

Supporting Information

Mechanochemical NH₄Cl-Mediated Hydrogen-Bonding Network

Reconstruction of HFIP: Enabling Yne-Allylic Substitutions

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1 General comments

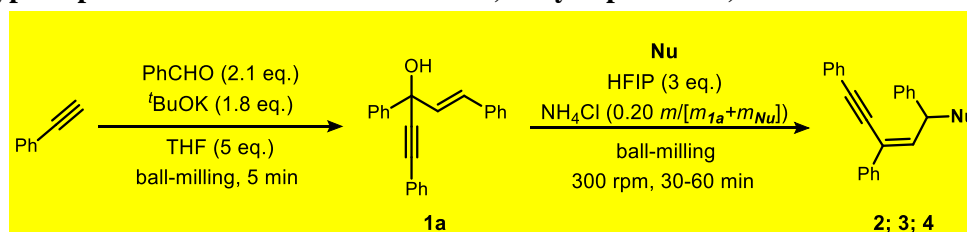
Commercially available reagents were purchased from Energy, Leyan, Bidepharm, Heowns or TCI, and used without further purification unless otherwise stated. All reactions were performed using grinding vessels in Changsha Vertical Planetary Ball Mill YXQM-0.4L. Both jars and balls were made of stainless steel or ZrO₂. Hexafluoroisopropanol and other alcohols for reactions were purchased from commercial suppliers.



¹H NMR and ¹³C NMR spectra were measured on Bruker Avance 400 MHz instrument and chemical shifts (δ) were reported in parts per million (ppm). Chemical shifts were reported in ppm on the δ scale relative to CHCl₃ ($\delta = 7.26$ for ¹H NMR, $\delta = 77.16$ for ¹³C NMR), CD₂Cl₂ ($\delta = 5.32$ for ¹H NMR, $\delta = 53.84$ for ¹³C NMR). Coupling constants were reported in Hz with multiplicities denoted as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). Single crystal X-ray diffraction analyses was carried out on SmartLab (9kW). High-resolution mass spectrometry (HRMS) data were obtained using an Agilent 6210 ESI/TOF mass spectrometer with molecular ions [M]⁺, [M+H]⁺, [M+Na]⁺, and [M+K]⁺ reported in *m/z* units.

All reactions were monitored by thin layer chromatography (TLC) and visualized by UV irradiation or stained with 10% ethanolic phosphomolybdic acid (PMA) followed by brief heating with a heating gun. Column chromatography was performed on silica gel (200-300 mesh) using a mixture of petroleum ether/ethyl/ dichlorometh acetate as the eluent.

2 Typical procedures for the formation of 1,3-enyne product 2, 3 and 4



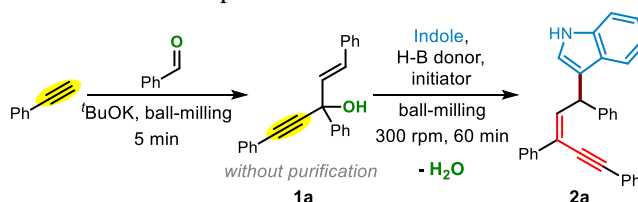
Phenylacetylene (1.2 mmol), benzaldehyde (2.4 mmol, 2.1 equiv) and ^tBuOK (2.16 mmol, 1.8 equiv) were placed in a ZrO₂ milling jar (50 mL) with 17 ZrO₂ balls (10 mm×2, 8 mm×5, 5 mm×10). Then THF (5 equiv) were added via a syringe. After the vessel was closed in air, the vessel was placed in the ball mill at 300 rpm. After 5 min, the jar was then opened. The mixture was extracted with ethyl acetate (5 mL × 3), and dried over anhydrous

Na₂SO₄ to get crude product **1a**.

Crude product **1a** (1.2 equiv), nucleophiles (1 mmol) and NH₄Cl [0.20 m/(m_{1a}+m_{Nu})] were added to a ZrO₂ milling jar. Then HFIP (3 equiv) were added via a syringe. After the jar was closed, the jar was placed in Changsha Vertical Planetary Ball Mill YXQM-0.4L grinding for 0.5-1 h. After grinding, the mixture was dissolved in dichloromethane followed by filtration, and the crude product was purified by flash chromatography on silica gel (PE/DCM, v:v = 5:1) to to give the corresponding products.

3 Typical procedures for the formation of 1,3-enyne product **5b-5l**

Table S1 The optimization of reaction conditions.

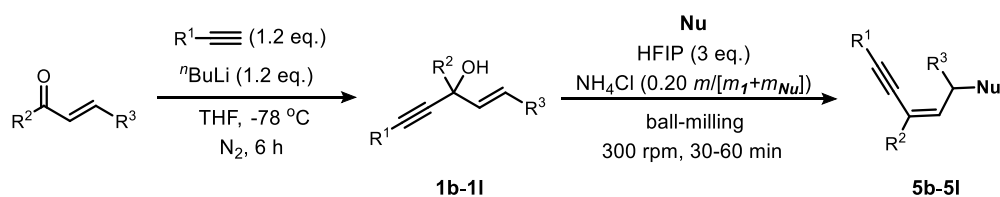


Entry	H-B donor (equiv)	Mediator [m/(m _{1a} +m _{Indole})]	Yield ^a [%]
1	BF ₃ ·Et ₂ O (2)	-	<5
2	TFA (2)	-	<5
3	ⁱ PrOH (2)	-	0
4	TFE (2)	-	8
5	HFIP (2)	-	13
6	HFIP (2)	NaCl (0.12)	39
7	HFIP (2)	NH ₄ Cl (0.12)	56
8	HFIP (2)	ⁿ Bu ₄ NCl (0.12)	40
9	HFIP (2)	NaOAc (0.12)	18
10	HFIP (2)	NH ₄ OAc (0.12)	27
11	HFIP (2)	NH ₄ Cl (0.2)	67
12^b	HFIP (3)	NH₄Cl (0.2)	87
13 ^c	HFIP (3)	NH ₄ Cl (0.2)	68
14	-	NH ₄ Cl (0.2)	0
15	HFIP (3)	NH₄F (0.2)	44
16	HFIP (3)	NH₄Br (0.2)	40
17	HFIP (3)	NH₄I (0.2)	77

General reaction conditions: **1a** (1.2 mmol), indole (1 mmol, 1 equiv), ball milling under air for 60 min.

Reactions were conducted in ZrO₂ milling jar (50 mL) at 300 rpm using 17 ZrO₂ balls: diameter 10 mm (2) + diameter 8 mm (5) + diameter 5 mm (10). ^aIsolated yield after silica gel column chromatography.

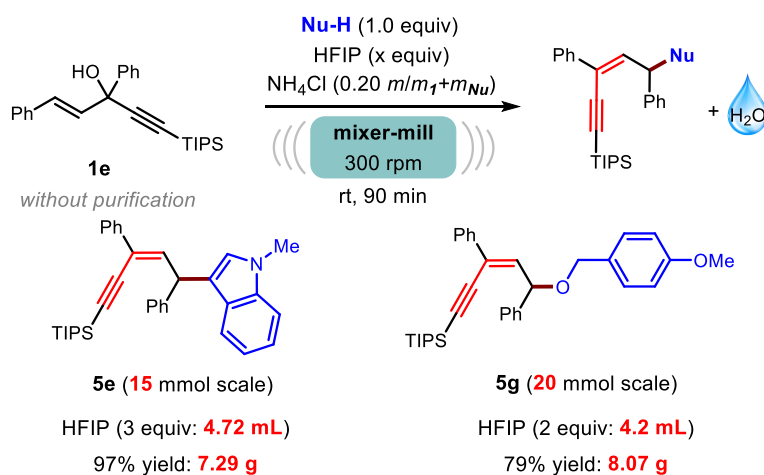
^bThe reaction was carried out for 30 min. ^cStainless-steel balls were used.



A solution of alkynes (18 mmol) in anhydrous THF (70 mL) was added to a flame dried two-necked round-bottom flask under nitrogen, followed by addition of *n*-BuLi (11.3 mL, 1.6 M in hexane, 18 mmol) with a syringe at -78 °C. The reaction mixture was stirred at 0 °C for 1 h, and then a solution of alkenyl ketone (15 mmol) in THF (30 mL) was added at -78 °C. After the reaction mixture was stirred at -78 °C for 5 h, it was quenched with NH₄Cl (30 mL). The organics were extracted with EtOAc (3 × 60 mL), washed with brine, dried over Na₂SO₄, filtered and concentrated under reduced pressure. The crude allylic alcohol was used for the next step without further purification.

Crude product **1b-1l** (1.2 equiv), nucleophiles (1 mmol) and NH₄Cl [0.20 m/(m_{1a}+m_{Nu})] were added to a ZrO₂ milling jar. Then HFIP (3 equiv) were added via a syringe. After the jar was closed, the jar was placed in Changsha Vertical Planetary Ball Mill YXQM-0.4L grinding for 0.5-1 h. After grinding, the mixture was dissolved in dichloromethane followed by filtration, and the crude product was purified by flash chromatography on silica gel (PE/DCM, v:v = 5:1) to give the corresponding products.

4 Scale-up reaction and synthetic transformations of **5e** and **5g**



100 mL ZrO₂ jar
17 ZrO₂ balls
1e + Nu + HFIP + NH₄Cl

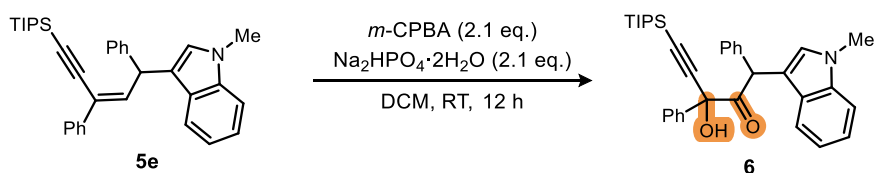
Planetary Ball Mill
300 rpm for 90 min

After reaction

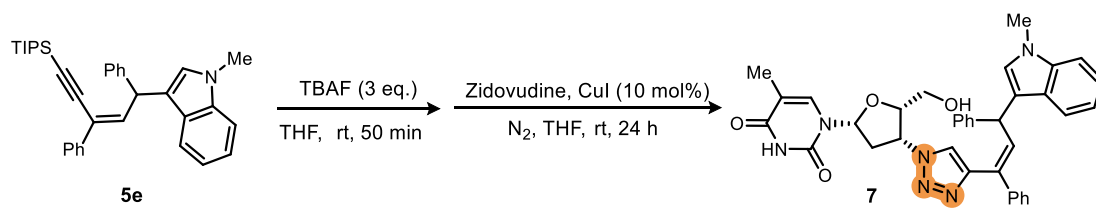
Filtration & recrystallization
5e

To a 100 mL ZrO₂ jar, equipped with 17 ZrO₂ balls (10 mm × 2, 8 mm × 5, 5 mm × 10), was added **1e** (7.02 g, 18 mmol, 1.2 equiv.), N-methylindole (1.97 g, 15 mmol, 1.0 equiv.), HFIP (4.72 mL, 45 mmol, 3.0 equiv.), and ammonium chloride (1.5 g). The jar was closed and mounted on the planetary mill, then milled at 300 rpm for 90 min. Upon completion, the crude reaction mixture was dissolved in a minimal amount of CH₂Cl₂ and subjected directly to filtration followed by recrystallization from DCM/PE to give **5e** as an off-white solid (7.29

g, 97%).

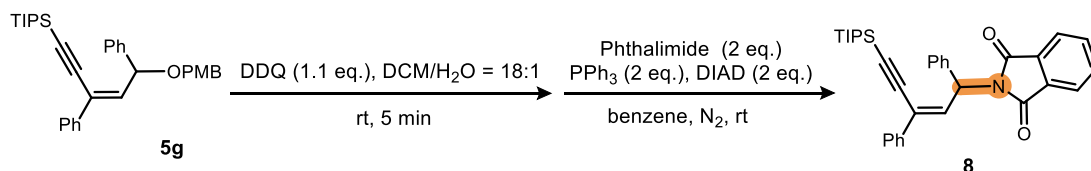


5e (75.5 mg, 0.15 mmol) was dissolved in DCM (2 mL) and the resulting solution was cooled to 0 °C. Then, *m*-CPBA (65 mg, 0.375 mmol) and Na₂HPO₄ · 2H₂O (66.8 mg, 0.375 mmol) were added in one portion. The reaction was kept at 0 °C for 2 h, at which point it was quenched with saturated Na₂CO₃ aqueous solution. This biphasic mixture was stirred for 10 min and was then washed with saturated NaHCO₃ and brine. The organic layer was dried over anhydrous Na₂SO₄. After the removal of solvent under vacuum, the crude material was purified by silica gel column chromatography (hexane/ethyl acetate = 3/1). The product **6** was obtained as a brown viscous solid (44.2 mg, 55% yield, *dr* = 6.5:1) on silica gel (petroleum ether/ethyl acetate, v:v = 20:3).



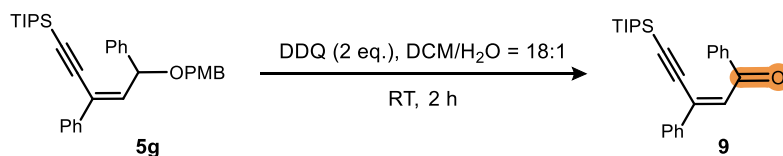
To a stirred solution of **5e** (100.6 mg, 0.2 mmol) in anhydrous THF (2 mL), TBAF (3 equiv) was then added dropwise via syringe. The reaction was stirred for 50 min and then quenched with a saturated aqueous ammonium chloride solution. The mixture was extracted with ethyl acetate (2 mL × 2). The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (petroleum ether/ethyl acetate, v: v = 20:1) on silica gel to afford the desired desilylation product.

To a 10 mL Schlenk tube, CuI (3 mg, 0.015 mmol) and the desilylation product (62.5 mg, 0.18 mmol) were dissolved in freshly distilled THF (1 mL) at room temperature under argon atmosphere, then the solution of Zidovudine (42.5 mg, 0.15 mmol) in anhydrous THF (0.5 mL) was added via syringe. After the reaction was completed as monitored by TLC, the solution was quenched carefully with saturated NH₄Cl solution and then warmed to room temperature. The product was extracted with ethyl acetate (5 mL × 3), and dried over anhydrous Na₂SO₄. After filtration and evaporation in vacuo, the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate, v: v = 1:1) to afford the product **7** (74 mg, 81% yield, >20:1 *dr*).



To a round bottom flask (10 mL) was charged with **5g** (46.8 mg, 0.2 mmol), DDQ (78 mg, 0.2 mmol) and DCM/H₂O (18:1, 3.8 mL). The reaction mixture was stirred at room temperature for 5 min. Then the resultant reaction mixture was quenched by saturated Na₂SO₃ and it was extracted with DCM (5 mL × 3) and washed with brine. The residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate, v:v = 100:1) to afford the debenzylation product.

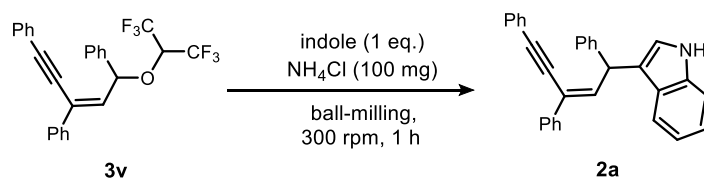
To a solution of debenzylation product (0.2 mmol), triphenylphosphine (105 mg, 2 equiv) and phthalimide (59 mg, 2 equiv) in anhydrous benzene (5 mL) was added a solution of diethyl azodicarboxylate (0.34 mL, 2 equiv) in anhydrous benzene (1 mL) over a period of 5 min, the reaction mixture was stirred for an additional 1 hour. Afterward, the resultant reaction mixture was quenched by water. The reaction mixture was extracted with ethyl acetate (5 mL × 3), and dried over anhydrous Na₂SO₄. The solvent was removed via rotary evaporation, yielding a viscous residue, the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate, v: v = 20:1) to afford the product **8** (38 mg, 37% yield).



To a round bottom flask (10 mL) was charged with **5g** (76.6 mg, 0.15 mmol), DDQ (71.5 mg, 0.315 mmol) and DCM/H₂O (18:1, 3.8 mL). The reaction mixture was stirred at room temperature for 2 hours. After that, the reaction was quenched by saturated Na₂SO₃ and it was extracted with DCM (5 mL × 3) and washed with brine. The residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate, v:v = 100:1) to afford the ketone product **9** (46.6 mg, 80% yield).

5 Control experiments and mechanistic studies

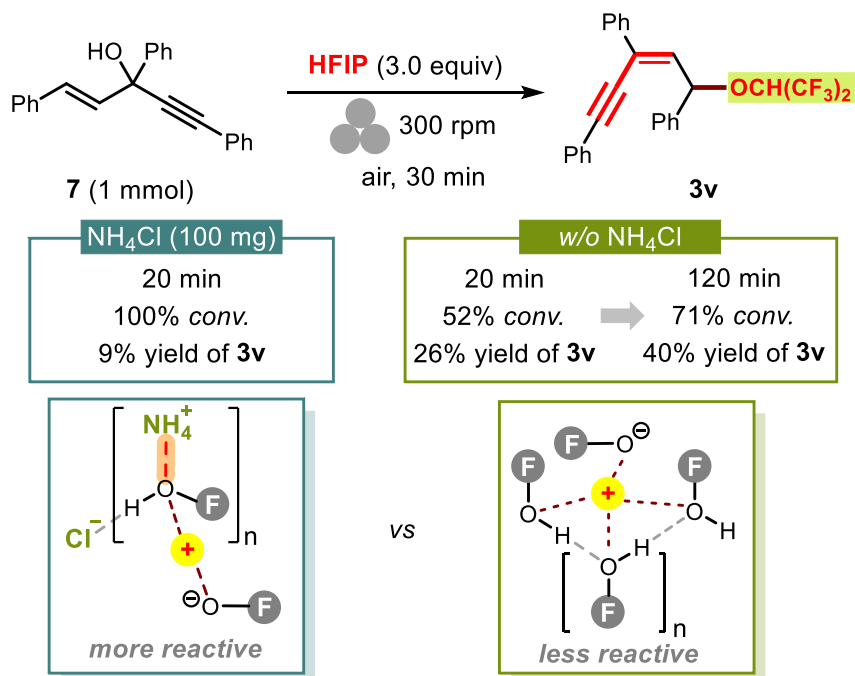
5.1 Attempted substitution reaction of **3v** with indole



The hexafluoroisopropoxylation product **3v** (1.2 mmol), indole (1 mmol, 1 equiv) and NH₄Cl (100 mg) were placed in a ZrO₂ milling jar (50 mL) using 17 ZrO₂ balls. After the

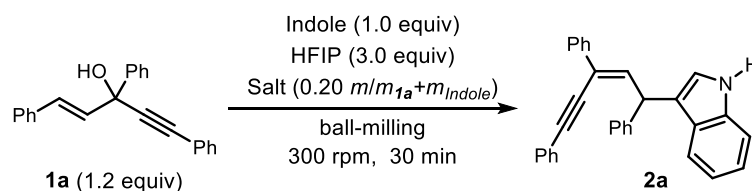
vessel was closed in air, the vessel was placed in the planetary ball mill at 300 rpm. After 60 min, the jar was then opened. After grinding, the mixture was monitored by TLC and the desired product **2a** was not detected.

5.2 Investigations on the effect of ammonium chloride on reaction efficiency

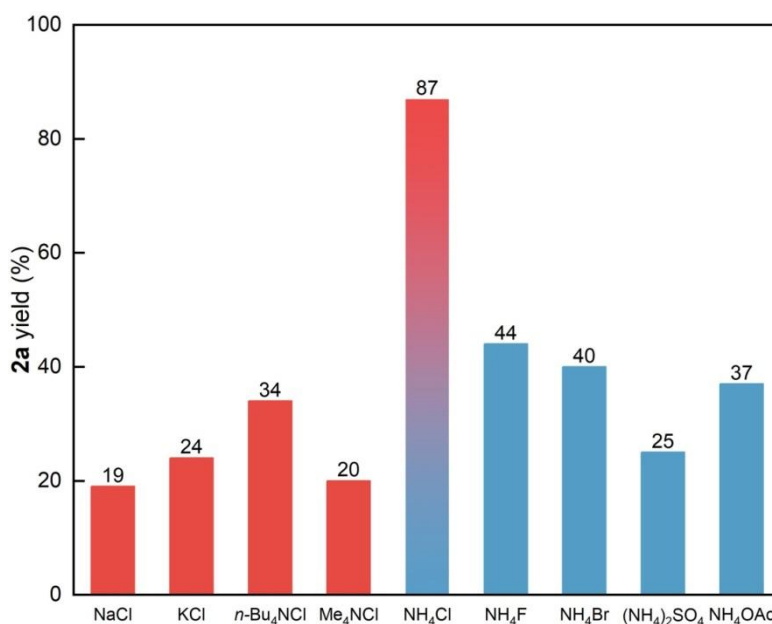


1a (1 mmol), NH₄Cl (100 mg) and HFIP (3 mmol) were added to a 50 mL ZrO₂ milling jar containing 17 ZrO₂ balls in air and the jar was placed in planetary ball mill. After grinding for 20 min, **1a** was completely consumed. After filtration and evaporation in vacuo, the residue was purified by flash chromatography on silica gel (petroleum ether/ethyl acetate, v:v = 100:1) to afford the product **3v** (41 mg, 9% yield). Under otherwise identical conditions but in the absence of NH₄Cl, the reactions were carried out for 20 min or 120 min, respectively. The yields and substrate conversion rates were then determined.

5.3 Investigation of the reactivity towards different ammonium salts and chlorides.

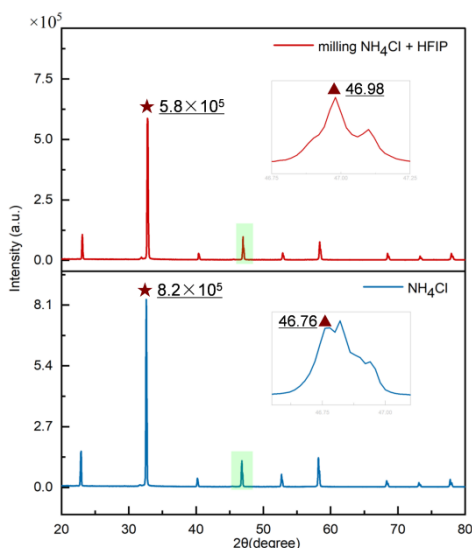


1a (1.2 mmol), indole (1 mmol, 1.0 equiv), HFIP (3 mmol), and salt (0.20 $m/m_{1a}+m_{indole}$) were added to a 50 mL ball mill jar. After grinding for 30 minutes, the mixture was dissolved in dichloromethane followed by filtration and purified by flash chromatography on silica gel (PE/DCM, v:v = 5:1) to afford the product **2a**. Herein, we examined nine different inorganic salts and NH₄Cl gives the highest yield of 1,3-enyne product.



5.4 XRD spectra of NH₄Cl or reaction between NH₄Cl and HFIP under ball-milling conditions.

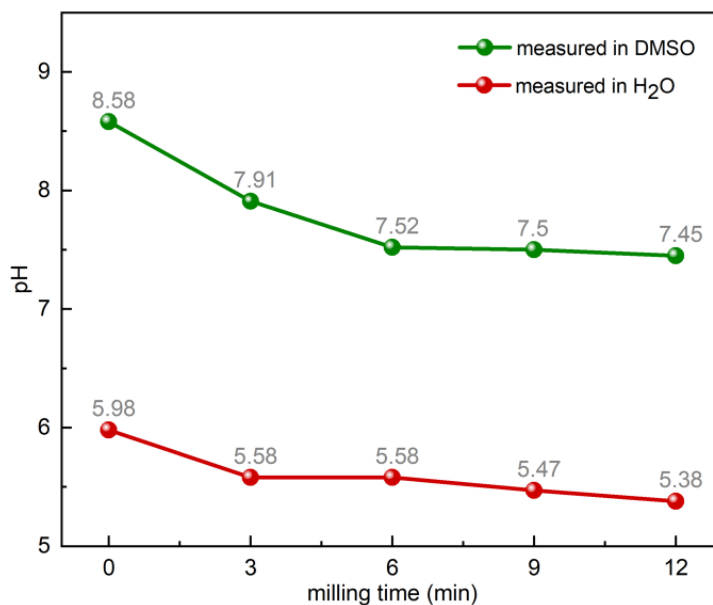
NH₄Cl (9.35 mmol, 500 mg) and HFIP (5 mmol, 1.57 mL) were placed in a ZrO₂ ball-milling jar (50 mL) loaded with grinding balls (ZrO₂). After the reaction was milled at 300 rpm for 10 min, the milled sample was collected for X-ray diffraction (XRD) analysis. Then another parallel experiment was furnished without HFIP. X-ray diffraction (XRD) further confirmed structural changes. NH₄Cl crystals exhibited distinct deviations in their diffraction patterns before and after milling.



5.5 Investigations of the changes in the acidity of HFIP caused by the introduction of NH₄Cl during ball milling

The pH measurement experiment was conducted using a pH meter. The electrode was first calibrated with standard buffer solutions (pH values of 4.0, 7.0, and 10.0), followed by rinsing

with distilled water. Subsequently, ammonium chloride and hexafluoroisopropanol were ground for different durations (0, 3, 6, 9, and 12 minutes). After each grinding period, 5 mL of DMSO (or 5 mL of water) was immediately added, and the solution was thoroughly homogenized before the pH value was measured and recorded. A line graph was then plotted to illustrate the relationship between the pH values and the grinding time.



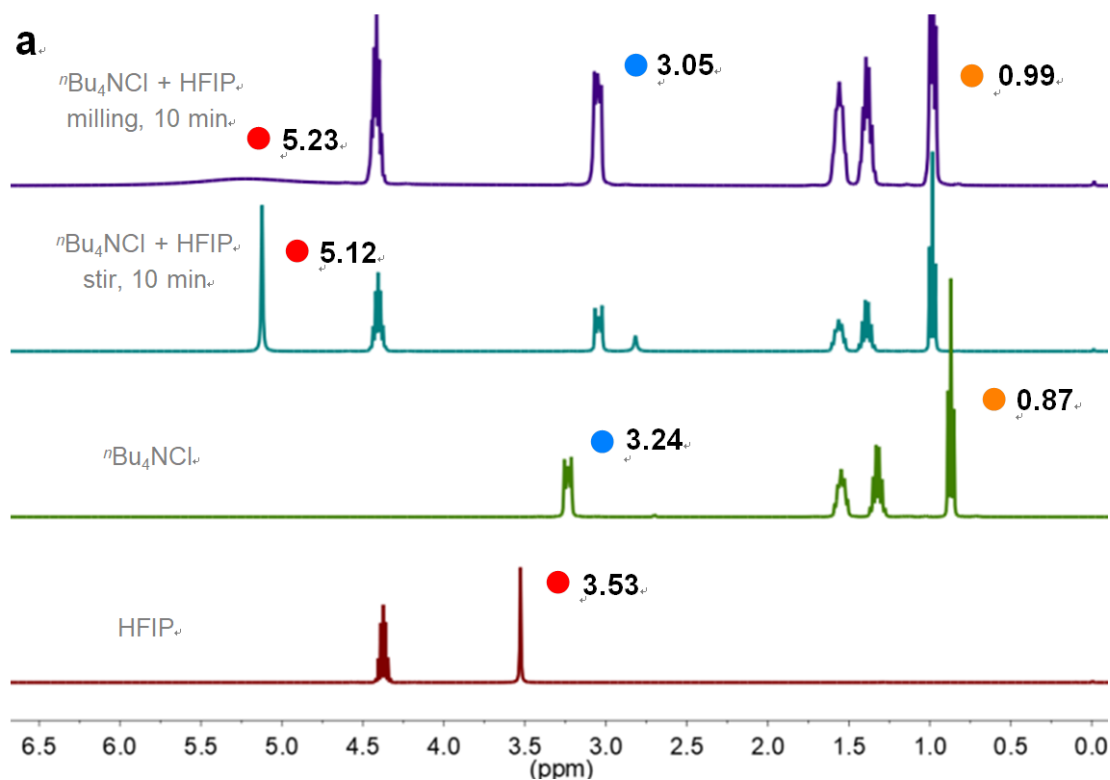
5.6 NMR experiments.

