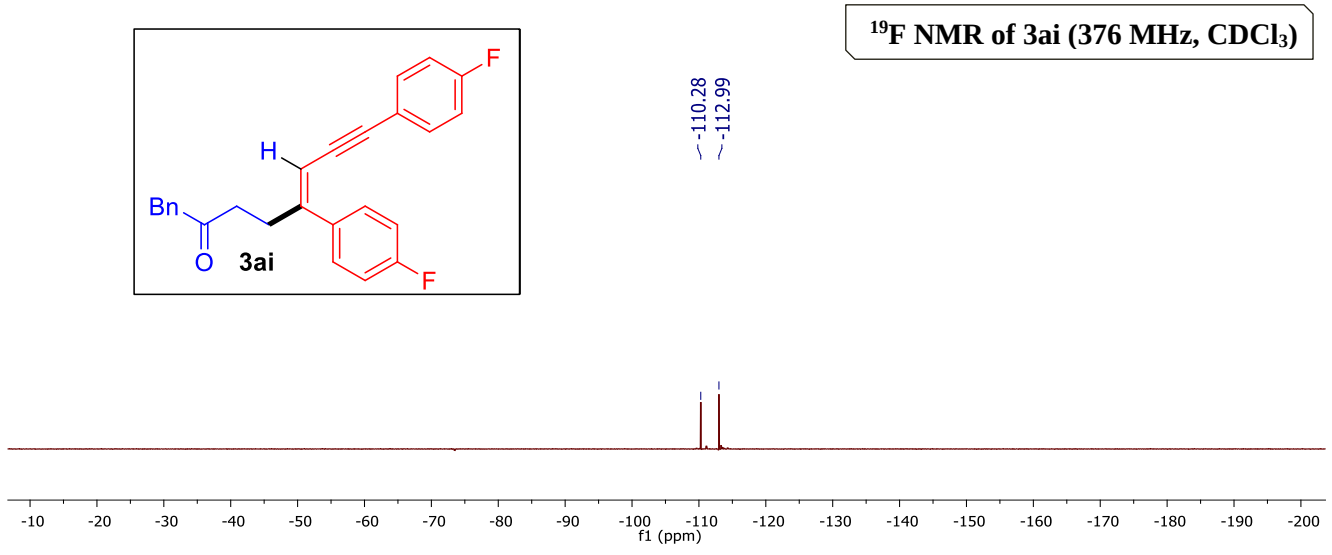
^{1}H NMR of 3ai (400 MHz, $CDCl_3$)

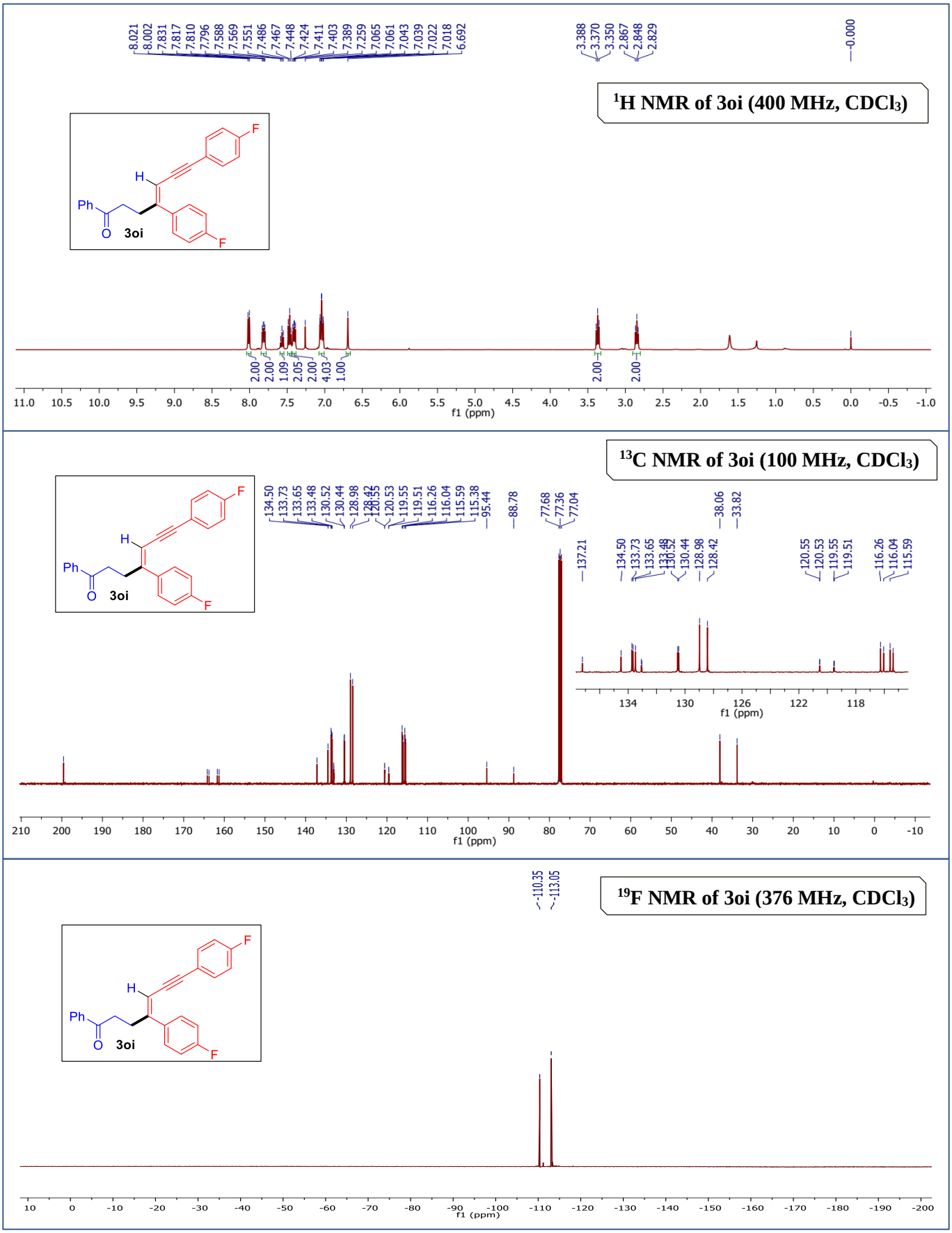


^{13}C NMR of 3ai (100 MHz, $CDCl_3$)

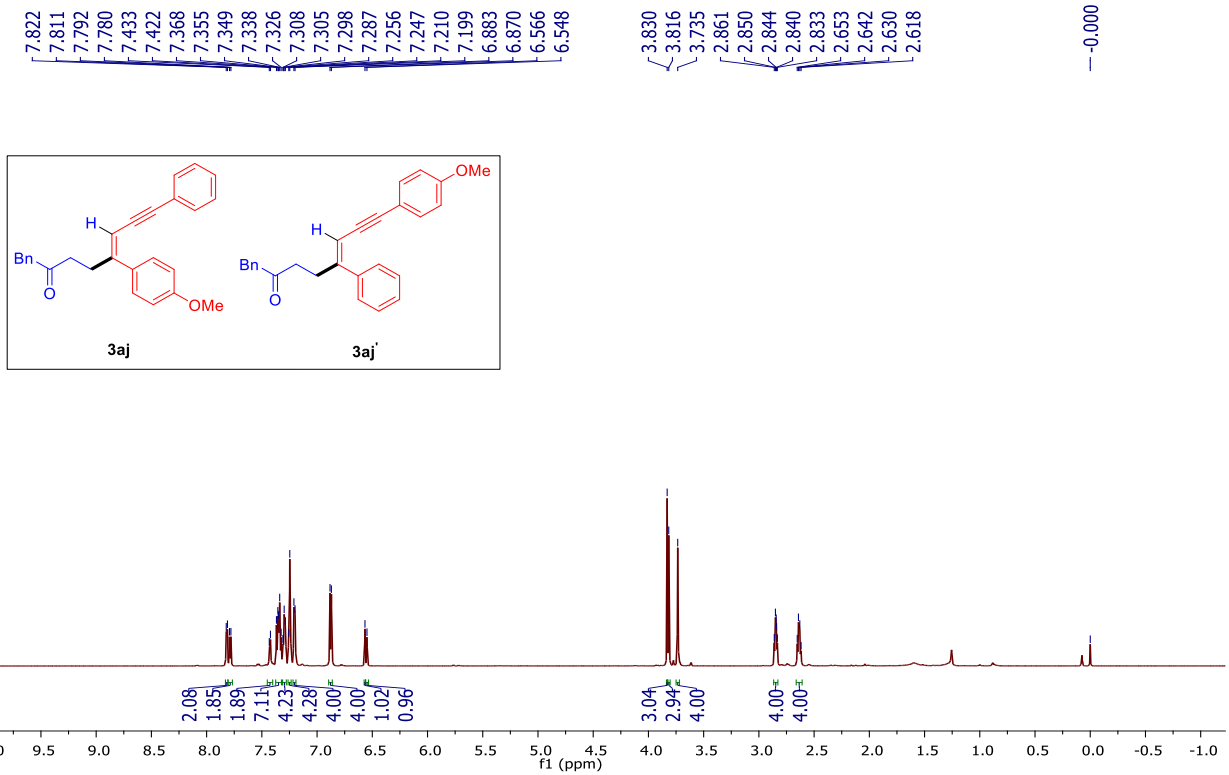


^{19}F NMR of 3ai (376 MHz, $CDCl_3$)

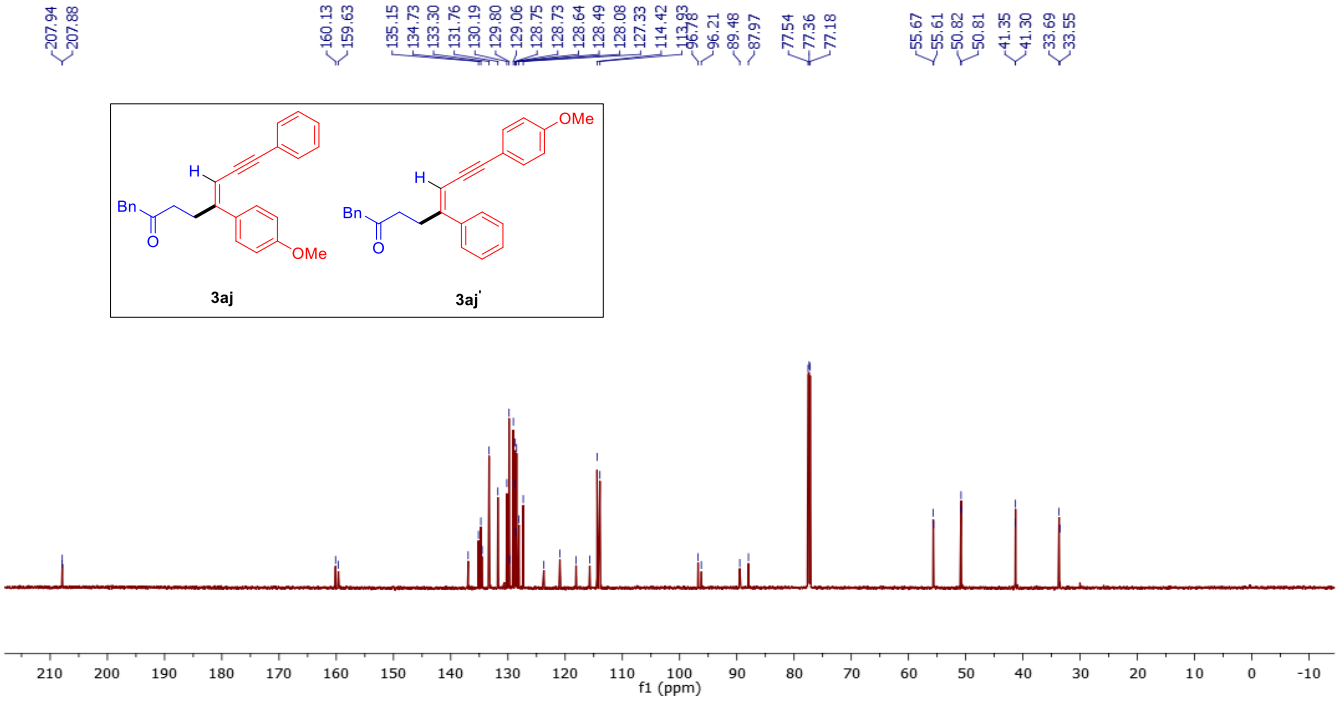



^{1}H NMR of 3oi (400 MHz, CDCl$_3$)
^{13}C NMR of 3oi (100 MHz, CDCl$_3$)
^{19}F NMR of 3oi (376 MHz, CDCl$_3$)
3oi
f1 (ppm)

^{1}H NMR of (3aj + 3aj') (400 MHz, $CDCl_3$)



^{13}C NMR of (3aj + 3aj') (100 MHz, $CDCl_3$)



7. Computational Studies

7.1. Methodology

The Gibbs free energy profiles were mapped at B3LYP-D3/6-31G(d,p) level of theory.[5-8] LANL2DZ[9] and SDD[10] pseudopotential was used for Pd atom. The LANL2DZ and SDD pseudopotentials have successfully been used in several studies to represent the electrons of Pd. [11-12] The B3LYP-D3/6-31G(d,p) level of theory has also been applied to investigate the mechanism of similar reactions successfully.[11] The solvent effects were incorporated in the system by using the SMD[13] solvation model with toluene as the solvent. The free energies were calculated at the experimental temperature of 373.15 K. All the calculations were performed using the Gaussian16 software package.[14] The stationary points on the potential energy surface were characterized by calculating the normal mode frequencies. A minima on the PES was characterized by 3*N*-6 positive frequencies whereas a transition state was characterized by one imaginary frequency and remaining 3*N*-7 positive frequencies. The intrinsic reaction coordinate (IRC) was followed on either side of the transition state to connect to the respective intermediates. It is known that the energetics of the reaction can change with the level of theory. We observe that the overall nature of the reaction energy profiles for the different pathways (**Path I-IV**) considered were similar when using SDD and LANL2DZ pseudopotentials. However, the relative energies of the intermediates and the transition states lowered when going from LANL2DZ to SDD potential. The energetics at the B3LYP-D3/6-31G(d,p)/LANL2DZ level of theory for the different stationary points for the reaction of **1a** + **2a** in the presence of **$Pd(PPh_3)_4$** is given in Table S1.

Table S1. Relative free energies (kcal/mol) obtained at the B3LYP-D3/6-31G(d,p)/LANL2DZ level of theory for the different stationary points for the reaction of **1a** + **2a** in the presence of **$Pd(PPh_3)_4$** . The energies are calculated with respect to **$Pd(PPh_3)_4$**.

Path I		**Path II**	
Stationary points	**ΔG (kcal/mol)**	**Stationary points**	**ΔG (kcal/mol)**
int1	-5.3	**int1_p2**	0.5
ts1	34.3	**int2_p2**	-2.0
int2	19.3	**int3_p2**	3.6
int3	33.5	**ts1_p2**	51.2
ts2	39.1	**int4_p2**	12.6
int4	16.2	**ts2_p2**	13.0
ts3	28.9		
int5	-4.8		
int6	-4.7		
ts4	12.7		
3aa_iso1	-48.8		

Path III		Path IV	
Stationary points	**ΔG (kcal/mol)**	**Stationary points**	**ΔG (kcal/mol)**
ts2_p3	20.2	**int2'**	37.5
		ts2_p4	47.3
		int4_p2	12.6

Transition State Theory (TST) rate constant calculations

The rate constant for a reaction can be written using the Eyring equation[15-16] as,

$$k = \frac{k_B T}{hc^o} exp(-\Delta G^{\ddagger}/RT)$$

where k_B is the Boltzman constant, T = reaction temperature, h = Planck's constant, c^o = standard state concentration, ΔG = effective barrier of the reaction, and R = gas constant. The standard state concentration was taken to be 1 M and the rate constant for the reaction was calculated at an experimental temperature of 373.15 K. The kinetic isotope was calculated by

$$\frac{k_H}{k_D} = \exp\left(-\frac{\Delta G_H{}^{\ddagger} - \Delta G_D{}^{\ddagger}}{RT}\right)$$

where, $\Delta G_H{}^{\ddagger}$ and $\Delta G_D{}^{\ddagger}$ are the effective barriers for the reaction pathway under consideration with H and isotopically substituted D at the alcoholic -OH site respectively.

7.2. Optimized structures of reactants and active catalyst

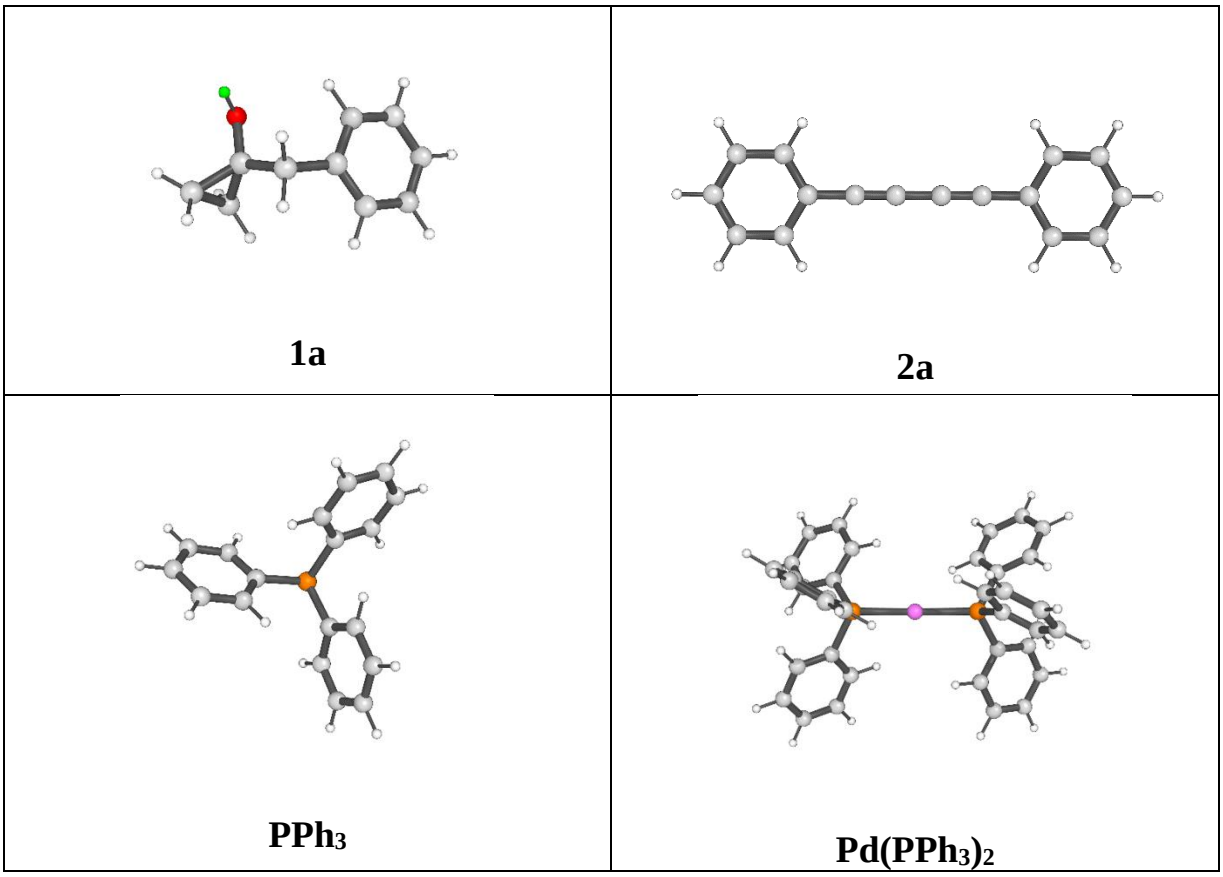


Figure S1. Optimized geometries for different stationary points obtained at the B3LYP-D3/6-31G(d,p) level of theory.