5.6.1 ¹H NMR of *n*-Bu₄NCl, HFIP and binary milling or stirring mixture.

¹H NMR (400 MHz, CDCl₃ with TMS)

¹H NMR experiments of binary milling mixture were performed according to the following procedure: At first, HFIP (105 μL, 1 mmol) and ⁿBu₄NCl (0.126 mmol) were placed in a ZrO₂ milling jar (25 mL) using ZrO₂ balls. After the vessel was closed in air, the vessel was placed in the planetary ball mill at 300 rpm. After 10 min, the resulting mixture was then diluted with CDCl₃ quickly. The samples were analyzed by ¹H NMR (400 MHz) with respect to the chemical shift of the hydroxyl proton of HFIP and ammonium moiety.

¹H NMR experiments of binary stirring mixture were performed according to the following procedure: At first, HFIP (105 μL, 1 mmol) and ⁿBu₄NCl (0.126 mmol) were placed in a nuclear magnetic tube. After mixing at room temperature for 10 min, the resulting mixture was then diluted with CDCl₃ quickly. The samples were analyzed by ¹H NMR (400 MHz) with respect to the chemical shift of the hydroxyl proton of HFIP and ammonium moiety.



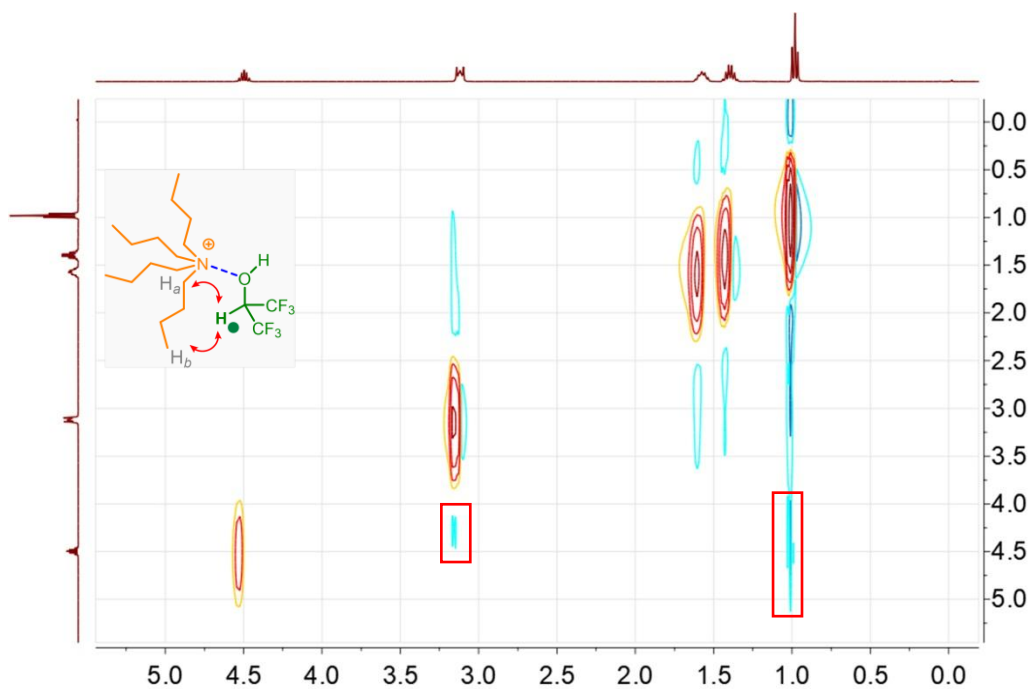
The most significant changes found in ^1H NMR, for the binary milling mixture compared to the individual species, are the downfield shift of the OH, from a frequency of 3.53 ppm (sharp signals) to 5.23 ppm (broad signals) ($\Delta = 1.70$) and the CH of HFIP, from a frequency of 4.38 ppm to 4.42 ppm ($\Delta = 0.04$). Additionally, upfield shift of the NCH_2 , from a frequency of 3.24 ppm to 3.05 ppm ($\Delta = 0.19$), and downfield shift of the CH_3 , from a frequency of 0.87 ppm to 0.99 ppm ($\Delta = 0.12$) were observed.

These data support a H-bonding reconstruction between the ammonium and HFIP. Meanwhile, both the OH and the CH of HFIP are deshielded, what might indicate not only the H-bonding reconstruction between the chloridion and OH, but also some degree of interaction between the cationic $n\text{-Bu}_4\text{N}^+$ and the hexafluoroisopropoxide moieties.

5.6.2 NOESY-2D experiment.

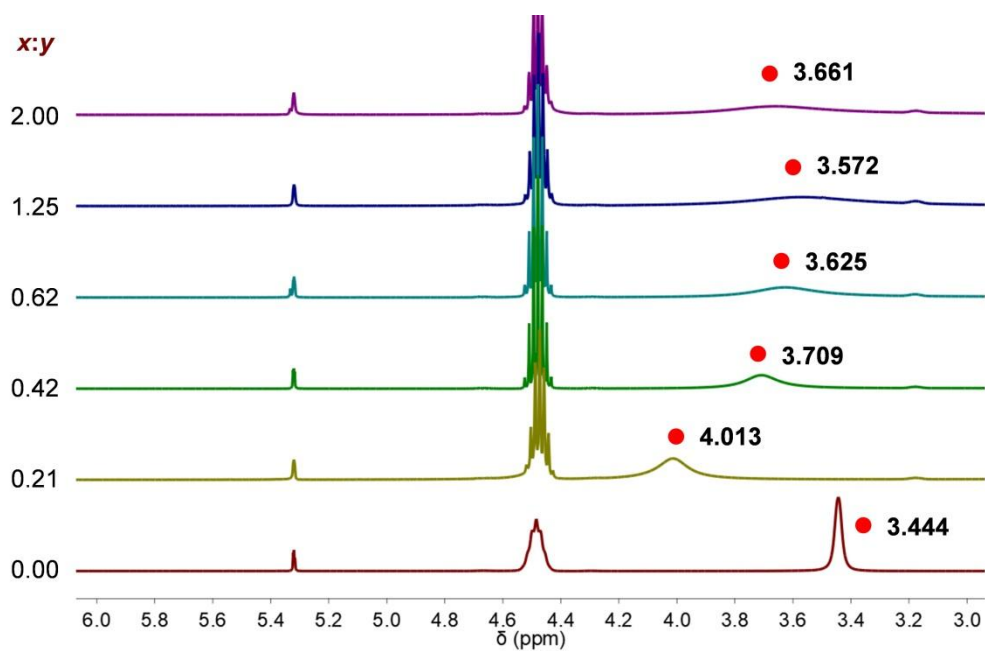
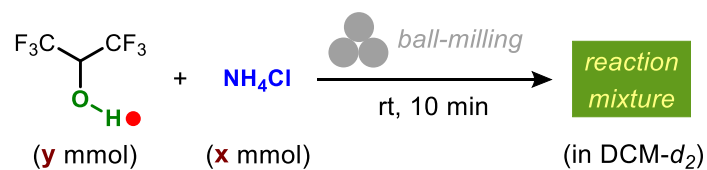
Additional support for the H-bonding reconstructions is found upon inspection of the NOESY-2D spectra of the milling mixture: HFIP (0.5 mmol) + $n\text{-Bu}_4\text{NCl}$ (0.126 mmol). Upon completion of the grinding process (10 minutes), CDCl_3 can be added to the mixture for the NOESY-2D experiment.

It was revealed that an apparent spatial correlation between both the H_a (NCH_2) and H_b (CH_3) of ammonium with the CH signals of HFIP.



5.6.3 NMR titration experiments.

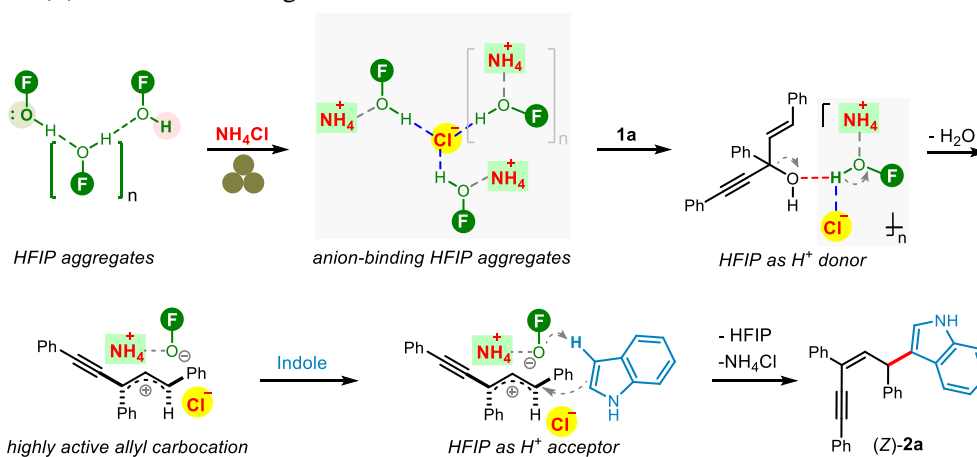
^1H NMR titration experiments were performed according to the following procedure: At first, HFIP (126 μL , 1 equiv) and various amount of NH_4Cl were placed in a ZrO_2 milling jar (50 mL) using 17 ZrO_2 balls. After the vessel was closed in air, the vessel was placed in the



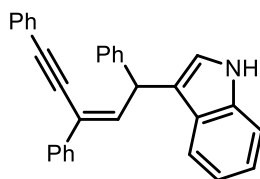
planetary ball mill at 300 rpm. After 10 min, the resulting mixture was then diluted with DCM- d_2 followed by filtration at the first opportunity. The samples were analyzed by ^1H NMR (400 MHz) with respect to the chemical shift of the hydroxyl proton of HFIP.

5.7 Proposed mechanism.

Based on the above results, we propose a cascade mechanism involving anion-binding H-bonding network reconstruction and NH_4Cl -facilitated allylic cation formation (Scheme 6). Under mechanical force, NH_4Cl and HFIP form a cooperative complex, dynamically binding by chloride anions to generate a more acidic aggregated state of HFIP. Alcohol **1a** is protonated by activated HFIP, forming a highly reactive allyl cation, for which the negative charge of corresponding counterion appearing partially offset via ammonium ion bonding to oxygen. Nucleophile then rapidly attacks the allyl cation, subsequent proton abstraction and aromatization by the conjugate base of HFIP yield the thermodynamically favored enyne product (**Z**)-**2a**, with HFIP regenerated.



6 ^1H , ^{13}C NMR and HRMS characterization data

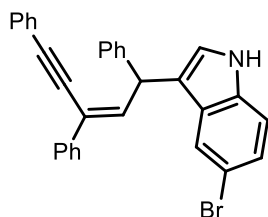


(Z)-3-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-indole (2a): 356.3 mg, 87% isolated yield, green viscous solid, $>20:1$ *Z/E*, R_f (PE/DCM = 5:1) = 0.3.

^1H NMR (400 MHz, CDCl_3) δ 7.96 (s, 1H), 7.73-7.69 (m, 2H), 7.55-7.48 (m, 3H), 7.43-7.41 (m, 2H), 7.35-7.21 (m, 10H), 7.18-7.15 (m, 1H), 7.05-7.01 (m, 1H), 6.94 (d, $J = 2.0$ Hz, 1H), 6.91 (d, $J = 10.0$ Hz, 1H), 5.83 (d, $J = 10.0$ Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 143.2, 139.7, 138.1, 136.8, 131.8, 128.7, 128.5, 128.4, 127.9, 127.0, 126.6, 126.5, 123.5, 123.3, 122.32, 122.28, 120.1, 119.7, 118.5, 111.3, 96.0, 86.9, 44.83.

HRMS (ESI $^+$): calcd. For $[\text{C}_{31}\text{H}_{25}\text{N}]^+$ ($M + \text{H}$) $^+$: 410.1909, found: 410.1912.

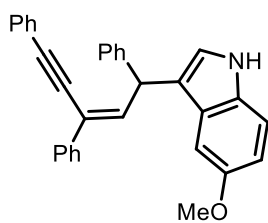


(Z)-5-Bromo-3-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-indole (2b): 429.8 mg, 88 % yield, brown solid, >20:1 *Z/E*, R_f (PE/DCM = 2:1) = 0.3.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.93 (s, 1H), 7.68-7.63 (m, 1H), 7.61 (d, J = 1.6 Hz, 1H), 7.52-7.49 (m, 2H), 7.36-7.17 (m, 12H), 7.14-7.11 (m, 1H), 6.90 (d, J = 1.6 Hz, 1H), 6.81 (d, J = 10.0 Hz, 1H), 5.73 (d, J = 10.0 Hz, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 142.8, 139.0, 137.9, 135.3, 131.8, 128.8, 128.7, 128.61, 128.55, 128.2, 128.0, 126.8, 126.5, 125.2, 123.53, 123.50, 123.2, 122.5, 118.2, 112.9, 112.7, 96.3, 86.7, 44.4.

HRMS (ESI^+): calcd. For $[\text{C}_{31}\text{H}_{24}\text{BrN}]^+$ ($\text{M} + \text{H}$) $^+$: 488.1014, found: 488.1015.

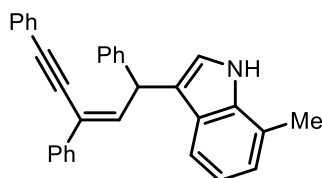


(Z)-5-Methoxy-3-(1,3,5-triphenylpent-2-en-1-yl)-1H-indole (2c): 246.2 mg, 56% yield, green solid, > 20:1 *Z/E*, R_f (PE/DCM = 2:1) = 0.3.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.95 (s, 2H), 7.75-7.73 (m, 2H), 7.60-7.57 (m, 3H), 7.50-7.48 (m, 2H), 7.41-7.35 (m, 6H), 7.34-7.29 (m, 2H), 7.29-7.26 (m, 1H), 7.05 (d, J = 2.4 Hz, 1H), 6.95-6.85 (m, 2H), 5.85 (d, J = 10.2 Hz, 1H), 3.71 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 154.0, 143.0, 139.7, 138.1, 131.8, 131.7, 128.7, 128.54, 128.52, 128.4, 127.9, 127.5, 126.7, 126.5, 123.5, 123.2, 123.1, 118.3, 112.6, 111.9, 101.7, 96.0, 87.0, 55.8, 44.8.

HRMS (ESI^+): calcd. For $[\text{C}_{32}\text{H}_{27}\text{NO}]^+$ ($\text{M} + \text{H}$) $^+$: 440.2016, found: 440.2011.

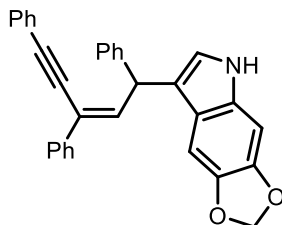


(Z)-7-Methyl-3-(1,3,5-triphenylpent-2-en-1-yl)-1H-indole (2d): 321.9 mg, 76% yield, green solid, > 20:1 *Z/E*, R_f (PE/DCM = 2:1) = 0.3.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.96 (s, 1H), 7.73-7.71 (m, 2H), 7.58-7.53 (m, 2H), 7.45-7.44 (m, 2H), 7.40-7.23 (m, 10H), 7.01-6.92 (m, 4H), 5.86 (d, J = 10.0 Hz, 1H), 2.50 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 143.3, 139.7, 138.1, 136.3, 131.8, 131.6, 128.6, 128.50, 128.49, 128.4, 127.9, 126.6, 126.5, 123.5, 123.2, 122.8, 122.0, 120.4, 119.9, 118.9, 117.9, 95.9, 86.9, 44.9, 16.8.

HRMS (ESI⁺): calcd. For $[\text{C}_{32}\text{H}_{27}\text{N}]^+$ (M + H)⁺: 424.2067, found: 424.2063.

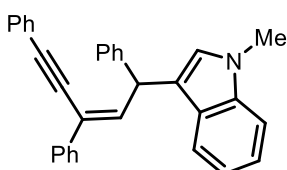


(Z)-7-(1,3,5-Triphenylpent-2-en-4-yn-1-yl)-5H-[1,3]dioxolo[4,5-f]indole (**2e**): 181.4 mg, 40% yield, brown liquid, > 20:1 Z/E, R_f (PE/DCM = 5:2) = 0.5.

^1H NMR (400 MHz, CDCl_3) δ 7.84 (s, 1H), 7.77-7.72 (m, 2H), δ 7.59-7.56 (m, 2H), 7.46-7.29 (m, 11H), 6.95 (s, 1H), 6.86 (d, J = 10.0 Hz, 1H), 6.76 (s, 1H), 6.24 (s, 1H), 5.90 (s, 2H), 5.72 (d, J = 10.0 Hz, 1H).

^{13}C NMR (100 MHz, CDCl_3) δ 144.5, 142.9, 141.3, 138.6, 137.6, 136.9, 131.8, 131.0, 129.1, 128.8, 128.61, 128.59, 128.5, 128.3, 127.4, 126.5, 124.5, 123.1, 122.3, 101.3, 100.5, 99.1, 96.2, 92.0, 86.4, 47.0.

HRMS (ESI⁺): calcd. For $[\text{C}_{32}\text{H}_{25}\text{NO}_2]^+$ (M + H)⁺: 454.1809, found: 454.1804.

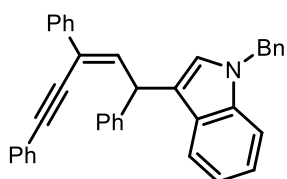


(Z)-1-Methyl-3-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-indole (**2f**): 402.4 mg, 95% yield, white solid, > 20:1 Z/E, R_f (PE/DCM = 2:1) = 0.3.

^1H NMR (400 MHz, CDCl_3) δ 7.77-7.75 (m, 2H), 7.62-7.54 (m, 3H), 7.50-7.48 (m, 2H), 7.42-7.24 (m, 11H), 7.10-7.06 (m, 1H), 6.96 (d, J = 10.0 Hz, 1H), 6.86 (s, 1H), 5.89 (d, J = 10.0 Hz, 1H), 3.78 (s, 3H).

^{13}C NMR (100 MHz, CDCl_3) δ 143.4, 139.8, 138.0, 137.5, 131.7, 128.7, 128.5, 128.3, 127.9, 127.3, 127.0, 126.6, 126.4, 123.5, 123.0, 121.8, 120.1, 119.1, 116.8, 109.4, 95.9, 86.9, 44.8, 32.8.

HRMS (ESI⁺): calcd. For $[\text{C}_{32}\text{H}_{25}\text{NNa}]^+$ (M + Na)⁺: 466.1885, found: 446.1879.



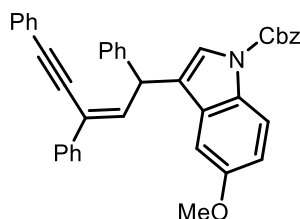
(Z)-1-Benzyl-3-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-indole (**2g**): 399.7 mg, 80% yield,

white solid, > 20:1 *Z/E*, R_f (PE/DCM = 2:1) = 0.3.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.71-7.69 (m, 2H), 7.53-7.51 (m, 3H), 7.45-7.43 (m, 2H), 7.34-7.29 (m, 7H), 7.27-7.20 (m, 6H), 7.17-7.10 (m, 1H), 7.10-7.04 (m, 2H), 7.03-7.00 (m, 1H), 6.94-6.88 (m, 2H), 5.86 (d, $J = 10.0$ Hz, 1H), 5.24 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 143.3, 139.7, 138.0, 137.7, 137.2, 131.8, 128.8, 128.7, 128.5, 128.3, 127.9, 127.7, 127.6, 126.7, 126.60, 126.58, 126.4, 123.4, 123.1, 122.0, 120.3, 119.4, 117.4, 109.9, 50.1, 44.8.

HRMS (ESI⁺): calcd. For $[\text{C}_{38}\text{H}_{29}\text{NNa}]^+$ ($M + \text{Na}$)⁺: 522.2198, found: 522.2201.

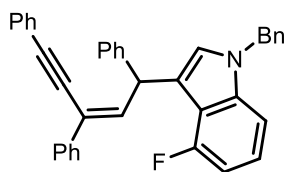


Benzyl (Z)-5-methoxy-3-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-indole-1-carboxylate (2h): 177.8 mg, 31% yield, yellow solid, > 20:1 *Z/E*, R_f (PE/DCM=5:2) = 0.4.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.04 (s, 1H), 7.71-7.69 (m, 2H), 7.55-7.52 (m, 2H), 7.48-7.46 (m, 2H), 7.43-7.25 (m, 15H), 6.93-6.89 (m, 2H), 6.81 (d, $J = 10.0$ Hz, 1H), 5.72 (d, $J = 10.0$ Hz, 1H), 5.43 (s, 2H), 3.67 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 156.0, 141.7, 137.9, 137.8, 135.4, 131.8, 128.90, 128.86, 128.8, 128.7, 128.60, 128.58, 128.3, 128.2, 127.0, 126.5, 124.2, 123.6, 123.2, 116.2, 113.4, 103.1, 96.5, 86.6, 68.7, 55.6, 44.5.

HRMS (ESI⁺): calcd. For $[\text{C}_{40}\text{H}_{31}\text{NO}_3\text{Na}]^+$ ($M + \text{Na}$)⁺: 596.2202, found: 596.2206.

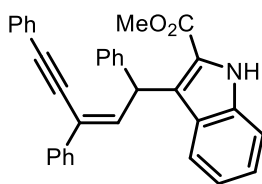


(Z)-1-Benzyl-4-fluoro-3-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-indole (2i): 429.6 mg, 83% yield, white solid, > 20:1 *Z/E*, R_f (PE/DCM = 5:2) = 0.65.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.73-7.66 (m, 2H), 7.51-7.48 (m, 2H), 7.38-7.37 (m, 2H), 7.35-7.15 (m, 12H), 7.09-7.03 (m, 2H), 7.03-6.94 (m, 4H), 6.72-6.65 (m, 1H), 6.03 (d, $J = 10.0$ Hz, 1H), 5.22 (s, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 157.1 (d, $J = 246.7$ Hz), 144.3, 139.9, 139.83 (d, $J = 1.6$ Hz), 139.80, 138.1, 137.2, 131.8, 128.9, 128.5, 128.4, 127.92, 127.88, 127.8, 126.7, 126.6, 126.42, 126.35, 123.1 (d, $J = 86.1$ Hz), 123.3, 122.6, 116.2 (d, $J = 20.1$ Hz), 115.8 (d, $J = 3.7$ Hz), 106.0 (d, $J = 3.6$ Hz), 104.9 (d, $J = 19.8$ Hz), 96.0, 86.9, 50.4, 44.8.

HRMS (ESI⁺): calcd. For [C₃₈H₂₈FNK]⁺ (M + K)⁺: 556.1843, found: 556.1838.

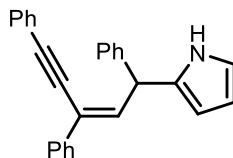


Methyl (Z)-3-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-indole-2-carboxylate (2j): 307.7 mg, 68% yield, brown solid, > 20:1 *Z/E*, **R_f**(PE/DCM = 5:2) = 0.4.

¹H NMR (400 MHz, CDCl₃) δ 9.15 (s, 1H), 7.81-7.79 (m, 2H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.61-7.59 (m, 2H), 7.48-7.42 (m, 3H), 7.42-7.27 (m, 11H), 7.14-7.10 (m, 1H), 6.86 (d, *J* = 9.8 Hz, 1H), 3.83 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 162.8, 143.0, 138.4, 138.1, 136.5, 131.8, 128.5, 128.44, 128.41, 128.0, 127.8, 127.0, 126.5, 126.3, 125.6, 124.9, 124.2, 123.8, 123.5, 122.7, 120.5, 112.2, 95.8, 86.9, 43.2.

HRMS (ESI⁺): calcd. For [C₃₃H₂₅NO₂Na]⁺ (M + Na)⁺: 490.1783, found: 490.1784.

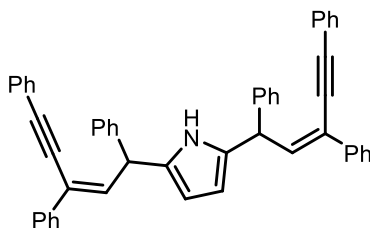


(Z)-2-(1,3,5-Triphenylpent-2-en-4-yn-1-yl)-1H-pyrrole (2k): 133.0 mg, 37% yield, brown solid, > 20:1 *Z/E*, **R_f**(PE/DCM = 5:2) = 0.5.

¹H NMR (400 MHz, CDCl₃) δ 8.02 (s, 1H), 7.78-7.76 (m, 2H), 7.63-7.60 (m, 2H), 7.47-7.40 (m, 9H), 7.38-7.31 (m, 2H), 6.87 (d, *J* = 10.0 Hz, 1H), 6.78-6.77 (m, 1H), 6.25 (q, *J* = 3.0 Hz, 1H), 6.10-6.06 (s, 1H), 5.67 (d, *J* = 9.6 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 141.8, 137.8, 137.7, 133.0, 131.8, 128.9, 128.7, 128.6, 128.5, 128.1, 127.2, 126.4, 123.9, 123.2, 117.5, 108.5, 106.5, 95.9, 86.5, 46.5.

HRMS (ESI⁺): calcd. For [C₂₇H₂₁NNa]⁺ (M + Na)⁺: 360.1756, found: 360.1756.



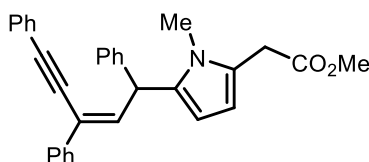
Bis((Z)-1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-pyrrole (2l): 241.2 mg, 37% yield, blue solid, > 20:1 *Z/E*, **R_f**(PE/DCM = 5:2) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.98 (s, 1H), 7.71-7.69 (m, 4H), 7.53-7.51 (m, 4H), 7.45-7.43 (m, 4H), 7.38-7.28 (m, 18H), 6.82 (d, *J* = 10.0 Hz, 2H), 5.98-5.96 (m, 2H), 5.61 (d, *J* = 10.0 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 141.8, 138.0, 137.8, 132.8, 131.8, 128.8, 128.6, 128.5, 128.4,

128.1, 127.1, 126.5, 123.7, 123.1, 106.6, 95.9, 86.6, 46.6.

HRMS (ESI⁺): calcd. For [C₅₀H₃₈N]⁺ (M + H)⁺: 652.3004, found: 652.3004.

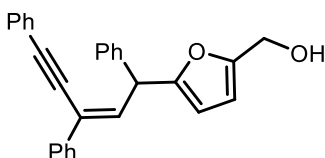


Methyl (Z)-2-(1-methyl-5-(1,3,5-triphenylpent-2-en-4-yn-1-yl)-1H-pyrrol-2-yl) acetate (2m): 320.8 mg, 72% yield, yellow solid, > 20:1 Z/E, **R_f** (PE/EA = 9:1) = 0.5.

¹H NMR (400 MHz, CDCl₃) δ 7.69-7.67 (m, 2H), 7.55-7.53 (m, 2H), 7.37-7.27 (m, 10H), 7.23-7.19 (m, 1H), 6.76 (d, *J* = 10.0 Hz, 1H), 6.04-5.96 (m, 2H), 5.59 (d, *J* = 10.0 Hz, 1H), 3.67 (s, 3H), 3.62 (s, 2H), 3.39 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 171.2, 142.3, 137.8, 133.9, 131.7, 128.8, 128.61, 128.57, 128.5, 128.1, 128.0, 126.8, 126.4, 125.2, 123.3, 123.1, 107.6, 106.4, 96.1, 86.7, 52.3, 45.6, 33.0, 31.1.

HRMS (ESI⁺): calcd. For [C₃₁H₂₈NO₂]⁺ (M + H)⁺: 446.2120, found: 446.2123.

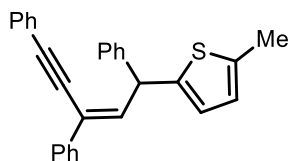


(Z)-5-(1,3,5-Triphenylpent-2-en-4-yn-1-yl)furan-2-yl) methanol (2n): 277.3 mg, 71% yield, brown solid, > 20:1 Z/E, **R_f** (PE/EA = 17:3) = 0.3.