7.3. Conformational isomers of product (3aa)

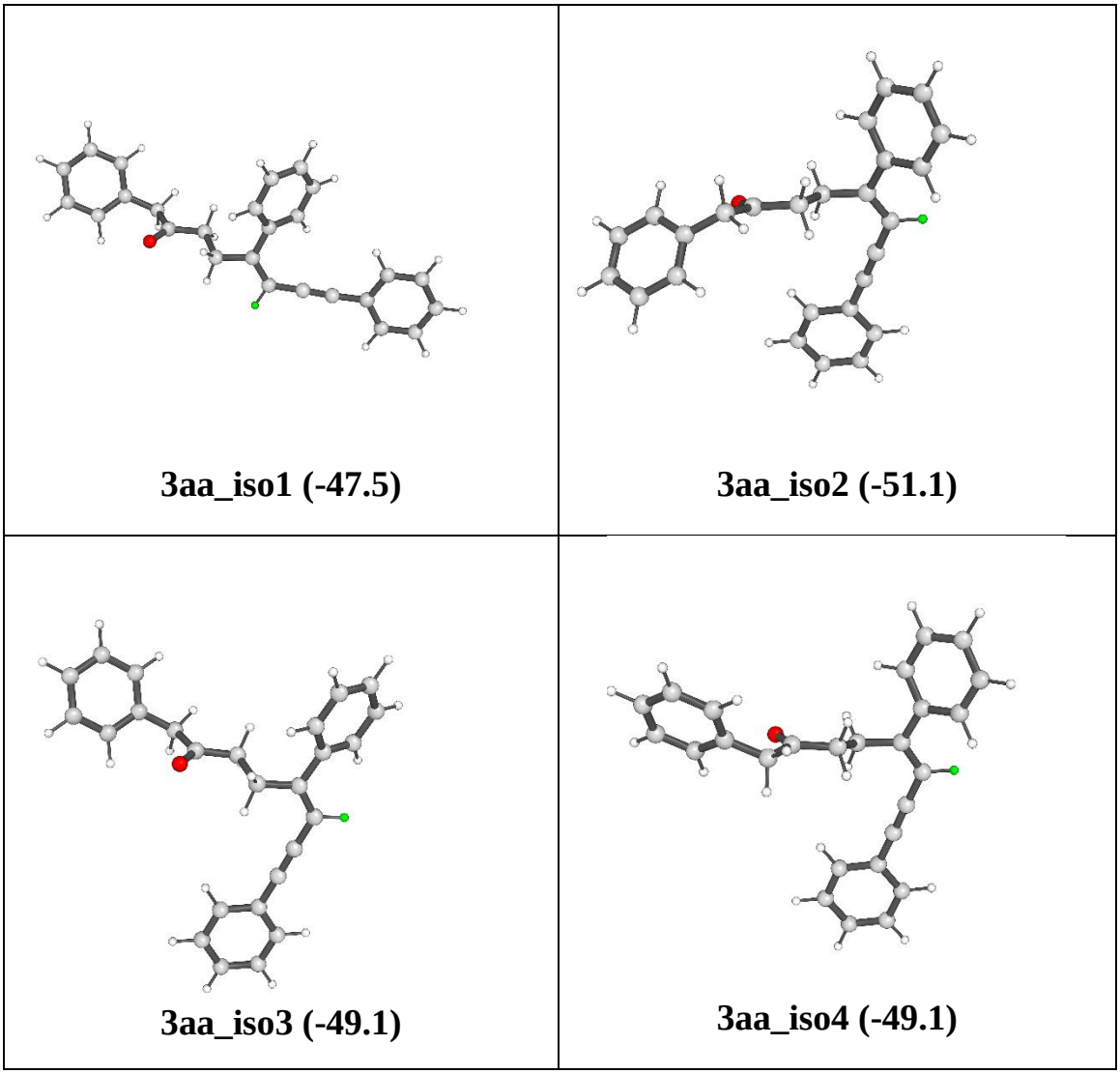


Figure S2. Different conformational isomers of product obtained due to C-C bond rotation and their energies (kcal/mol) with respect to **$Pd(PPh_3)_4$**.

7.4. Alternative pathways proposed for the reaction

Path II

1,3-diyne coordination → ligand exchange with cyclopropanol → syn-addition → β-carbon elimination → reductive elimination

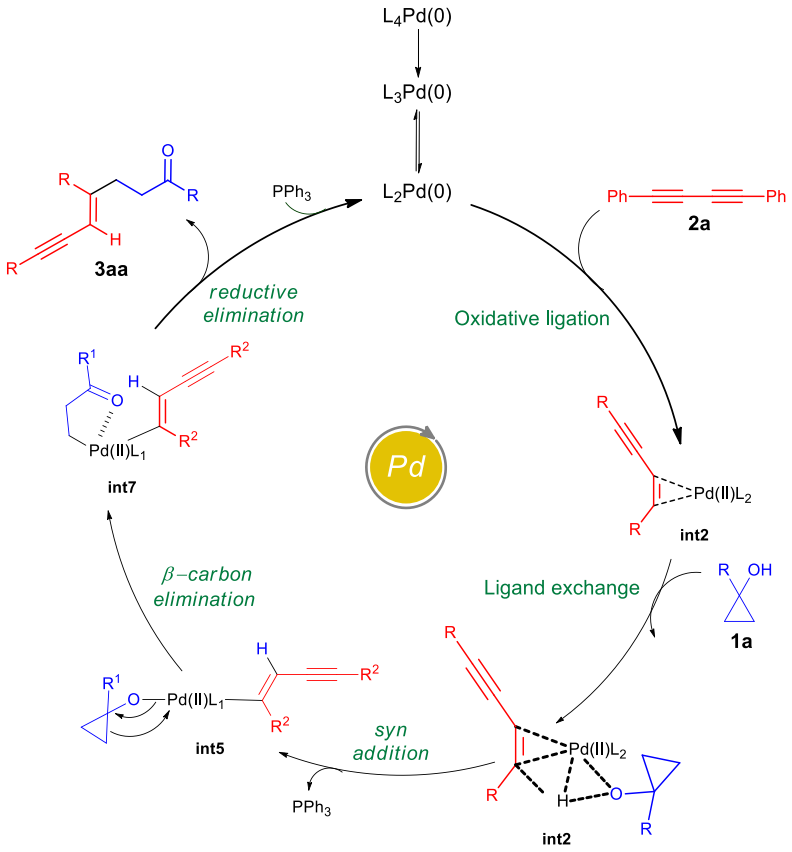


Figure S3. Catalytic cycle proposed for the reaction following **Path II**.

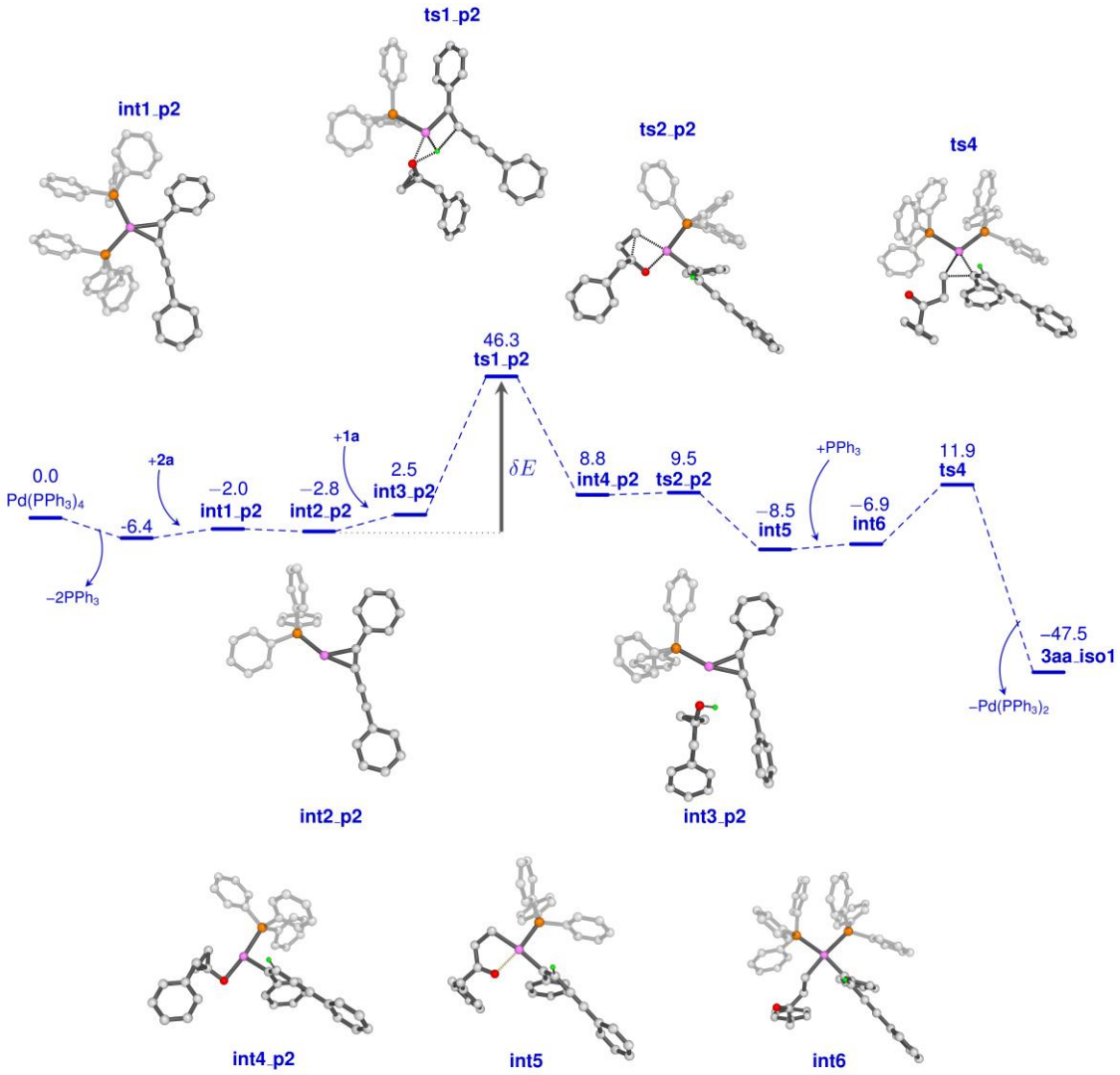


Figure S4. Gibbs Free energy profile mapped for the reaction mechanism (**Path II)** proposed in the catalytic cycle. The relative energies (kcal/mol) are calculated with respect to **Pd(PPh$_3$)$_4$**.

This pathway involves the alkyne coordination to the active catalyst Pd(PPh$_3$)$_2$ via **int1_p2**. This is then followed by the formation of an intermediate **int3_p2** due to the interaction of **1a** with **int2_p2**. The concerted O-H bond dissociation and C-C bond formation results in **int4_p2** via transition state **ts1_p2** with a barrier of 46.3 kcal/mol. The β-carbon elimination from **int4_p2** leads to the formation of a stable homoenolate intermediate **int5**. The addition of a PPh$_3$ leads to the formation of **int6** which further undergoes reductive elimination to form the product via **ts4**.

Path III

oxidative addition → β-carbon elimination → 1,3-diyne coordination → syn-addition → reductive elimination

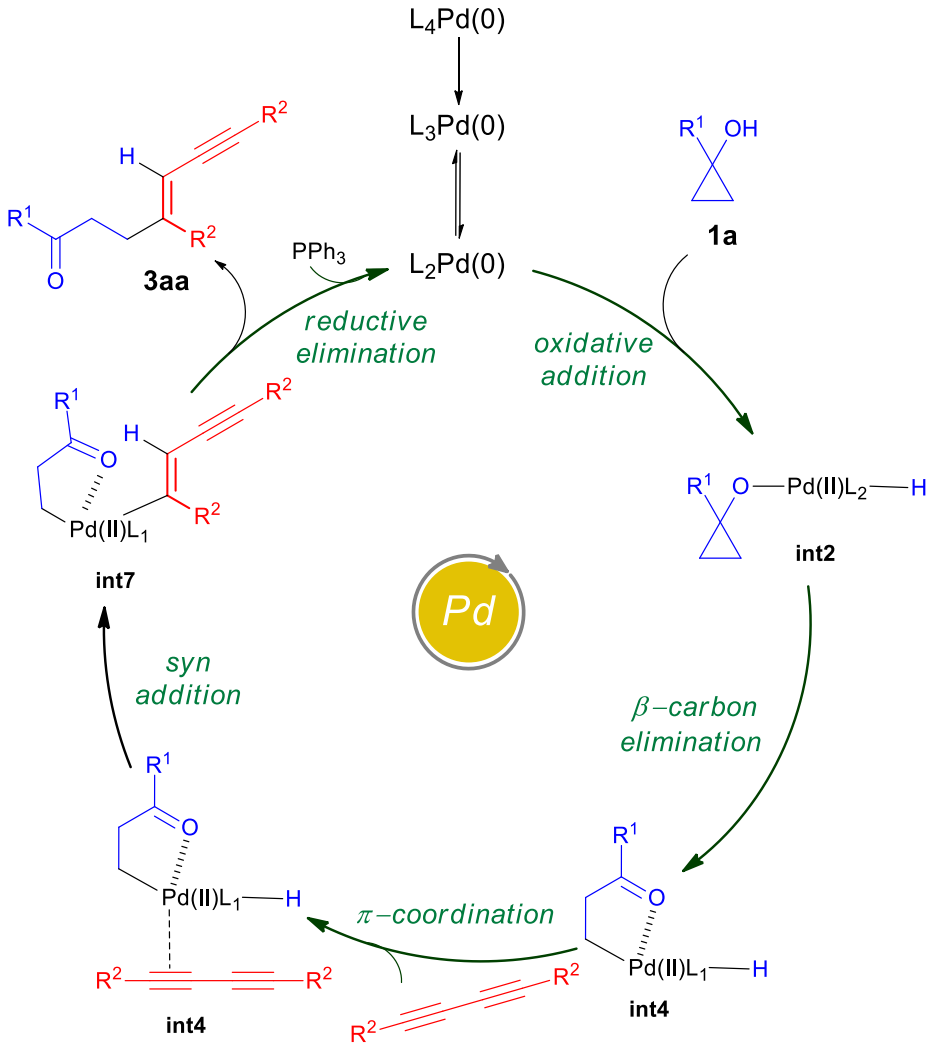


Figure S5. Catalytic cycle for the reaction following **Path III**.

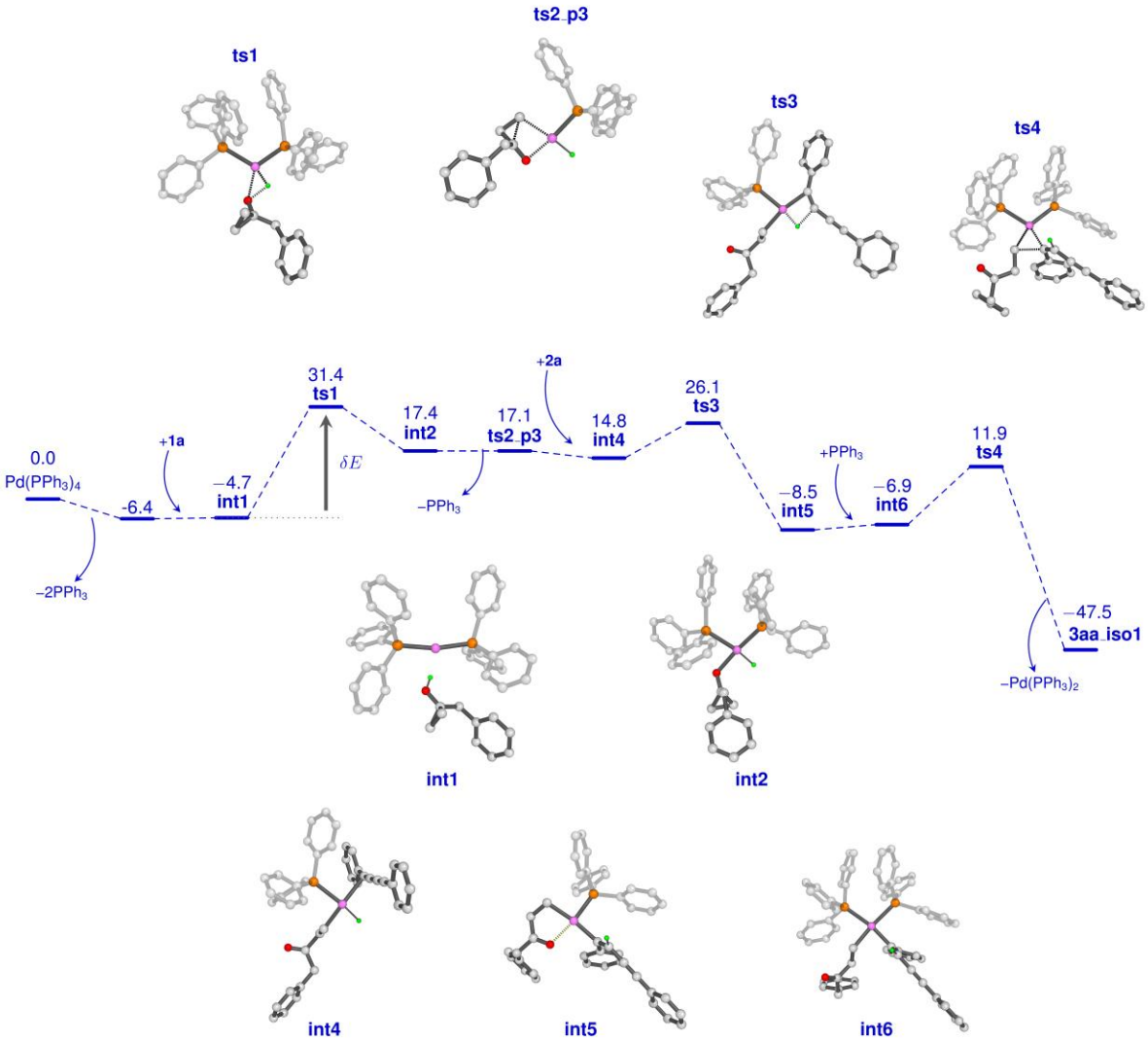


Figure S6. Gibbs free energy profile mapped for the reaction mechanism (**Path III)** proposed in the catalytic cycle. The relative energies (kcal/mol) are calculated with respect to **Pd(PPh$_3$)$_4$**.

The reaction starts by the interaction of the cyclopropanol with the active catalyst Pd(PPh$_3$)$_2$ via intermediate **int1**. The oxidative addition then leads to the formation of **int2** via **ts1** with a barrier of 31.4 kcal/mol. This is then followed by the β-carbon elimination to yield **int4** with the addition of the alkyne **2a**. The *syn* addition then occurs via **ts3** to form a stable homoenolate intermediate **int5**. Further addition of **PPh$_3$** followed by reductive elimination leads to the formation of products.

Path IV

oxidative addition → 1,3-diyne coordination → syn-addition → β-carbon elimination → reductive elimination

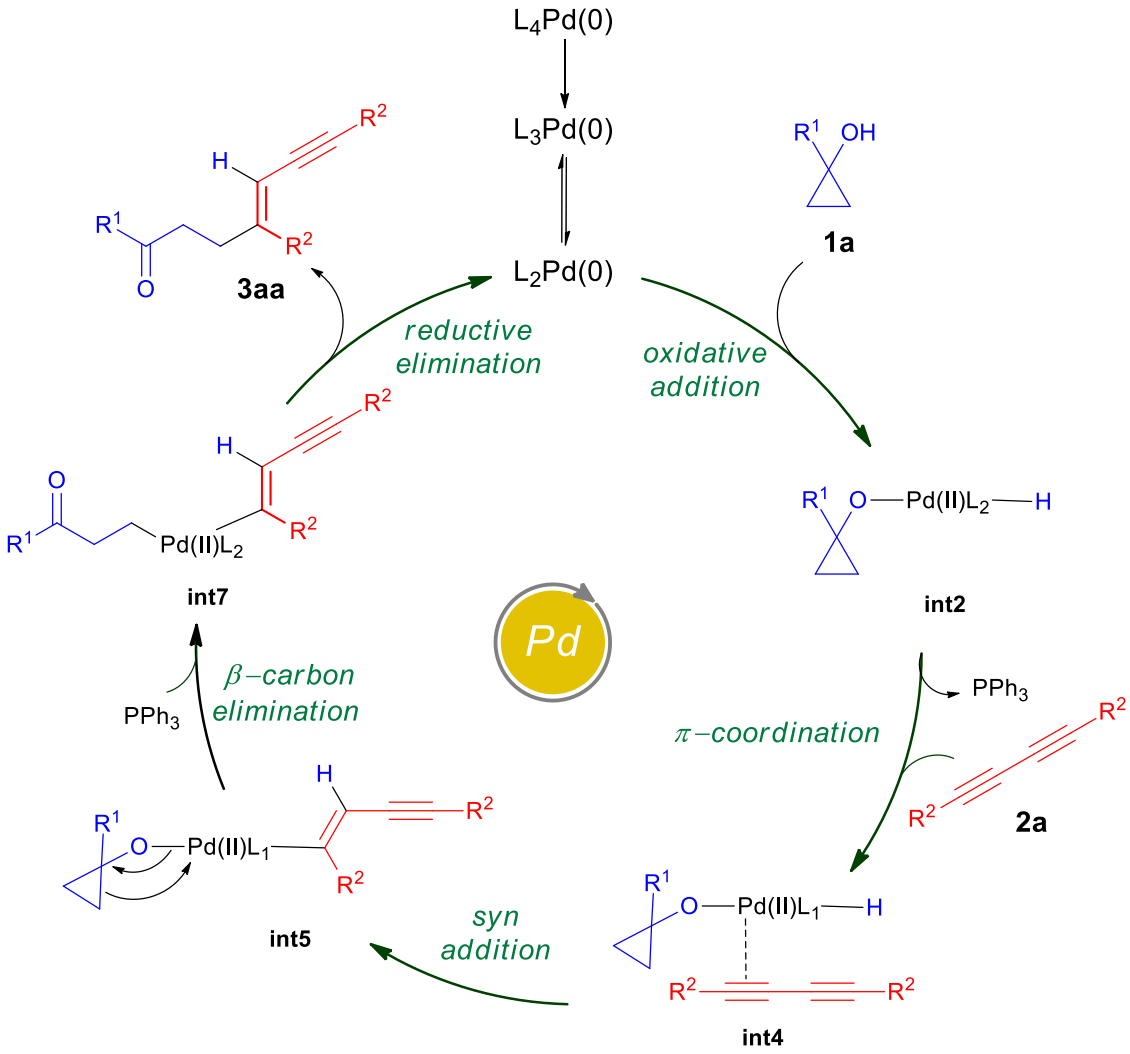


Figure S7. Catalytic cycle for proposed for the reaction following **Path IV**.

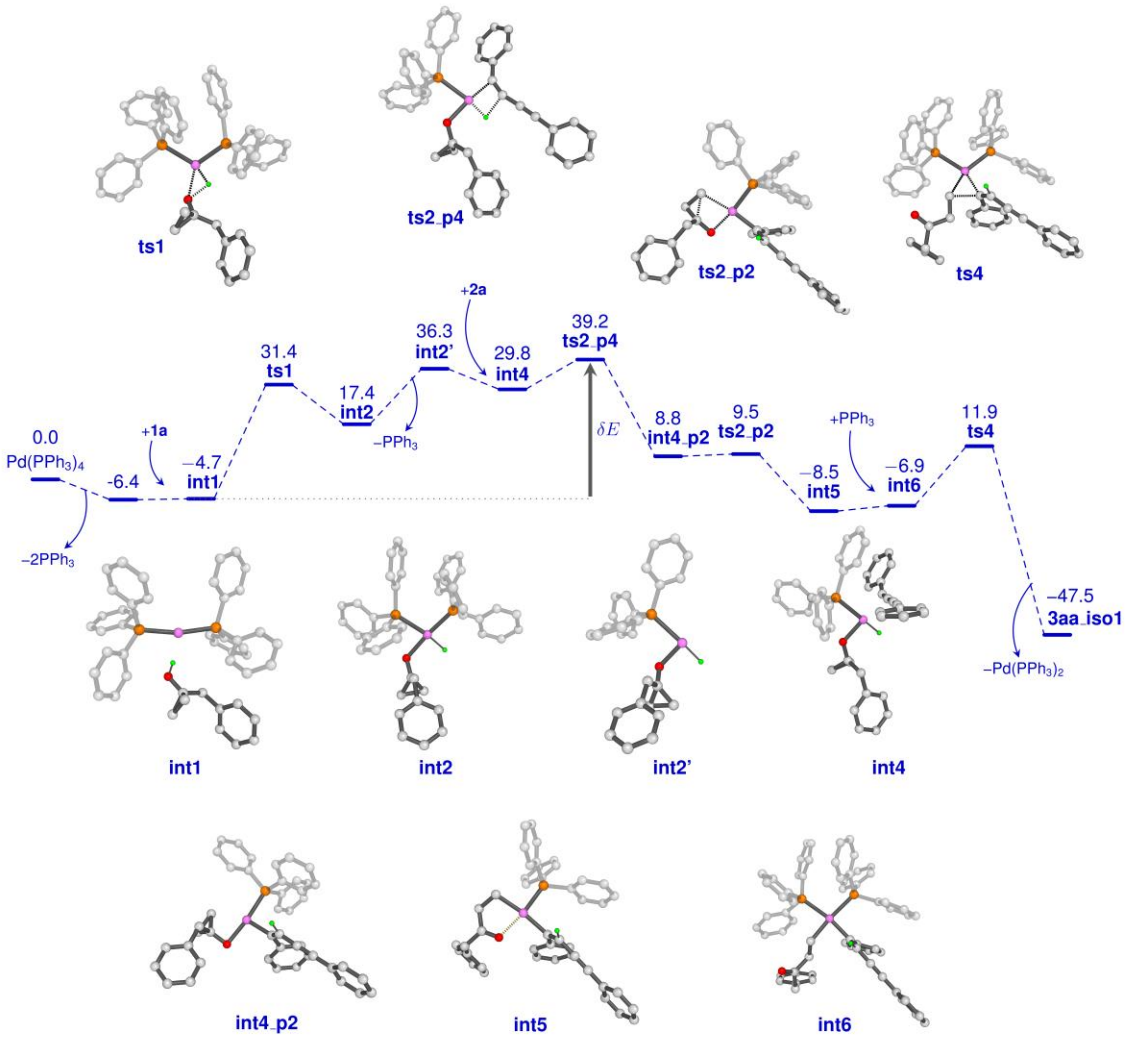


Figure S8. Gibbs Free energy profile mapped for the reaction mechanism (**Path IV)** proposed in the catalytic cycle. The relative energies (kcal/mol) are calculated with respect to **Pd(PPh3)4**.

This pathway involves the oxidative addition of **1a** to the active catalyst **Pd(PPh3)2** via transition state **ts1**. This is followed by the coordination of the alkyene leading to the formation of intermediate **int4**. The syn addition further occurs via **ts2_p4** to yield **int4_p2**. The β-carbon elimination form **int4_p2** leads to the formation of **int5** which after addition of PPh_3 forms intermediate **int6**. The reductive elimination then occurs from **int6** to form the **3aa_iso1**.

7.5. Geometrical parameters of stationary points

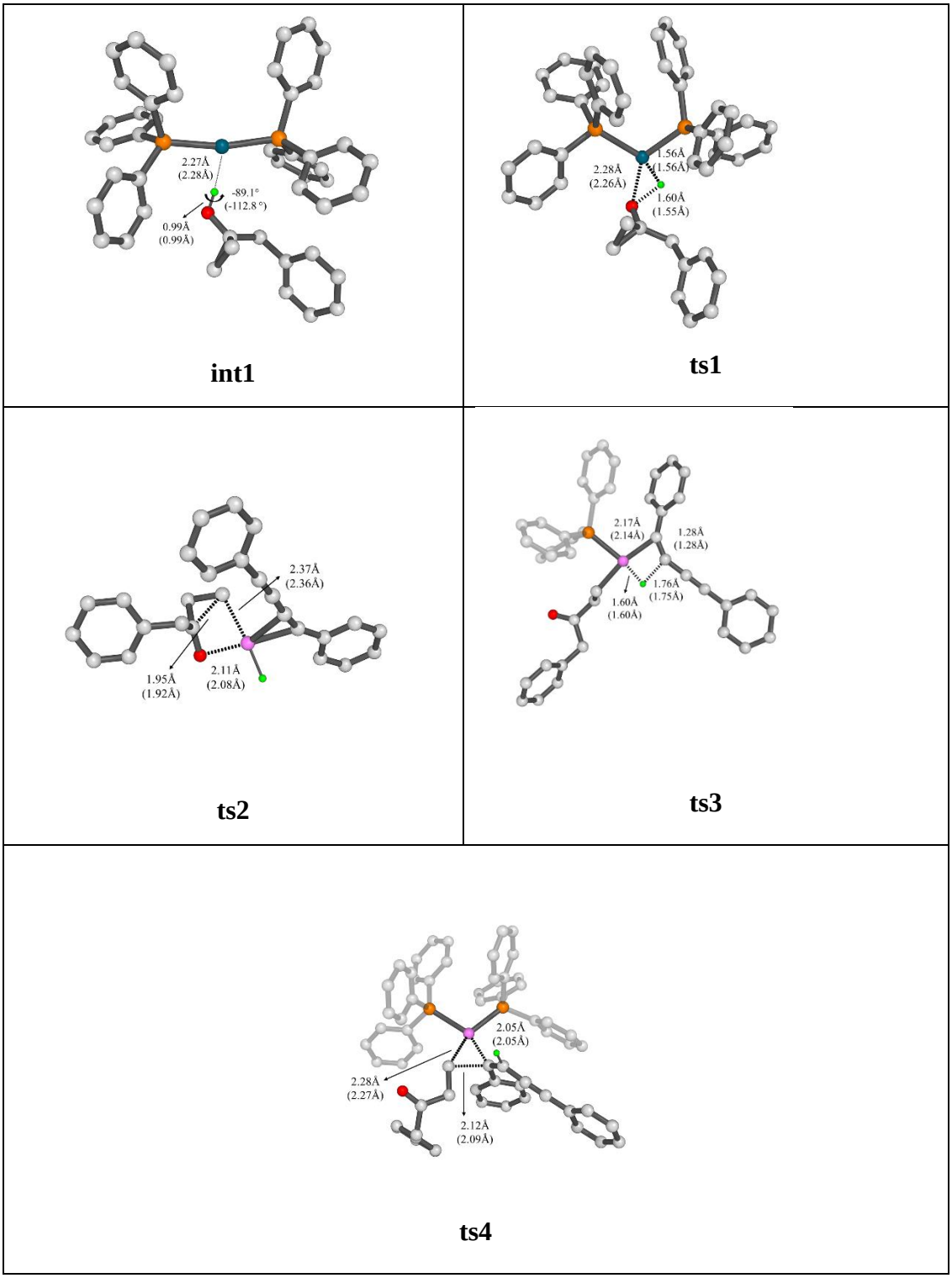


Figure S9. The values in parantheses are obtained using SDD peudopotential for Pd and the others are obtained using LANL2DZ pseudopotential at B3LYP-D3/6-31G(d,p) level of theory

7.6. Substituent Effect

To understand the substituent effect on the reaction mechanism, the Gibbs free energy for the stationary points of the reactions involving *p*-Me-phenylcyclopropanol, and *p*-CF_3-phenylcyclopropanol were calculated at the B3LYP-D3/6-31G(d,p) level of theory using LANL2DZ and SDD pseudopotential for Pd and results are given in Table S2. In addition, the Gibbs free energy for the stationary points of the reactions involving diyene-paraF, and diyen-paraOCH_3 were also calculated at the B3LYP-D3/6-31G(d,p) level of theory using LANL2DZ and SDD pseudopotential for Pd and results are given in Table S3.

Table S2: The Gibbs free energy for the important stationary points of the reactions involving *p*-Me-phenylcyclopropanol, and *p*-CF_3-phenylcyclopropanol calculated at the B3LYP-D3/6-31G(d,p)/LANL2DZ level of theory. The energy in parentheses were calculated by optimizing the geometries at B3LYP-D3/6-31G(d,p)/SDD level of theory. The relative energies are reported here with respect to **$Pd(PPh_3)_4$.**

Stationary points	**ΔG (kcal/mol) *p*-CF_3-phenylcyclopropanol**	**ΔG (kcal/mol) *p*-CH_3-phenylcyclopropanol**
int1	-4.3 (-4.5)	-5.0 (-5.8)
ts2	38.1 (34.4)	36.7 (32.6)
ts3	30.2 (26.3)	27.7 (22.1)
int5	-2.7 (-7.4)	-6.8 (-9.7)
ts4	14.6 (14.5)	13.9 (11.3)
3aa_iso1	-49.7 (-48.5)	-51.6 (-50.3)

Table S3: The Gibbs free energy for the important stationary points of the reactions involving diyne-para-F, and diyne-para-OCH_3 calculated at the B3LYP-D3/6-31G(d,p)/LANL2DZ level of theory. The energy in parentheses were calculated by optimizing the geometries at B3LYP-D3/6-31G(d,p)/SDD level of theory. The relative energies are reported here with respect to **$Pd(PPh_3)_4$.**

Stationary point	**ΔG (kcal/mol) (4-fluorophenyl)buta-1,3-diyne**	**ΔG (kcal/mol) (4-methoxyphenyl)buta-1,3-diyne**
int1	-5.3 (-4.7)	-5.3 (-4.7)
ts2	41.2 (36.9)	41.3 (37.2)
int5	-4.2 (-6.7)	-2.2 (-4.6)
ts4	14.3 (13.6)	17.6 (16.5)
3aa_iso1	-47.7 (-46.4)	-48.7 (-47.4)

7.7. Cartesian coordinates for the optimized geometries of stationary points at B3LYP-D3/6-31G(d,p) level of theory using SDD pseudopotential for Pd:

1a

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C	-3.23294600	-0.54365900	0.04556800
C	-2.22435600	-0.81700200	-1.05859000
C	-1.89124300	0.14693000	0.03492700
H	-4.09626500	0.06283000	-0.21223400
H	-3.41910600	-1.31795200	0.78496800
H	-2.42556700	-0.39172800	-2.03650900
H	-1.71128900	-1.77422100	-1.07155100
C	-0.84040500	-0.21348700	1.08006500
H	-0.97357600	0.45601700	1.94145500
H	-1.03702400	-1.22811600	1.44171300
C	0.57891200	-0.11972900	0.56187200
C	1.17111500	1.12648500	0.31080500
C	1.32088700	-1.27687400	0.29239700
C	2.46837800	1.21196000	-0.19358400
H	0.60013800	2.03009800	0.49788400
C	2.62082300	-1.19573500	-0.21163800
H	0.87818900	-2.25154500	0.48400300
C	3.19912600	0.05035800	-0.45619300
H	2.91040700	2.18657800	-0.38193200
H	3.18046500	-2.10558400	-0.41084500
H	4.21092200	0.11713500	-0.84598500
O	-1.86752400	1.49701000	-0.37401500
H	-2.19884900	2.02492700	0.36738000

2a

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C	1.90118800	0.00008400	-0.00009500
C	3.32249200	0.00003600	0.00001400
C	4.03679300	1.21644600	0.00021000
C	4.03670100	-1.21643500	-0.00019200
C	5.42846000	1.20976500	0.00024200
H	3.48924500	2.15329400	0.00033900
C	5.42836700	-1.20986300	-0.00016800
H	3.48907700	-2.15323900	-0.00039100
C	6.12804500	-0.00007400	0.00005900

H	5.96963200	2.15125800	0.00041000
H	5.96947000	-2.15139600	-0.00033000
H	7.21401300	-0.00011500	0.00008500
C	0.67955700	0.00010700	-0.00016900
C	-0.67955700	0.00008700	-0.00005900
C	-1.90118800	-0.00000400	-0.00002200
C	-3.32249200	-0.00001700	0.00001100
C	-4.03675300	1.21642700	-0.00018200
C	-4.03674000	-1.21645400	0.00022000
C	-5.42841500	1.20979800	-0.00017600
H	-3.48916300	2.15325000	-0.00035400
C	-5.42841200	-1.20983000	0.00023400
H	-3.48915900	-2.15328300	0.00037600
C	-6.12804600	-0.00002200	0.00003500
H	-5.96956100	2.15130600	-0.00034400
H	-5.96954200	-2.15134800	0.00039600
H	-7.21401300	-0.00002400	0.00003800

$Pd(PPh_3)_2$

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Pd	-0.00068900	0.00544000	-0.03611700
P	2.29914500	0.00178900	-0.01368800
P	-2.30039700	0.00029100	-0.01578500
C	-3.09265500	1.61332500	-0.44176000
C	-4.30197900	1.72005200	-1.14439800
C	-2.44245300	2.78546200	-0.02095400
C	-4.85165000	2.97527700	-1.41610600
H	-4.81428800	0.82553600	-1.48481000
C	-2.99869000	4.03709000	-0.28442700
H	-1.49537200	2.70878700	0.50784400
C	-4.20386200	4.13463400	-0.98507700
H	-5.78649700	3.04528100	-1.96554200
H	-2.48603000	4.93555000	0.04791400
H	-4.63279500	5.10965600	-1.19899700
C	-3.10403900	-1.18861700	-1.17724100
C	-4.30570200	-1.85440400	-0.89347400
C	-2.47134300	-1.41776200	-2.41029400
C	-4.86588600	-2.72760700	-1.82881200
H	-4.80334200	-1.69645400	0.05837700
C	-3.03805800	-2.28254500	-3.34662400
H	-1.52917500	-0.91958300	-2.62619900
C	-4.23593300	-2.94101600	-3.05664400
H	-5.79472500	-3.24123000	-1.59612900