¹H NMR (400 MHz, CDCl₃) δ 7.78-7.76 (m, 2H), 7.63-7.61 (m, 2H), 7.44-7.30 (m, 11H), 6.87 (d, *J* = 9.6 Hz, 1H), 6.30 (d, *J* = 3.2 Hz, 1H), 6.20 (d, *J* = 3.0 Hz, 1H), 5.70 (d, *J* = 10.0 Hz, 1H), 4.56 (s, 2H), 2.21 (s, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 155.6, 153.6, 141.3, 137.6, 135.9, 131.7, 128.8, 128.7, 128.5, 128.2, 128.0, 127.0, 126.4, 124.6, 123.1, 108.7, 107.5, 96.3, 86.3, 57.5, 46.9.

HRMS (ESI⁺): calcd. For [C₂₈H₂₂O₂Na]⁺ (M + Na)⁺: 413.1520, found: 413.1517.

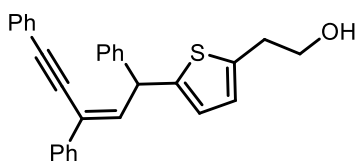


(Z)-2-Methyl-5-(1,3,5-triphenylpent-2-en-4-yn-1-yl) thiophene (2o): 304.6 mg, 78% yield, yellow solid, > 20:1 Z/E, **R_f** (PE/EA = 19:1) = 0.3.

¹H NMR (400 MHz, CDCl₃) δ 7.80-7.78 (m, 2H), 7.64-7.62 (m, 2H), 7.50-7.48 (m, 2H), 7.46-7.40 (m, 7H), 7.39-7.31 (m, 2H), 6.91 (d, *J* = 10.0 Hz, 1H), 6.75-6.68 (m, 2H), 5.81 (d, *J* = 10.0 Hz, 1H), 2.51 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 144.8, 143.2, 138.9, 138.5, 137.8, 131.8, 128.8, 128.6, 128.54, 128.52, 128.2, 128.1, 127.1, 126.5, 124.9, 124.8, 123.9, 123.3, 96.1, 86.5, 48.3, 15.5.

HRMS (ESI⁺): calcd. For [C₂₈H₂₂SNa]⁺ (M + Na)⁺: 413.1338, found: 413.1340.

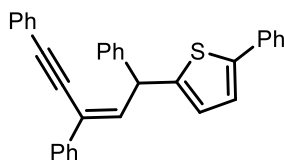


(Z)-2-(5-(1,3,5-Triphenylpent-2-en-4-yn-1-yl)thiophen-2-yl) ethan-1-ol (2p): 201.9 mg, 48% yield, brown solid, > 20:1 *Z/E*, **R_f**(PE/EA = 17:3) = 0.3.

¹H NMR (400 MHz, CDCl₃) δ 7.77-7.75 (m, 2H), 7.61-7.58 (m, 2H), 7.46-7.29 (m, 11H), 6.88 (d, *J* = 9.6 Hz, 1H), 6.78-6.75 (m, 2H), 5.78 (d, *J* = 10.0 Hz, 1H), 3.85 (t, *J* = 6.4 Hz, 2H), 3.03 (t, *J* = 6.4 Hz, 2H), 1.78 (s, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 145.9, 143.0, 139.9, 138.2, 137.6, 131.8, 128.8, 128.6, 128.54, 128.52, 128.2, 127.1, 126.5, 125.5, 124.8, 124.0, 123.2, 96.2, 86.3, 63.4, 48.3, 33.7.

HRMS (ESI⁺): calcd. For [C₂₉H₂₄OSNa]⁺ (M + Na)⁺: 443.1443, found: 443.1446.

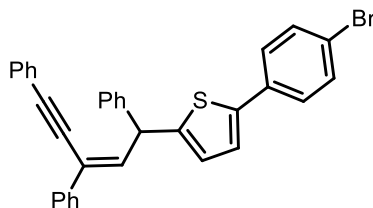


(Z)-2-Phenyl-5-(1,3,5-triphenylpent-2-en-4-yn-1-yl) thiophene (2q): 402.8 mg, 89% yield, light yellow liquid, > 20:1 *Z/E*, **R_f**(PE/DCM = 5:1) = 0.3.

¹H NMR (400 MHz, CDCl₃) δ 7.74-7.70 (m, 2H), 7.56-7.53 (m, 4H), 7.44-7.42 (m, 2H), 7.38-7.24 (m, 11H), 7.23-7.19 (m, 1H), 7.16 (d, *J* = 3.6 Hz, 1H), 6.87-6.83 (m, 2H), 5.78 (d, *J* = 10.0 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 146.9, 143.4, 142.8, 138.1, 137.6, 134.6, 131.8, 128.92, 128.88, 128.7, 128.58, 128.55, 128.3, 127.4, 127.2, 126.5, 126.1, 125.67, 124.30, 123.19, 122.87, 96.31, 86.32, 77.48, 77.16, 76.84, 48.40.

HRMS (ESI⁺): calcd. For C₃₃H₂₄S⁺ (M + H)⁺: 453.1677, found: 453.1678.

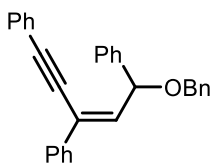


(Z)-2-(4-Bromophenyl)-5-(1,3,5-triphenylpent-2-en-4-yn-1-yl) thiophene (2r): 281.7 mg, 53% yield, white solid, > 20:1 *Z/E*, **R_f**(PE/DCM = 9:1) = 0.5.

¹H NMR (400 MHz, CDCl₃) δ 7.78-7.77 (m, 2H), 7.62-7.59 (m, 2H), 7.50-7.31 (m, 15H), 7.20 (d, *J* = 3.6 Hz, 1H), 6.91-6.89 (m, 2H), 5.83 (d, *J* = 10.0 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃) δ 147.6, 142.7, 142.0, 137.8, 137.6, 133.5, 132.0, 131.8, 128.9, 128.7, 128.60, 128.56, 128.3, 128.2, 127.3, 127.1, 126.5, 126.2, 124.5, 123.3, 123.2, 121.1, 96.4, 86.3, 48.4.

HRMS (ESI⁺): calcd. For [C₃₃H₂₅S]⁺ (M + H)⁺: 531.0782, found: 531.0770.

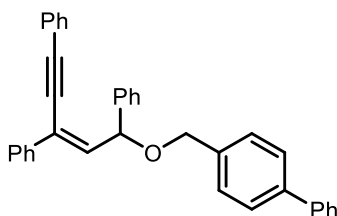


(Z)-5-(Benzyloxy) pent-3-en-1-yn-1,3,5-triyl tribenzene (3a): 332.4 mg, 83% yield, yellow liquid, > 20:1 *Z/E*, **R_f** (PE/DCM = 7:3) = 0.5.

¹H NMR (400 MHz, CDCl₃) δ 7.79-7.78 (m, 2H), 7.65-7.63 (m, 2H), 7.54-7.50 (m, 4H), 7.48-7.30 (m, 12H), 6.68 (d, *J* = 9.2 Hz, 1H), 5.88 (d, *J* = 9.2 Hz, 1H), 4.77 (q, *J* = 12.4 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 141.2, 138.5, 137.2, 137.1, 131.8, 128.72, 128.70, 128.54, 128.51, 128.48, 128.4, 128.0, 127.8, 127.6, 126.7, 126.5, 125.4, 123.0, 96.5, 86.3, 79.4, 70.5.

HRMS (ESI⁺): calcd. For [C₃₀H₂₄ONa]⁺ (M + Na)⁺: 423.1725, found: 423.1724.

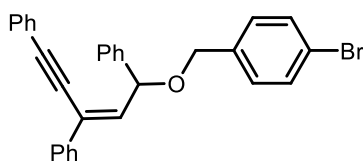


(Z)-4-(((1,3,5-Triphenylpent-2-en-4-yn-1-yl) oxy) methyl)-1,1'-biphenyl (3b): 371.4 mg, 78% yield, brown liquid, > 20:1 *Z/E*, **R_f** (PE/EA=19:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.81-7.79 (m, 2H), 7.67-7.62 (m, 6H), 7.59-7.57 (m, 2H), 7.52-7.36 (m, 14H), 6.70 (d, *J* = 8.8 Hz, 1H), 5.91 (d, *J* = 9.2 Hz, 1H), 4.87-4.79 (m, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 141.1, 141.0, 140.6, 137.6, 137.1, 131.7, 128.8, 128.73, 128.69, 128.6, 128.5, 128.4, 127.9, 127.3, 127.24, 127.18, 126.7, 126.5, 125.5, 123.0, 96.5, 86.3, 79.2, 70.2.

HRMS (ESI⁺): calcd. For [C₃₆H₂₈ONa]⁺ (M + Na)⁺: 499.2038, found: 499.2036.

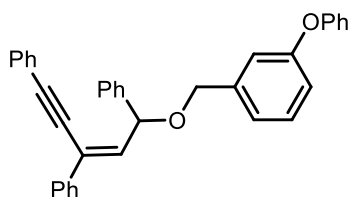


(Z)-5-(((4-Bromobenzyl)oxy) pent-3-en-1-yn-1,3,5-triyl)tribenzene (3c): 350.0 mg, 73% yield, yellow solid, > 20:1 *Z/E*, **R_f** (PE/EA = 19:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.7-7.72 (m, 2H), 7.56-7.55 (m, 2H), 7.47-7.39 (m, 11H), 7.36-7.31 (m, 4H), 6.59 (d, *J* = 9.2 Hz, 1H), 5.78 (d, *J* = 9.2 Hz, 1H), 4.67 (q, *J* = 12.4 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 140.9, 137.6, 137.0, 136.7, 131.7, 131.6, 129.7, 128.82, 128.77, 128.62, 128.59, 128.5, 128.0, 126.6, 126.5, 125.7, 122.9, 121.6, 96.6, 86.1, 79.2, 69.6.

HRMS (ESI⁺): calcd. For [C₃₀H₂₄BrO]⁺ (M + H)⁺: 479.1011, found: 479.1109.

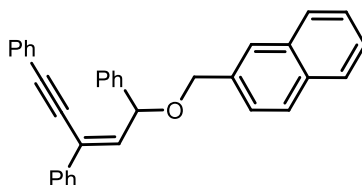


(Z)-5-((3-Phenoxybenzyl) oxy) pent-3-en-1-yne-1,3,5-triyl tribenzene (3d): 295.6 mg, 60% yield, orange liquid, > 20:1 *Z/E*, R_f (PE/EA = 19:1) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.74-7.72 (m, 2H), 7.58-7.56 (m, 2H), 7.52-7.50 (m, 2H), 7.43-7.30 (m, 12H), 7.21-7.19 (m, 1H), 7.14-7.10 (m, 2H), 7.02-7.01 (m, 2H), 6.96-6.94 (m, 1H), 6.62-6.60 (m, 1H), 5.83 (d, $J = 9.2$ Hz, 1H), 4.70 (q, $J = 12.4$ Hz, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 157.6, 157.2, 141.0, 140.7, 137.1, 137.0, 131.8, 129.82, 129.78, 128.76, 128.7, 128.6, 128.5, 127.9, 126.7, 126.5, 125.5, 123.4, 123.0, 122.6, 119.2, 118.1, 117.9, 96.6, 86.2, 79.6, 70.1.

HRMS (ESI⁺): calcd. For $[\text{C}_{36}\text{H}_{28}\text{O}_2\text{Na}]^+$ ($M + \text{Na}$)⁺: 515.1987, found: 515.1987.

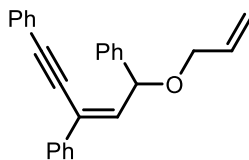


(Z)-2-(((1,3,5-Triphenylpent-2-en-4-yn-1-yl) oxy) methyl) naphthalene (3e): 360.5 mg, 80% yield, orange liquid, > 20:1 *Z/E*, R_f (PE/EA = 19:1) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.83-7.77 (m, 3H), 7.73-7.68 (m, 3H), 7.56-7.53 (m, 3H), 7.44-7.32 (m, 6H), 7.30-7.16 (m, 7H), 6.61 (d, $J = 9.2$ Hz, 1H), 5.82 (d, $J = 9.2$ Hz, 1H), 4.84 (q, $J = 12.4$ Hz, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.1, 137.14, 137.05, 135.9, 133.4, 133.1, 131.6, 128.7, 128.59, 128.56, 128.4, 128.3, 128.1, 127.9, 127.8, 126.9, 126.7, 126.5, 126.11, 126.08, 125.9, 125.5, 122.9, 96.5, 86.2, 79.1, 70.5.

HRMS (ESI⁺): calcd. For $[\text{C}_{34}\text{H}_{26}\text{ONa}]^+$ ($M + \text{Na}$)⁺: 473.1881, found: 473.1884.

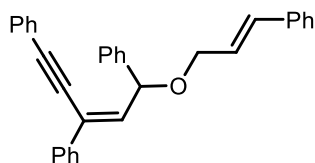


(Z)-5-(Allyloxy) pent-3-en-1-yne-1,3,5-triyl tribenzene (3f): 122.7 mg, 35% yield, yellow liquid, > 20:1 *Z/E*, R_f (PE/EA = 19:1) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.73-7.71 (m, 2H), 7.61-7.58 (m, 2H), 7.55-7.54 (m, 1H), 7.43-7.29 (m, 9H), 6.56 (d, $J = 9.2$ Hz, 1H), 6.08-5.99 (m, 1H), 5.77 (d, $J = 9.2$ Hz, 1H), 5.41-5.36 (m, 1H), 5.25-5.22 (m, 1H), 4.22-4.11 (m, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.2, 137.3, 137.2, 134.9, 131.7, 128.8, 128.7, 128.62, 128.56, 128.4, 127.8, 126.7, 126.5, 125.2, 123.2, 117.4, 96.5, 92.8, 86.4, 79.6, 69.6.

HRMS (ESI⁺): calcd. For [C₂₆H₂₂ONa]⁺ (M + Na)⁺: 373.1568, found: 373.1566.

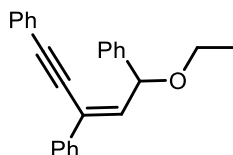


((Z)-5-(Cinnamyloxy) pent-3-en-1-yne-1,3,5-triyl) tribenzene (3g): 260.2 mg, 61% yield, yellow liquid, > 20:1 *Z/E*, **R_f** (PE/EA = 19:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.71-7.69 (m, 2H), 7.55-7.53 (m, 2H), 7.47-7.45 (m, 2H), 7.39-7.25 (m, 12H), 7.23-7.18 (m, 2H), 6.67-6.61 (m, 1H), 6.56 (d, *J* = 8.8 Hz, 1H), 6.41-6.35 (m, 1H), 5.82 (d, *J* = 8.8 Hz, 1H), 4.44-4.33(m, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 141.2, 137.2, 137.1, 136.8, 133.0, 131.7, 128.8, 128.7, 128.59, 128.55, 128.53, 128.4, 127.9, 127.7, 126.7, 126.5, 126.1, 125.4, 123.0, 96.6, 86.3, 79.2, 69.2.

HRMS (ESI⁺): calcd. For [C₃₂H₂₆ONa]⁺ (M + Na)⁺: 449.1881, found: 449.1882.

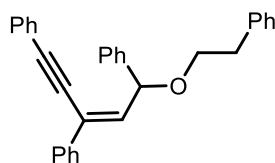


(Z)-5-Ethoxypent-3-en-1-yne-1,3,5-triyl) tribenzene (3h): 264.0 mg, 78% yield, yellow viscous solid, > 20:1 *Z/E*, **R_f** (PE/EA = 19:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.72-7.70 (m, 2H), 7.61-7.58 (m, 2H), 7.55-7.53 (m, 2H), 7.43-7.35 (m, 7H), 7.33-7.25 (m, 2H), 6.56 (d, *J* = 9.2 Hz, 1H), 5.70 (d, *J* = 9.2 Hz, 1H), 3.76-3.59 (m, 2H), 1.32 (t, *J* = 7.2 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 141.5, 137.7, 137.3, 131.7, 128.8, 128.7, 128.6, 128.5, 128.3, 127.8, 126.6, 126.5, 124.9, 123.2, 96.4, 86.4, 80.2, 64.3, 15.6.

HRMS (ESI⁺): calcd. For [C₂₅H₂₃O]⁺ (M + H)⁺: 339.1749, found: 339.1747.

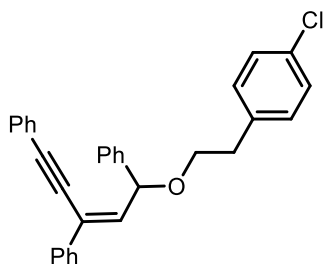


(Z)-5-Phenethoxypent-3-en-1-yne-1,3,5-triyl) tribenzene (3i): 273.4 mg, 66% isolated yield, yellow solid, >20:1 *Z/E*, **R_f** (PE/EA = 19:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.66-7.64 (m, 2H), 7.55-7.53 (m, 2H), 7.48-7.46 (m, 2H), 7.36-7.31 (m, 7H), 7.29-7.22 (m, 6H), 7.20-7.16 (m, 1H), 6.47 (d, *J* = 8.8 Hz, 1H), 5.71 (d, *J* = 9.2 Hz, 1H), 3.88-3.74 (m, 2H), 2.99 (t, *J* = 7.2 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 141.3, 139.1, 137.5, 137.1, 131.7, 129.2, 128.8, 128.7, 128.6, 128.5, 128.4, 128.4, 127.8, 126.5, 126.4, 126.3, 125.1, 123.2, 96.5, 86.3, 80.4, 69.8, 36.67.

HRMS (ESI⁺): calcd. For [C₃₁H₂₆ONa]⁺ (M + Na)⁺: 437.1881, found: 431.1877.

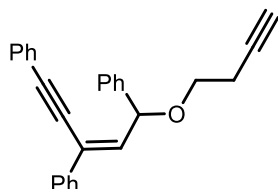


(Z)-5-(4-Chlorophenoxy) pent-3-en-1-yne-1,3,5-triyl tribenzene (3j): 211.0 mg, 47% isolated yield, yellow solid, >20:1 Z/E, R_f (PE/EA = 19:1) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.65-7.63 (m, 2H), 7.55-7.53 (m, 2H), 7.45-7.43 (m, 2H), 7.38-7.32 (m, 7H), 7.30-7.20 (m, 4H), 7.16-7.14 (m, 2H), 6.42 (d, J = 8.8 Hz, 1H), 5.67 (d, J = 8.8 Hz, 1H), 3.85-3.71 (m, 2H), 2.93 (t, J = 6.8 Hz, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.2, 137.8, 137.3, 137.1, 132.0, 131.7, 130.5, 128.8, 128.7, 128.63, 128.55, 128.5, 128.4, 127.8, 126.5, 126.4, 125.2, 123.1, 96.5, 86.3, 80.4, 69.5, 36.0.

HRMS (ESI^+): calcd. For $[\text{C}_{31}\text{H}_{25}\text{ClONa}]^+$ ($M + \text{Na}$) $^+$: 471.1492, found: 471.1495.

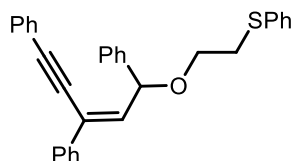


(Z)-5-(But-3-yn-1-yloxy) pent-3-en-1-yne-1,3,5-triyl tribenzene (3k): 115.9 mg, 32% isolated yield, yellow solid, >20:1 Z/E, R_f (PE/EA = 19:1) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.74-7.71 (m 2H), 7.62-7.60 (m, 2H), 7.56-7.54 (m, 2H), 7.42-7.37 (m, 7H), 7.35-7.29 (m, 2H), 6.56 (d, J = 8.8 Hz, 1H), 5.75 (d, J = 9.2 Hz, 1H), 3.83-3.70 (m, 2H), 2.62-2.58 (m, 2H), 2.01 (t, J = 2.4 Hz, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.0, 137.1, 137.0, 131.7, 128.8, 128.7, 128.63, 128.55, 128.5, 127.9, 126.6, 126.5, 125.3, 123.1, 96.6, 86.2, 81.5, 80.5, 69.5, 66.9, 20.2.

HRMS (ESI^+): calcd. For $[\text{C}_{27}\text{H}_{22}\text{ONa}]^+$ ($M + \text{Na}$) $^+$: 385.1568, found: 385.1563.

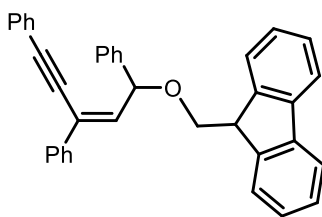


(Z)-Phenyl (2-((1,3,5-triphenylpent-2-en-4-yn-1-yl) oxy) ethyl) sulfane (3l): 245.4 mg, 55% isolated yield, orange solid, >20:1 Z/E, R_f (PE/EA = 20:1) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.67-7.65 (m, 2H), 7.54-7.52 (m, 2H), 7.49-7.55 (m, 2H), 7.36-7.28 (m, 11H), 7.21-7.17 (m, 2H), 7.13-7.09 (m, 1H), 6.50 (d, J = 9.2 Hz, 1H), 5.69 (d, J = 9.2 Hz, 1H), 3.87-3.75 (m, 2H), 3.21 (t, J = 6.8 Hz, 2H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 141.0, 137.1, 137.0, 136.2, 131.7, 129.4, 129.0, 128.8, 128.7, 128.6, 128.5, 128.4, 127.9, 126.6, 126.5, 126.1, 125.4, 123.0, 96.6, 86.2, 80.5, 67.5, 33.6.

HRMS (ESI⁺): calcd. For [C₃₁H₂₆OSNa]⁺ (M + Na)⁺: 469.1602, found: 469.1611.

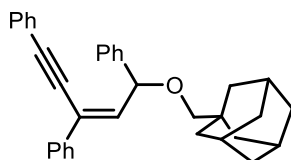


(Z)-9-(((1,3,5-Triphenylpent-2-en-4-yn-1-yl) oxy) methyl)-9H-fluorene (3m): 293.2 mg, 60% isolated yield, yellow solid, >20:1 *Z/E*, **R_f** (PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.80-7.78 (m, 3H), 7.74-7.72 (m, 3H), 7.66-7.64 (m, 2H), 7.56-7.54 (m, 2H), 7.47-7.32 (m, 13H), 6.64 (d, *J* = 8.8 Hz, 1H), 5.89 (d, *J* = 8.8 Hz, 1H), 4.39 (t, *J* = 7.6 Hz, 1H), 3.95 (d, *J* = 7.6 Hz, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 145.2, 144.9, 141.4, 141.3, 141.2, 137.4, 137.2, 131.7, 128.8, 128.7, 128.6, 128.4, 127.8, 127.5, 127.1, 127.0, 126.6, 126.5, 125.6, 125.5, 125.4, 123.0, 119.9, 96.6, 86.3, 80.9, 71.7, 48.3.

HRMS (ESI⁺): calcd. For [C₃₇H₂₈ONa]⁺ (M + Na)⁺: 511.2038, found: 511.2037.

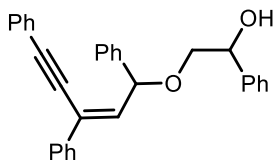


(1R,3R,5S)-1-(((Z)-1,3,5-Triphenylpent-2-en-4-yn-1-yl) oxy) methyl) adamantane (3n): 238.5 mg, 52% isolated yield, colorless viscous solid, >20:1 *Z/E*, **R_f** (PE/EA = 20:1) = 0.4.

¹H NMR (400 MHz, CDCl₃) δ 7.75-7.73 (m, 2H), 7.63-7.61 (m, 2H), 7.58-7.56 (m, 2H), 7.43-7.38 (m, 7H), 7.35-7.29 (m, 2H), 6.52 (d, *J* = 9.2 Hz, 1H), 5.65 (d, *J* = 8.8 Hz, 1H), 3.27-3.16 (m, 2H), 2.05-1.99 (m, 3H), 1.78-1.67 (m, 12H).

¹³C NMR (100 MHz, CDCl₃) δ 141.9, 138.5, 137.3, 131.7, 128.7, 128.6, 128.5, 128.3, 127.5, 126.4, 124.6, 123.3, 96.2, 86.6, 80.4, 79.7, 40.0, 37.4, 34.4, 28.5.

HRMS (ESI⁺): calcd. For [C₃₄H₃₅O]⁺ (M + H)⁺: 459.2688, found: 459.2685.



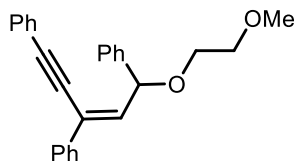
(Z)-1-Phenyl-2-(((1,3,5-triphenylpent-2-en-4-yn-1-yl) oxy) ethan-1-ol (3o): 176.5 mg, 41% isolated yield, yellow liquid, *dr* = 1:1, >20:1 *Z/E*, **R_f** (PE/EA = 10:1) = 0.3.

¹H NMR (400 MHz, CDCl₃) δ 7.74-7.42 (m, 5H), 7.62-7.54 (m, 11H), 7.41-7.30 (m, 34H), 6.59-6.57 (m, 2H), 5.83-5.79 (m, 2H), 5.07-5.04 (m, 2H), 3.88-3.76 (m, 2H), 3.72-3.63 (m, 2H), 3.04 (s, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 140.79, 140.76, 140.2, 137.0, 136.6, 136.5, 131.8, 131.7, 128.9, 128.8, 128.6, 128.6, 128.52, 128.46, 128.1, 128.0, 127.9, 126.6, 126.6, 126.5, 126.4,

126.1, 125.8, 125.5, 122.9, 96.9, 96.8, 86.2, 86.1, 81.1, 80.8, 74.6, 74.4, 73.2, 72.9.

HRMS (ESI⁺): calcd. For [C₃₁H₂₆O₂Na]⁺ (M + Na)⁺: 453.1830, found: 453.1823.

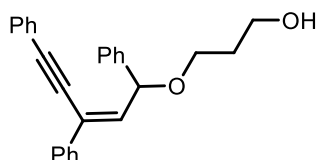


(Z)-5-(2-Methoxyethoxy) pent-3-en-1-yn-1,3,5-triyl tribenzene (3p): 125.3 mg, 34% isolated yield, yellow liquid, >20:1 *Z/E*, **R_f** (PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.74-7.72 (m, 2H), 7.63-7.60 (m, 2H), 7.58-7.56 (m, 2H), 7.44-7.31 (m, 7H), 7.34-7.29 (m, 2H), 6.63-6.60 (m, 1H), 5.77 (d, *J* = 8.8 Hz, 1H), 3.86-3.73 (m, 2H), 3.68-3.66 (m, 2H), 3.45-3.42 (m, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 141.1, 137.3, 137.2, 131.7, 128.8, 128.7, 128.6, 128.5, 128.3, 127.8, 126.7, 126.4, 125.0, 123.1, 96.5, 86.3, 80.8, 72.1, 68.1, 59.2.

HRMS (ESI⁺): calcd. For [C₂₆H₂₄O₂Na]⁺ (M + Na)⁺: 391.1674, found: 391.1677.

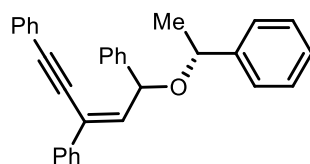


(Z)-3-((1,3,5-Triphenylpent-2-en-4-yn-1-yl)oxy) propan-1-ol (3q): 165.8 mg, 45% isolated yield, light yellow liquid, >20:1 *Z/E*, **R_f** (PE/EA = 5:1) = 0.2.

¹H NMR (400 MHz, CDCl₃) δ 7.76-7.74 (m, 2H), 7.65-7.63 (m, 2H), 7.57-7.55 (m, 2H), 7.47-7.39 (m, 7H), 7.37-7.32 (m, 2H), 6.57 (d, *J* = 8.8 Hz, 1H), 5.74 (d, *J* = 8.8 Hz, 1H), 3.91-3.85 (m, 3H), 3.80-3.75 (m, 1H), 2.52 (s, 1H), 2.00-1.94 (m, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 141.0, 137.1, 137.0, 131.7, 128.8, 128.7, 128.6, 128.5, 128.4, 127.9, 126.5, 126.4, 125.4, 123.0, 96.6, 86.2, 80.8, 67.8, 61.8, 32.4.

HRMS (ESI⁺): calcd. For [C₂₆H₂₄O₂Na]⁺ (M + Na)⁺: 391.1674, found: 391.1673.