H	-2.53910300	-2.45013800	-4.29712200
H	-4.67299600	-3.62184200	-3.78180800
C	-3.05467200	-0.42718600	1.61534600
C	-4.24255500	0.14607300	2.09253700
C	-2.39720300	-1.38826200	2.40134700
C	-4.76420300	-0.23870100	3.33011100
H	-4.75997900	0.89609700	1.50239000
C	-2.92540400	-1.77790600	3.63198600
H	-1.46576900	-1.82147200	2.04484400
C	-4.10958400	-1.20203800	4.10007200
H	-5.68274100	0.21582900	3.69117000
H	-2.40729000	-2.52305700	4.22934100
H	-4.51659500	-1.49870200	5.06273800
C	3.05930600	-0.70387900	1.51472700
C	4.25445500	-1.43818600	1.51609400
C	2.39822300	-0.47407700	2.73278300
C	4.77995800	-1.92813400	2.71419300
H	4.77444900	-1.63248400	0.58314500
C	2.93046800	-0.95545500	3.92875600
H	1.46120000	0.07768200	2.73460700
C	4.12195900	-1.68563900	3.92157400
H	5.70411000	-2.49954800	2.70214200
H	2.40976500	-0.76950900	4.86407500
H	4.53201300	-2.06862100	4.85194600
C	3.08613900	1.66690500	-0.14925000
C	2.44883200	2.62097600	-0.95969500
C	4.28177200	2.01233300	0.49833700
C	3.00413400	3.88903100	-1.13056200
H	1.51221600	2.36396400	-1.44862900
C	4.83051900	3.28635700	0.33348300
H	4.78381300	1.29060100	1.13527500
C	4.19557100	4.22504700	-0.48227100
H	2.50137700	4.61732000	-1.76092000
H	5.75445600	3.54409700	0.84398200
H	4.62365000	5.21574000	-0.60750000
C	3.10368300	-0.95964600	-1.36961700
C	2.46494800	-2.13584200	-1.79636200
C	4.31169800	-0.58246900	-1.97457000
C	3.03199100	-2.92675000	-2.79554600
H	1.51831400	-2.42196500	-1.34435000
C	4.87220400	-1.37094800	-2.98238700
H	4.81469200	0.32799100	-1.66377300
C	4.23643300	-2.54456600	-3.39225000
H	2.52825700	-3.83476700	-3.11528100
H	5.80624400	-1.06626900	-3.44651900
H	4.67410700	-3.15549400	-4.17686000

PPh_3

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P	-0.00061200	0.00045600	-1.24624900
C	0.57968000	-1.55784100	-0.43081900
C	0.19095600	-2.77144400	-1.02225200
C	1.37496900	-1.59566600	0.72465500
C	0.57208000	-3.99138200	-0.46395900
H	-0.41454000	-2.76033700	-1.92533600
C	1.76567500	-2.81738600	1.27653300
H	1.68961000	-0.66998900	1.19578900
C	1.36331100	-4.01700900	0.68672800
H	0.25899800	-4.92060200	-0.93165700
H	2.38304100	-2.83034600	2.17056500
H	1.66829100	-4.96623600	1.11796500
C	1.05979300	1.28157200	-0.43126000
C	0.69300200	1.99534200	0.71977700
C	2.30819700	1.54533200	-1.01935300
C	1.55671700	2.94425900	1.27066100
H	-0.26821200	1.81022600	1.18842200
C	3.17514600	2.48487100	-0.46191100
H	2.60297800	1.01057600	-1.91906800
C	2.79975000	3.18907100	0.68442400
H	1.25773700	3.49031100	2.16119100
H	4.13880500	2.67315200	-0.92682200
H	3.47016600	3.92747900	1.11488600
C	-1.64003200	0.27717600	-0.43046400
C	-2.49808700	1.21822800	-1.02372100
C	-2.06930600	-0.39089600	0.72643100
C	-3.74549500	1.49751600	-0.46584900
H	-2.18654500	1.73558700	-1.92792900
C	-3.32303900	-0.11915600	1.27782100
H	-1.42397800	-1.12450200	1.19890200
C	-4.16217600	0.82673300	0.68619100
H	-4.39477000	2.23147000	-0.93484900
H	-3.64225500	-0.64615900	2.17278800
H	-5.13700100	1.03662400	1.11708600

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C	0.61752300	-0.54268000	0.61568500
C	1.57261100	-1.50446500	0.51354500
H	1.26289400	-2.54222700	0.63093800
C	2.95652900	-1.30059900	0.30587100
C	4.15411200	-1.15662300	0.13518000
C	0.89740200	0.90647900	0.44442400
C	1.73329800	1.37276700	-0.58696500
C	0.30198500	1.85694800	1.29434700
C	1.98308800	2.73466600	-0.74622000
H	2.17706100	0.66156900	-1.27407200
C	0.55817200	3.21849500	1.13849500
H	-0.35040400	1.52982800	2.09766800
C	1.40102400	3.66392600	0.11862600
H	2.62731000	3.07023700	-1.55408900
H	0.09809300	3.93186200	1.81627800
H	1.59692600	4.72506800	-0.00517700
C	5.53877700	-0.90812000	-0.07787100
C	6.45301600	-1.97007600	-0.23346200
C	6.01485000	0.41879600	-0.14076700
C	7.80348700	-1.70781100	-0.44712700
H	6.09157800	-2.99233100	-0.18516600
C	7.36710600	0.66919800	-0.35487200
H	5.31288700	1.23760400	-0.01857900
C	8.26569100	-0.39037200	-0.50873300
H	8.49857400	-2.53398600	-0.56551700
H	7.72238700	1.69460300	-0.40071800
H	9.32015900	-0.19049500	-0.67478100
C	-0.81123600	-0.94634500	0.90523600
H	-0.86717300	-2.02489700	1.07993300
H	-1.16504300	-0.47649500	1.82992600
C	-1.77463300	-0.56135000	-0.22497500
H	-1.70253800	0.51267600	-0.44678500
H	-1.50946100	-1.06920200	-1.16166800
C	-3.23028000	-0.84791200	0.09822900
C	-4.19402600	-0.75278100	-1.09058300
H	-3.81599500	-0.00634700	-1.79743900
H	-4.10499300	-1.72128500	-1.60570300
C	-5.63008400	-0.47577500	-0.72264500
C	-6.38560300	-1.42541000	-0.02084600
C	-6.22895400	0.74337700	-1.06099100
C	-7.70944100	-1.16224700	0.32871300
H	-5.92820800	-2.36973200	0.25653400
C	-7.55508600	1.00914500	-0.71359100
H	-5.65356200	1.49042200	-1.60257300
C	-8.29932900	0.05614300	-0.01724100

H	-8.28172100	-1.90895800	0.87208500
H	-8.00466200	1.95949200	-0.98757600
H	-9.33151500	0.25960400	0.25331100
O	-3.59907300	-1.15265700	1.21679900

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C	-2.75913700	1.32797500	0.14116100
H	-3.73532400	1.63550200	0.51016300
C	-2.56843800	0.03670500	-0.24372200
C	-1.76912100	2.33530900	0.08969200
C	-0.92121700	3.21022200	0.05605600
C	0.09465000	4.20492000	-0.00068600
C	1.38849800	3.87297100	-0.45537200
C	-0.17042100	5.53221300	0.39557800
C	2.38360000	4.84455800	-0.51017600
H	1.59741100	2.85276900	-0.76179300
C	0.83273200	6.49557300	0.33723900
H	-1.16431100	5.79247000	0.74549100
C	2.11113600	6.15718100	-0.11490400
H	3.37544100	4.57676100	-0.86248400
H	0.61683600	7.51459400	0.64500700
H	2.89052500	6.91217000	-0.15925400
C	-3.65117500	-0.96329500	-0.08058800
C	-3.78995700	-2.04155700	-0.97576600
C	-4.56478900	-0.87833900	0.98879800
C	-4.81347500	-2.97576100	-0.82421700
H	-3.10654700	-2.14134500	-1.81235400
C	-5.58725700	-1.81184300	1.13959900
H	-4.45192900	-0.08763500	1.72371700
C	-5.71897800	-2.86554100	0.23228100
H	-4.90405400	-3.79116700	-1.53629100
H	-6.27409500	-1.72456700	1.97671300
H	-6.51291800	-3.59670600	0.35279600
C	-1.24271000	-0.42182000	-0.80529500
H	-0.60640900	0.43966700	-1.01370400
H	-1.38301700	-0.93007600	-1.76544500
C	-0.50693900	-1.36702700	0.15284700
H	-0.33794100	-0.87496200	1.12098500
H	-1.10872800	-2.25700400	0.38079600
C	0.84382700	-1.82116900	-0.36942400
C	1.54710200	-2.89496300	0.47208500
H	1.21049800	-2.81671500	1.51095100

H	1.14977800	-3.85113600	0.09964800
O	1.32190400	-1.38538900	-1.39975900
C	3.05316300	-2.87618200	0.38585300
C	3.70680600	-3.21126200	-0.80829100
C	3.82425500	-2.50393800	1.49337900
C	5.09846500	-3.17767000	-0.88931600
H	3.11858600	-3.49078900	-1.67622500
C	5.21800400	-2.47128400	1.41549700
H	3.32984900	-2.23966400	2.42508900
C	5.85918300	-2.80782300	0.22273800
H	5.59037700	-3.44041500	-1.82170500
H	5.80053700	-2.18340500	2.28620100
H	6.94337700	-2.78414800	0.15950500

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C	2.25847300	2.07476600	-0.00344100
H	2.80048500	2.98691900	-0.24439900
C	0.93079900	2.14800700	0.28476700
C	3.02379800	0.88667200	-0.00138300
C	3.70424500	-0.12463600	-0.01203000
C	4.47702700	-1.31943300	-0.02113300
C	3.88384100	-2.55532700	0.31222100
C	5.84492300	-1.28996100	-0.36378800
C	4.64055300	-3.72344700	0.30101400
H	2.83206700	-2.58313600	0.57911900
C	6.59214500	-2.46440100	-0.37243200
H	6.30672500	-0.34181200	-0.62014100
C	5.99509000	-3.68376800	-0.04109000
H	4.17233000	-4.66846300	0.56060100
H	7.64467100	-2.42862900	-0.63811900
H	6.58194600	-4.59748000	-0.04858900
C	0.21331300	3.44236800	0.18853500
C	0.57731000	4.40837800	-0.77059300
C	-0.86887700	3.73938600	1.03927700
C	-0.09082600	5.62746700	-0.85492100
H	1.37329500	4.18787800	-1.47487800
C	-1.53726200	4.95976900	0.95404700
H	-1.18014000	3.02090100	1.79007800
C	-1.15098500	5.91152100	0.00899000
H	0.20804500	6.35165300	-1.60743500
H	-2.36135600	5.16699300	1.63074600
H	-1.67552000	6.85993700	-0.06013100

C	0.14542000	0.91950600	0.67950800
H	-0.36706400	1.07628400	1.63435800
H	0.82545800	0.07998000	0.83912400
C	-0.89849100	0.53202400	-0.37555900
H	-1.57833200	1.37093200	-0.58134000
H	-0.41945600	0.30292200	-1.33658200
C	-1.76020900	-0.64756600	0.03812000
C	-2.61044300	-1.26112400	-1.08083800
H	-2.87032800	-0.47923300	-1.80232000
H	-1.92841500	-1.94141100	-1.61308400
O	-1.75522500	-1.08901200	1.17178300
C	-3.83887000	-1.99972500	-0.61146100
C	-3.72242400	-3.18074300	0.13478800
C	-5.11812500	-1.50894200	-0.89834400
C	-4.85914000	-3.85562900	0.57810500
H	-2.73559500	-3.56441200	0.37280100
C	-6.25835000	-2.18354800	-0.45700700
H	-5.22308100	-0.59222000	-1.47370000
C	-6.13159100	-3.35969000	0.28297800
H	-4.75202500	-4.77000400	1.15497400
H	-7.24323200	-1.78973700	-0.69209200
H	-7.01673500	-3.88729700	0.62674500

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C	-2.25849000	2.07476100	-0.00346300
H	-2.80051600	2.98690500	-0.24442600
C	-0.93081900	2.14802500	0.28475700
C	-3.02379300	0.88665400	-0.00140300
C	-3.70421900	-0.12466800	-0.01204400
C	-4.47697800	-1.31948000	-0.02113900
C	-3.88376700	-2.55536100	0.31222000
C	-5.84487600	-1.29003700	-0.36378900
C	-4.64045700	-3.72349600	0.30102200
H	-2.83199200	-2.58314900	0.57911400
C	-6.59207600	-2.46449200	-0.37242400
H	-6.30669800	-0.34189800	-0.62014600
C	-5.99499600	-3.68384500	-0.04107700
H	-4.17221400	-4.66850200	0.56061300
H	-7.64460300	-2.42874100	-0.63810700
H	-6.58183500	-4.59756800	-0.04856800

C	-0.21334900	3.44239700	0.18853100
C	0.86882000	3.73943600	1.03929100
C	-0.57734200	4.40839500	-0.77061000
C	1.53719000	4.95982800	0.95406600
H	1.18008000	3.02096200	1.79010300
C	0.09077800	5.62749400	-0.85493300
H	-1.37330800	4.18788000	-1.47491200
C	1.15091700	5.91156900	0.00899600
H	2.36126800	5.16706900	1.63077900
H	-0.20808800	6.35167100	-1.60745900
H	1.67544000	6.85999200	-0.06012200
C	-0.14542800	0.91953500	0.67951000
H	-0.82545800	0.08000400	0.83913300
H	0.36705600	1.07632500	1.63435700
C	0.89848600	0.53205400	-0.37555600
H	0.41945200	0.30294800	-1.33657900
H	1.57832300	1.37096600	-0.58133700
C	1.76021000	-0.64752900	0.03812900
C	2.61044400	-1.26108900	-1.08082800
H	1.92841100	-1.94136400	-1.61308400
H	2.87034100	-0.47919600	-1.80230200
O	1.75522800	-1.08896600	1.17179500
C	3.83886100	-1.99970900	-0.61145300
C	5.11812300	-1.50894400	-0.89834100
C	3.72240200	-3.18072900	0.13479100
C	6.25834000	-2.18356900	-0.45701000
H	5.22309000	-0.59222300	-1.47369500
C	4.85910900	-3.85563300	0.57810100
H	2.73556800	-3.56438400	0.37280500
C	6.13156700	-3.35971100	0.28297100
H	7.24322700	-1.78977100	-0.69209900
H	4.75198300	-4.77000800	1.15496600
H	7.01670400	-3.88733300	0.62673200

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P	-1.19937700	1.76877100	0.04082200
C	-2.34011600	1.38161600	1.43910100
C	-2.27340400	1.65071600	-1.45548100
C	-0.91932200	3.58561700	0.21255100
C	-1.75049200	1.04349100	2.66943700
C	-3.73795600	1.36488200	1.32773500

C	-2.18133600	0.48676500	-2.23442700
C	-3.18528200	2.65110600	-1.82876000
C	0.18836700	4.14112000	-0.44860000
C	-1.76139600	4.42535600	0.95613900
C	-2.54231600	0.69941800	3.76365500
H	-0.66710000	1.02654400	2.75521500
C	-4.52887800	1.00629800	2.42228100
H	-4.21460100	1.60996400	0.38477600
C	-3.00542400	0.31172500	-3.34791700
H	-1.46496300	-0.28125400	-1.95949100
C	-4.00500600	2.47618400	-2.94484800
H	-3.25435800	3.56718200	-1.24981500
C	0.43921800	5.51117200	-0.38024000
H	0.85766000	3.49197100	-1.00718900
C	-1.50305800	5.79636100	1.02981300
H	-2.61599800	4.01108000	1.48213500
C	-3.93437300	0.67351600	3.64014900
H	-2.07224900	0.43206900	4.70574200
H	-5.60947200	0.97723800	2.31605900
C	-3.92103600	1.30458800	-3.70249900
H	-2.92968000	-0.59858700	-3.93567600
H	-4.70819800	3.25600300	-3.22379400
C	-0.40590200	6.34183700	0.36065100
H	1.30051300	5.92784700	-0.89494200
H	-2.16019700	6.43668100	1.61184300
H	-4.55129800	0.38603600	4.48675500
H	-4.56046100	1.17139700	-4.57063000
H	-0.20561200	7.40787100	0.42168800
Pd	0.74351200	0.52808600	-0.01483800
P	2.82851100	-0.46842000	-0.04861200
C	3.43989500	-1.09554200	1.57333300
C	4.14253600	0.70576600	-0.60058800
C	3.05983500	-1.91975500	-1.16587400
C	4.35093500	-2.15688300	1.68590600
C	2.97524100	-0.46703800	2.73914100
C	3.80583800	1.64049700	-1.59419200
C	5.44977200	0.69298500	-0.09348000
C	2.23468600	-3.03888100	-0.95554000
C	3.98606500	-1.94109100	-2.21740600
C	4.79219500	-2.57591100	2.94234900
H	4.71065200	-2.66038500	0.79380600
C	3.42273000	-0.88333700	3.99328100
H	2.25445200	0.34244200	2.65599500
C	4.75957500	2.53654100	-2.07722300
H	2.79058500	1.66219600	-1.98286200
C	6.39975700	1.59919200	-0.56996400

H	5.72833000	-0.01973600	0.67614400
C	2.33973700	-4.15550500	-1.78311800
H	1.50781400	-3.02779600	-0.14799100
C	4.08121700	-3.06064800	-3.04931900
H	4.63538300	-1.08912600	-2.39099000
C	4.33078900	-1.93963600	4.09701000
H	5.49449200	-3.40146300	3.01836000
H	3.05374400	-0.39059900	4.88849100
C	6.05857300	2.51994500	-1.56277700
H	4.48601600	3.25212100	-2.84765200
H	7.40771900	1.58358500	-0.16463600
C	3.26078800	-4.16870600	-2.83514100
H	1.69410300	-5.01250800	-1.61174100
H	4.80151200	-3.06422000	-3.86293300
H	4.67242000	-2.27043200	5.07385800
H	6.79970200	3.22380600	-1.93105000
H	3.33619900	-5.03706000	-3.48370800
H	-0.12934600	-1.40096800	0.84057100
O	-0.33447800	-2.32395200	1.11966900
C	-1.49509700	-2.74878200	0.44065100
C	-1.40690500	-2.87629500	-1.05845500
C	-1.38850600	-4.11216300	-0.17511600
H	-0.47241400	-2.57497800	-1.52114900
H	-2.29762600	-2.69173600	-1.65040600
H	-2.26851100	-4.74887600	-0.17813400
H	-0.44309300	-4.63017500	-0.04429300
C	-2.77139800	-2.29220000	1.15400100
H	-2.76476800	-2.74659700	2.15170800
H	-2.68826600	-1.21272500	1.30257500
C	-4.06950900	-2.59880500	0.44685600
C	-4.77955800	-3.78062600	0.70010300
C	-4.58265400	-1.70589400	-0.50649400
C	-5.96422700	-4.06656100	0.01693200
H	-4.40120000	-4.47903400	1.44270600
C	-5.76335800	-1.98819200	-1.19395100
H	-4.04671400	-0.78490900	-0.71159500
C	-6.45934100	-3.17186900	-0.93446200
H	-6.50130700	-4.98713200	0.22986600
H	-6.13721700	-1.28194400	-1.93078500
H	-7.38076000	-3.39361600	-1.46599400