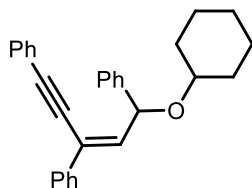
((Z)-5-((R)-1-Phenylethoxy) pent-3-en-1-yn-1,3,5-triyl) tribenzene (3r): 221.4 mg, 51% isolated yield, yellow liquid, *dr* = 1:1, >20:1 *Z/E*, **R_f** (PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.75-7.73 (m, 2H), 7.59-7.57 (m, 2H), 7.48-7.46 (m, 4H), 7.40-7.16 (m, 32H), 6.54 (d, *J* = 9.2 Hz, 1H), 6.52 (d, *J* = 9.2 Hz, 1H), 5.67 (d, *J* = 9.2 Hz, 1H), 5.62 (d, *J* = 9.2 Hz, 1H), 4.78 (q, *J* = 6.4 Hz, 1H), 4.55 (q, *J* = 6.4 Hz, 1H), 1.53 (d, *J* = 6.4 Hz, 3H), 1.50 (d, *J* = 6.4 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 144.1, 144.0, 141.44, 141.43, 137.44, 137.41, 137.20, 137.18, 131.8, 131.7, 128.8, 128.62, 128.59, 128.54, 128.53, 128.46, 128.40, 128.37, 128.3, 128.2,

127.9, 127.53, 127.49, 127.4, 126.9, 126.8, 126.54, 126.48, 126.47, 126.46, 126.0, 123.8, 123.1, 122.9, 96.2, 96.1, 86.3, 86.1, 78.1, 76.7, 75.2, 75.1, 24.6, 24.4.

HRMS (ESI⁺): calcd. For [C₃₁H₂₆ONa]⁺ (M + Na)⁺: 437.1881, found: 437.1881.

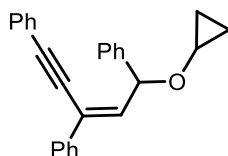


(Z)-5-(Cyclohexyloxy) pent-3-en-1-yn-1,3,5-triyl tribenzene (3s): 78.5 mg, 20% isolated yield, yellow viscous solid, >20:1 Z/E, **R_f** (PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.71-7.69 (m, 2H), 7.57-7.54 (m, 2H), 7.53-7.51 (m, 2H), 7.39-7.33 (m, 7H), 7.30-7.23 (m, 2H), 6.55 (d, *J* = 9.2 Hz, 1H), 5.86 (d, *J* = 9.2 Hz, 1H), 3.56-3.49 (m, 1H), 2.02-2.00 (m, 2H), 1.77-1.72 (m, 2H), 1.57-1.41 (m, 3H), 1.29-1.20 (m, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 142.1, 138.3, 137.3, 131.7, 128.7, 128.62, 128.59, 128.5, 128.3, 127.6, 126.6, 126.5, 124.4, 123.3, 96.0, 86.5, 75.1, 33.1, 32.5, 26.0, 24.4.

HRMS (ESI⁺): calcd. For [C₂₉H₂₉O]⁺ (M + H)⁺: 393.2218, found: 393.2218.

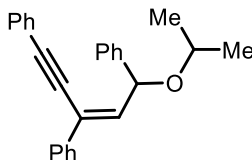


(Z)-5-(Cyclopropoxy)pent-3-en-1-yn-1,3,5-triyl tribenzene (3t): 73.6 mg, 21% isolated yield, yellow viscous solid, >20:1 Z/E, **R_f** (PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.75-7.73 (m, 2H), 7.64-7.61 (m, 2H), 7.55-7.54 (m, 2H), 7.46-7.38 (m, 7H), 7.35-7.30 (m, 2H), 6.60 (d, *J* = 9.2 Hz, 1H), 5.84 (d, *J* = 9.2 Hz, 1H), 3.53-3.49 (m, 1H), 0.85-0.74 (m, 2H), 0.62-0.53 (m, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 141.2, 137.2, 137.1, 131.7, 128.8, 128.7, 128.63, 128.55, 128.4, 127.8, 126.7, 126.5, 125.1, 123.2, 96.4, 86.3, 80.8, 52.1, 6.5, 6.1.

HRMS (ESI⁺): calcd. For [C₂₆H₂₂ONa]⁺ (M + Na)⁺: 373.1568, found: 373.1571.



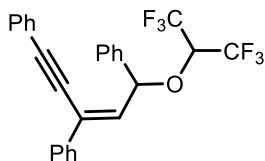
(Z)-5-(Isopropoxy)pent-3-en-1-yn-1,3,5-triyl tribenzene (3u): 95.2 mg, 27% isolated yield, yellow liquid, >20:1 Z/E, **R_f** (PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.73-7.71 (m, 2H), 7.61-7.58 (m, 2H), 7.55-7.54 (m, 2H), 7.43-7.36 (m, 7H), 7.33-7.27 (m, 2H), 6.54 (d, *J* = 9.2 Hz, 1H), 5.85 (d, *J* = 9.2 Hz, 1H), 3.92-3.83 (m, 1H), 1.30 (t, *J* = 5.6 Hz, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 142.0, 138.2, 137.3, 131.7, 128.7, 128.6, 128.5, 128.3, 127.6,

126.6, 126.5, 124.5, 123.3, 96.1, 86.5, 77.4, 69.2, 22.9, 22.5.

HRMS (ESI⁺): calcd. For [C₂₆H₂₄ONa]⁺ (M + Na)⁺: 375.1725, found: 375.1724.

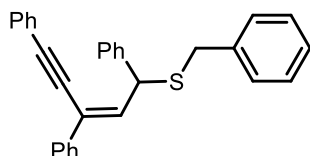


(Z)-5-((1,1,1,3,3,3-Hexafluoropropan-2-yl)oxy)pent-3-en-1-yn-1,3,5-triyl tribenzene (3v): 73.7 mg, 16% isolated yield, light yellow liquid, >20:1 *Z/E*, **R_f**(PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.75-7.73 (m, 2H), 7.59-7.57 (m, 2H), 7.53-7.51 (m, 2H), 7.44-7.36 (m, 9H), 6.52 (d, *J* = 9.6 Hz, 1H), 6.18 (d, *J* = 9.6 Hz, 1H), 4.50 (septet, *J* = 6.0 Hz, 1H).

¹³C NMR (100 MHz, CDCl₃) 138.3, 136.5, 132.5, 131.8, 129.3, 129.2, 128.99, 128.96, 128.82, 128.79, 128.75, 126.8, 126.7, 122.4, 97.6, 85.1, 82.9, 73.3, 73.0, 72.6, 72.3, 72.0.

HRMS (ESI⁺): calcd. For [C₂₆H₁₉F₆O]⁺ (M + H)⁺: 461.1340, found: 461.1343.

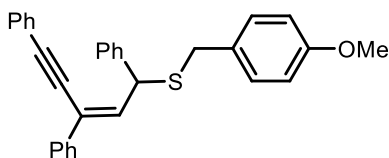


(Z)-Benzyl (1,3,5-triphenylpent-2-en-4-yn-1-yl) sulfane (4a): 304.1 mg, 73% isolated yield, light yellow liquid, >20:1 *Z/E*, **R_f**(PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.69-7.66 (m, 2H), 7.46-7.44 (m, 2H), 7.42-7.39 (m, 2H), 7.37-7.26 (m, 10H), 7.25-7.23 (m, 1H), 7.20-7.13 (m, 3H), 6.64 (d, *J* = 10.4 Hz, 1H), 5.33 (d, *J* = 10.4 Hz, 1H), 3.84-3.71 (m, 2H).

¹³C NMR (100 MHz, CDCl₃) δ 139.9, 138.4, 137.3, 136.7, 131.8, 129.1, 128.9, 128.7, 128.6, 128.54, 128.46, 128.3, 128.0, 127.6, 126.9, 126.5, 124.1, 123.1, 96.8, 86.2, 49.9, 36.3.

HRMS (ESI⁺): calcd. For [C₃₀H₂₅S]⁺ (M + H)⁺: 417.1677, found: 417.1677.

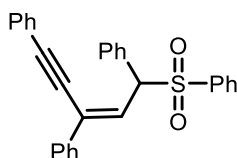


(Z)-(4-Methoxybenzyl) (1,3,5-triphenylpent-2-en-4-yn-1-yl) sulfane (4b): 330.5 mg, 74% isolated yield, white solid, >20:1 *Z/E*, **R_f**(PE/EA = 20:1) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.79-7.76 (m, 2H), 7.55-7.53 (m, 2H), 7.51-7.49 (m, 2H), 7.47-7.31 (m, 11H), 6.81-6.79 (m, 2H), 6.74 (d, *J* = 10.4 Hz, 1H), 5.40 (d, *J* = 10.4 Hz, 1H), 3.89-3.76 (m, 2H), 3.73 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 158.6, 140.0, 137.3, 136.8, 131.8, 130.3, 130.2, 128.9, 128.6, 128.54, 128.45, 128.3, 128.0, 127.6, 126.4, 123.9, 123.1, 113.9, 96.7, 86.3, 55.2, 49.6, 35.6.

HRMS (ESI⁺): calcd. For [C₃₁H₂₆OSNa]⁺ (M + Na)⁺: 469.1602, found: 469.1599.

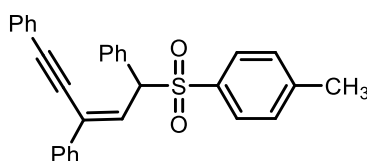


(Z)-3-(5-(Phenylsulfonyl) pent-3-en-1-yn-1,3,5-triyl) tribenzene (4c): 195.5 mg, 45% isolated yield, white solid, >20:1 Z/E, R_f (PE/EA = 20:1) = 0.3.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.87-7.85 (m, 2H), 7.61-7.59 (m, 2H), 7.57-7.54 (m, 3H), 7.45-7.39 (m, 10H), 7.37-7.33 (m, 2H), 6.82 (d, J = 10.4 Hz, 1H), 5.64 (d, J = 10.8 Hz, 1H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 138.0, 136.9, 133.8, 131.70, 131.65, 130.3, 130.1, 129.3, 129.2, 129.1, 128.99, 128.95, 128.8, 128.7, 128.6, 126.62, 126.57, 122.4, 97.4, 85.0, 73.3.

HRMS (ESI^+): calcd. For $[\text{C}_{29}\text{H}_{22}\text{O}_2\text{SNa}]^+$ ($\text{M} + \text{Na}$) $^+$: 457.1238, found: 457.1233.

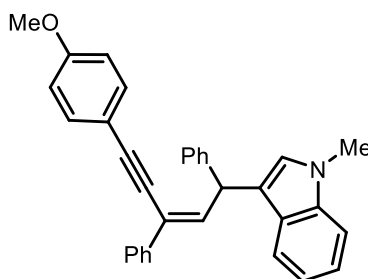


(Z)-3-(5-(Tosyl)pent-3-en-1-yn-1,3,5-triyl) tribenzene (4d): 197.4 mg, 44% isolated yield, white solid, >20:1 Z/E, R_f (PE/EA = 20:1) = 0.3.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.72-7.70 (m, 2H), 7.62-7.60 (m, 2H), 7.54-7.52 (m, 2H), 7.44-7.35 (m, 11H), 7.19 (d, J = 8.0 Hz, 2H), 6.81 (d, J = 10.8 Hz, 1H), 5.60 (d, J = 10.8 Hz, 1H), 2.35 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 144.7, 137.0, 135.1, 132.0, 131.7, 130.07, 130.05, 129.5, 129.3, 129.1, 129.04, 128.96, 128.9, 128.7, 128.6, 127.0, 126.6, 122.6, 97.3, 85.1, 73.3, 21.7.

HRMS (ESI^+): calcd. For $[\text{C}_{30}\text{H}_{25}\text{O}_2\text{S}]^+$ ($\text{M} + \text{H}$) $^+$: 449.1575, found: 449.1572.

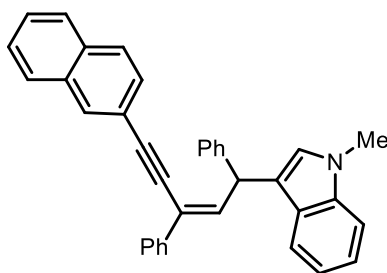


(Z)-3-(5-(4-Methoxyphenyl)-1,3-diphenylpent-2-en-4-yn-1-yl)-1-methyl-1H-indole (5b): 226.8 mg, 50% isolated yield, white solid, >20:1 Z/E, R_f (PE/DCM = 5:2) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.71-7.69 (m, 2H), 7.52-7.50 (m, 1H), 7.47-7.42 (m, 4H), 7.34-7.27 (m, 4H), 7.26-7.17 (m, 4H), 7.03-6.99 (m, 1H), 6.88-6.84 (m, 3H), 6.80-6.77 (m, 1H), 5.83 (d, J = 10.0 Hz, 1H), 3.77 (s, 3H), 3.68 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 159.8, 143.5, 139.1, 138.2, 137.5, 133.2, 128.6, 128.5, 128.3, 127.8, 127.4, 127.0, 126.5, 126.4, 123.2, 121.8, 120.2, 119.0, 116.9, 115.6, 114.1, 109.3, 85.6, 55.4, 44.7, 32.8.

HRMS (ESI^+): calcd. For $[\text{C}_{33}\text{H}_{27}\text{NONa}]^+$ ($\text{M} + \text{Na}$) $^+$: 476.1990, found: 476.1995.



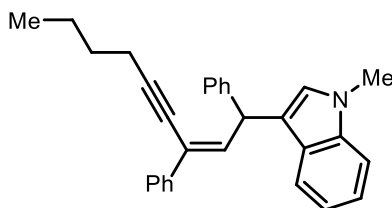
(Z)-1-Methyl-3-(5-(naphthalen-2-yl)-1,3-diphenylpent-2-en-4-yn-1-yl)-1H-indole (5c):

293.6 mg, 62% isolated yield, white solid, >20:1 *Z/E*, R_f (PE/DCM = 5:2) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.01 (s, 1H), 7.77-7.73 (m, 5H), 7.56-7.54 (m, 2H), 7.47-7.43 (m, 4H), 7.36-7.14 (m, 8H), 7.05-7.01 (m, 1H), 6.95-6.93 (m, 1H), 6.80 (s, 1H), 5.90 (d, J = 10.0 Hz, 1H), 3.67 (s, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 143.4, 140.0, 138.1, 137.6, 133.1, 133.0, 131.6, 128.7, 128.5, 128.4, 128.2, 127.90, 127.88, 127.4, 127.1, 126.8, 126.7, 126.6, 126.5, 123.2, 121.8, 120.8, 120.2, 119.1, 116.9, 109.4, 96.4, 87.3, 44.9, 32.8.

HRMS (ESI^+): calcd. For $[\text{C}_{36}\text{H}_{28}\text{N}]^+$ ($\text{M} + \text{H}$) $^+$: 474.2222, found: 474.2217.

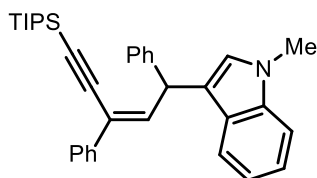


(Z)-3-(1,3-Diphenylnon-2-en-4-yn-1-yl)-1-methyl-1H-indole (5d): 391.5 mg, 97% isolated yield, white solid, >20:1 *Z/E*, R_f (PE/DCM = 5:2) = 0.5.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 7.64-7.61 (m, 2H), 7.47-7.45 (m, 1H), 7.39-7.37 (m, 2H), 7.31-7.27 (m, 5H), 7.24-7.17 (m, 3H), 7.03-6.99 (m, 1H), 6.77-6.75 (m, 2H), 5.72 (d, J = 10.0 Hz, 1H), 3.72 (s, 3H), 2.49 (t, J = 6.8 Hz, 2H), 1.64-1.58 (m, 2H), 1.52-1.47 (m, 2H), 0.93 (t, J = 7.6 Hz, 3H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 143.7, 138.7, 138.3, 137.5, 128.6, 128.32, 128.30, 127.6, 127.5, 127.0, 126.4, 123.4, 121.7, 120.3, 119.0, 117.1, 109.3, 100.1, 97.1, 77.9, 44.5, 32.8, 31.1, 22.2, 19.5, 13.8.

HRMS (ESI^+): calcd. For $[\text{C}_{30}\text{H}_{29}\text{NNa}]^+$ ($\text{M} + \text{Na}$) $^+$: 426.2198, found: 426.2198.



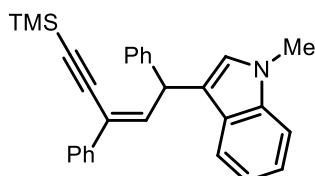
(Z)-3-(1,3-Diphenyl-5-(triisopropylsilyl)pent-2-en-4-yn-1-yl)-1-methyl-1H-indole (5e):

488.7 mg, 97% isolated yield, white solid, >20:1 *Z/E*, R_f (PE/DCM = 5:2) = 0.4.

¹H NMR (400 MHz, CDCl₃) δ 7.69-7.66 (m, 2H), 7.55-7.53 (m, 1H), 7.43-7.40 (m, 2H), 7.35-7.30 (m, 4H), 7.29-7.0 (m, 4H), 7.05-7.01 (m, 1H), 6.90 (d, *J* = 10.0 Hz, 1H), 6.77 (s, 1H), 5.85 (d, *J* = 10.4 Hz, 1H), 3.74 (s, 3H), 1.17-1.14 (m, 21H).

¹³C NMR (100 MHz, CDCl₃) δ 143.3, 140.4, 137.9, 137.5, 128.6, 128.4, 128.3, 127.8, 127.4, 126.9, 126.5, 126.4, 123.2, 121.8, 120.2, 119.0, 116.9, 109.2, 104.1, 97.8, 44.8, 32.7, 18.9, 11.6.

HRMS (ESI⁺): calcd. For [C₃₅H₄₂NSi]⁺ (*M* + *H*)⁺: 504.3087, found: 504.3078.

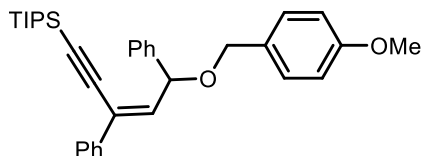


(Z)-3-(1,3-Diphenyl-5-(trimethylsilyl)pent-2-en-4-yn-1-yl)-1-methyl-1H-indole (5f): 352.5 mg, 84% isolated yield, white solid, >20:1 *Z/E*, *R_f* (PE/DCM = 5:2) = 0.4.

¹H NMR (400 MHz, CDCl₃) δ 7.86-7.84 (m, 2H), 7.78-7.76 (m, 1H), 7.64-7.63 (m, 2H), 7.55-7.40 (m, 8H), 7.28-7.24 (m, 1H), 7.12 (d, *J* = 10.0 Hz, 1H), 6.95 (s, 1H), 6.02 (d, *J* = 10.0 Hz, 1H), 3.85 (s, 3H), 0.52 (s, 9H).

¹³C NMR (100 MHz, CDCl₃) δ 143.4, 140.7, 137.7, 137.5, 128.6, 128.4, 128.3, 127.8, 127.4, 126.9, 126.6, 126.4, 123.0, 121.8, 120.1, 119.1, 116.9, 109.3, 102.5, 101.4, 44.6, 32.7, 0.2.

HRMS (ESI⁺): calcd. For [C₂₉H₃₀NSi]⁺ (*M* + *H*)⁺: 420.2148, found: 420.2146.

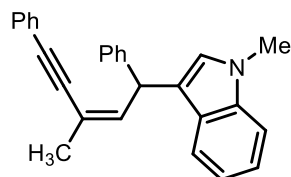


(Z)-Triisopropyl(5-((4-methoxybenzyl)oxy)-3,5-diphenylpent-3-en-1-yn-1-yl)silane (5g): 408.6 mg, 80% isolated yield, pale yellow liquid, >20:1 *Z/E*, *R_f* (PE/DCM = 5:2) = 0.4.

¹H NMR (400 MHz, CDCl₃) δ 7.65-7.63 (m, 2H), 7.54-7.52 (m, 2H), 7.35-7.22 (m, 8H), 6.86-6.84 (m, 2H), 6.55 (d, *J* = 9.2 Hz, 1H), 5.79 (d, *J* = 9.2 Hz, 1H), 4.62-4.55 (m, 2H), 3.74 (s, 3H), 1.21-1.06 (s, 21H).

¹³C NMR (100 MHz, CDCl₃) δ 159.2, 141.3, 138.1, 137.0, 130.7, 129.3, 128.6, 128.4, 128.3, 127.8, 126.6, 126.4, 125.1, 113.9, 103.5, 98.7, 79.7, 70.4, 55.3, 18.9, 11.5.

HRMS (ESI⁺): calcd. For [C₃₄H₄₂O₂SiNa]⁺ (*M* + *Na*)⁺: 533.2852, found: 533.2854.

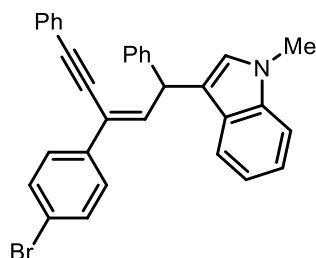


(Z)-1-Methyl-3-(3-methyl-1,5-diphenylpent-2-en-4-yn-1-yl)-1H-indole (5h): 122.9 mg, 34% isolated yield, pale yellow liquid, *Z/E* = 3.6:1, *R_f* (PE/DCM = 5:2) = 0.65.

¹H NMR (400 MHz, CDCl₃) δ 7.48-7.45 (m, 3.2H), 7.42-7.36 (m, 3.1H), 7.32-7.25 (m, 8.9H), 7.22-7.17 (m, 2.9H), 7.03-6.98 (m, 1.3H), 6.81 (s, 0.28H), 6.75 (s, 1H), 6.45-6.42 (m, 0.28H), 6.22-6.20 (m, 1H), 5.59 (d, *J* = 10.0 Hz, 1H), 5.20 (d, *J* = 10.0 Hz, 0.28H), 3.70-3.69 (s, 4H), 2.04 (d, *J* = 1.6 Hz, 0.84H), 2.00 (d, *J* = 1.6 Hz, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 143.9, 143.7, 140.4, 139.8, 137.5, 131.7, 131.6, 128.63, 128.55, 128.43, 128.36, 128.2, 128.0, 127.3, 127.1, 126.9, 126.5, 126.4, 123.7, 121.8, 121.748, 120.2, 119.9, 118.98, 118.95, 117.8, 117.2, 116.7, 109.4, 109.3, 93.6, 92.6, 88.9, 86.9, 44.4, 42.2, 32.8, 23.3, 17.8.

RMS (ESI⁺): calcd. For [C₂₇H₂₃NNa]⁺ (M + Na)⁺: 384.1728, found: 384.1726.



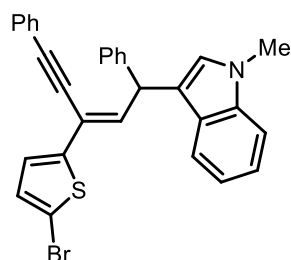
(Z)-3-(3-(4-Bromophenyl)-1,5-diphenylpent-2-en-4-yn-1-yl)-1-methyl-1H-indole (5i):

452.2 mg, 90% isolated yield, white solid, >20:1 *Z/E*, **R_f** (PE/DCM = 5:2) = 0.5.

¹H NMR (400 MHz, CDCl₃) δ 7.60-7.51 (m, 5H), 7.49-7.44 (m, 4H), 7.38-7.31 (m, 6H), 7.29-7.22 (m, 2H), 7.07-7.04 (m, 1H), 6.92 (d, *J* = 10.0 Hz, 1H), 6.82 (s, 1H), 5.83 (d, *J* = 10.0 Hz, 1H), 3.76 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 143.1, 140.2, 137.6, 137.1, 131.8, 131.6, 128.72, 128.66, 128.6, 128.3, 128.1, 127.4, 127.1, 126.7, 123.3, 122.1, 121.90, 121.85, 120.1, 119.2, 116.7, 109.4, 96.4, 86.3, 44.9, 32.9.

HRMS (ESI⁺): calcd. For [C₃₂H₂₅BrN]⁺ (M + H)⁺: 502.1170, found: 502.1163.



(E)-3-(3-(5-Bromothiophen-2-yl)-1,5-diphenylpent-2-en-4-yn-1-yl)-1-methyl-1H-indole

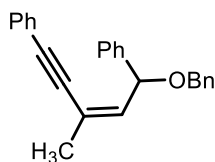
(5j): 508.5 mg, 30% isolated yield, yellow liquid, >20:1 *Z/E*, **R_f** (PE/DCM = 5:2) = 0.6.

¹H NMR (400 MHz, CDCl₃) δ 7.58-7.56 (m, 2H), 7.51-7.49 (m, 1H), 7.44-7.42 (m, 2H), 7.40-7.32 (m, 6H), 7.30-7.23 (m, 2H), 7.12-7.10 (m, 1H), 7.09-7.05 (m, 1H), 6.98-6.97 (m, 1H), 6.83 (s, 1H), 6.75 (d, *J* = 10.0 Hz, 1H), 5.76 (d, *J* = 10.0 Hz, 1H), 3.77 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 144.3, 142.9, 138.0, 137.5, 131.8, 130.4, 128.8, 128.7, 128.6, 128.3, 127.3, 127.0, 126.7, 125.0, 122.8, 121.9, 120.0, 119.2, 116.9, 116.3, 111.3, 109.4, 95.7.

85.0, 44.5, 32.8.

HRMS (ESI⁺): calcd. For [C₃₀H₂₃NSBr]⁺(M + H)⁺: 507.0656, found: 507.0575.

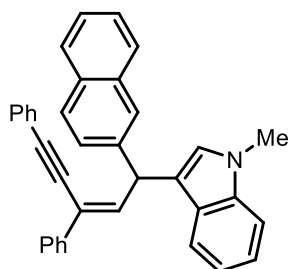


(Z)-5-(Benzyloxy)-3-methylpent-3-en-1-yne-1,5-diyl dibenzene (5k): 277.5 mg, 82% isolated yield, colorless liquid, *Z/E* = 9:1, **R_f**(PE/EA = 20:1) = 0.3.

¹H NMR (400 MHz, CDCl₃) δ 7.47-7.45 (m, 3.2H), 7.38-7.19 (m, 15.6H), 7.07 (s, 1.8H), 6.16 (d, *J* = 7.2 Hz, 0.11H), 5.88 (d, *J* = 10.0 Hz, 1H), 5.53 (d, *J* = 9.2 Hz, 1H), 5.14 (d, *J* = 8.8 Hz, 1H), 4.63-4.55 (m, 2.4H), 1.97 (s, 3H), 1.93 (s, 0.33H).

¹³C NMR (100 MHz, CDCl₃) δ 141.5, 138.6, 137.8, 131.61, 131.56, 128.7, 128.6, 128.44, 128.39, 128.37, 128.3, 127.9, 127.8, 127.6, 127.5, 126.8, 126.5, 123.2, 121.0, 94.1, 88.2, 79.1, 77.4, 70.2, 23.3.

HRMS (ESI⁺): calcd. For [C₂₅H₂₂ONa]⁺(M + Na)⁺: 361.1568, found: 361.1571.

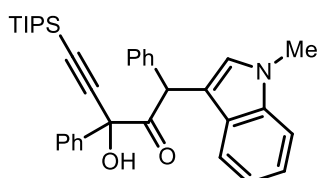


(Z)-1-Methyl-3-(1-(naphthalen-2-yl)-3,5-diphenylpent-2-en-4-yn-1-yl)-1H-indole (5l): 322.0 mg, 68% isolated yield, white solid, >20:1 *Z/E*, **R_f**(PE/DCM = 5:2) = 0.5.

¹H NMR (400 MHz, CDCl₃) δ 7.89-7.81 (m, 1H), 7.79-7.71 (m, 5H), 7.58-7.52 (m, 4H), 7.42-7.40 (m, 2H), 7.35-7.23 (m, 7H), 7.21-7.17 (m, 1H), 7.02-6.97 (m, 2H), 6.83-6.77 (m, 1H), 6.01-5.98 (m, 1H), 3.69 (s, 3H).

¹³C NMR (100 MHz, CDCl₃) δ 140.9, 139.6, 138.1, 137.6, 133.8, 132.5, 131.8, 128.5, 128.3, 128.0, 127.9, 127.7, 127.5, 127.20, 127.17, 126.5, 126.4, 126.0, 125.6, 123.5, 123.3, 121.9, 120.2, 119.2, 116.8, 109.4, 96.2, 87.0, 44.9, 32.8.