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P	-0.00998600	1.96450500	-0.22228000
C	0.82138000	3.29063400	-1.20614500
C	0.81617800	2.06326600	1.42842600
C	-1.68961800	2.67086700	0.05841300
C	1.27955500	3.00440600	-2.49876600
C	0.98547400	4.58919600	-0.69605000
C	1.84594800	1.14610500	1.69698400
C	0.47336000	3.00335900	2.41202700
C	-2.45188300	2.26455700	1.16721700
C	-2.29234400	3.48020100	-0.91843900
C	1.89287800	3.99621900	-3.26906900
H	1.15890200	2.00121800	-2.89741700
C	1.60287900	5.57592300	-1.46265400
H	0.63471700	4.83103600	0.30231600
C	2.52142600	1.17143200	2.91755000
H	2.10375100	0.39891400	0.95193800
C	1.14528100	3.02294400	3.63591800
H	-0.33201900	3.70901300	2.23549500
C	-3.78205600	2.66306400	1.29533200
H	-2.01135400	1.63280800	1.92994100
C	-3.62592300	3.87309900	-0.78805800
H	-1.72236300	3.80323400	-1.78407700
C	2.05752100	5.28118200	-2.75192000
H	2.24374000	3.75970500	-4.26957600
H	1.73000300	6.57486900	-1.05480900
C	2.17061200	2.10956400	3.89158700
H	3.31347300	0.45214500	3.10581200
H	0.86441000	3.75221500	4.39063600
C	-4.37513200	3.46531300	0.31778800
H	-4.35431400	2.33428700	2.15770100
H	-4.07709900	4.50009600	-1.55216200
H	2.53920800	6.05147200	-3.34768000
H	2.68987100	2.12617100	4.84567100
H	-5.41345000	3.76894400	0.41590700
Pd	0.09750300	-0.17040100	-1.00923100
P	-1.76619300	-1.47355000	-0.13014300
C	-3.39111700	-1.27867100	-0.97515200
C	-2.14307200	-1.11876600	1.63794900
C	-1.46460200	-3.28852200	-0.15201700
C	-4.30216100	-2.33109800	-1.15235900
C	-3.72445300	0.00075500	-1.44980600
C	-1.05137200	-0.89321400	2.49359400
C	-3.44342700	-0.98804000	2.14418000
C	-0.67942800	-3.79914100	-1.19926600
C	-1.98119300	-4.16776100	0.81265400

C	-5.52573200	-2.10412500	-1.78601000
H	-4.05770200	-3.32792000	-0.79931000
C	-4.95189400	0.22601200	-2.07275500
H	-3.02547200	0.82070500	-1.32614800
C	-1.25584200	-0.53634000	3.82565500
H	-0.03947400	-0.96676300	2.10666700
C	-3.64688100	-0.62639700	3.47864700
H	-4.29780700	-1.14820900	1.49442000
C	-0.43982300	-5.17159600	-1.29055000
H	-0.22536100	-3.12029400	-1.91630000
C	-1.72913200	-5.53780700	0.72235300
H	-2.57811600	-3.78218900	1.63392700
C	-5.85456500	-0.82616400	-2.24389900
H	-6.22179200	-2.92743800	-1.92131000
H	-5.19697700	1.22326800	-2.42653000
C	-2.55626800	-0.39499700	4.31961200
H	-0.40106900	-0.34786700	4.46855300
H	-4.65958000	-0.52023000	3.85810300
C	-0.96330400	-6.04206900	-0.33196300
H	0.16911900	-5.55721200	-2.10345000
H	-2.13156600	-6.21085600	1.47451100
H	-6.80750000	-0.65298300	-2.73628600
H	-2.71762700	-0.10304100	5.35350400
H	-0.76783800	-7.10864700	-0.40012500
H	1.45336900	0.03165100	-1.75939400
O	1.63019400	-1.49031100	-2.01431900
C	2.72682900	-1.78656800	-1.21537600
C	2.49242200	-2.33025300	0.17742800
C	2.96139500	-3.25174900	-0.93396800
H	1.45357400	-2.41917200	0.48378000
H	3.19410500	-2.09217100	0.97250200
H	3.98114600	-3.62476700	-0.88731800
H	2.23414900	-3.94291000	-1.34675000
C	3.91370100	-0.84973300	-1.49797000
H	4.18610500	-0.98650600	-2.55130400
H	3.52786200	0.17432800	-1.40368700
C	5.13095300	-1.00376400	-0.61948400
C	6.14073000	-1.92652100	-0.93061500
C	5.26842300	-0.24162000	0.55116600
C	7.24447900	-2.09515800	-0.09201300
H	6.05975300	-2.51400700	-1.84178400
C	6.37049400	-0.40539200	1.39217400
H	4.50665000	0.49277500	0.79815900
C	7.36191400	-1.33725000	1.07535400
H	8.01552900	-2.81520300	-0.35317500
H	6.45783000	0.19958000	2.29108000

H	8.22157400	-1.46570400	1.72726300

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P	0.58300800	-1.94750600	-0.16848400
C	0.22407600	-3.37795900	-1.27699800
C	-0.09372300	-2.44340400	1.47468600
C	2.41483800	-2.06669400	0.02011700
C	-0.09683000	-3.13881900	-2.62107100
C	0.33097100	-4.70115800	-0.82308300
C	-1.37359100	-1.98622300	1.83288400
C	0.61142600	-3.26021100	2.37260900
C	3.05605900	-1.50178200	1.13476700
C	3.19981300	-2.61106500	-1.00981900
C	-0.30257300	-4.20631500	-3.49774000
H	-0.19778300	-2.11750700	-2.97595400
C	0.11286500	-5.76537200	-1.69793900
H	0.57558700	-4.90476600	0.21453400
C	-1.93394300	-2.33857200	3.06075300
H	-1.92302000	-1.34208000	1.15343100
C	0.04985600	-3.60648800	3.60296000
H	1.60588100	-3.61522200	2.12306300
C	4.44849100	-1.47551400	1.21126200
H	2.47285100	-1.08681200	1.94762700
C	4.59272800	-2.57973600	-0.92998400
H	2.72694400	-3.05798900	-1.87821300
C	-0.20102900	-5.52011600	-3.03733500
H	-0.55191500	-4.00827300	-4.53624200
H	0.18755400	-6.78587300	-1.33301100
C	-1.22218100	-3.14686000	3.95038400
H	-2.92315600	-1.97329400	3.32193200
H	0.60973500	-4.23455400	4.29014000
C	5.22146600	-2.00870800	0.17821100
H	4.92434000	-1.03017400	2.07983600
H	5.18510400	-3.00495500	-1.73531000
H	-0.37065600	-6.35027200	-3.71719700
H	-1.65513300	-3.41525100	4.90989600
H	6.30572800	-1.98152100	0.23704500
Pd	-0.40118200	0.01901300	-0.83808600
P	1.15835100	1.74100200	-0.10108200

C	2.73583300	1.93411200	-1.02808800
C	1.66028000	1.47404800	1.65128600
C	0.47936600	3.44694100	-0.10800800
C	3.49131300	3.11805500	-0.98500800
C	3.19744200	0.85756800	-1.79811500
C	0.70346400	0.91159300	2.51286200
C	2.94181900	1.75218000	2.14627600
C	-0.04533000	3.93047700	-1.31811200
C	0.46636900	4.27112000	1.02506200
C	4.69545800	3.20982500	-1.68321400
H	3.13411600	3.96820000	-0.41162400
C	4.40503300	0.94984100	-2.49186800
H	2.61364000	-0.05384400	-1.85056300
C	1.02517000	0.62092500	3.83856800
H	-0.28638500	0.67363500	2.13674400
C	3.26304600	1.45933000	3.47346300
H	3.69889000	2.17298400	1.49334400
C	-0.55020400	5.22730600	-1.39407900
H	-0.07862000	3.28338700	-2.18680900
C	-0.05512200	5.56555100	0.94779000
H	0.86359200	3.90939600	1.96802100
C	5.15639600	2.12460500	-2.43414400
H	5.27191900	4.12990800	-1.64431500
H	4.75364500	0.10371700	-3.07673900
C	2.30944400	0.88852200	4.31988900
H	0.27920500	0.16809900	4.48494700
H	4.26281400	1.67025700	3.84295600
C	-0.55900600	6.04683300	-0.26114300
H	-0.95443600	5.59186400	-2.33416000
H	-0.06148100	6.19605000	1.83263600
H	6.09418900	2.19919000	-2.97761700
H	2.56635800	0.65113900	5.34836800
H	-0.96241900	7.05391100	-0.32083000
H	-1.50455200	-1.01725500	-1.24212000
O	-1.71025700	1.50024100	-1.41770100
C	-2.95444000	1.46388900	-0.82930500
C	-3.04846500	1.70052200	0.66749700
C	-3.47388200	2.78610200	-0.30387200
H	-2.10132100	1.84455100	1.17937200
H	-3.81925500	1.20475400	1.25150400
H	-4.53711200	3.00224600	-0.38116600
H	-2.81579500	3.64054500	-0.42313800
C	-3.93846300	0.50905500	-1.53233000
H	-4.14380300	0.92696000	-2.52543000
H	-3.38940900	-0.42713900	-1.69003800
C	-5.22929500	0.21110000	-0.81198100

C	-6.38710300	0.97115700	-1.03261200
C	-5.29048100	-0.82640700	0.13309000
C	-7.56538700	0.71123300	-0.32869500
H	-6.36220100	1.77204000	-1.76761200
C	-6.46480400	-1.09123300	0.83851700
H	-4.40402800	-1.43151600	0.30993800
C	-7.60846900	-0.32052300	0.61127900
H	-8.45104100	1.31234600	-0.51795200
H	-6.48976900	-1.90223000	1.56210500
H	-8.52498300	-0.52602400	1.15765900

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Pd	0.26110900	0.47174200	-2.01338700
P	1.66416100	-0.05675000	-0.08152600
O	-0.94251800	1.53318800	-0.81932600
C	-2.28865600	1.25234500	-0.79158300
C	-3.13820400	2.47630400	-0.46806100
C	-3.15917600	1.87056200	-1.85325600
H	-2.59553200	3.40567500	-0.32825900
H	-4.00602700	2.34061300	0.17141300
H	-4.05758500	1.34339700	-2.16273200
H	-2.62325100	2.39123500	-2.64160800
C	-2.61353100	-0.12308000	-0.19607500
H	-2.19087300	-0.86657300	-0.88474200
H	-2.04737000	-0.20656000	0.73657300
C	-4.06791100	-0.43068800	0.05890300
C	-4.87694300	-0.99367500	-0.93929900
C	-4.65006400	-0.14493700	1.30313000
C	-6.22861800	-1.25477600	-0.70619700
H	-4.43807700	-1.23149300	-1.90528700
C	-6.00077500	-0.40445500	1.54134800
H	-4.03123400	0.27898100	2.09035100
C	-6.79599700	-0.95906400	0.53543900
H	-6.83749300	-1.69273700	-1.49271600
H	-6.43168000	-0.17756700	2.51301600
H	-7.84707600	-1.16380700	0.71936500
C	2.35201800	1.37212200	0.84473400
C	1.59311100	2.55469100	0.88478100
C	3.58477100	1.31631200	1.51205700
C	2.06574200	3.66108300	1.59244800
H	0.63483500	2.59403800	0.37420900

C	4.05350300	2.42988000	2.21070300
H	4.18033400	0.40904500	1.48492900
C	3.29523200	3.60225800	2.25297700
H	1.47399000	4.57172800	1.62167300
H	5.01093200	2.38063000	2.72179900
H	3.66284700	4.46773500	2.79721100
C	3.10741500	-1.13476200	-0.43501500
C	3.80444000	-0.90876600	-1.63370700
C	3.54068500	-2.15352400	0.42729500
C	4.91850500	-1.68217900	-1.96078100
H	3.47902300	-0.11949200	-2.30821600
C	4.65239500	-2.92943700	0.09452900
H	3.00742200	-2.34293800	1.35364500
C	5.34240500	-2.69517400	-1.09734200
H	5.45025100	-1.49793300	-2.88980300
H	4.97984200	-3.71671600	0.76762700
H	6.20596200	-3.30207500	-1.35389100
C	0.66312500	-0.98684500	1.14568700
C	0.32889100	-0.46050300	2.39976800
C	0.10686100	-2.21435000	0.74642500
C	-0.55401400	-1.14787600	3.23745400
H	0.74335700	0.48959900	2.72023300
C	-0.76399300	-2.90204100	1.58855000
H	0.34620000	-2.62516700	-0.23100600
C	-1.10301300	-2.36564600	2.83459300
H	-0.81267000	-0.72640600	4.20472200
H	-1.19151000	-3.84719800	1.26668400
H	-1.79524000	-2.89359800	3.48396500
H	-0.71187500	0.76054200	-3.21286400

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Pd	-0.28301500	0.28787900	-1.07289900
P	-0.52228400	-0.90520900	1.01858900
H	0.06388800	1.08787600	-2.40680700
C	-2.17080000	-0.94508700	-2.10790500
C	-2.05610200	-1.87582400	1.33799100
C	-3.27857000	-1.20874800	1.15089800
C	-2.06895500	-3.22018400	1.73485900
C	-4.48713400	-1.87692900	1.34336300
H	-3.28472100	-0.16596400	0.84841400
C	-3.28092800	-3.88866300	1.92303700

H	-1.13675100	-3.75279100	1.88838700
C	-4.49132000	-3.22255600	1.72254900
H	-5.42417700	-1.34913700	1.19000200
H	-3.27626100	-4.93170600	2.22713000
H	-5.43254000	-3.74602100	1.86464100
C	-0.40230600	0.13216800	2.53187600
C	-0.32752500	1.52605300	2.40088300
C	-0.42544700	-0.43838800	3.81535600
C	-0.26753300	2.33734900	3.53687300
H	-0.31870000	1.97194700	1.41032300
C	-0.36069400	0.37304200	4.94651900
H	-0.49534100	-1.51670400	3.92656400
C	-0.28067700	1.76259500	4.80818300
H	-0.21058100	3.41634400	3.42520000
H	-0.37629100	-0.07628900	5.93546600
H	-0.23249700	2.39358500	5.69126100
C	0.85648100	-2.11141400	1.13207800
C	0.86454300	-3.19030100	0.22769200
C	1.97833300	-1.89353200	1.94220200
C	1.96113200	-4.04680200	0.16249000
H	0.01695400	-3.35745900	-0.42876600
C	3.08269200	-2.74571100	1.86051300
H	2.00664300	-1.05079600	2.62394200
C	3.07548700	-3.82517400	0.97835600
H	1.94881300	-4.87920400	-0.53550200
H	3.95318600	-2.55085400	2.47890500
H	3.93680200	-4.48415800	0.91621000
C	-2.70194500	0.14036000	-1.86462600
C	-3.34501100	1.31135000	-1.61052200
C	-3.93002400	2.35290300	-1.35613200
C	-1.78138100	-2.29686200	-2.35531700
C	-2.49891100	-3.34657600	-1.74619200
C	-0.65792900	-2.59104500	-3.15438700
C	-2.09332800	-4.66513300	-1.93859800
H	-3.34791200	-3.11556300	-1.11244700
C	-0.26781000	-3.91380500	-3.34248300
H	-0.09819900	-1.77464100	-3.59786700
C	-0.98068100	-4.95275700	-2.73465700
H	-2.64282600	-5.46805000	-1.45643700
H	0.60004500	-4.13489000	-3.95654900
H	-0.66716500	-5.98273100	-2.87805200
C	-4.58903500	3.57585000	-1.06104000
C	-5.80422500	3.57883200	-0.34455100
C	-4.03062500	4.80213800	-1.47993000
C	-6.44124200	4.78246900	-0.05660300
H	-6.23389000	2.63560300	-0.02232300

C	-4.67781900	5.99868500	-1.18520300
H	-3.09604700	4.79874200	-2.03167700
C	-5.88201900	5.99346900	-0.47499600
H	-7.37638300	4.77649900	0.49564100
H	-4.24181200	6.93852800	-1.51080100
H	-6.38304300	6.93002900	-0.24818200
C	1.64869800	0.86591900	-0.56479300
H	1.80983800	1.89877200	-0.88815700
H	1.74099000	0.84033500	0.52611000
C	2.71374800	-0.06472900	-1.17937400
H	2.66839500	-0.02199600	-2.27214200
H	2.55419900	-1.09740900	-0.85877600
C	4.08390300	0.37340300	-0.68130600
O	4.53306800	0.00116300	0.38795000
C	4.82575700	1.36681600	-1.58442300
H	5.03851700	0.84330300	-2.52604100
H	4.10687400	2.15489900	-1.84837100
C	6.08140100	1.95104200	-0.99198200
C	7.34401200	1.62123200	-1.49736000
C	6.00400200	2.83340900	0.09513100
C	8.50384000	2.16310100	-0.93747600
H	7.42037100	0.93455800	-2.33722100
C	7.15828700	3.37617300	0.65779800
H	5.02951900	3.09060400	0.50268500
C	8.41422300	3.04321100	0.14177100
H	9.47537800	1.89737400	-1.34556100
H	7.07934900	4.05882200	1.49968300
H	9.31435300	3.46682200	0.57868100

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C	6.59804500	-3.15358400	-0.73337600
C	5.83451000	-4.13290100	-0.09455100
C	4.51737600	-3.86146100	0.28452900
C	3.93700000	-2.61100700	0.03103300
C	4.71540300	-1.63824200	-0.61741800
C	6.03317700	-1.90190300	-0.99375400
C	2.51184600	-2.30660500	0.41996800
C	1.43128600	-2.51315100	-0.65551700
C	1.77933600	-2.48331100	-2.12361900
C	1.40269300	-3.79580900	-1.45061600
O	0.19586700	-2.02207900	-0.26900200

Pd	-0.10413300	0.01387100	-0.32209300
P	-2.37692100	-0.56033000	0.28948100
H	1.40878700	0.18184300	-0.67585700
H	0.42006900	-4.20676000	-1.66286100
H	2.19094500	-4.52980800	-1.29905400
H	2.81084400	-2.34948300	-2.43757100
H	1.03616400	-2.02398100	-2.76952400
H	2.44525800	-1.25442900	0.72385600
H	2.22174600	-2.90343400	1.29338200
H	3.93155900	-4.62565000	0.78961900
H	4.27750600	-0.66533600	-0.82710600
H	6.26577600	-5.10845400	0.11436500
H	6.61789100	-1.12942800	-1.48643100
H	7.62409300	-3.36236400	-1.02352600
C	-0.20069200	2.10413700	-0.54448100
C	-3.63053200	0.77123400	0.46654600
C	-3.32366200	1.84429200	1.32022400
C	-4.85517800	0.76706300	-0.21319900
C	-4.22628000	2.89053300	1.49193700
H	-2.37027300	1.86426000	1.84102000
C	-5.75635800	1.82165500	-0.04364200
H	-5.10986500	-0.05499900	-0.87386100
C	-5.44496700	2.88268800	0.80675100
H	-3.97215700	3.71923400	2.14583300
H	-6.70207600	1.81020400	-0.57825500
H	-6.14472900	3.70393300	0.93242700
C	-2.47429600	-1.42504300	1.91686400
C	-1.43745100	-2.30252900	2.27686100
C	-3.56420200	-1.24947900	2.78492100
C	-1.49728000	-2.98851300	3.49052700
H	-0.60644700	-2.44358700	1.58877700
C	-3.61388700	-1.93955800	3.99775900
H	-4.37284500	-0.57601400	2.52133500
C	-2.58051900	-2.80831200	4.35389800
H	-0.69113100	-3.66472300	3.76205300
H	-4.46081300	-1.79554700	4.66297000
H	-2.62002300	-3.34201100	5.29957000
C	-3.10665600	-1.73715500	-0.91462000
C	-2.68779600	-1.67296400	-2.25195100
C	-4.07835800	-2.67791900	-0.54306000
C	-3.24175600	-2.52704100	-3.20584500
H	-1.91363000	-0.96757500	-2.54014900
C	-4.62774000	-3.53389100	-1.49866700
H	-4.40112300	-2.74644000	0.49127400
C	-4.21213300	-3.45866500	-2.83028200
H	-2.90551900	-2.47360900	-4.23734300