HRMS (ESI⁺): calcd. For [C₃₆H₂₈N]⁺(M + H)⁺: 474.2222, found: 474.2217.



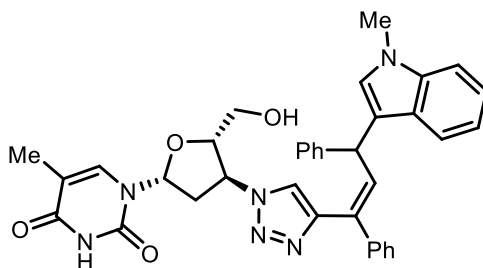
3-Hydroxy-1-(1-methyl-1H-indol-3-yl)-1,3-diphenyl-5-(triisopropylsilyl) pent-4-yn-2-one (6): 44.2 mg, 55% isolated yield, brown viscous solid, *dr* = 7:1, **R_f**(PE/EA = 20:3) = 0.3.

¹H NMR (400 MHz, CDCl₃) δ 8.16 (s, 0.14H), 7.96-7.94 (m, 0.14H), 7.90-7.88 (m, 1H), 7.75

(s, 1H), 7.67-7.62 (m, 2.5H), 7.55-7.50 (m, 1.4H), 7.43-7.17 (m, 13.8H), 7.05-7.02 (1, 1.3H), 6.00-5.98 (m, 1.2H), 3.27 (s, 0.43H), 3.02 (s, 3H), 1.18-1.16 (m, 24H).

^{13}C NMR (100 MHz, CDCl_3) δ 199.5, 162.5, 140.7, 137.1, 136.9, 134.7, 132.7, 129.4, 129.2, 129.0, 128.9, 128.51, 128.49, 128.4, 128.3, 128.0, 127.9, 126.5, 125.4, 103.6, 98.6, 58.8, 34.1, 18.9, 11.5.

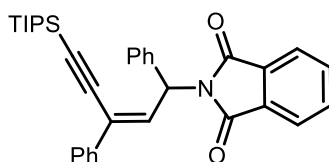
HRMS (ESI⁺): calcd. For $[\text{C}_{35}\text{H}_{41}\text{NO}_2\text{SiNa}]^+$ (M + Na)⁺: 558.2804, found: 558.2806.



1-((2R,4R,5S)-5-(Hydroxymethyl)-4-(4-((Z)-3-(1-methyl-1H-indol-3-yl)-1,3diphenylprop-1-en-1-yl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)-dione (7): 49.8 mg, 81% isolated yield, white solid, >20:1 Z/E, R_f (PE/EA = 5:4) = 0.4.

^1H NMR (400 MHz, CDCl_3) δ 9.98-9.95 (m, 1H), 7.50-7.45 (m, 1H), 7.39-7.32 (m, 3H), 7.29-7.1 (m, 12H), 6.94-6.92 (m, 1H), 6.81 (d, J = 10.0 Hz, 1H), 6.56-6.53 (m, 1H), 6.15-6.14 (m, 1H), 5.61 (d, J = 10.0 Hz, 1H), 5.27-5.23 (m, 1H), 4.36 (s, 1H), 3.85-3.82 (m, 1H), 3.66-3.65 (m, 3H), 3.61-3.57 (m, 1H), 2.82-2.73 (m, 2H), 1.78 (s, 3H).

The spectroscopic data was in accordance with that reported in the literature.^[1]

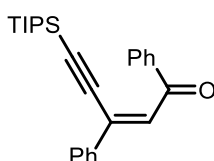


(Z)-2-(1,3-Diphenyl-5-(triisopropylsilyl) pent-2-en-4-yn-1-yl) isoindoline-1,3-dione (8): 38 mg, 37% isolated yield, white solid, >20:1 Z/E, R_f (PE/EA = 20:1) = 0.3.

^1H NMR (400 MHz, CDCl_3) δ 7.85-7.83 (m 2H), 7.75-7.73 (m, 2H), 7.71-7.69 (m, 2H), 7.52-7.50 (m, 2H), 7.44 (d, J = 9.6 Hz, 1H), 7.39-7.23 (m, 6H), 6.83 (d, J = 9.6 Hz, 1H), 1.15-1.12 (m, 21H).

^{13}C NMR (100 MHz, CDCl_3) δ 167.9, 139.1, 137.1, 134.1, 132.3, 132.2, 128.8, 128.5, 127.9, 127.5, 127.2, 126.6, 123.4, 102.4, 100.5, 54.8, 18.8, 11.4.

HRMS (ESI⁺): calcd. For $[\text{C}_{34}\text{H}_{37}\text{NO}_2\text{SiNa}]^+$ (M + Na)⁺: 542.2491, found: 542.2491.



(Z)-1,3-Diphenyl-5-(triisopropylsilyl) pent-2-en-4-yn-1-one (9): 46.6 mg, 80% isolated

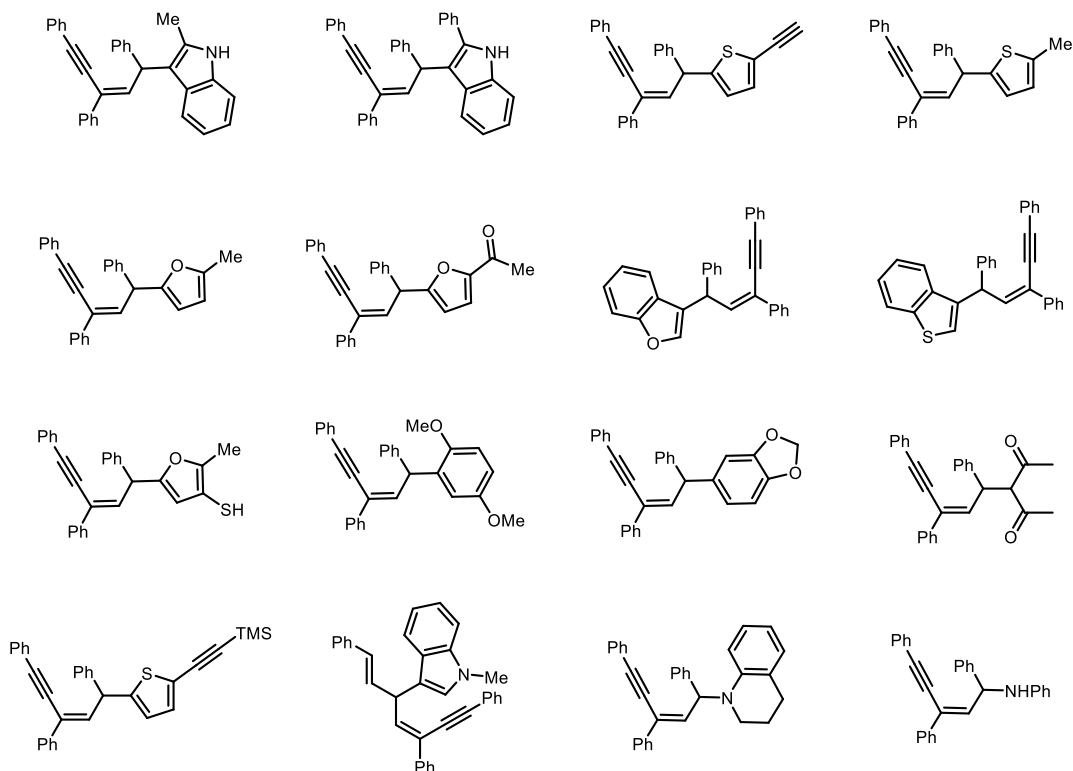
yield, yellow liquid, >20:1 Z/E, R_f (PE/DCM = 5:2) = 0.6.

$^1\text{H NMR}$ (400 MHz, CDCl_3) δ 8.05-8.00 (m, 2H), 7.87-7.81 (m, 2H), 7.59-7.53 (m, 1H), 7.50-7.41 (m, 5H), 7.39 (s, 1H), 1.09 (s, 21H).

$^{13}\text{C NMR}$ (100 MHz, CDCl_3) δ 191.1, 138.2, 137.5, 133.5, 133.0, 129.8, 129.6, 129.01, 128.97, 128.7, 128.6, 127.2, 105.1, 103.6, 18.8, 11.4.

HRMS (ESI^+): calcd. For $[\text{C}_{26}\text{H}_{33}\text{OSi}]^+$ ($\text{M} + \text{H}$) $^+$: 389.2301, found: 389.2305.

Unsuccessful examples



7 X-ray crystallographic analysis

Method for single crystals growth: **2a** (20 mg) was dissolved in ethyl acetate/hexane (v:v = 1:4, 4 mL) in a vial at room temperature. The vial was properly sealed with parafilm and kept at room temperature to allow the slow evaporation of the solvents until the single crystal was appeared.

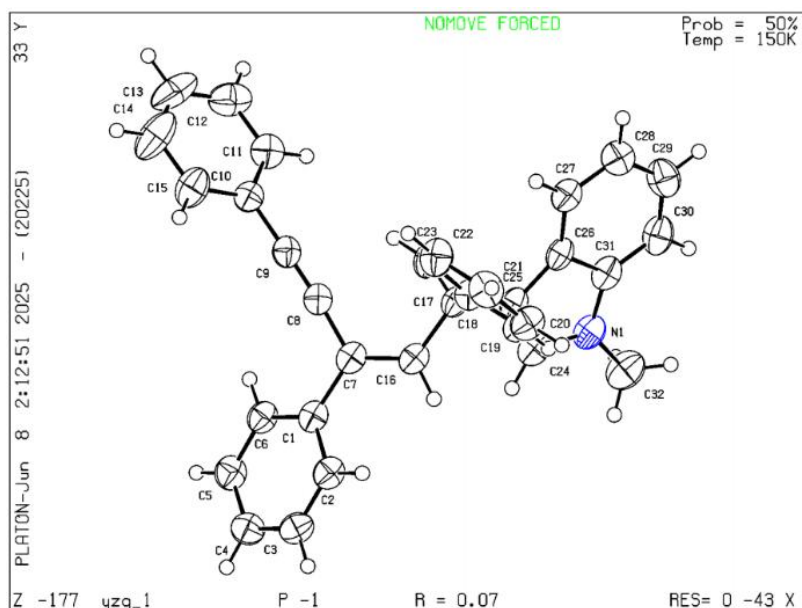


Table 1 Crystal data and structure refinement for YZQ_1.

Identification code	YZQ_1
Empirical formula	C ₃₂ H ₂₅ N
Formula weight	423.53
Temperature/K	149.95(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.2035(6)
b/Å	10.3335(8)
c/Å	11.6404(8)
α/°	94.054(6)
β/°	105.675(5)
γ/°	95.557(5)
Volume/Å ³	1170.12(14)
Z	2
ρ _{calc} /cm ³	1.202
μ/mm ⁻¹	0.524
F(000)	448.0
Crystal size/mm ³	0.15 × 0.12 × 0.1

Radiation	Cu K α ($\lambda = 1.54184$)
2 Θ range for data collection/	$^{\circ}7.93$ to 149.54
Index ranges	$-8 \leq h \leq 12, -12 \leq k \leq 12, -14 \leq l \leq 14$
Reflections collected	11437
Independent reflections	4464 [$R_{\text{int}} = 0.0366, R_{\text{sigma}} = 0.0309$]
Data/restraints/parameters	4464/0/299
Goodness-of-fit on F^2	1.047
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0659, wR_2 = 0.1775$
Final R indexes [all data]	$R_1 = 0.0758, wR_2 = 0.1856$
Largest diff. peak/hole / e \AA^{-3}	0.29/-0.24

Crystal Data for $C_{32}H_{25}N$ ($M = 423.53$ g/mol): triclinic, space group P-1 (no. 2), $a = 10.2035(6)$ \AA , $b = 10.3335(8)$ \AA , $c = 11.6404(8)$ \AA , $\alpha = 94.054(6)^{\circ}$, $\beta = 105.675(5)^{\circ}$, $\gamma = 95.557(5)^{\circ}$, $V = 1170.12(14)$ \AA^3 , $Z = 2$, $T = 149.95(10)$ K, $\mu(\text{Cu K}\alpha) = 0.524$ mm^{-1} , $D_{\text{calc}} = 1.202$ g/cm^3 , 11437 reflections measured ($7.93^{\circ} \leq 2\Theta \leq 149.54^{\circ}$), 4464 unique ($R_{\text{int}} = 0.0366$, $R_{\text{sigma}} = 0.0309$) which were used in all calculations. The final R_1 was 0.0659 ($I > 2\sigma(I)$) and wR_2 was 0.1856 (all data).

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for YZQ_1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N ₁	1564.9(16)	7187.2(17)	6993.0(16)	46.4(4)
C ₁	6487.6(18)	7267.0(19)	4620.8(17)	38.6(4)
C ₂	6588(2)	8582.6(19)	4404.9(18)	43.4(5)
C ₃	6656(2)	8943(2)	3301.2(19)	47.3(5)
C ₄	6628(2)	8002(2)	2382.2(19)	48.2(5)
C ₅	6582(2)	6702(2)	2599.4(19)	48.1(5)
C ₆	6522(2)	6336(2)	3704.4(18)	42.3(5)
C ₇	6281.0(19)	6843.5(18)	5761.7(17)	38.9(4)
C ₈	6831.4(19)	5672.4(19)	6141.6(17)	38.9(4)
C ₉	7319.6(19)	4676.5(19)	6398.7(17)	39.8(4)
C ₁₀	7863.6(19)	3472.8(19)	6658.8(16)	39.5(4)

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for YZQ_1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U(\text{eq})$
C ₁₁	7039(2)	2413(2)	6869.5(19)	49.5(5)
C ₁₂	7550(3)	1242(2)	7076(2)	63.9(7)
C ₁₃	8876(3)	1103(3)	7083(3)	76.4(9)
C ₁₄	9698(3)	2141(3)	6886(3)	82.6(9)
C ₁₅	9210(2)	3320(3)	6688(2)	59.7(6)
C ₁₆	5568.8(19)	7488.0(19)	6389.6(17)	39.7(4)
C ₁₇	5328.7(18)	7129.3(18)	7546.5(17)	37.5(4)
C ₁₈	6309.8(18)	8066.4(18)	8572.6(17)	37.3(4)
C ₁₉	5961(2)	9256(2)	8934.3(19)	44.8(5)
C ₂₀	6914(2)	10132(2)	9794(2)	49.9(5)
C ₂₁	8201(2)	9810(2)	10306.9(19)	49.9(5)
C ₂₂	8551(2)	8610(2)	9974(2)	52.5(6)
C ₂₃	7607(2)	7740(2)	9109.8(19)	45.9(5)
C ₂₄	2756(2)	7368.0(19)	6649.2(19)	43.5(5)
C ₂₅	3848.1(19)	7096.6(17)	7540.0(17)	38.0(4)
C ₂₆	3306.5(19)	6717.1(17)	8497.8(17)	38.1(4)
C ₂₇	3890(2)	6331.8(19)	9633.8(18)	43.2(5)
C ₂₈	3057(2)	6024(2)	10355(2)	51.2(5)
C ₂₉	1640(2)	6093(2)	9968(2)	56.8(6)
C ₃₀	1034(2)	6459(2)	8850(2)	52.4(6)
C ₃₁	1874(2)	6780.3(19)	8126.8(19)	42.7(5)
C ₃₂	212(2)	7429(3)	6294(2)	64.4(7)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for YZQ_1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N ₁	32.8(8)	47.8(10)	51.2(10)	-0.6(8)	0.8(7)	5.3(7)
C ₁	32.9(9)	39.0(10)	37.8(10)	-4.2(7)	1.9(7)	3.6(7)
C ₂	45.7(11)	37.5(10)	41.5(11)	-5.1(8)	5.6(8)	3.3(8)
C ₃	46.3(11)	39.7(10)	51.3(12)	3.7(9)	7.1(9)	2.8(8)
C ₄	47.5(11)	52.0(12)	41.7(11)	3.9(9)	7.7(9)	3.1(9)
C ₅	51.4(12)	48.2(12)	41.1(11)	-5.3(9)	9.1(9)	6.2(9)
C ₆	42.9(10)	37.6(10)	42.9(11)	-2.9(8)	7.4(8)	5.7(8)
C ₇	33.3(9)	37.1(9)	39.6(10)	-4.5(7)	1.6(7)	2.1(7)
C ₈	34.6(9)	42.3(10)	36.8(10)	-1.9(8)	7.1(8)	2.9(8)
C ₉	37.2(10)	43.5(11)	36.3(10)	-2.1(8)	8.5(8)	3.9(8)
C ₁₀	38.4(10)	42.6(10)	33.3(9)	-1.1(7)	3.7(7)	5.8(8)
C ₁₁	47.5(12)	49.0(12)	46.6(12)	-2.3(9)	7.9(9)	0.4(9)
C ₁₂	88.9(19)	42.2(12)	50.4(13)	0.3(10)	5.5(12)	0.7(12)
C ₁₃	86(2)	52.9(15)	70.0(17)	-0.8(12)	-18.9(14)	30.7(14)
C ₁₄	47.4(14)	72.2(19)	110(2)	-9.5(16)	-9.4(14)	24.6(13)
C ₁₅	37.6(11)	60.0(14)	75.1(16)	-1.9(12)	6.3(10)	8.1(10)
C ₁₆	37.4(10)	36.4(10)	40.3(10)	-1.8(8)	3.3(8)	6.3(7)
C ₁₇	34.5(9)	34.5(9)	40.4(10)	-2.9(7)	5.9(7)	6.7(7)
C ₁₈	33.9(9)	37.8(10)	37.8(10)	-0.5(7)	8.0(7)	1.3(7)
C ₁₉	41.0(10)	39.3(10)	47.6(11)	-1.9(8)	2.5(8)	6.5(8)
C ₂₀	56.0(13)	37.5(11)	50.0(12)	-6.2(9)	8.1(10)	2.9(9)
C ₂₁	42.9(11)	53.3(12)	44.7(11)	-6.9(9)	4.8(9)	-7.7(9)
C ₂₂	34.0(10)	63.2(14)	52.4(13)	-4.8(10)	2.4(9)	2.8(9)
C ₂₃	35.6(10)	48.8(11)	49.7(12)	-5.4(9)	7.6(8)	7.9(8)
C ₂₄	39.7(10)	40.4(10)	44.5(11)	-2.2(8)	3.7(8)	4.5(8)
C ₂₅	35.5(9)	31.6(9)	42.1(10)	-6.9(7)	5.2(8)	4.2(7)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for YZQ_1. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C ₂₆	35.1(9)	29.8(9)	44.5(10)	-7.7(7)	5.6(8)	4.9(7)
C ₂₇	41.0(10)	40.0(10)	43.1(11)	-4.2(8)	4.5(8)	5.8(8)
C ₂₈	51.4(12)	50.1(12)	49.2(12)	0.2(9)	11.4(10)	2.3(9)
C ₂₉	51.8(13)	58.4(14)	59.9(14)	-3.0(11)	20.9(11)	-4.5(10)
C ₃₀	36.0(10)	50.5(12)	66.4(14)	-7.8(10)	12.0(10)	1.5(9)
C ₃₁	36.2(10)	36.8(10)	49.4(11)	-5.4(8)	5.6(8)	2.5(7)
C ₃₂	38.6(12)	73.5(17)	71.0(16)	7.0(13)	-2.8(11)	10.4(11)

Table 4 Bond Lengths for YZQ_1.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
N ₁	C ₂₄	1.379(3)	C ₁₄	C ₁₅	1.372(4)
N ₁	C ₃₁	1.377(3)	C ₁₆	C ₁₇	1.497(3)
N ₁	C ₃₂	1.455(3)	C ₁₇	C ₁₈	1.539(2)
C ₁	C ₂	1.399(3)	C ₁₇	C ₂₅	1.506(3)
C ₁	C ₆	1.395(3)	C ₁₈	C ₁₉	1.381(3)
C ₁	C ₇	1.488(3)	C ₁₈	C ₂₃	1.388(3)
C ₂	C ₃	1.380(3)	C ₁₉	C ₂₀	1.394(3)
C ₃	C ₄	1.386(3)	C ₂₀	C ₂₁	1.372(3)
C ₄	C ₅	1.383(3)	C ₂₁	C ₂₂	1.381(3)
C ₅	C ₆	1.381(3)	C ₂₂	C ₂₃	1.389(3)
C ₇	C ₈	1.431(3)	C ₂₄	C ₂₅	1.369(3)
C ₇	C ₁₆	1.348(3)	C ₂₅	C ₂₆	1.434(3)
C ₈	C ₉	1.208(3)	C ₂₆	C ₂₇	1.399(3)
C ₉	C ₁₀	1.429(3)	C ₂₆	C ₃₁	1.417(3)
C ₁₀	C ₁₁	1.393(3)	C ₂₇	C ₂₈	1.378(3)

Table 4 Bond Lengths for YZQ_1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C ₁₀	C ₁₅	1.389(3)	C ₂₈	C ₂₉	1.403(3)
C ₁₁	C ₁₂	1.375(3)	C ₂₉	C ₃₀	1.379(3)
C ₁₂	C ₁₃	1.372(4)	C ₃₀	C ₃₁	1.388(3)
C ₁₃	C ₁₄	1.368(5)			

Table 5 Bond Angles for YZQ_1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C ₂₄	N ₁	C ₃₂	125.8(2)	C ₁₆	C ₁₇	C ₁₈	108.13(15)
C ₃₁	N ₁	C ₂₄	108.68(16)	C ₁₆	C ₁₇	C ₂₅	112.69(16)
C ₃₁	N ₁	C ₃₂	125.49(19)	C ₂₅	C ₁₇	C ₁₈	113.28(15)
C ₂	C ₁	C ₇	122.04(17)	C ₁₉	C ₁₈	C ₁₇	121.77(17)
C ₆	C ₁	C ₂	117.94(19)	C ₁₉	C ₁₈	C ₂₃	118.92(17)
C ₆	C ₁	C ₇	119.96(18)	C ₂₃	C ₁₈	C ₁₇	119.24(17)
C ₃	C ₂	C ₁	120.95(18)	C ₁₈	C ₁₉	C ₂₀	120.41(19)
C ₂	C ₃	C ₄	120.4(2)	C ₂₁	C ₂₀	C ₁₉	120.3(2)
C ₅	C ₄	C ₃	119.1(2)	C ₂₀	C ₂₁	C ₂₂	119.84(19)
C ₆	C ₅	C ₄	120.71(19)	C ₂₁	C ₂₂	C ₂₃	120.0(2)
C ₅	C ₆	C ₁	120.76(19)	C ₁₈	C ₂₃	C ₂₂	120.52(19)
C ₈	C ₇	C ₁	116.44(17)	C ₂₅	C ₂₄	N ₁	110.42(19)
C ₁₆	C ₇	C ₁	122.48(18)	C ₂₄	C ₂₅	C ₁₇	128.82(19)
C ₁₆	C ₇	C ₈	121.03(18)	C ₂₄	C ₂₅	C ₂₆	106.19(17)
C ₉	C ₈	C ₇	176.0(2)	C ₂₆	C ₂₅	C ₁₇	124.96(17)
C ₈	C ₉	C ₁₀	177.7(2)	C ₂₇	C ₂₆	C ₂₅	133.85(18)
C ₁₁	C ₁₀	C ₉	120.30(18)	C ₂₇	C ₂₆	C ₃₁	118.76(19)
C ₁₅	C ₁₀	C ₉	121.29(19)	C ₃₁	C ₂₆	C ₂₅	107.39(17)
C ₁₅	C ₁₀	C ₁₁	118.4(2)	C ₂₈	C ₂₇	C ₂₆	119.12(19)
C ₁₂	C ₁₁	C ₁₀	120.2(2)	C ₂₇	C ₂₈	C ₂₉	121.1(2)

Table 4 Bond Lengths for YZQ_1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å		
C ₁₃	C ₁₂	C ₁₁	120.6(2)	C ₃₀	C ₂₉	C ₂₈	121.1(2)
C ₁₄	C ₁₃	C ₁₂	119.6(2)	C ₂₉	C ₃₀	C ₃₁	117.8(2)
C ₁₃	C ₁₄	C ₁₅	120.6(3)	N ₁	C ₃₁	C ₂₆	107.31(18)
C ₁₄	C ₁₅	C ₁₀	120.5(2)	N ₁	C ₃₁	C ₃₀	130.64(19)
C ₇	C ₁₆	C ₁₇	125.55(18)	C ₃₀	C ₃₁	C ₂₆	122.0(2)

Table 6 Torsion Angles for YZQ_1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N ₁	C ₂₄	C ₂₅	C ₁₇	178.38(17)	C ₁₇	C ₂₅	C ₂₆	C ₂₇	1.9(3)
N ₁	C ₂₄	C ₂₅	C ₂₆	0.3(2)	C ₁₇	C ₂₅	C ₂₆	C ₃₁	-178.21(16)
C ₁	C ₂	C ₃	C ₄	0.0(3)	C ₁₈	C ₁₇	C ₂₅	C ₂₄	121.9(2)
C ₁	C ₇	C ₁₆	C ₁₇	-179.43(17)	C ₁₈	C ₁₇	C ₂₅	C ₂₆	-60.3(2)
C ₂	C ₁	C ₆	C ₅	-3.3(3)	C ₁₈	C ₁₉	C ₂₀	C ₂₁	-1.2(3)
C ₂	C ₁	C ₇	C ₈	-150.75(18)	C ₁₉	C ₁₈	C ₂₃	C ₂₂	-1.7(3)
C ₂	C ₁	C ₇	C ₁₆	31.8(3)	C ₁₉	C ₂₀	C ₂₁	C ₂₂	-0.3(3)
C ₂	C ₃	C ₄	C ₅	-2.4(3)	C ₂₀	C ₂₁	C ₂₂	C ₂₃	0.8(4)
C ₃	C ₄	C ₅	C ₆	2.0(3)	C ₂₁	C ₂₂	C ₂₃	C ₁₈	0.2(3)
C ₄	C ₅	C ₆	C ₁	0.9(3)	C ₂₃	C ₁₈	C ₁₉	C ₂₀	2.2(3)
C ₆	C ₁	C ₂	C ₃	2.9(3)	C ₂₄	N ₁	C ₃₁	C ₂₆	0.4(2)
C ₆	C ₁	C ₇	C ₈	32.3(3)	C ₂₄	N ₁	C ₃₁	C ₃₀	-179.2(2)
C ₆	C ₁	C ₇	C ₁₆	-145.14(19)	C ₂₄	C ₂₅	C ₂₆	C ₂₇	-179.9(2)
C ₇	C ₁	C ₂	C ₃	-174.17(18)	C ₂₄	C ₂₅	C ₂₆	C ₃₁	0.0(2)
C ₇	C ₁	C ₆	C ₅	173.80(18)	C ₂₅	C ₁₇	C ₁₈	C ₁₉	-38.1(3)
C ₇	C ₁₆	C ₁₇	C ₁₈	102.6(2)	C ₂₅	C ₁₇	C ₁₈	C ₂₃	145.19(19)
C ₇	C ₁₆	C ₁₇	C ₂₅	-131.43(19)	C ₂₅	C ₂₆	C ₂₇	C ₂₈	180.0(2)
C ₈	C ₇	C ₁₆	C ₁₇	3.3(3)	C ₂₅	C ₂₆	C ₃₁	N ₁	-0.3(2)