H	-5.37676000	-4.26233700	-1.20137200
H	-4.63730000	-4.12993200	-3.57110400
C	1.03377200	1.88680500	-0.28436400
C	2.34451700	2.23093400	-0.04761500
C	3.51823000	2.47942000	0.17917800
C	-1.20810700	3.09770400	-0.82330200
C	-1.10087700	4.38609800	-0.26291200
C	-2.29936300	2.80079900	-1.65881900
C	-2.07064000	5.34805600	-0.53249700
H	-0.26070400	4.61541400	0.38548100
C	-3.25832600	3.77120400	-1.93334500
H	-2.38545700	1.80413500	-2.07737600
C	-3.15038800	5.04431900	-1.36725900
H	-1.98406500	6.33713700	-0.09172900
H	-4.09962700	3.52884700	-2.57507900
H	-3.90660400	5.79640200	-1.57269600
C	4.88731400	2.76126100	0.43523100
C	5.37770600	4.08161100	0.35694700
C	5.77429600	1.71445800	0.76661100
C	6.72308300	4.34202200	0.60223900
H	4.69707100	4.88771200	0.10201500
C	7.11775100	1.98827400	1.00617100
H	5.40239700	0.69726300	0.82704000
C	7.59644500	3.29931600	0.92580600
H	7.09240000	5.36148700	0.53920100
H	7.79204800	1.17457400	1.25677300
H	8.64555300	3.50793000	1.11427700

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Pd	-1.16081800	0.22632300	0.38490600
O	-1.65166400	2.09485900	1.09710300
C	-3.66033700	0.51602900	1.02566500
C	-4.00603100	1.79647400	1.76779100
H	-4.35905800	0.13604000	0.28815400
H	-3.18083500	-0.25107400	1.63334800
H	-4.97905600	2.23737200	1.56621100
H	-3.68085300	1.85997300	2.80186300
C	0.82159900	0.53080000	0.37029600
C	1.46016100	0.89821800	-0.76981100
H	0.90058000	0.95585600	-1.70131100
P	-0.91512800	-1.93229400	-0.36602000

C	-2.94806900	1.95134500	0.73230100
C	-3.34468400	2.60083500	-0.60265000
H	-2.64127000	2.24798700	-1.36613800
H	-4.34661600	2.27051500	-0.89791200
C	-3.30219000	4.11046300	-0.51733200
C	-2.07125700	4.78237600	-0.46718200
C	-4.48122000	4.86380900	-0.45039800
C	-2.02466400	6.17174100	-0.35332700
H	-1.15422200	4.20274300	-0.50215800
C	-4.43750200	6.25574400	-0.33767900
H	-5.44280600	4.35680900	-0.49216700
C	-3.20760200	6.91401000	-0.28861400
H	-1.06301900	6.67658700	-0.31469200
H	-5.36300200	6.82370100	-0.29045500
H	-3.16993400	7.99660200	-0.20267600
C	1.47805100	0.33297300	1.67854900
C	2.61635600	-0.48737800	1.79440900
C	0.94235500	0.90422200	2.85067100
C	3.19747600	-0.73292600	3.03831200
H	3.04295400	-0.93303900	0.90250700
C	1.53282800	0.66473000	4.09018600
H	0.06263200	1.53595900	2.76965500
C	2.65796500	-0.15983200	4.19219900
H	4.06959700	-1.37792700	3.10522800
H	1.11155800	1.12209400	4.98156700
H	3.11011000	-0.35167000	5.16139300
C	2.84288600	1.20272200	-0.85351500
C	4.03544500	1.43984300	-0.93666300
C	5.43699600	1.68173800	-0.95622100
C	6.10774900	1.99778300	-2.15625800
C	6.18388100	1.59789000	0.23918600
C	7.48246700	2.22126200	-2.15648800
H	5.53890700	2.06504000	-3.07851800
C	7.55779100	1.82288700	0.22719300
H	5.67029900	1.35637800	1.16475100
C	8.21321200	2.13496100	-0.96788900
H	7.98629000	2.46473000	-3.08786600
H	8.12016900	1.75622800	1.15447900
H	9.28505700	2.31122900	-0.97250300
C	-0.18329400	-3.06788500	0.87413000
C	0.34212600	-4.31965400	0.51120400
C	-0.15243100	-2.67397500	2.22005300
C	0.88073300	-5.16252100	1.48289600
H	0.33838700	-4.63027200	-0.52905500
C	0.38987400	-3.51939200	3.18907900
H	-0.52513500	-1.69570000	2.50617000

C	0.90579200	-4.76301200	2.82233300
H	1.28603600	-6.12782200	1.19349400
H	0.42512800	-3.19353900	4.22408900
H	1.33484700	-5.41775100	3.57552900
C	0.11565100	-2.18063600	-1.86941900
C	-0.44640000	-2.28451400	-3.14965000
C	1.51433100	-2.16861000	-1.73555800
C	0.37719000	-2.36912600	-4.27441300
H	-1.52335600	-2.30863100	-3.27675800
C	2.33234100	-2.25469300	-2.86061700
H	1.96365400	-2.09527800	-0.75209700
C	1.76572500	-2.35075900	-4.13383600
H	-0.07064000	-2.45370300	-5.26048000
H	3.41133800	-2.23541400	-2.73978800
H	2.40344500	-2.41293200	-5.01090900
C	-2.56256100	-2.63667700	-0.79018100
C	-3.44760100	-1.83570100	-1.53412000
C	-2.97436800	-3.91504800	-0.38776500
C	-4.70919300	-2.31421100	-1.88732600
H	-3.14909000	-0.83476700	-1.83377900
C	-4.24352500	-4.38504900	-0.73196500
H	-2.31141100	-4.54476000	0.19575600
C	-5.11037600	-3.59018200	-1.48390400
H	-5.37975000	-1.68730300	-2.46794900
H	-4.55289200	-5.37568200	-0.41121400
H	-6.09622100	-3.96032600	-1.75002700

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Pd	-1.10978000	0.21734500	0.44731800
O	-1.66112600	2.08658600	1.20535900
C	-3.42556200	0.10288500	1.09954400
C	-3.93594000	1.37456100	1.76316800
H	-4.05110500	-0.33836700	0.33185600
H	-2.97796900	-0.60723200	1.79245800
H	-4.95696800	1.67101600	1.53029500
H	-3.67842100	1.48763200	2.81358600
C	0.88626900	0.58107200	0.37851300
C	1.49323000	1.01079100	-0.75848100
H	0.91498800	1.07186800	-1.67911300
P	-0.82307600	-1.89977600	-0.36666500
C	-2.88732700	1.79802800	0.81178700

C	-3.34128200	2.32405400	-0.55703100
H	-2.52104400	2.18049600	-1.26784100
H	-4.20319300	1.75268500	-0.91475700
C	-3.69717200	3.79322800	-0.45445000
C	-2.68819700	4.75232700	-0.27930500
C	-5.03130400	4.21771000	-0.49343200
C	-3.00926700	6.10326700	-0.14910400
H	-1.65330300	4.42676700	-0.23322100
C	-5.35493500	5.57074100	-0.36463600
H	-5.82266500	3.48436100	-0.63187900
C	-4.34386000	6.51742000	-0.19185200
H	-2.21676200	6.83441400	-0.01428300
H	-6.39510500	5.88345800	-0.40077900
H	-4.59253200	7.57046500	-0.09279300
C	1.58902700	0.37475900	1.66286100
C	2.77467400	-0.38277600	1.73153600
C	1.04680400	0.86730600	2.86807900
C	3.38932500	-0.64614800	2.95572200
H	3.21317000	-0.76542300	0.81652300
C	1.67067900	0.61340600	4.08846300
H	0.13484000	1.45594100	2.82983100
C	2.84025700	-0.15135300	4.14093300
H	4.29765600	-1.24250600	2.98244500
H	1.24057500	1.01255800	5.00344800
H	3.31919300	-0.35641700	5.09442900
C	2.85862100	1.38225800	-0.86212400
C	4.03634800	1.68108800	-0.96112100
C	5.42308600	1.99498400	-0.99749700
C	6.05409100	2.38552200	-2.19733000
C	6.19677000	1.91075700	0.18094400
C	7.41513000	2.68078200	-2.21387600
H	5.46507700	2.45345200	-3.10681800
C	7.55672800	2.20759600	0.15276900
H	5.71412900	1.61231800	1.10655800
C	8.17228700	2.59348600	-1.04198200
H	7.88754000	2.98129500	-3.14510700
H	8.13937300	2.13962700	1.06741500
H	9.23330200	2.82570700	-1.05922500
C	-0.10075000	-3.04853600	0.86825200
C	0.41328100	-4.30176400	0.49330300
C	-0.05023900	-2.66120800	2.21511600
C	0.95703600	-5.15303600	1.45435300
H	0.39755400	-4.60574200	-0.54887000
C	0.49935500	-3.51419300	3.17374500
H	-0.41139700	-1.68109900	2.50925600
C	1.00140600	-4.75975400	2.79534800

H	1.35290000	-6.11938900	1.15553700
H	0.55077500	-3.19247400	4.20942200
H	1.43548200	-5.42076800	3.54013300
C	0.27632300	-2.09047200	-1.83248100
C	-0.22156600	-2.15846800	-3.14106300
C	1.66675900	-2.07750000	-1.63145200
C	0.65626000	-2.20417600	-4.22678100
H	-1.29010400	-2.18602000	-3.32363100
C	2.53913900	-2.12502800	-2.71688300
H	2.06703200	-2.03179400	-0.62557300
C	2.03596000	-2.18345600	-4.01874000
H	0.25680900	-2.26050000	-5.23542400
H	3.61085700	-2.10422900	-2.54304600
H	2.71596900	-2.21510500	-4.86517300
C	-2.42472600	-2.64731900	-0.88465900
C	-3.27219300	-1.87741800	-1.70151400
C	-2.84161800	-3.92411500	-0.48484400
C	-4.49689500	-2.38632700	-2.13175500
H	-2.97487200	-0.87325600	-1.99136100
C	-4.07643700	-4.42479700	-0.90512000
H	-2.21069100	-4.53056100	0.15575600
C	-4.90254500	-3.66252200	-1.73180100
H	-5.13747400	-1.78262400	-2.76820500
H	-4.38993300	-5.41413000	-0.58430100
H	-5.86084300	-4.05632500	-2.05781200

int5

84

Pd	-1.00656800	0.11589500	-0.96016900
O	-0.90552300	2.07328700	-1.99895100
C	-3.02815000	0.36266500	-1.57839700
C	-3.25539200	1.88349800	-1.64635100
H	-3.09918000	-0.06957300	-2.58632500
H	-3.81485400	-0.10539100	-0.97744300
H	-4.10240700	2.19903300	-2.27474300
H	-3.47447900	2.29135300	-0.64580500
C	1.03579300	0.15315000	-0.47143500
C	1.95417600	-0.47013700	-1.26404600
H	1.59891200	-1.09636700	-2.08374700

P	-1.44735500	-1.79409700	0.11740000
C	-2.01742700	2.61624400	-2.08226800
C	-2.08505500	4.06921900	-2.50674200
H	-1.25927700	4.26557400	-3.19581800
H	-3.03281500	4.27519900	-3.01068200
C	-1.94836300	4.92222800	-1.25189400
C	-0.68231300	5.14654000	-0.69344100
C	-3.07967800	5.43525300	-0.60502600
C	-0.55075400	5.88053300	0.48628200
H	0.19893400	4.73952500	-1.18045300
C	-2.94807900	6.16753200	0.57689400
H	-4.06567600	5.26553400	-1.03035000
C	-1.68355400	6.39111400	1.12577400
H	0.43712600	6.05041700	0.90413200
H	-3.83308200	6.56461400	1.06612000
H	-1.58072800	6.96179200	2.04423100
C	1.42049200	0.95011700	0.71402100
C	2.38208900	0.49788600	1.64391500
C	0.77326900	2.17252900	0.99638300
C	2.67744900	1.23010500	2.79405600
H	2.88744600	-0.44303800	1.46034500
C	1.07961900	2.91141000	2.13772100
H	0.03265700	2.55156700	0.29999100
C	2.03060300	2.44241400	3.04836400
H	3.41669100	0.85020200	3.49523800
H	0.56672800	3.85301700	2.31562600
H	2.26271200	3.01197500	3.94423200
C	3.36635200	-0.37688600	-1.14958500
C	4.58083400	-0.30333500	-1.05934100
C	5.98466700	-0.17952000	-0.87181200
C	6.89801200	-0.89355000	-1.67666900
C	6.49188000	0.66648600	0.13953800
C	8.26978800	-0.76371200	-1.47369200
H	6.51686500	-1.54596500	-2.45634200
C	7.86508500	0.78849800	0.33409400
H	5.79358900	1.21865900	0.76108400
C	8.76066600	0.07621500	-0.46974400
H	8.95975600	-1.32015400	-2.10237800
H	8.23942400	1.44383900	1.11600400
H	9.83138700	0.17543200	-0.31545800
C	-2.24443900	-1.50401200	1.74950900
C	-2.28247300	-2.50661500	2.73318100
C	-2.83022400	-0.25832900	2.01999700
C	-2.90892700	-2.26906700	3.95664900
H	-1.81307600	-3.46773100	2.54799600
C	-3.45355200	-0.02334500	3.24641000

H	-2.78376000	0.52625600	1.27158900
C	-3.49628800	-1.02789500	4.21473300
H	-2.93137100	-3.05110600	4.71020500
H	-3.89734300	0.94765800	3.44664900
H	-3.97779800	-0.84286700	5.17078500
C	-0.03206100	-2.89632200	0.52502900
C	0.25813300	-4.04438600	-0.22366200
C	0.82973000	-2.52143500	1.56891000
C	1.39587200	-4.80226400	0.06508800
H	-0.39706300	-4.35287500	-1.03148700
C	1.95939700	-3.28366600	1.85690100
H	0.62580800	-1.62682400	2.14743200
C	2.24809300	-4.42462900	1.10288000
H	1.61173700	-5.68982000	-0.52297900
H	2.61955000	-2.97990800	2.66421900
H	3.13355000	-5.01376300	1.32361800
C	-2.59614500	-2.88294100	-0.82587400
C	-2.42593800	-2.96348000	-2.21800500
C	-3.60548600	-3.64036000	-0.21630300
C	-3.23847200	-3.80052500	-2.98226700
H	-1.66048700	-2.36220400	-2.70071300
C	-4.42679600	-4.46654400	-0.98665800
H	-3.76158600	-3.58452000	0.85554100
C	-4.24306800	-4.55223500	-2.36760500
H	-3.09321100	-3.85685700	-4.05728400
H	-5.21118000	-5.04276900	-0.50408400
H	-4.88306800	-5.19658500	-2.96363200

int6

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Pd	-0.31011700	-0.09714100	-0.50935600
P	-0.59935900	-2.25705700	0.51797000
P	-2.59849500	0.60487100	-0.64679200
C	1.73905700	-0.28074900	-0.35158600
C	2.49923100	-0.65719000	-1.42027600
H	1.99358900	-0.86471900	-2.36313000
C	0.14376300	1.59183600	-1.72575500
H	-0.76375100	2.01609700	-2.16256700
H	0.74138000	1.18864100	-2.55182400
C	-1.82319000	-3.23575800	-0.46336400
C	-2.70257300	-4.17833200	0.08651800

C	-1.88513700	-2.97615600	-1.84298200
C	-3.62569600	-4.84016200	-0.72500300
H	-2.69765400	-4.37699600	1.15179800
C	-2.80670900	-3.63932900	-2.65412300
H	-1.22634000	-2.22975200	-2.27622700
C	-3.68354200	-4.57127300	-2.09463500
H	-4.30878800	-5.55984600	-0.28235600
H	-2.85067400	-3.41113900	-3.71496700
H	-4.41100800	-5.08030000	-2.72047000
C	-1.17936300	-2.31659300	2.26080800
C	-1.19811500	-3.49872100	3.02260200
C	-1.60779900	-1.12185900	2.85457100
C	-1.66054500	-3.48374900	4.33773500
H	-0.83273700	-4.42634800	2.59324900
C	-2.07140300	-1.10766100	4.17112800
H	-1.57641200	-0.20211600	2.28213300
C	-2.10216000	-2.28843100	4.91294000
H	-1.67057200	-4.40355700	4.91563700
H	-2.40668000	-0.17404800	4.61321600
H	-2.46082600	-2.27886700	5.93833300
C	0.88236800	-3.35808000	0.51644400
C	1.24019000	-4.05246600	-0.65037100
C	1.73057300	-3.42765200	1.63142600
C	2.41328700	-4.80398300	-0.69677100
H	0.60342800	-4.00908600	-1.52811300
C	2.89963200	-4.19001000	1.58486900
H	1.49011500	-2.88103200	2.53634200
C	3.24662500	-4.87771400	0.42212400
H	2.67606500	-5.33249900	-1.60877100
H	3.54494800	-4.23006700	2.45794200
H	4.16105100	-5.46272400	0.38468300
C	-3.92864100	-0.11268100	0.42141900
C	-4.34749100	0.50248800	1.61111600
C	-4.49002500	-1.35199800	0.07033900
C	-5.28877700	-0.11442800	2.43699400
H	-3.94615800	1.46745200	1.89961900
C	-5.43066500	-1.96474500	0.89725300
H	-4.20007700	-1.84001600	-0.85294000
C	-5.82927100	-1.35220500	2.08692800
H	-5.59960000	0.37789100	3.35427600
H	-5.84587700	-2.92559300	0.60807100
H	-6.55903000	-1.83284500	2.73226300
C	-3.34194900	0.48813300	-2.32660500
C	-2.52232300	0.16997100	-3.41992700
C	-4.71539700	0.69268500	-2.54106800
C	-3.06362700	0.06275000	-4.70230100

H	-1.46146900	0.00493400	-3.26591200
C	-5.25393100	0.58502600	-3.82315700
H	-5.36562500	0.92710200	-1.70384600
C	-4.42901100	0.26922000	-4.90598700
H	-2.41664600	-0.18311600	-5.53950400
H	-6.31752400	0.74509200	-3.97569600
H	-4.85013200	0.18309800	-5.90370100
C	-2.62632400	2.39561900	-0.20627800
C	-1.94098000	2.78496400	0.95903400
C	-3.21751400	3.38147500	-1.00504600
C	-1.86148100	4.12749600	1.32442800
H	-1.44434400	2.03454900	1.56819000
C	-3.12748300	4.72849600	-0.64312000
H	-3.73289600	3.10837900	-1.91942600
C	-2.45282300	5.10386300	0.51842100
H	-1.30493300	4.41552200	2.21071900
H	-3.57772000	5.48418400	-1.28051500
H	-2.36990400	6.15200900	0.78866200
C	0.90819700	2.70625000	-1.03083200
H	0.38186900	3.04364900	-0.12938100
H	1.88610900	2.36477800	-0.67355500
C	1.12410500	3.96474800	-1.85027900
C	2.11080500	4.99006300	-1.25746600
H	3.11120700	4.54419800	-1.33231500
H	2.08613100	5.87212700	-1.90288900
C	1.81935100	5.35655900	0.18256400
C	0.93872200	6.40675900	0.47788300
C	2.37775100	4.63287100	1.24654600
C	0.62978900	6.73224600	1.80002100
H	0.49245400	6.97089400	-0.33715000
C	2.06375800	4.94947400	2.56902900
H	3.05612500	3.80994300	1.03967100
C	1.18933900	6.00240400	2.85189700
H	-0.04761400	7.55618500	2.00857800
H	2.51062900	4.37571000	3.37586700
H	0.95277300	6.25648900	3.88147800
O	0.57432200	4.18350200	-2.91501400
C	2.29999700	0.00038700	0.99203500
C	3.40307300	-0.70383100	1.52167300
C	1.69315300	0.96274400	1.82792900
C	3.87885700	-0.44635200	2.80716600
H	3.86812900	-1.48032200	0.92951100
C	2.17328800	1.22758900	3.10949600
H	0.83722500	1.51295700	1.45454700
C	3.27169800	0.52328100	3.60914300
H	4.72278900	-1.01693700	3.18700300

H	1.68430400	1.98393700	3.71748000
H	3.64367100	0.72142300	4.61069200
C	3.91114500	-0.77427800	-1.47257900
C	5.12460100	-0.87657300	-1.55068400
C	6.54161900	-0.99046800	-1.54194800
C	7.27622600	-0.60144100	-0.39968200
C	7.24321900	-1.49579400	-2.65726700
C	8.66332900	-0.71887800	-0.37932800
H	6.74227900	-0.20844700	0.46018400
C	8.63104500	-1.60828900	-2.62647200
H	6.68654000	-1.79639800	-3.53958500
C	9.34781000	-1.22197600	-1.49007200
H	9.21408500	-0.41504200	0.50681700
H	9.15648100	-1.99911500	-3.49363500
H	10.43028500	-1.31060000	-1.47076100

ts4

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Pd	0.41626500	-0.12380600	0.28841900
P	0.24872400	-2.36300700	-0.46593900
P	2.79651900	0.36141300	0.48605000
C	-1.56002900	0.38527400	0.44377300
C	-2.34972300	-0.07034000	1.48241500
H	-1.85232200	-0.30395500	2.42312300
C	-0.27112500	1.82268900	1.24352300
H	0.52724100	2.33253700	0.69951500
H	0.10183800	1.50623400	2.21904500
C	0.95712400	-3.46666000	0.84683300
C	1.56829200	-4.70404700	0.59495700
C	0.92336100	-2.98948100	2.16911100
C	2.13223400	-5.44137300	1.63801700
H	1.63517300	-5.08708400	-0.41644000
C	1.47940000	-3.73148200	3.21231400
H	0.48477100	-2.01635900	2.37380000
C	2.08937700	-4.95916000	2.94836300
H	2.61053000	-6.39319900	1.42348900
H	1.44865600	-3.34016200	4.22517700
H	2.53481200	-5.53318200	3.75593300
C	1.09805500	-2.84513000	-2.02833100
C	0.93244800	-4.10055400	-2.64113000
C	1.94995600	-1.90886300	-2.63157000
C	1.62819200	-4.41685400	-3.80776300

H	0.24364400	-4.82447900	-2.21692500
C	2.64806100	-2.22625500	-3.79808200
H	2.06920200	-0.93010000	-2.18200400
C	2.49334300	-3.48257600	-4.38448400
H	1.49118600	-5.39102500	-4.26885300
H	3.31396600	-1.49164300	-4.24116800
H	3.03657500	-3.73207800	-5.29168800
C	-1.46131400	-3.01518800	-0.67716800
C	-2.23806700	-3.27572900	0.46435800
C	-2.06935600	-3.10217000	-1.94048600
C	-3.58444800	-3.61998700	0.34445900
H	-1.79429400	-3.20396700	1.45169700
C	-3.41135400	-3.46747400	-2.05784600
H	-1.50105400	-2.87649000	-2.83631600
C	-4.17601800	-3.71865400	-0.91684300
H	-4.17488800	-3.79616700	1.23837500
H	-3.86255300	-3.53478900	-3.04400500
H	-5.22657900	-3.97925400	-1.00674600
C	4.10386100	-0.73947600	-0.20742600
C	5.08163200	-0.29183400	-1.10855500
C	4.05440600	-2.10729700	0.11119000
C	5.98553800	-1.19350600	-1.67535700
H	5.13831700	0.75763300	-1.37681100
C	4.96629300	-3.00274100	-0.44506200
H	3.29267900	-2.47768000	0.78631900
C	5.93213600	-2.54913800	-1.34599700
H	6.73332800	-0.83207700	-2.37599600
H	4.90591700	-4.05579900	-0.18611000
H	6.63447500	-3.24755900	-1.79204500
C	3.28720800	0.63877600	2.24465100
C	2.76941400	1.76146400	2.91900900
C	4.04627800	-0.29320700	2.96880800
C	3.00668600	1.93824400	4.28206800
H	2.18326300	2.50744000	2.39324000
C	4.27834800	-0.11119900	4.33380100
H	4.46566300	-1.16198000	2.47373700
C	3.75820400	1.00186900	4.99619200
H	2.59890800	2.81252100	4.78152400
H	4.87240600	-0.84165900	4.87635300
H	3.94028800	1.14124300	6.05810200
C	3.12938000	1.98352700	-0.32436600
C	2.34938000	2.33100500	-1.43976000
C	4.12682700	2.87003400	0.11066500
C	2.56267800	3.53729300	-2.10799400
H	1.56141400	1.66151100	-1.77408400
C	4.33575800	4.07853100	-0.55576600

H	4.73524300	2.61947200	0.97395700
C	3.55571700	4.41358300	-1.66554700
H	1.94026300	3.79815000	-2.95839000
H	5.10760700	4.75869400	-0.20672900
H	3.71908600	5.35676200	-2.17948400
C	-1.37546500	2.85790500	1.45778200
H	-1.96493600	3.04885600	0.55810600
H	-2.09457100	2.51842200	2.21493800
C	-0.79881700	4.18216000	1.93772700
C	-1.57793400	5.43356800	1.53083900
H	-2.64668800	5.28708500	1.72048200
H	-1.21829800	6.27071800	2.13584400
C	-1.33892800	5.68195400	0.05048800
C	-0.05137600	6.00784100	-0.40149000
C	-2.36347100	5.51895800	-0.89040200
C	0.19918700	6.18561600	-1.76205900
H	0.75653000	6.10774400	0.31838100
C	-2.11334500	5.69373600	-2.25340100
H	-3.36112700	5.24782100	-0.55524700
C	-0.83154100	6.03011400	-2.69351500
H	1.20151700	6.43946900	-2.09373000
H	-2.91969600	5.56110600	-2.96900400
H	-0.63642800	6.16912900	-3.75328900
O	0.25134200	4.27035300	2.55381800
C	-2.08234800	0.73954300	-0.90243500
C	-3.11009800	-0.01956400	-1.49900000
C	-1.51299400	1.77794100	-1.67162600
C	-3.55244300	0.25704400	-2.79245900
H	-3.54521600	-0.84660200	-0.95575200
C	-1.96851600	2.06317900	-2.95726300
H	-0.71038600	2.37661100	-1.25828400
C	-2.99229100	1.30308100	-3.52839400
H	-4.33610600	-0.35866200	-3.22624700
H	-1.52077300	2.88582100	-3.50745600
H	-3.34394400	1.52009400	-4.53336800
C	-3.74412400	-0.24420900	1.46679700
C	-4.95040700	-0.44644800	1.46300100
C	-6.33947200	-0.70669400	1.34552600
C	-7.01659900	-0.41807800	0.13761300
C	-7.07642100	-1.27143600	2.41053300
C	-8.37548900	-0.68859600	0.00689400
H	-6.45806800	0.01712200	-0.68555200
C	-8.43582600	-1.53741300	2.26781000
H	-6.56754600	-1.49735500	3.34280800
C	-9.09397000	-1.24910400	1.06829000
H	-8.87888100	-0.46042300	-0.92900200

H	-8.98586100	-1.97269500	3.09799100
H	-10.15466500	-1.45766300	0.96192400

int1_p2

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Pd	0.20889200	0.50494600	-0.09370600
C	0.05375500	2.58392700	0.05247000
C	-1.14415800	2.11483700	-0.05953700
C	-2.51107900	2.22967900	-0.10453400
C	-3.73360600	2.23972900	-0.15334600
C	-5.14948400	2.14820500	-0.21646200
C	-5.96409500	3.29964100	-0.24488400
C	-5.76199000	0.87642300	-0.25806900
C	-7.34980100	3.17805300	-0.31392900
H	-5.49752500	4.27938600	-0.21284300
C	-7.14753500	0.76698300	-0.32784800
H	-5.13709400	-0.00933800	-0.24037900
C	-7.94664200	1.91426200	-0.35579400
H	-7.96713200	4.07184600	-0.33508700
H	-7.60488800	-0.21798700	-0.36312800
H	-9.02793900	1.82470200	-0.41020000
C	0.83028600	3.79540100	0.19384800
C	0.27910000	5.04009500	-0.17936600
C	2.14386900	3.76417500	0.69741400
C	1.02592800	6.20880900	-0.05663600
H	-0.73422100	5.07199000	-0.56908100
C	2.88297400	4.93751800	0.82756300
H	2.57026300	2.81288500	0.99133300
C	2.33066600	6.16336700	0.44673100
H	0.59020100	7.15930300	-0.35286200
H	3.89418400	4.89232700	1.22262600
H	2.91040500	7.07734400	0.54110600
P	-1.16106700	-1.42695500	0.05093800
P	2.49022300	-0.06707800	-0.17429200
C	-0.45880400	-3.12425800	-0.12437600
C	0.48926600	-3.53978800	0.82700700
C	-0.79967600	-3.99900600	-1.16428500
C	1.05329900	-4.81034800	0.75961400

H	0.77929800	-2.86756900	1.62969800
C	-0.22296200	-5.27047100	-1.23741300
H	-1.52359300	-3.69888800	-1.91440100
C	0.69616800	-5.68238600	-0.27334700
H	1.78297100	-5.11528000	1.50360600
H	-0.50017700	-5.93850400	-2.04837100
H	1.14150800	-6.67155500	-0.32973600
C	-2.60104300	-1.44287600	-1.10877400
C	-3.68968800	-2.31622900	-0.94348300
C	-2.60612000	-0.54860400	-2.18785000
C	-4.75298500	-2.30029500	-1.84587200
H	-3.70876300	-3.00815200	-0.10751700
C	-3.67468000	-0.52922700	-3.08790600
H	-1.77911000	0.14503100	-2.30900600
C	-4.74786600	-1.40442000	-2.91956100
H	-5.58878500	-2.98040600	-1.70654200
H	-3.67124000	0.17913200	-3.91122500
H	-5.58251300	-1.38343500	-3.61446100
C	-1.98558400	-1.54628300	1.70997200
C	-2.38686300	-2.76968800	2.27233500
C	-2.25421500	-0.36055600	2.41170900
C	-3.04744400	-2.80298200	3.50140500
H	-2.17663100	-3.70131600	1.75719200
C	-2.92003000	-0.39600600	3.63799500
H	-1.94491100	0.59159100	1.99610600
C	-3.31790600	-1.61642000	4.18668600
H	-3.34934000	-3.75793300	3.92295900
H	-3.12253100	0.53277700	4.16393200
H	-3.83205800	-1.64392900	5.14338800
C	3.30103500	0.28884800	1.44787600
C	4.56910900	0.87140800	1.58782400
C	2.56786000	-0.02726000	2.60509100
C	5.09261400	1.12800500	2.85772000
H	5.14673000	1.13936800	0.70974900
C	3.09814200	0.21687500	3.87121800
H	1.56970800	-0.44691100	2.50927300
C	4.36232200	0.79818700	4.00059200
H	6.07265900	1.58776700	2.95101000
H	2.51816800	-0.03317400	4.75519300
H	4.77125500	1.00051300	4.98646500
C	3.49219800	0.85679000	-1.42832700
C	4.79912000	0.46541500	-1.76854000
C	2.93109300	1.96910900	-2.07089500
C	5.53403100	1.18989800	-2.70672200
H	5.24123100	-0.41153500	-1.30557100
C	3.66720200	2.69253900	-3.01180200

H	1.91593100	2.26539200	-1.83427600
C	4.97047000	2.30810200	-3.32803200
H	6.54401400	0.87736600	-2.95744800
H	3.21711600	3.55449200	-3.49608900
H	5.54295900	2.86981200	-4.06101300
C	3.04292200	-1.78919700	-0.54597800
C	4.00615700	-2.47400800	0.20649900
C	2.50119400	-2.40590900	-1.68543400
C	4.43253000	-3.74669800	-0.18456400
H	4.43354200	-2.01414500	1.09184400
C	2.93422400	-3.66999600	-2.07793400
H	1.73481700	-1.89302400	-2.26065700
C	3.90400400	-4.34340700	-1.32854000
H	5.18208400	-4.26682500	0.40588900
H	2.50338000	-4.13754400	-2.95812600
H	4.23596000	-5.33240000	-1.63171200

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Pd	-0.45224900	-0.20393200	-0.01982700
C	-1.36664200	1.64194200	-0.04136800
C	-2.33817600	0.81594800	-0.02016700
C	-3.61409300	0.32533100	-0.01819700
C	-4.74050800	-0.15378400	-0.01497600
C	-6.05948800	-0.68201900	-0.01142200
C	-7.17384000	0.17113500	0.14304500
C	-6.27840400	-2.06844000	-0.16279400
C	-8.46407400	-0.35141700	0.14597000
H	-7.01073900	1.23794600	0.25944700
C	-7.57318900	-2.57992300	-0.15980500
H	-5.42498000	-2.72863800	-0.28195100
C	-8.66933900	-1.72600000	-0.00560400
H	-9.31304200	0.31560700	0.26594700
H	-7.72850200	-3.64856100	-0.27794500
H	-9.67784200	-2.12936100	-0.00352600
C	-0.83640600	2.98299200	-0.03661100
C	-1.69393200	4.06688000	0.24790400
C	0.52112000	3.24047200	-0.30702900
C	-1.19905200	5.36788900	0.26394000
H	-2.74144800	3.87201400	0.45719600
C	1.00691000	4.54585900	-0.29198800
H	1.17964200	2.41014000	-0.53591100
C	0.15179600	5.61316700	-0.00450200

H	-1.86841300	6.19408900	0.48699700
H	2.05617200	4.72882400	-0.50605400
H	0.53352400	6.63005400	0.00967700
P	1.80739200	-0.73484100	0.01034500
C	2.68621500	-0.32951200	1.58031900
C	3.73226100	-1.10997000	2.09439600
C	2.29294800	0.82932900	2.26998300
C	4.37592900	-0.73415800	3.27575600
H	4.04455600	-2.01127500	1.57601700
C	2.94451900	1.20660700	3.44389500
H	1.47468300	1.43221500	1.88598600
C	3.98586700	0.42443500	3.95034300
H	5.18187300	-1.34837600	3.66774800
H	2.63199600	2.10573000	3.96745500
H	4.48737600	0.71388700	4.86955500
C	2.20841600	-2.51232400	-0.26580800
C	3.29796000	-2.94986500	-1.03256900
C	1.36818900	-3.46470500	0.33522800
C	3.54337100	-4.31589800	-1.19057700
H	3.95397700	-2.22734500	-1.50780100
C	1.62032000	-4.82766100	0.18221600
H	0.51617200	-3.13530000	0.92596700
C	2.70838900	-5.25569200	-0.58316200
H	4.38853800	-4.64412500	-1.78922000
H	0.96398400	-5.55408200	0.65293600
H	2.90112000	-6.31730400	-0.70939000
C	2.79464300	0.15493900	-1.26944800
C	2.17620900	0.43419500	-2.49924500
C	4.11941100	0.56799300	-1.06180000
C	2.87379000	1.10134300	-3.50605100
H	1.14120400	0.14112700	-2.65574900
C	4.81268500	1.24264600	-2.06915000
H	4.60968300	0.36953400	-0.11394200
C	4.19297800	1.50881400	-3.29190600
H	2.38272500	1.31394800	-4.45139400
H	5.83669200	1.56170700	-1.89584300
H	4.73291200	2.03773100	-4.07223400

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C	1.01412300	2.67711300	0.03216100
C	-0.22385400	2.58162300	-0.28166100

C	-1.56257100	2.76100400	-0.48143600
C	-2.77731500	2.74479900	-0.65608800
Pd	0.68162600	0.67128400	-0.37232200
P	2.26347100	-1.01335000	-0.20331600
O	-1.47476900	-0.42374600	-1.06693100
H	-1.81306200	0.44013600	-1.35679700
C	-2.42419800	-0.93838000	-0.13313700
C	-1.83366000	-1.75628300	0.96841100
C	-2.38933100	-0.37028000	1.25725500
H	-0.75461600	-1.87309100	0.97719100
H	-2.39640900	-2.61564400	1.32050100
H	-3.32234600	-0.29208300	1.80587900
H	-1.67220800	0.42431500	1.43738800
C	-3.71990200	-1.32325700	-0.84744900
H	-4.03528000	-0.45419700	-1.43848800
H	-3.48029500	-2.12320100	-1.55820400
C	-4.85942300	-1.74018600	0.05176800
C	-5.74876700	-0.77842900	0.55354100
C	-5.04006800	-3.07960700	0.42245000
C	-6.78912300	-1.14571000	1.40761700
H	-5.62353500	0.26213100	0.26992100
C	-6.07976700	-3.45015600	1.27840200
H	-4.36370800	-3.83654400	0.03270300
C	-6.95717100	-2.48343200	1.77454500
H	-7.46982000	-0.38591200	1.78233800
H	-6.20645900	-4.49367600	1.55387200
H	-7.76811600	-2.77110000	2.43793600
C	2.17431500	-1.93605800	1.39420500
C	1.77826000	-1.22011000	2.53705500
C	2.47031900	-3.30200800	1.51629000
C	1.69260400	-1.85450400	3.77634100
H	1.52510800	-0.16692600	2.44643200
C	2.37535900	-3.93660400	2.75676100
H	2.76957000	-3.87445300	0.64417800
C	1.98890800	-3.21521900	3.88820800
H	1.38333700	-1.28874700	4.65069200
H	2.60190700	-4.99623600	2.83701700
H	1.91226000	-3.71232000	4.85114800
C	2.19232100	-2.34562400	-1.47898400
C	3.32470000	-3.06662900	-1.88978100
C	0.94346000	-2.65200100	-2.04347000
C	3.20698600	-4.08403500	-2.83840800
H	4.29887400	-2.83212000	-1.47143800
C	0.82959800	-3.67374200	-2.98766200
H	0.06510700	-2.08267700	-1.75363200
C	1.95934000	-4.39164900	-3.38633400

H	4.09043300	-4.63440600	-3.15026400
H	-0.14144100	-3.90116700	-3.41900400
H	1.87008000	-5.18223800	-4.12626400
C	4.02000800	-0.45916300	-0.29550800
C	4.36076800	0.42676200	-1.33163600
C	5.00258300	-0.83912700	0.62849900
C	5.66123600	0.91268400	-1.44741200
H	3.59432300	0.75254500	-2.03024000
C	6.30355500	-0.33845900	0.51842500
H	4.75608000	-1.51950800	1.43741700
C	6.63592300	0.53412400	-0.51861300
H	5.90986500	1.60099600	-2.25009600
H	7.05567200	-0.63422100	1.24468400
H	7.64676500	0.92360500	-0.60061400
C	2.12212800	3.52268400	0.41006400
C	1.99869400	4.92636000	0.33500500
C	3.33605600	2.97016900	0.85646200
C	3.06474400	5.74592900	0.69467200
H	1.06352700	5.35725600	-0.01034800
C	4.39880800	3.79617600	1.21583200
H	3.43297600	1.89265600	0.90750500
C	4.26868000	5.18493900	1.13529100
H	2.95849500	6.82539200	0.63078400
H	5.33136700	3.35136900	1.55117400
H	5.09920800	5.82820300	1.41233100
C	-4.19400700	2.70623000	-0.76653100
C	-4.81588500	2.24143200	-1.94605900
C	-5.00521400	3.08731500	0.32466400
C	-6.20395000	2.15798300	-2.02477300
H	-4.19962000	1.94926900	-2.79085200
C	-6.39230600	2.99969300	0.23426300
H	-4.53336200	3.44106300	1.23571700
C	-6.99744500	2.53434100	-0.93724500
H	-6.66795700	1.79365900	-2.93666600
H	-7.00350500	3.29218800	1.08330100
H	-8.07904500	2.46259700	-1.00119800