Table 6 Torsion Angles for YZQ_1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C ₉	C ₁₀	C ₁₁	C ₁₂	177.62(19)	C ₂₅	C ₂₆	C ₃₁	C ₃₀	179.43(18)
C ₉	C ₁₀	C ₁₅	C ₁₄	-177.1(2)	C ₂₆	C ₂₇	C ₂₈	C ₂₉	-0.1(3)
C ₁₀	C ₁₁	C ₁₂	C ₁₃	0.3(4)	C ₂₇	C ₂₆	C ₃₁	N ₁	179.65(16)
C ₁₁	C ₁₀	C ₁₅	C ₁₄	1.8(4)	C ₂₇	C ₂₆	C ₃₁	C ₃₀	-0.7(3)
C ₁₁	C ₁₂	C ₁₃	C ₁₄	0.2(4)	C ₂₇	C ₂₈	C ₂₉	C ₃₀	0.6(4)
C ₁₂	C ₁₃	C ₁₄	C ₁₅	0.3(5)	C ₂₈	C ₂₉	C ₃₀	C ₃₁	-1.1(3)
C ₁₃	C ₁₄	C ₁₅	C ₁₀	-1.3(4)	C ₂₉	C ₃₀	C ₃₁	N ₁	-179.2(2)
C ₁₅	C ₁₀	C ₁₁	C ₁₂	-1.3(3)	C ₂₉	C ₃₀	C ₃₁	C ₂₆	1.2(3)
C ₁₆	C ₁₇	C ₁₈	C ₁₉	87.5(2)	C ₃₁	N ₁	C ₂₄	C ₂₅	-0.4(2)
C ₁₆	C ₁₇	C ₁₈	C ₂₃	-89.2(2)	C ₃₁	C ₂₆	C ₂₇	C ₂₈	0.1(3)
C ₁₆	C ₁₇	C ₂₅	C ₂₄	-1.3(3)	C ₃₂	N ₁	C ₂₄	C ₂₅	177.6(2)
C ₁₆	C ₁₇	C ₂₅	C ₂₆	176.49(16)	C ₃₂	N ₁	C ₃₁	C ₂₆	-177.6(2)
C ₁₇	C ₁₈	C ₁₉	C ₂₀	-174.45(19)	C ₃₂	N ₁	C ₃₁	C ₃₀	2.7(4)
C ₁₇	C ₁₈	C ₂₃	C ₂₂	175.0(2)					

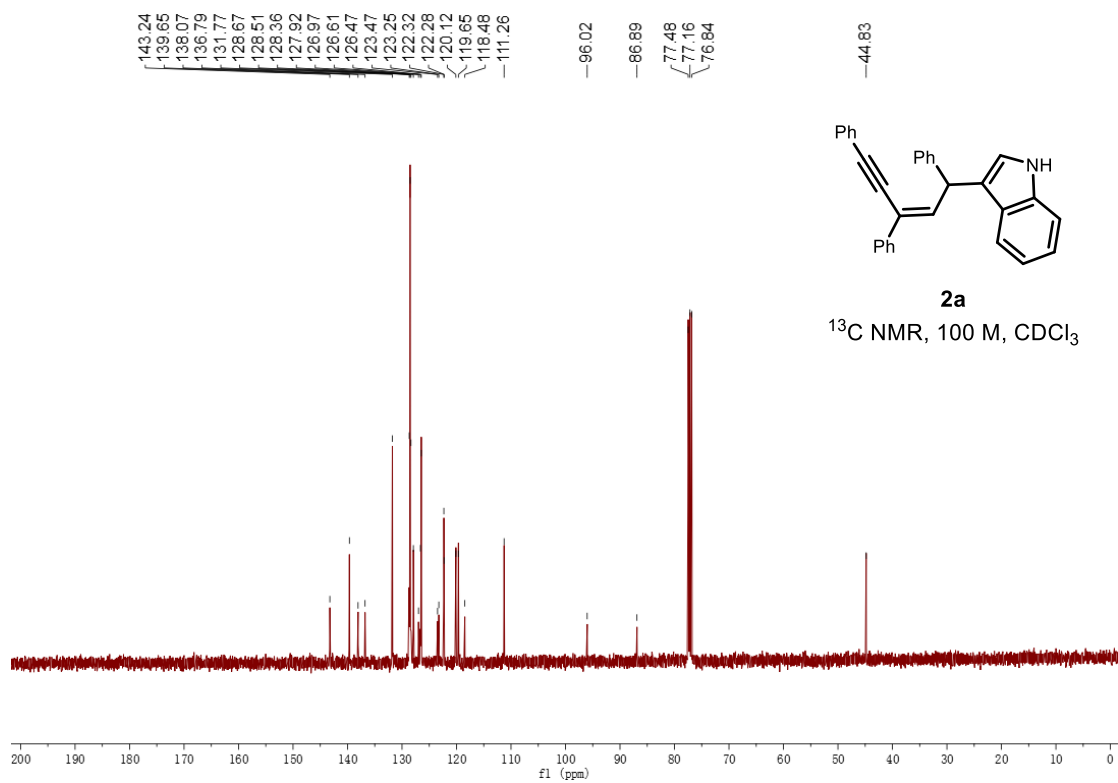
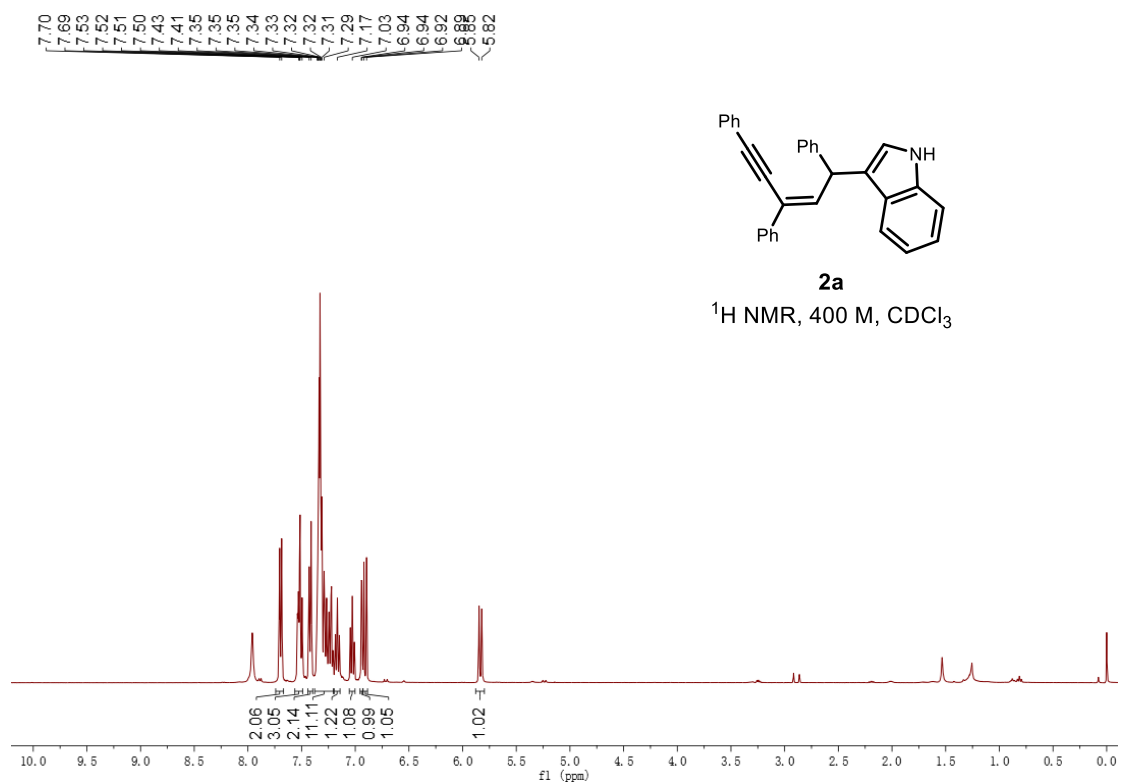
Table 7 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for YZQ_1.

Atom	x	y	z	U(eq)
H ₂	6608.71	9237.72	5026.95	52
H ₃	6723.27	9840.74	3170.63	57
H ₄	6640.2	8246.71	1613.43	58
H ₅	6591.18	6053.29	1981.86	58
H ₆	6504.61	5439.87	3842.18	51
H ₁₁	6120.5	2498.85	6870.38	59
H ₁₂	6980.12	521.7	7215.49	77
H ₁₃	9222.09	289.85	7224.23	92

Table 7 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for YZQ_1.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H ₁₄	10614.45	2044.59	6886.85	99
H ₁₅	9797.15	4038.66	6568.78	72
H ₁₆	5186.94	8233.06	6071.01	48
H ₁₇	5589.67	6229.24	7660.68	45
H ₁₉	5065.13	9478.89	8594.59	54
H ₂₀	6670.97	10954.8	10026.75	60
H ₂₁	8850.65	10410.31	10889.86	60
H ₂₂	9438.39	8380.41	10335.06	63
H ₂₃	7850.97	6914.68	8885	55
H ₂₄	2810.08	7642.26	5899.83	52
H ₂₇	4847.73	6283.14	9904.85	52
H ₂₈	3447.74	5759.95	11126.36	61
H ₂₉	1090.31	5883.59	10486	68
H ₃₀	73.26	6491.37	8582.93	63
H _{32A}	-307.79	6602.74	5876.21	97
H _{32B}	308.14	8037.32	5705.21	97
H _{32C}	-274.77	7808.1	6829.88	97

8 ^1H , ^{13}C NMR and HRMS characterization data



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1361 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

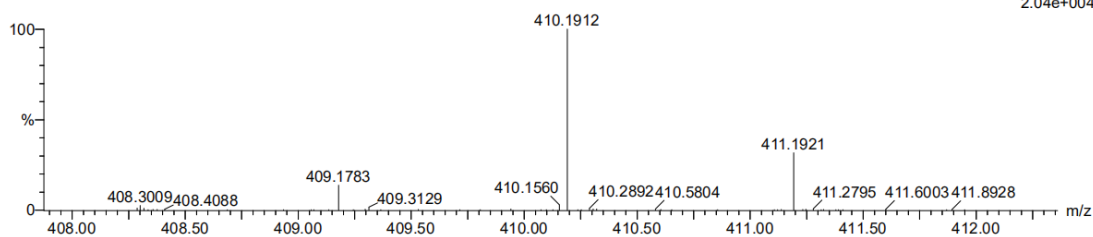
Elements Used:

C: 31-31 H: 24-24 N: 0-50 O: 0-50 Na: 0-3

32

250109-11-723-2-11 28 (0.090)

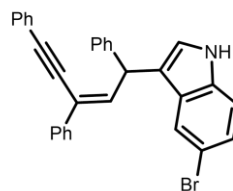
1: TOF MS ES+
2.04e+004



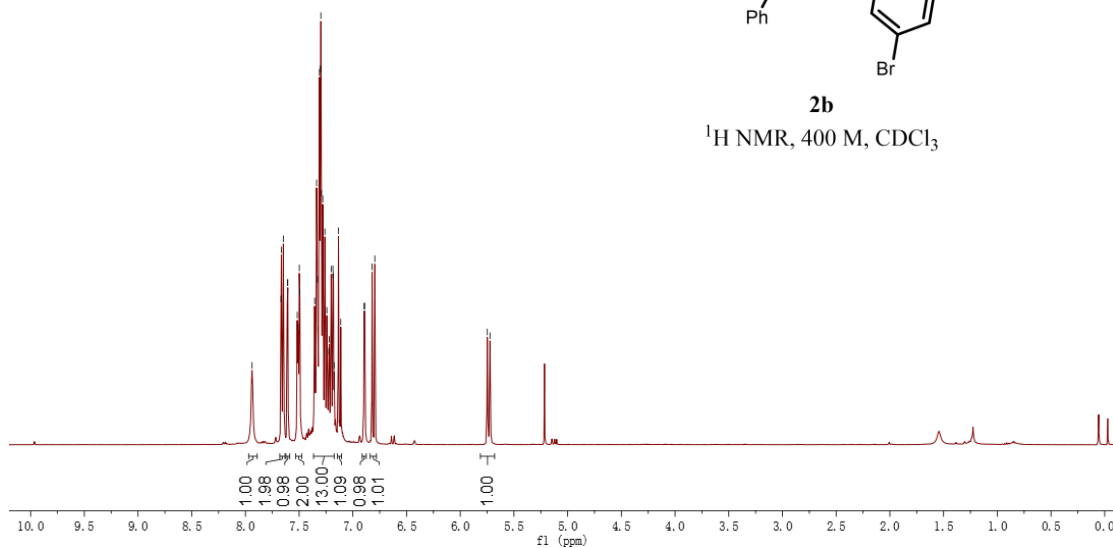
Minimum: -1.5
Maximum: 5.0 10.0 50.0

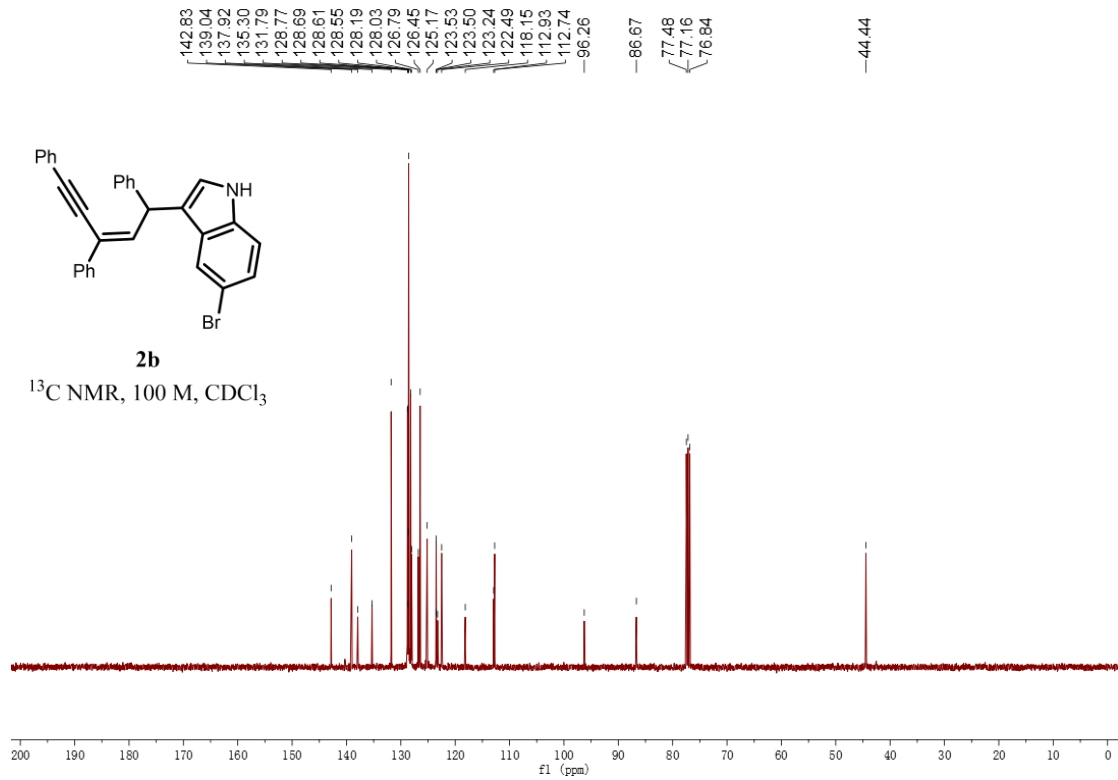
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
410.1912	410.1909	0.3	0.7	20.5	209.8	n/a	n/a	C31 H24 N

7.67
7.67
7.65
7.61
7.50
7.49
7.36
7.34
7.33
7.31
7.30
7.30
7.29
7.28
7.26
7.20
7.18
7.13
7.13
6.89
6.89
6.82
6.82
5.72



¹H NMR, 400 M, CDCl₃





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2708 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

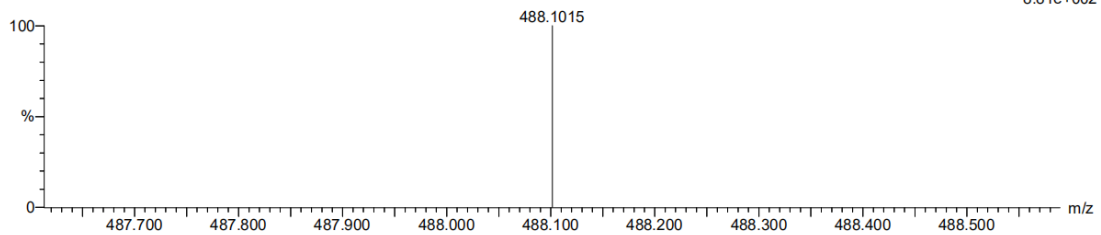
Elements Used:

C: 31-31 H: 23-23 N: 0-50 O: 0-50 Na: 0-3 Br: 1-3

32

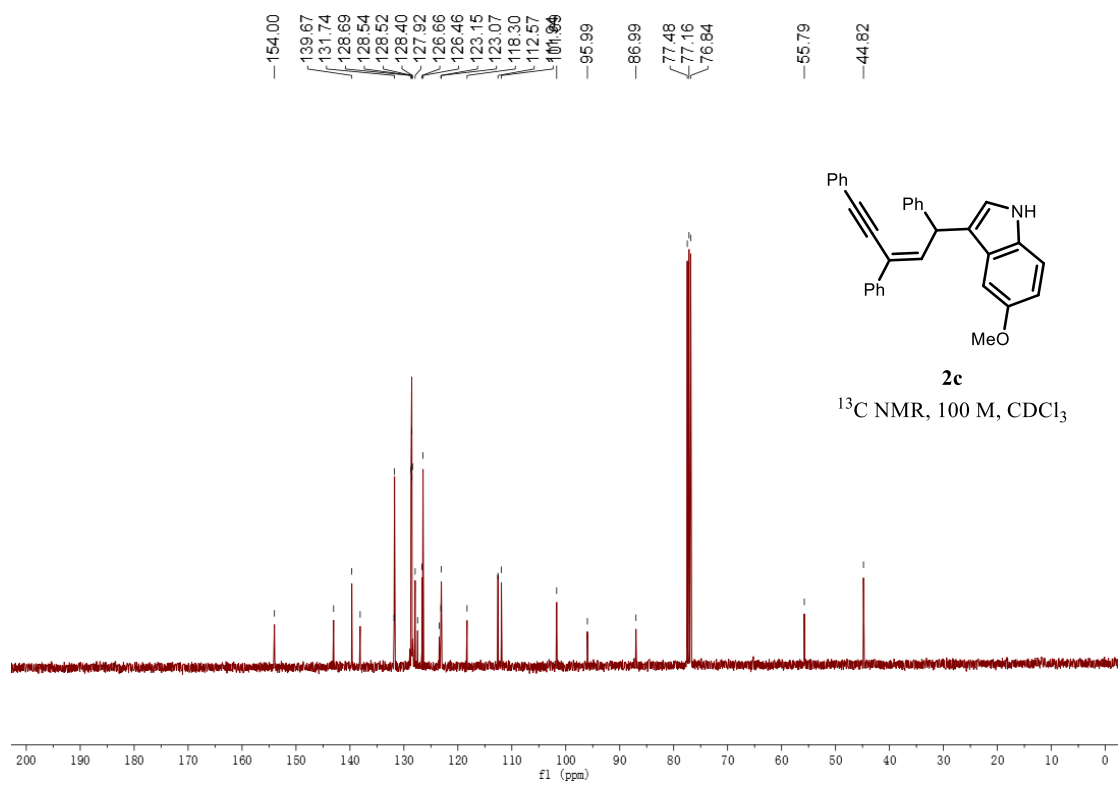
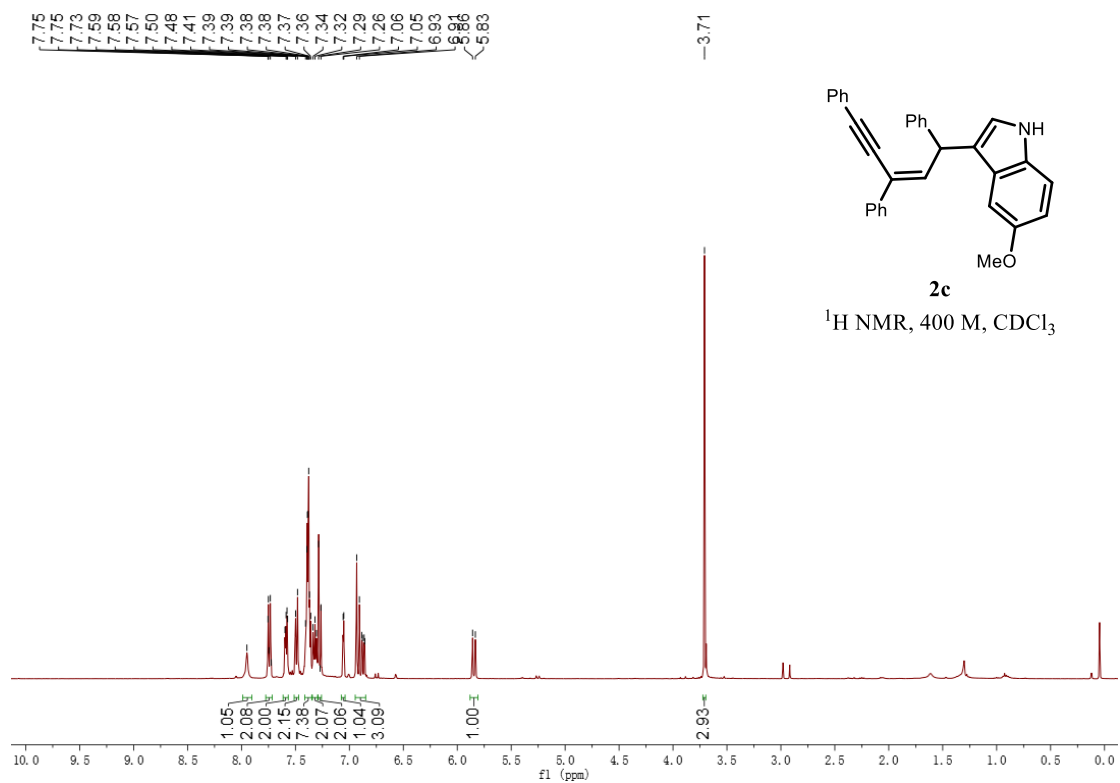
250109-11-723-2-10 21 (0.077)

1: TOF MS ES+
8.81e+002



Minimum: -1.5
 Maximum: 10.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
488.1015	488.1014	0.1	0.2	20.5	24.7	n/a	n/a	C31 H23 N Br



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1567 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

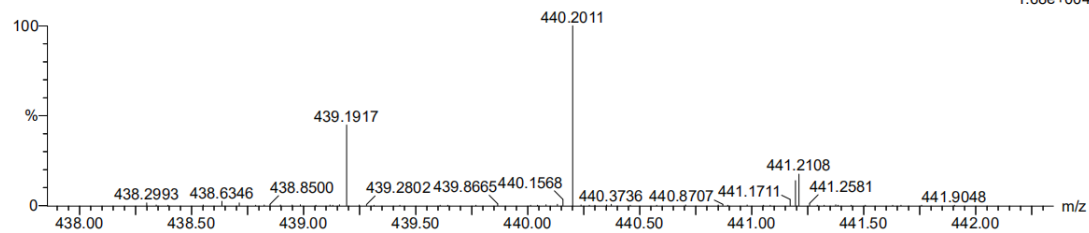
Elements Used:

C: 32-32 H: 26-26 N: 0-50 O: 0-50 Na: 0-3

32

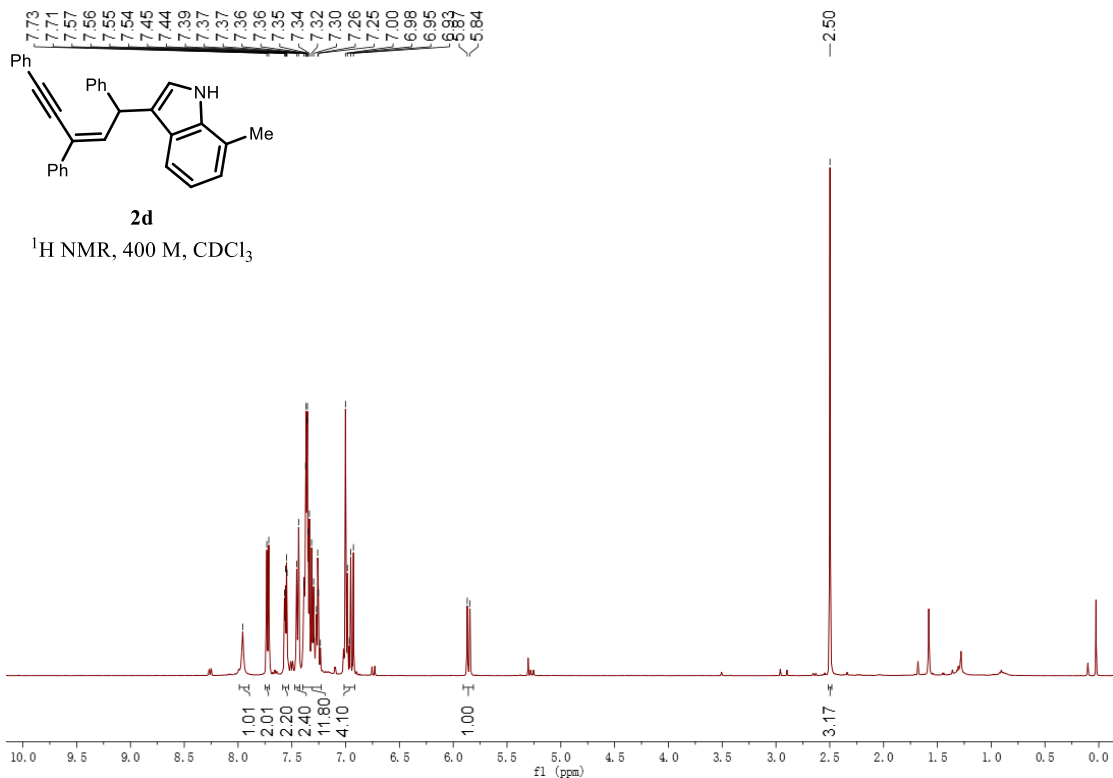
250109-11-723-2-8 26 (0.086)

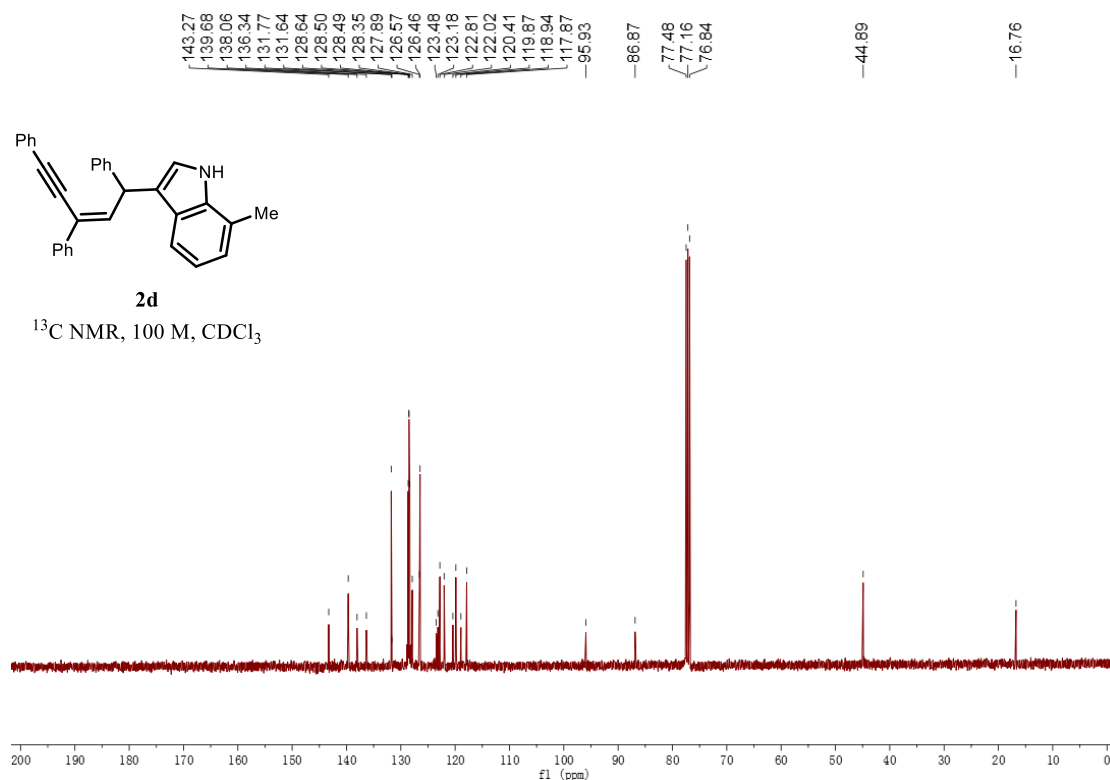
1: TOF MS ES+
1.68e+004



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
440.2011	440.2014	-0.3	-0.7	20.5	237.6	n/a	n/a	C32 H26 N O