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C	0.18619800	2.15955800	-0.03737800
C	-1.02394800	1.86321400	-0.32830800
C	-2.37816700	2.08386900	-0.41306900

C	-3.58935600	2.22638800	-0.48431200
Pd	0.19593500	0.13232700	-0.58153600
P	2.48854300	-0.60446100	-0.18333500
O	-0.63790200	-1.78749600	-1.17861000
H	-1.14461000	-0.12439100	-1.28747200
C	-1.66029500	-2.27159300	-0.37455200
C	-1.46315000	-3.68155200	0.13423500
C	-1.38365100	-2.50664700	1.09173000
H	-0.53415600	-4.17030800	-0.14335100
H	-2.32805700	-4.33651600	0.20218800
H	-2.18652400	-2.38245200	1.81284600
H	-0.39760300	-2.21837900	1.44363400
C	-3.04296800	-1.80776000	-0.85344000
H	-2.99805600	-0.71040900	-0.91441000
H	-3.16868200	-2.17409500	-1.87910900
C	-4.23079700	-2.19987200	-0.00969300
C	-4.63777500	-1.39359100	1.06529400
C	-4.94739600	-3.37786900	-0.26599200
C	-5.72604800	-1.75403200	1.86132700
H	-4.10077400	-0.47000700	1.26580100
C	-6.03471600	-3.74425500	0.53014400
H	-4.65081700	-4.00819300	-1.10080700
C	-6.42751700	-2.93310600	1.59723900
H	-6.02945200	-1.11086900	2.68296800
H	-6.57817200	-4.66015900	0.31344200
H	-7.27657300	-3.21428300	2.21415400
C	2.68133400	-1.37777700	1.47512600
C	1.87220600	-0.90668400	2.52227000
C	3.60116800	-2.40566700	1.73217500
C	1.99421300	-1.43994200	3.80592700
H	1.13650500	-0.13105000	2.32791300
C	3.71649400	-2.94147400	3.01613100
H	4.22305000	-2.79144700	0.93053800
C	2.91679700	-2.45849500	4.05455700
H	1.35995000	-1.06896500	4.60588900
H	4.42961700	-3.73929000	3.20345900
H	3.00624900	-2.88041400	5.05152500
C	3.10971300	-1.87889900	-1.35630500
C	4.46284300	-1.96063900	-1.72330500
C	2.19372200	-2.81227000	-1.87030100
C	4.89574400	-2.97083100	-2.58378000
H	5.17760400	-1.23868100	-1.34143100
C	2.63704500	-3.81960300	-2.72929800
H	1.14021400	-2.73180100	-1.61149200
C	3.98475600	-3.90323300	-3.08571900
H	5.94433500	-3.02665800	-2.86283700

H	1.92270600	-4.53556300	-3.12648100
H	4.32411600	-4.68740000	-3.75693700
C	3.78959900	0.69146500	-0.25037800
C	3.70099200	1.64065400	-1.28090700
C	4.84238600	0.77518600	0.67080800
C	4.65131400	2.65349700	-1.39001700
H	2.87374700	1.59566600	-1.98441100
C	5.79022700	1.79559000	0.56218000
H	4.92153700	0.05211000	1.47641000
C	5.69615600	2.73518000	-0.46565800
H	4.56540300	3.38949800	-2.18387700
H	6.59998900	1.85605400	1.28406500
H	6.42933500	3.53294000	-0.54305100
C	1.13291300	3.17804900	0.35421400
C	1.09375500	4.44104200	-0.26885100
C	2.10156400	2.93305600	1.34291500
C	2.00899700	5.42811300	0.08974800
H	0.34903200	4.63070300	-1.03582300
C	3.00492600	3.92850000	1.70468500
H	2.14247200	1.95849300	1.81521000
C	2.96670100	5.17594900	1.07610100
H	1.97420600	6.39640800	-0.40161900
H	3.75106400	3.72371400	2.46616900
H	3.68122400	5.94648800	1.35089300
C	-4.99903700	2.40160300	-0.55060400
C	-5.83934000	1.30759800	-0.84778100
C	-5.57683200	3.66621300	-0.31012900
C	-7.21995100	1.47893900	-0.89537000
H	-5.40149400	0.33186700	-1.02543100
C	-6.95868700	3.82578400	-0.36437800
H	-4.93247700	4.50916800	-0.08103700
C	-7.78390100	2.73517700	-0.65537600
H	-7.85642300	0.62750400	-1.11783000
H	-7.39410600	4.80325000	-0.17766600
H	-8.86169600	2.86430400	-0.69390700

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C	5.89106100	-3.18433500	-0.32777700
C	4.77285600	-3.64091300	-1.03156400
C	3.57909300	-2.92059900	-0.99589900
C	3.48575900	-1.73172400	-0.25751500

C	4.61031800	-1.28345100	0.44661100
C	5.80714700	-2.00317100	0.41129900
C	2.17315300	-0.97403800	-0.19478200
C	1.16940100	-1.76700300	0.64735400
C	1.26026300	-1.65300700	2.12345300
C	0.18374300	-0.62341700	1.83510600
Pd	-1.01214300	-1.18467400	-0.12648300
C	-2.73581000	0.06002800	-0.13660400
O	0.43203600	-2.67414800	0.06849700
H	0.49447800	0.41622900	1.80479900
H	-0.77325200	-0.81467500	2.31775300
H	2.20726000	-1.27344100	2.50635500
H	0.91560900	-2.53670100	2.65736100
H	1.75587000	-0.84056600	-1.19767400
H	2.33137700	0.01575200	0.24210100
H	2.70692400	-3.27937400	-1.53512300
H	4.55103300	-0.36120700	1.01997800
H	4.83095800	-4.55931300	-1.60925800
H	6.67208400	-1.64011000	0.95980000
H	6.82107800	-3.74512200	-0.35722900
H	-1.77408100	-1.81650700	-1.35421500
C	-1.77162600	0.87310300	-0.16650400
C	-0.90713600	1.92488200	-0.17087500
C	-0.09499000	2.83906600	-0.16756500
C	0.86335500	3.88672700	-0.16156600
C	2.11503000	3.70383700	-0.78804800
C	3.05921900	4.72625700	-0.77127500
C	2.77292300	5.93977000	-0.13872100
C	1.53442300	6.12983700	0.48142800
C	0.58271100	5.11419400	0.47498500
H	2.32934900	2.76215900	-1.28372700
H	4.01996300	4.57761300	-1.25530300
H	3.51233400	6.73520100	-0.12987200
H	1.31058800	7.07213400	0.97277500
H	-0.37937100	5.25529600	0.95707700
C	-4.13677100	-0.26350700	-0.14841900
C	-5.07561200	0.79054500	-0.14895200
C	-4.59362500	-1.59379600	-0.14537500
C	-6.43804400	0.51083300	-0.15018300
H	-4.72297600	1.81736500	-0.15118800
C	-5.96049800	-1.86239900	-0.14945900
H	-3.86754200	-2.39936900	-0.14694300
C	-6.88488900	-0.81495000	-0.15088700
H	-7.15405300	1.32755100	-0.15323800
H	-6.30433500	-2.89249300	-0.15088200
H	-7.94975400	-1.02887000	-0.15269700

int4

84

Pd	-0.28301500	0.28787900	-1.07289900
P	-0.52228400	-0.90520900	1.01858900
H	0.06388800	1.08787600	-2.40680700
C	-2.17080000	-0.94508700	-2.10790500
C	-2.05610200	-1.87582400	1.33799100
C	-3.27857000	-1.20874800	1.15089800
C	-2.06895500	-3.22018400	1.73485900
C	-4.48713400	-1.87692900	1.34336300
H	-3.28472100	-0.16596400	0.84841400
C	-3.28092800	-3.88866300	1.92303700
H	-1.13675100	-3.75279100	1.88838700
C	-4.49132000	-3.22255600	1.72254900
H	-5.42417700	-1.34913700	1.19000200
H	-3.27626100	-4.93170600	2.22713000
H	-5.43254000	-3.74602100	1.86464100
C	-0.40230600	0.13216800	2.53187600
C	-0.32752500	1.52605300	2.40088300
C	-0.42544700	-0.43838800	3.81535600
C	-0.26753300	2.33734900	3.53687300
H	-0.31870000	1.97194700	1.41032300
C	-0.36069400	0.37304200	4.94651900
H	-0.49534100	-1.51670400	3.92656400
C	-0.28067700	1.76259500	4.80818300
H	-0.21058100	3.41634400	3.42520000
H	-0.37629100	-0.07628900	5.93546600
H	-0.23249700	2.39358500	5.69126100
C	0.85648100	-2.11141400	1.13207800
C	0.86454300	-3.19030100	0.22769200
C	1.97833300	-1.89353200	1.94220200
C	1.96113200	-4.04680200	0.16249000
H	0.01695400	-3.35745900	-0.42876600
C	3.08269200	-2.74571100	1.86051300
H	2.00664300	-1.05079600	2.62394200
C	3.07548700	-3.82517400	0.97835600
H	1.94881300	-4.87920400	-0.53550200
H	3.95318600	-2.55085400	2.47890500
H	3.93680200	-4.48415800	0.91621000
C	-2.70194500	0.14036000	-1.86462600

C	-3.34501100	1.31135000	-1.61052200
C	-3.93002400	2.35290300	-1.35613200
C	-1.78138100	-2.29686200	-2.35531700
C	-2.49891100	-3.34657600	-1.74619200
C	-0.65792900	-2.59104500	-3.15438700
C	-2.09332800	-4.66513300	-1.93859800
H	-3.34791200	-3.11556300	-1.11244700
C	-0.26781000	-3.91380500	-3.34248300
H	-0.09819900	-1.77464100	-3.59786700
C	-0.98068100	-4.95275700	-2.73465700
H	-2.64282600	-5.46805000	-1.45643700
H	0.60004500	-4.13489000	-3.95654900
H	-0.66716500	-5.98273100	-2.87805200
C	-4.58903500	3.57585000	-1.06104000
C	-5.80422500	3.57883200	-0.34455100
C	-4.03062500	4.80213800	-1.47993000
C	-6.44124200	4.78246900	-0.05660300
H	-6.23389000	2.63560300	-0.02232300
C	-4.67781900	5.99868500	-1.18520300
H	-3.09604700	4.79874200	-2.03167700
C	-5.88201900	5.99346900	-0.47499600
H	-7.37638300	4.77649900	0.49564100
H	-4.24181200	6.93852800	-1.51080100
H	-6.38304300	6.93002900	-0.24818200
C	1.64869800	0.86591900	-0.56479300
H	1.80983800	1.89877200	-0.88815700
H	1.74099000	0.84033500	0.52611000
C	2.71374800	-0.06472900	-1.17937400
H	2.66839500	-0.02199600	-2.27214200
H	2.55419900	-1.09740900	-0.85877600
C	4.08390300	0.37340300	-0.68130600
O	4.53306800	0.00116300	0.38795000
C	4.82575700	1.36681600	-1.58442300
H	5.03851700	0.84330300	-2.52604100
H	4.10687400	2.15489900	-1.84837100
C	6.08140100	1.95104200	-0.99198200
C	7.34401200	1.62123200	-1.49736000
C	6.00400200	2.83340900	0.09513100
C	8.50384000	2.16310100	-0.93747600
H	7.42037100	0.93455800	-2.33722100
C	7.15828700	3.37617300	0.65779800
H	5.02951900	3.09060400	0.50268500
C	8.41422300	3.04321100	0.14177100
H	9.47537800	1.89737400	-1.34556100
H	7.07934900	4.05882200	1.49968300
H	9.31435300	3.46682200	0.57868100

ts3

84

Pd	-0.50115100	0.30460900	0.16077200
P	-0.43982700	-2.03642400	0.18656600
H	-0.25806200	1.87818600	0.27013500
C	-2.55709100	0.78966900	-0.16656400
C	-2.00067300	-3.01114000	0.12788700
C	-2.99116100	-2.67910800	1.06661000
C	-2.22808700	-4.06931200	-0.76130200
C	-4.18430900	-3.39507800	1.11805600
H	-2.83131500	-1.84815600	1.74794000
C	-3.43132700	-4.77877200	-0.71451400
H	-1.47335700	-4.34405900	-1.49057900
C	-4.40918200	-4.44465900	0.22282600
H	-4.94625000	-3.12020200	1.84090100
H	-3.59931000	-5.59553000	-1.41107400
H	-5.34476800	-4.99567100	0.25418800
C	0.34809900	-2.74929400	1.68947700
C	0.70099800	-1.91858400	2.76157300
C	0.54414400	-4.13596100	1.79987100
C	1.25304300	-2.46512200	3.92251500
H	0.54518000	-0.84687600	2.68306500
C	1.10342300	-4.67721000	2.95592800
H	0.25688200	-4.79063200	0.98209000
C	1.45925500	-3.84175000	4.01918100
H	1.52237600	-1.81293500	4.74836800
H	1.25709200	-5.75001000	3.02966200
H	1.89221200	-4.26540300	4.92095000
C	0.56425300	-2.60648100	-1.23838400
C	0.05517100	-2.38489400	-2.53122700
C	1.87009400	-3.09120200	-1.09414400
C	0.82769000	-2.67425100	-3.65369400
H	-0.94590200	-1.98225700	-2.65770800
C	2.64774900	-3.36390900	-2.22237100
H	2.29407400	-3.23950800	-0.10763900
C	2.12887700	-3.16392200	-3.50051800
H	0.41947000	-2.50714200	-4.64644500
H	3.66570900	-3.71799400	-2.09487200
H	2.73717900	-3.37553500	-4.37509400
C	-1.99396800	1.92212400	0.04516900

C	-2.08431100	3.29991400	0.10933900
C	-2.15856400	4.51572900	0.17230300
C	-3.80630200	0.12091100	-0.44373400
C	-4.95033700	0.39677000	0.33008400
C	-3.89721700	-0.82231400	-1.48351400
C	-6.15027400	-0.26108700	0.06663100
H	-4.88356600	1.12031600	1.13694700
C	-5.10491500	-1.45754600	-1.75620500
H	-3.01137700	-1.04754500	-2.06701400
C	-6.23351200	-1.18644800	-0.97746300
H	-7.02464700	-0.04573000	0.67456700
H	-5.15995900	-2.18283000	-2.56243600
H	-7.17085300	-1.69633400	-1.18032100
C	-2.26046000	5.93245800	0.23973800
C	-3.50585700	6.57035800	0.05966200
C	-1.11584200	6.71912100	0.48746200
C	-3.59763700	7.95788400	0.12655700
H	-4.38782000	5.96753200	-0.13238700
C	-1.22004200	8.10588700	0.55174900
H	-0.15640900	6.23085700	0.62672400
C	-2.45815800	8.72958200	0.37213200
H	-4.56107300	8.43940400	-0.01396300
H	-0.33261300	8.70226700	0.74299500
H	-2.53462700	9.81180400	0.42306400
C	1.63466000	0.27949100	0.29991600
H	1.97271800	1.02731200	1.02599200
H	1.99696900	-0.68849400	0.65807100
C	2.26631900	0.55590700	-1.08262700
H	1.97667200	1.54918300	-1.44330600
H	1.93625600	-0.19067200	-1.81035900
C	3.77823000	0.45356100	-0.96203000
O	4.36911700	-0.60612600	-1.07647500
C	4.49939600	1.76300500	-0.61562900
H	4.36573900	2.43520600	-1.47377400
H	3.93854800	2.22894000	0.20638200
C	5.95697400	1.61995400	-0.26281000
C	6.95619500	2.19254200	-1.05775300
C	6.33904100	0.90055200	0.87896200
C	8.30555400	2.05905900	-0.71998700
H	6.67605200	2.74909000	-1.94913400
C	7.68380600	0.76388700	1.21968000
H	5.57311200	0.44133300	1.49858800
C	8.67342300	1.34469900	0.42078800
H	9.06684800	2.51327400	-1.34861400
H	7.96146300	0.20281700	2.10802400
H	9.72178200	1.23925900	0.68615100

ts2_p3

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Pd	0.42389300	-0.06605800	-1.03878400
O	2.37652200	-0.33824400	-1.72680200
C	1.38871200	-1.86664900	0.21666500
C	2.78759000	-2.24892000	-0.24519000
H	1.22981300	-1.75375900	1.28385800
H	0.59047100	-2.38514200	-0.31244500
H	3.49987000	-2.53032100	0.52843800
H	2.82887500	-2.88574400	-1.12579500
P	-1.61317300	0.12370800	-0.08523000
C	2.64681800	-0.80287900	-0.52147600
C	3.25074300	0.16998700	0.50232500
H	2.74751800	1.13611500	0.39160700
H	3.06957900	-0.18898800	1.51984500
C	4.73996300	0.31943300	0.26396800
C	5.21011900	0.97512800	-0.88396700
C	5.67215100	-0.22079200	1.15898500
C	6.57885400	1.08877100	-1.12626500
H	4.49177200	1.38200700	-1.58931500
C	7.04393900	-0.10680500	0.91923700
H	5.32175600	-0.72959600	2.05422300
C	7.50112700	0.54872800	-0.22497100
H	6.92709100	1.59968700	-2.01995700
H	7.75293100	-0.52889900	1.62654100
H	8.56730400	0.63991000	-0.41351300
C	-3.02901400	-0.27687600	-1.18758100
C	-4.34704100	0.06708500	-0.84842900
C	-2.78658400	-0.98513900	-2.37354500
C	-5.40377000	-0.29685300	-1.68238100
H	-4.55025900	0.62365800	0.06106600
C	-3.84774600	-1.35164000	-3.20387000
H	-1.76628400	-1.23635900	-2.64889800
C	-5.15609900	-1.00850000	-2.85963300
H	-6.42011100	-0.02244100	-1.41459900
H	-3.64873400	-1.89738100	-4.12164600
H	-5.98107500	-1.28870100	-3.50847300
C	-2.00035200	1.78608300	0.60350400
C	-2.83967600	1.94890400	1.71829900
C	-1.46855000	2.92298300	-0.02504900
C	-3.14504200	3.22653300	2.18906500

H	-3.24798400	1.08104500	2.22621100
C	-1.77936700	4.19852100	0.44816500
H	-0.80889200	2.80481600	-0.87869200
C	-2.61687000	4.35309200	1.55470900
H	-3.79356000	3.33983300	3.05315200
H	-1.36008700	5.07052400	-0.04542100
H	-2.85293300	5.34673100	1.92486700
C	-1.82307500	-1.00920200	1.35018400
C	-1.05044500	-0.77606900	2.50172200
C	-2.64625200	-2.14206400	1.29820900
C	-1.11702000	-1.64956600	3.58544900
H	-0.40095600	0.09398600	2.54940700
C	-2.70301100	-3.02074900	2.38366700
H	-3.24816600	-2.33954500	0.41717600
C	-1.94367100	-2.77605200	3.52799900
H	-0.52223200	-1.45312800	4.47294900
H	-3.34653100	-3.89442100	2.33272600
H	-1.99204300	-3.45920000	4.37106100
H	-0.09934800	0.96539700	-2.09623100

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