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1459 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

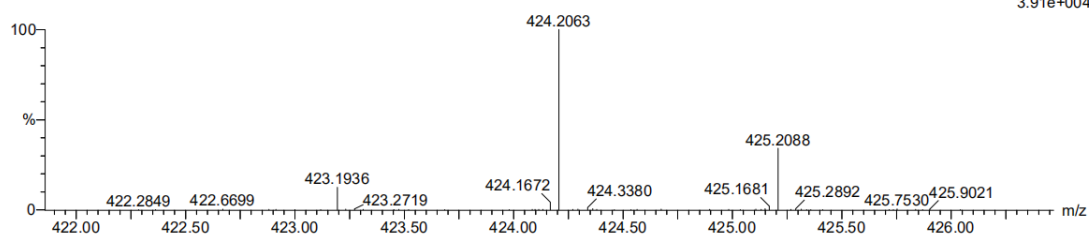
Elements Used:

C: 32-32 H: 26-26 N: 0-50 O: 0-50 Na: 0-3

32

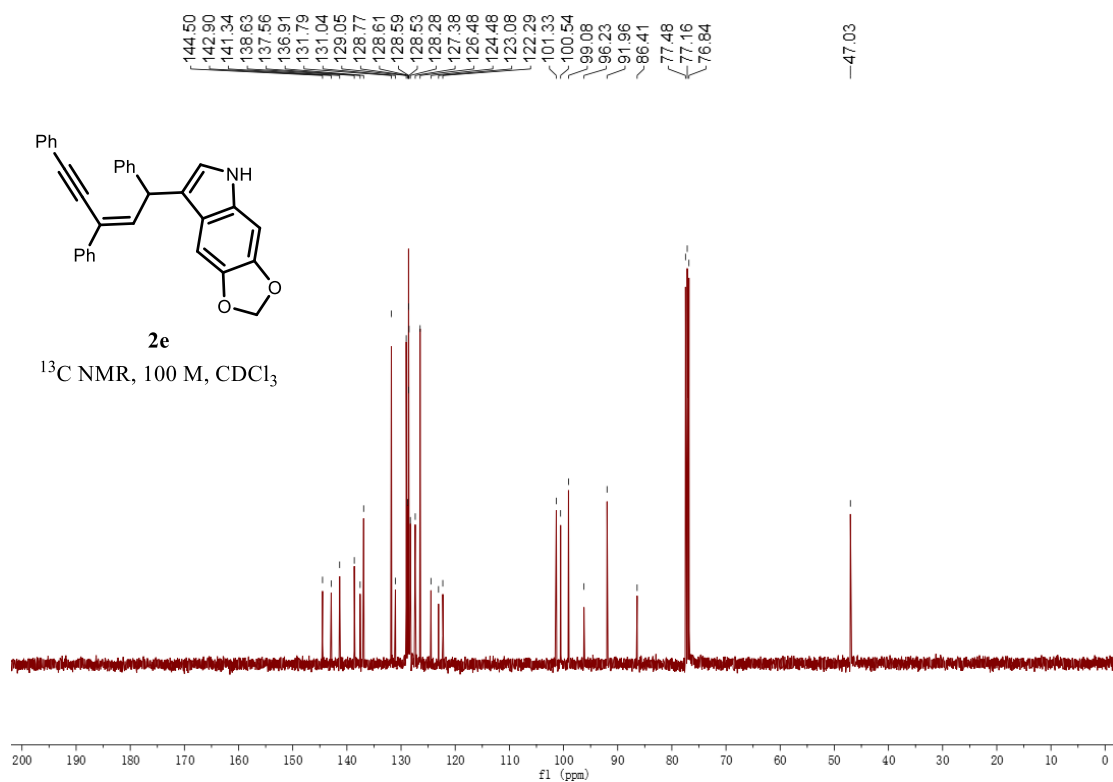
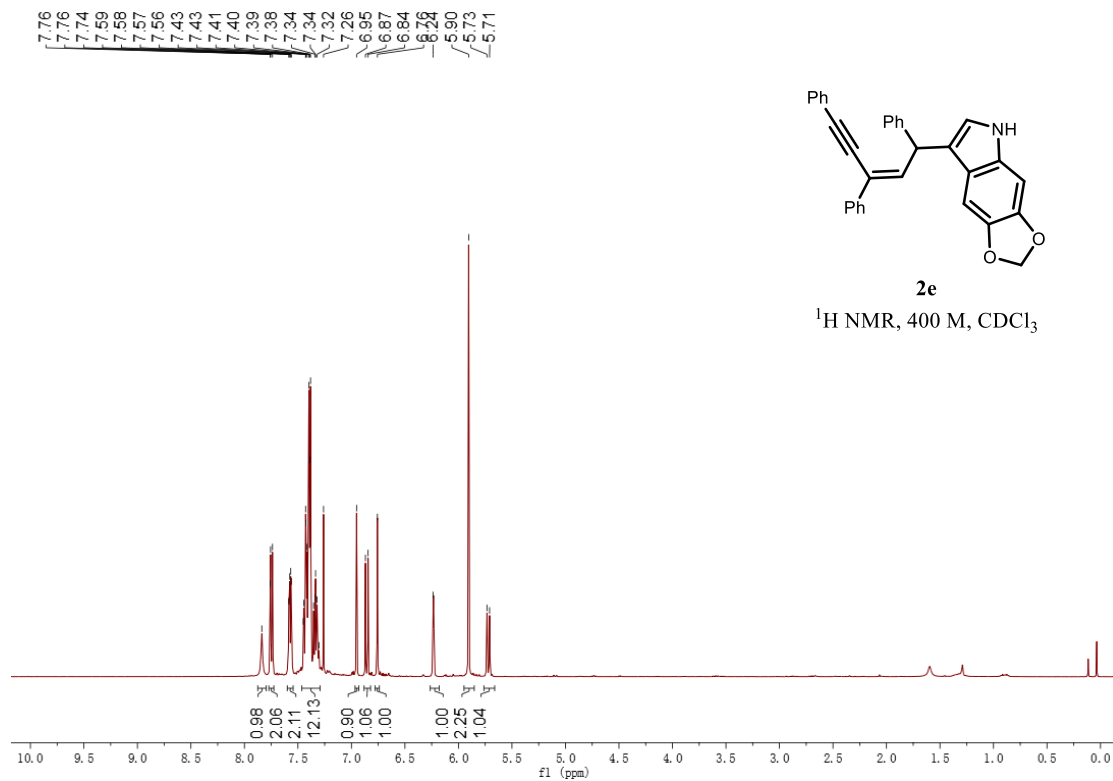
250109-11-723-2-4 27 (0.088)

1: TOF MS ES+
3.91e+004



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
424.2063	424.2065	-0.2	-0.5	20.5	265.1	n/a	n/a	C ₃₂ H ₂₆ N



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1306 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

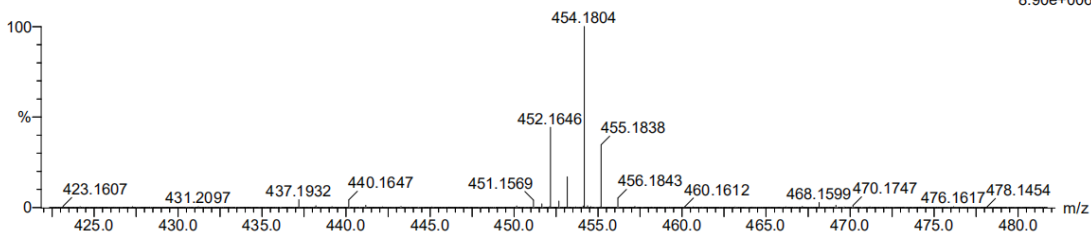
Elements Used:

C: 32-32 H: 24-24 N: 0-100 O: 0-100 Na: 0-2

7

250403-12-761-2-YQZ-25 14 (0.143)

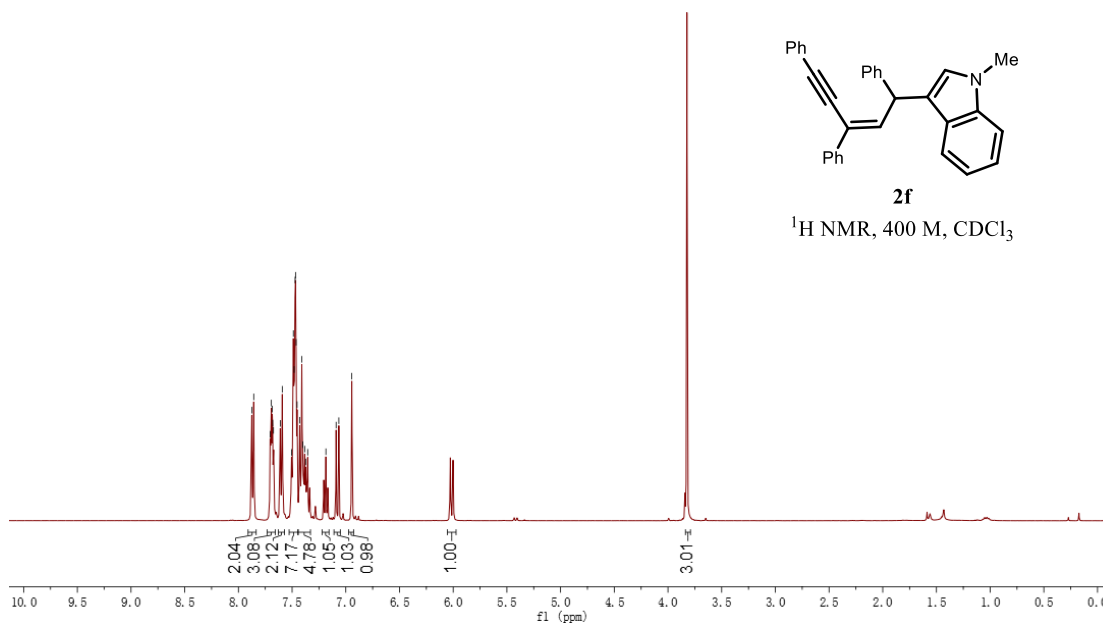
1: TOF MS ES+
8.90e+006

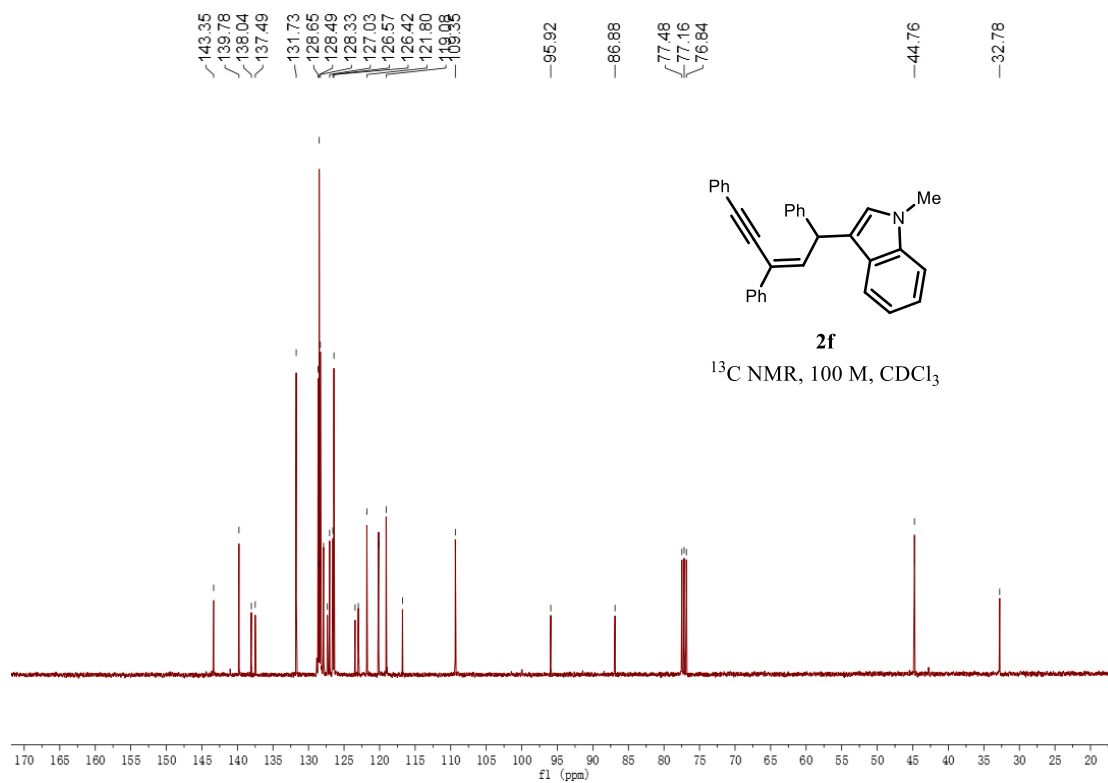


Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
454.1804	454.1807	-0.3	-0.7	21.5	1197.6	n/a	n/a	C32 H24 N O2

7.88
7.86
7.70
7.69
7.69
7.68
7.67
7.61
7.59
7.51
7.49
7.48
7.47
7.47
7.46
7.45
7.43
7.41
7.40
7.38
7.37
7.35
7.19
7.08
7.06
6.94





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1608 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

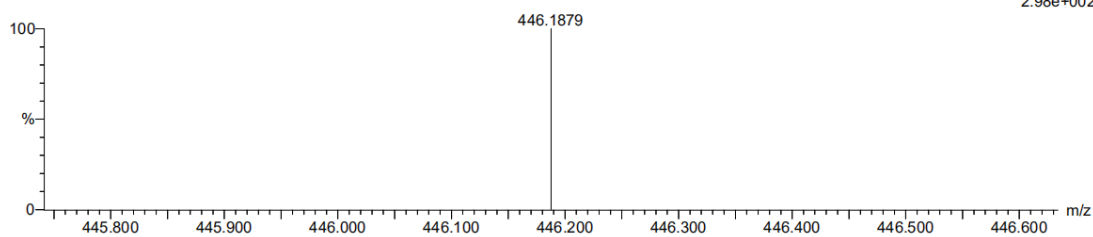
Elements Used:

C: 32-32 H: 25-25 N: 0-50 O: 0-50 Na: 0-3

25

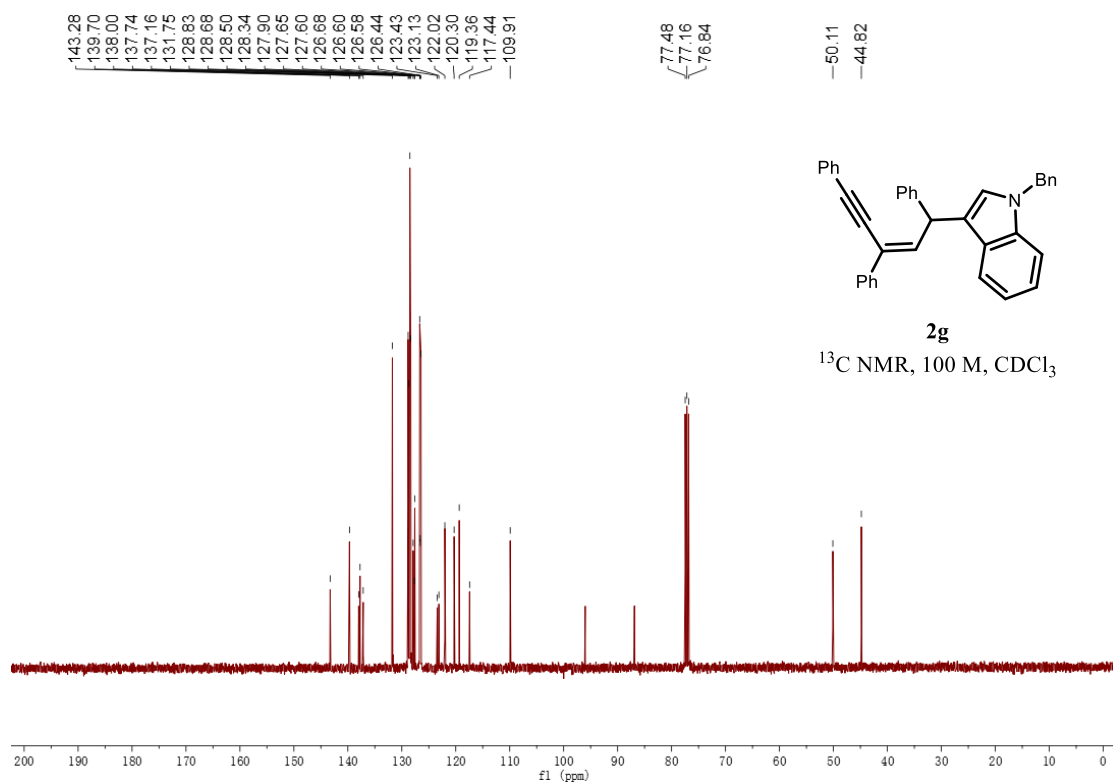
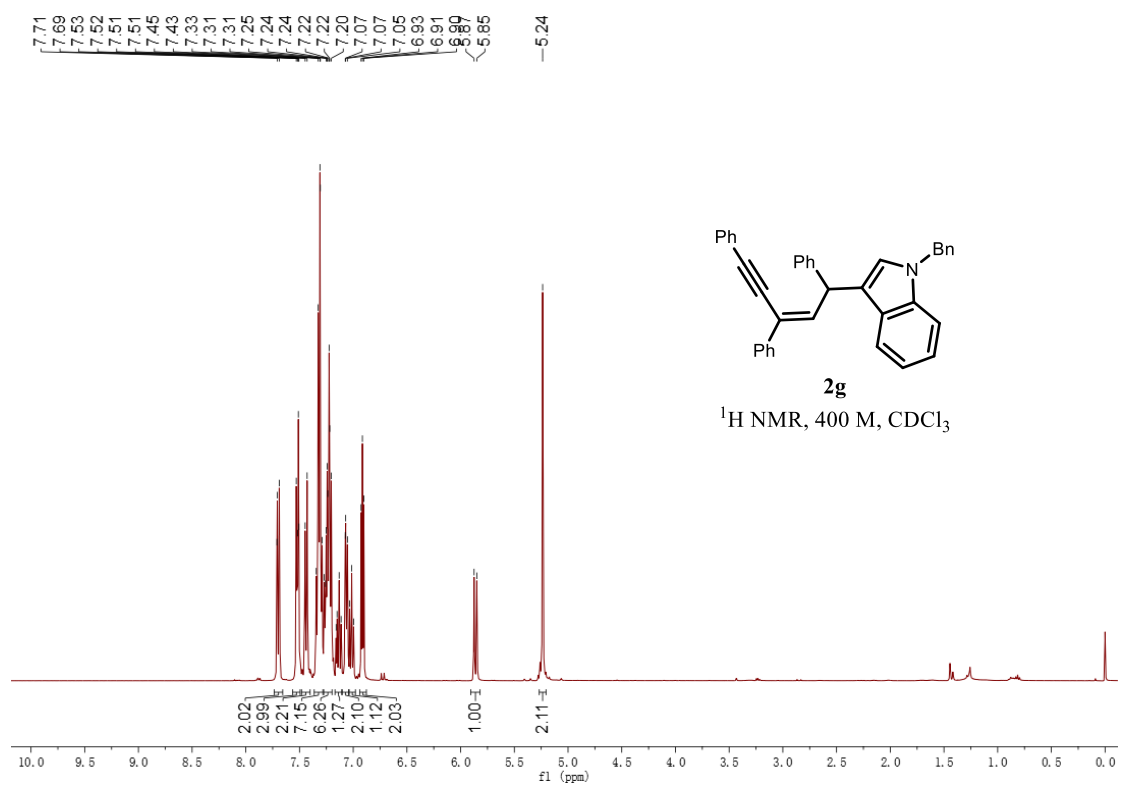
250109-11-723-2-1 20 (0.075)

1: TOF MS ES+
2.98e+002



Minimum: -1.5
Maximum: 5.0 10.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
446.1879	446.1885	-0.6	-1.3	20.5	21.3	n/a	n/a	C32 H25 N Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2235 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

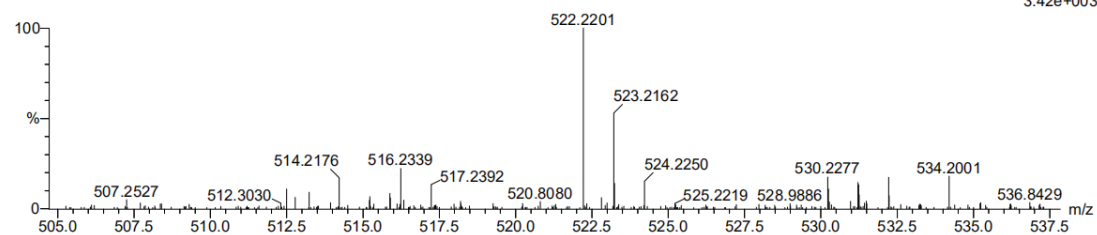
Elements Used:

C: 38-38 H: 29-29 N: 0-50 O: 0-50 Na: 0-3

32

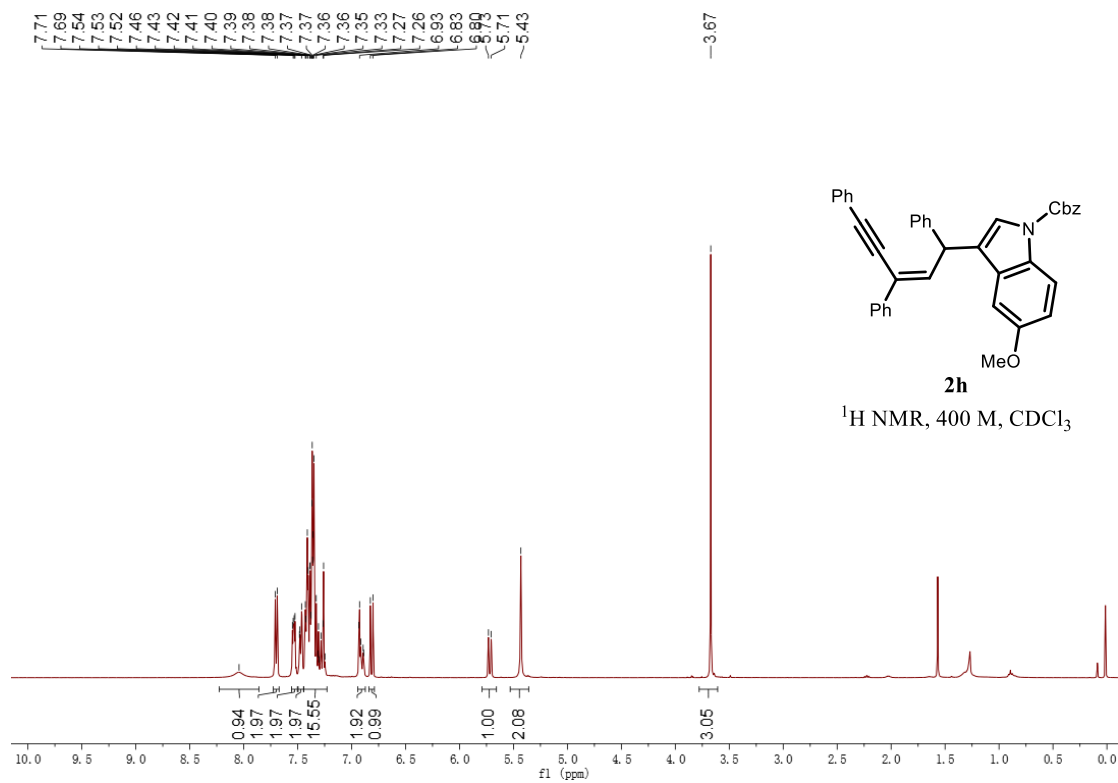
250109-11-723-2-9 33 (0.100)

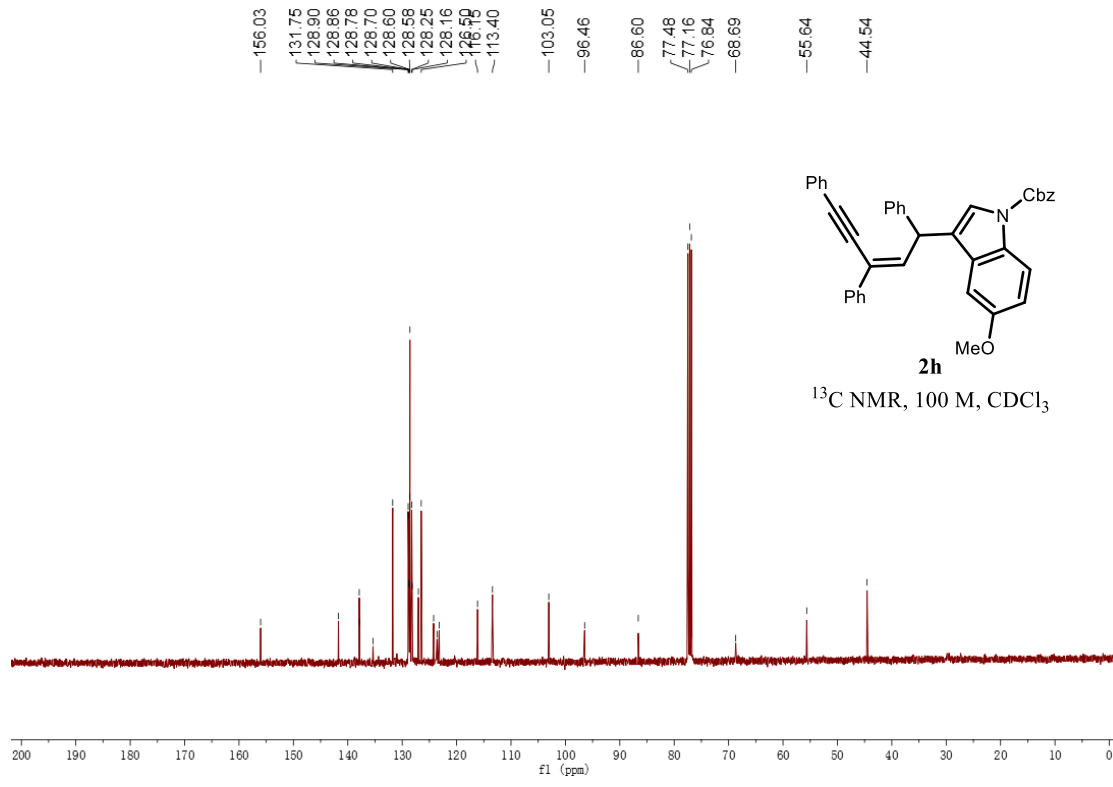
1: TOF MS ES+
3.42e+003



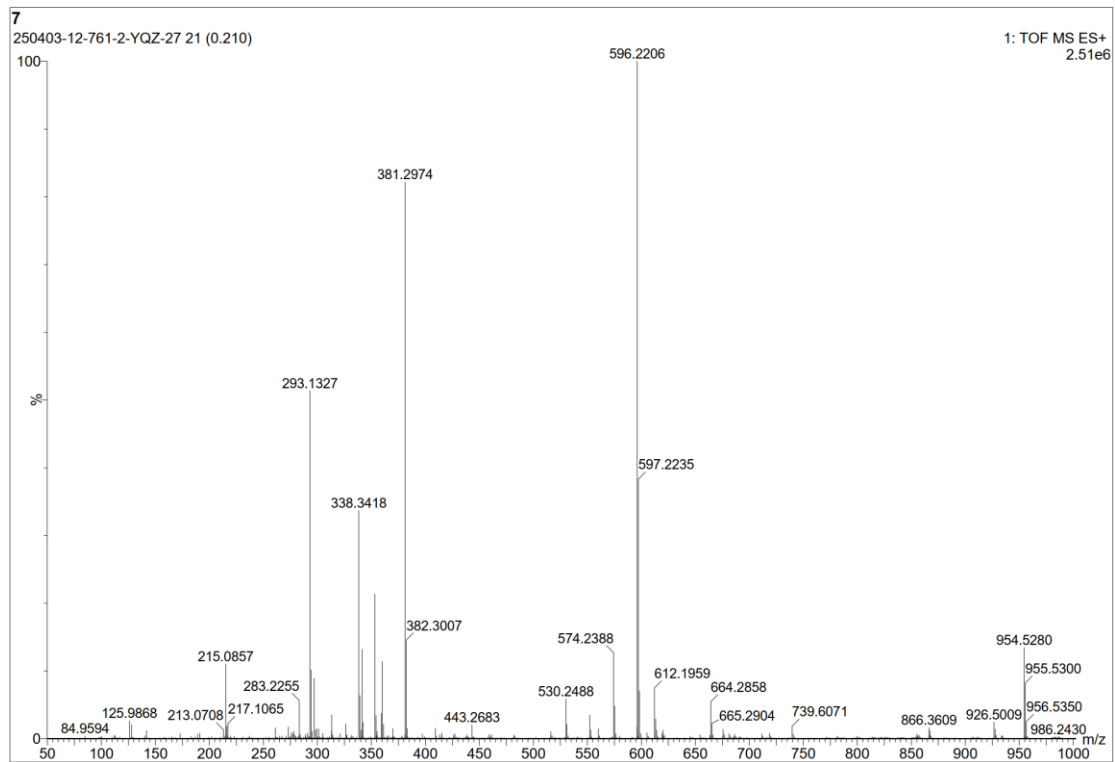
Minimum: -1.5
Maximum: 5.0 10.0 50.0

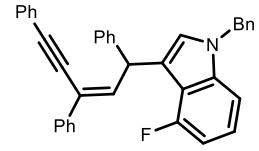
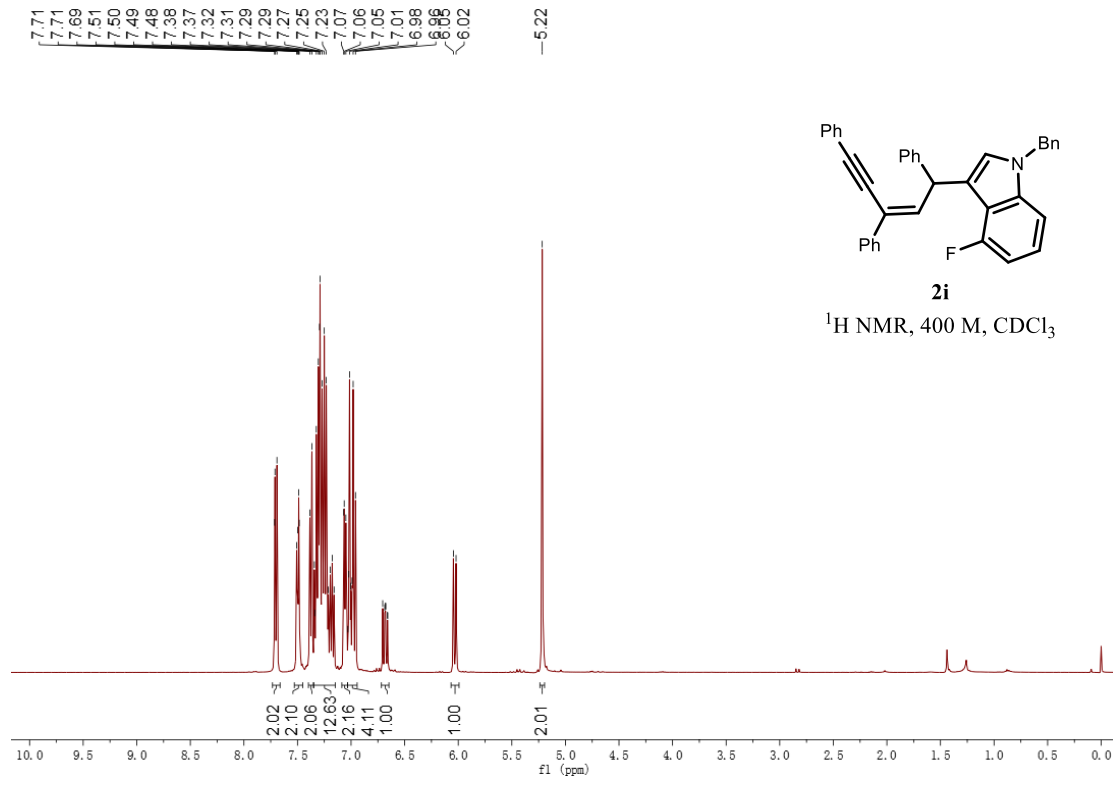
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
522.2201	522.2198	0.3	0.6	24.5	189.7	n/a	n/a	C38 H29 N Na





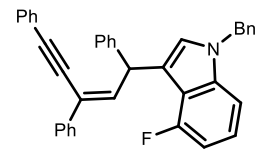
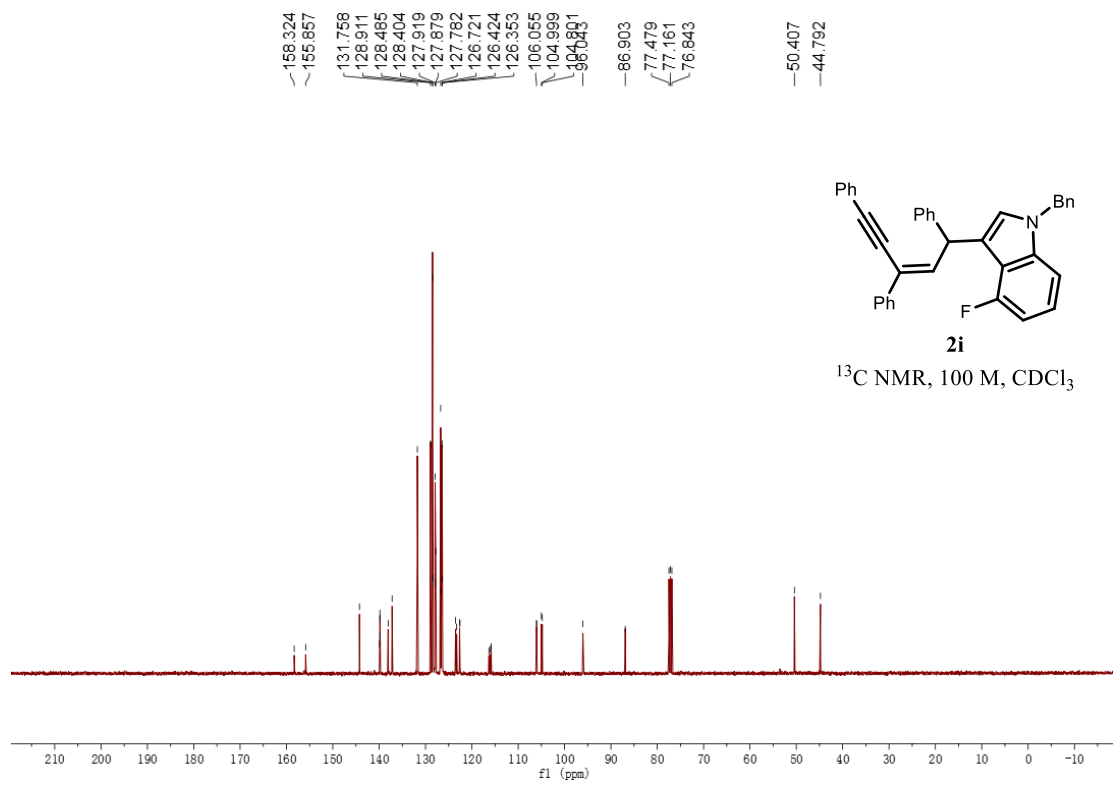
HRMS spectrum





2i

^1H NMR, 400 M, CDCl_3



2i

^{13}C NMR, 100 M, CDCl_3

HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2041 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

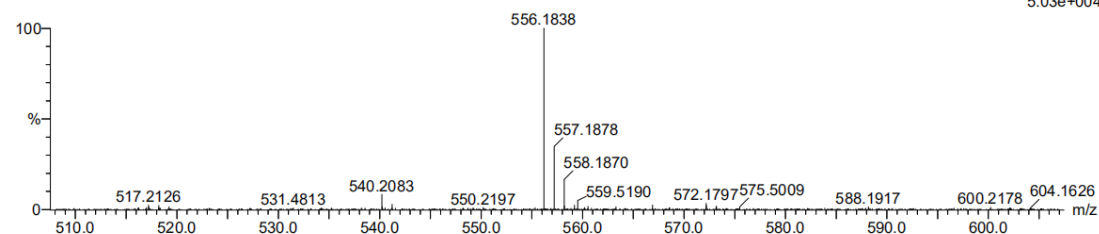
Elements Used:

C: 38-38 H: 28-28 N: 0-50 O: 0-50 Na: 0-3 K: 1-1 F: 1-1

32

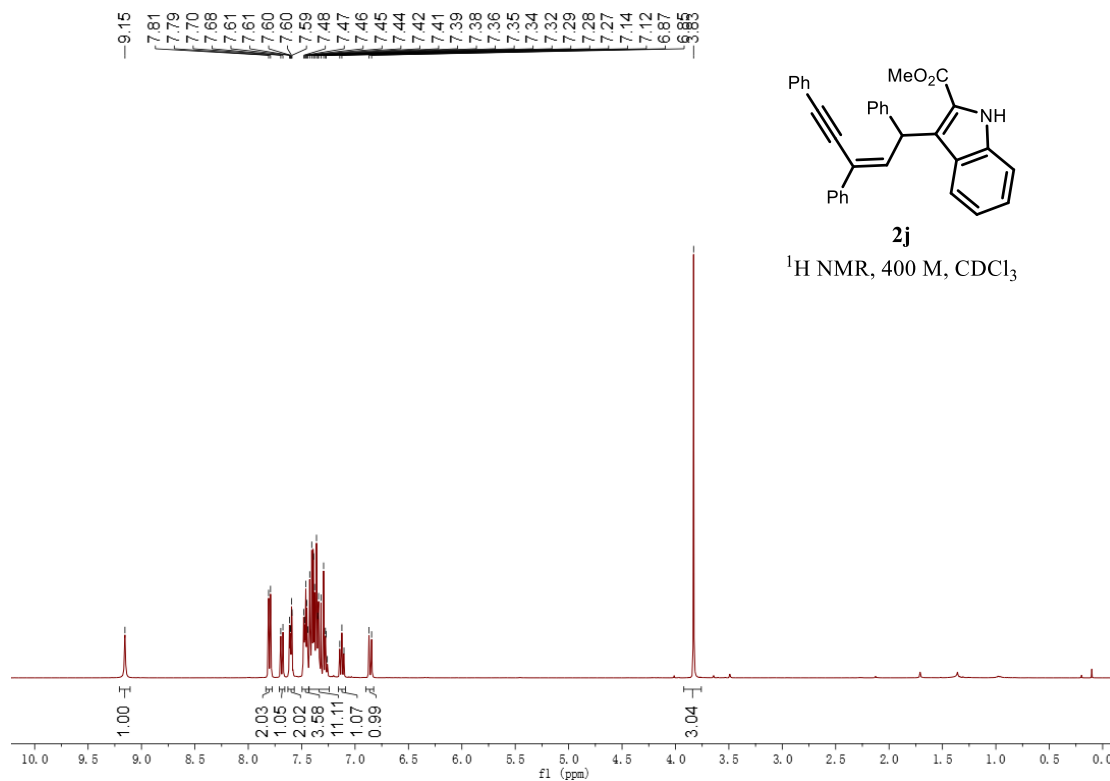
250109-11-723-2-12 39 (0.111)

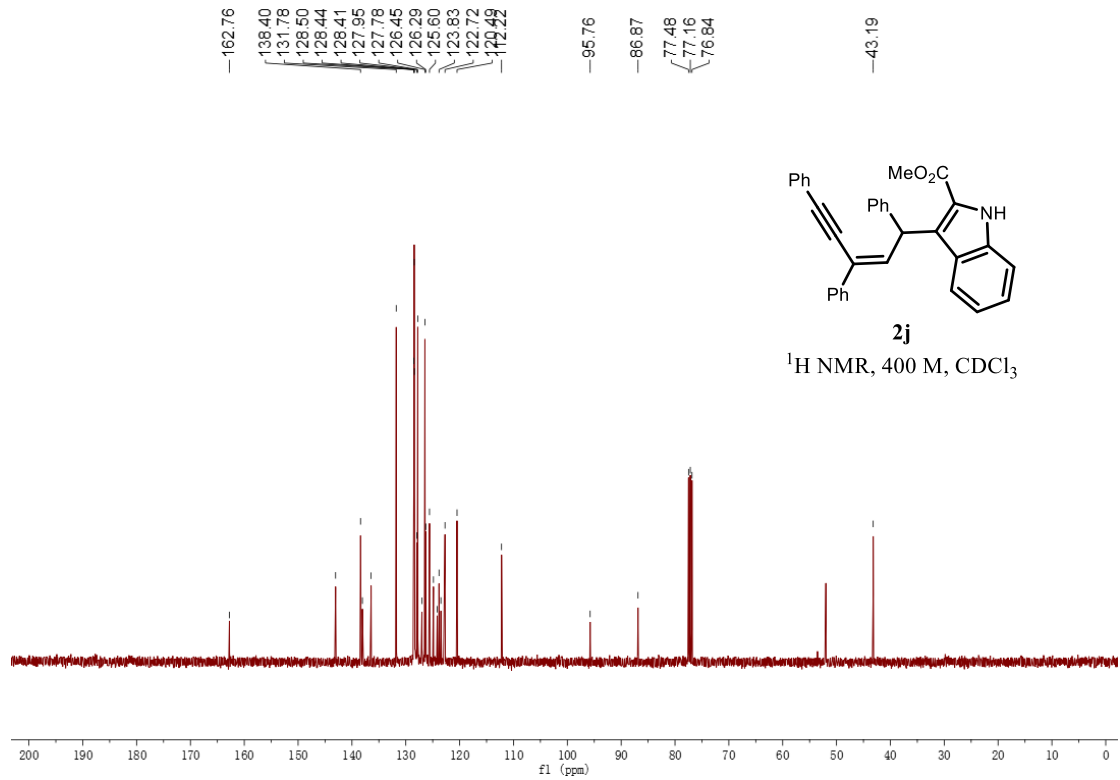
1: TOF MS ES+
5.03e+004



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
556.1838	556.1843	-0.5	-0.9	24.5	331.6	n/a	n/a	C38 H28 N K F





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1504 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

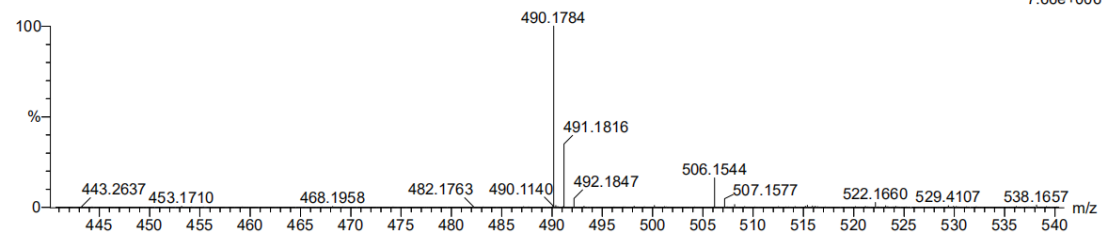
Elements Used:

C: 33-33 H: 25-25 N: 0-100 O: 0-100 Na: 0-2

7

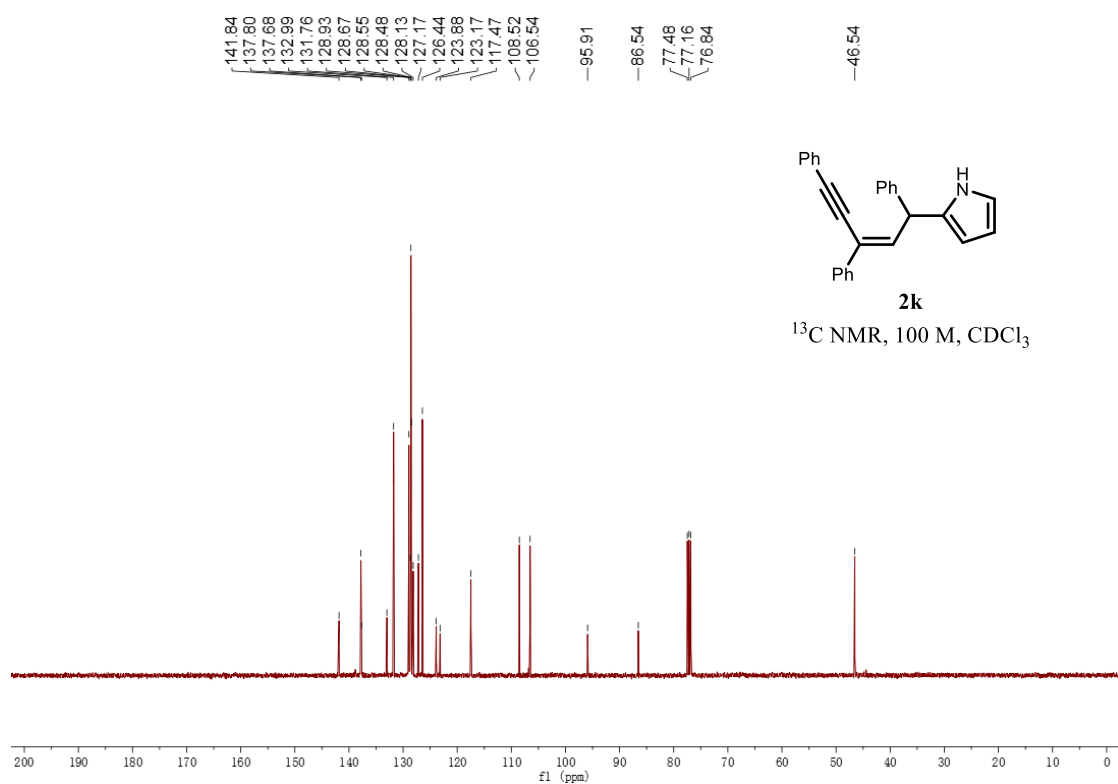
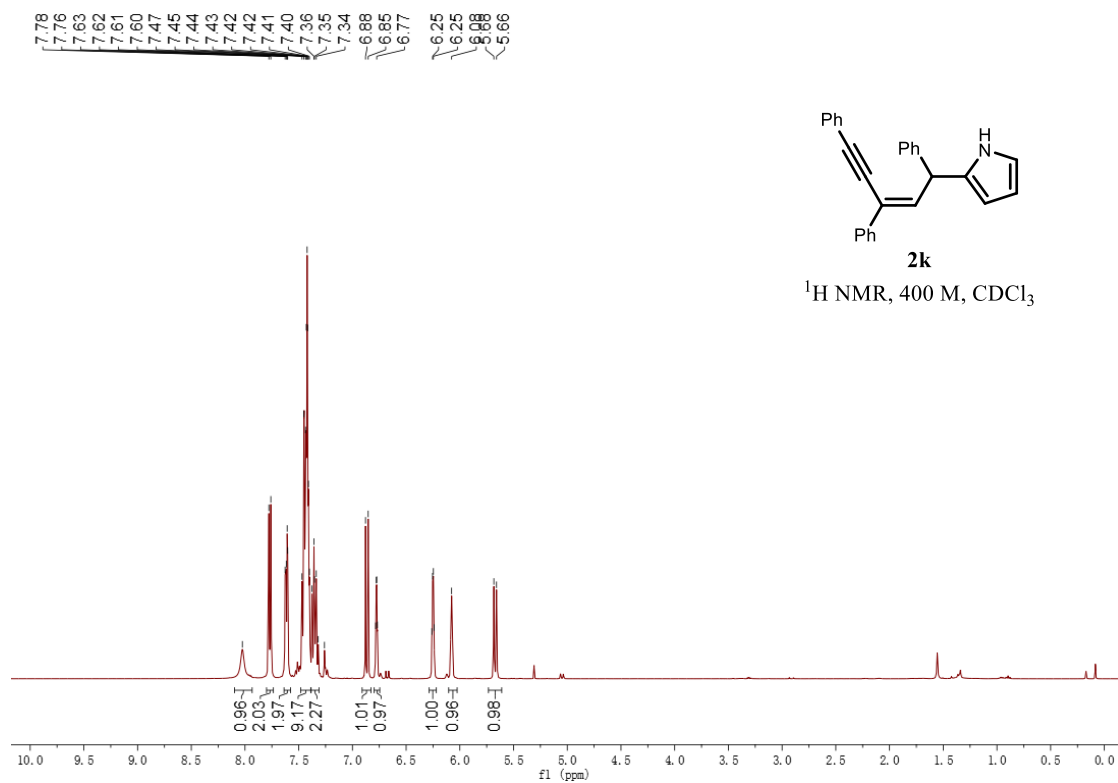
250403-12-761-2-YQZ-24 13 (0.135)

1: TOF MS ES+
7.66e+006



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
490.1784	490.1783	0.1	0.2	21.5	1039.2	n/a	n/a	C33 H25 N O2 Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1035 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

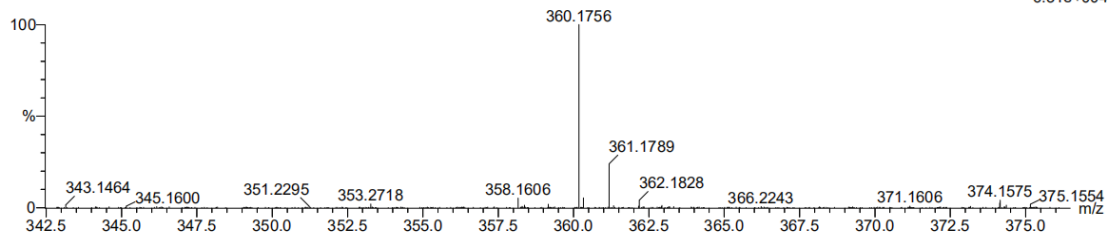
Elements Used:

C: 27-27 H: 22-22 N: 0-50 O: 0-50 Na: 0-3

32

250109-11-723-2-6 34 (0.101)

1: TOF MS ES+
6.31e+004

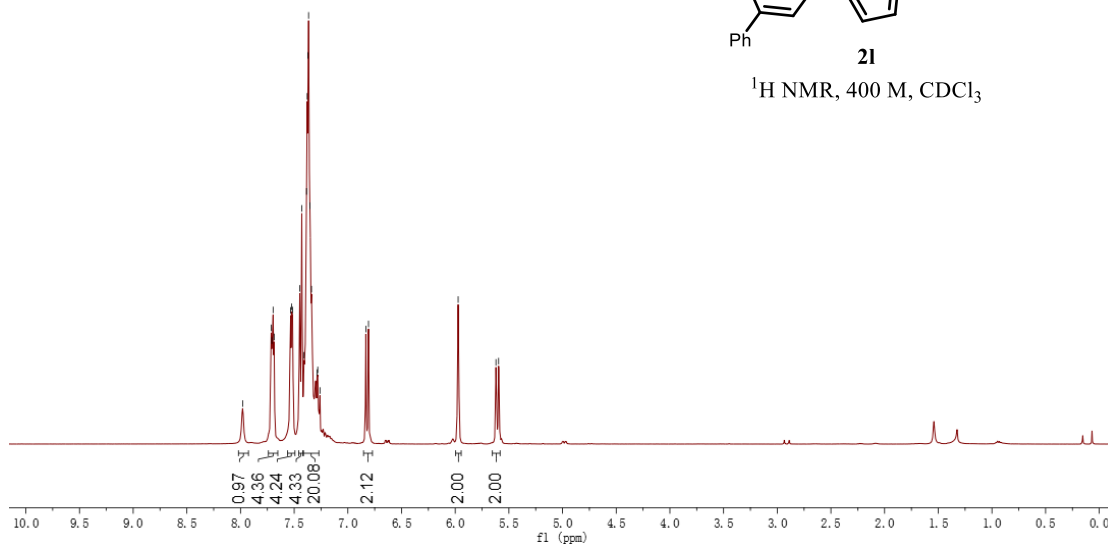
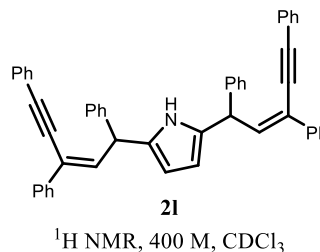


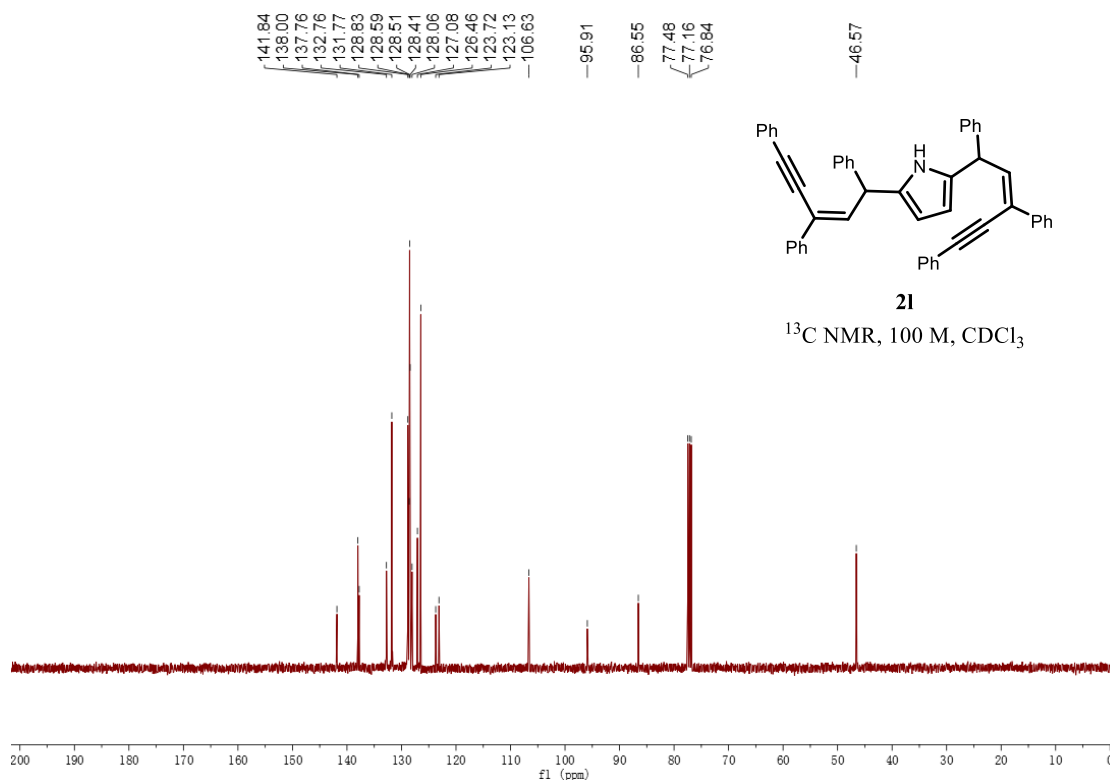
Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
360.1756	360.1752	0.4	1.1	17.5	298.0	n/a	n/a	C27 H22 N

7.71
7.70
7.69
7.53
7.52
7.51
7.45
7.43
7.41
7.38
7.37
7.37
7.35
7.34
7.28
6.83
6.81

-5.97
5.62
5.60





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3565 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

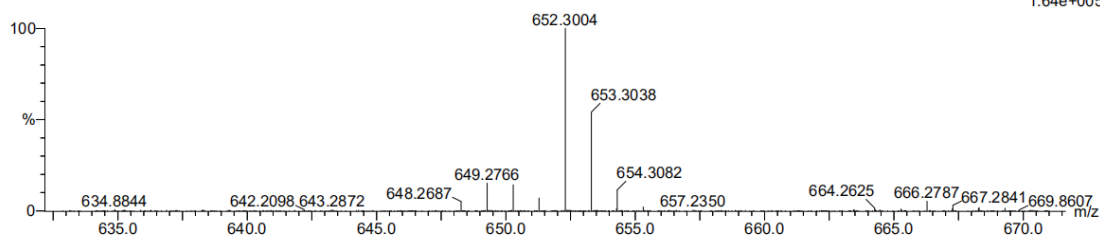
Elements Used:

C: 50-50 H: 38-38 N: 0-50 O: 0-50 Na: 0-3

32

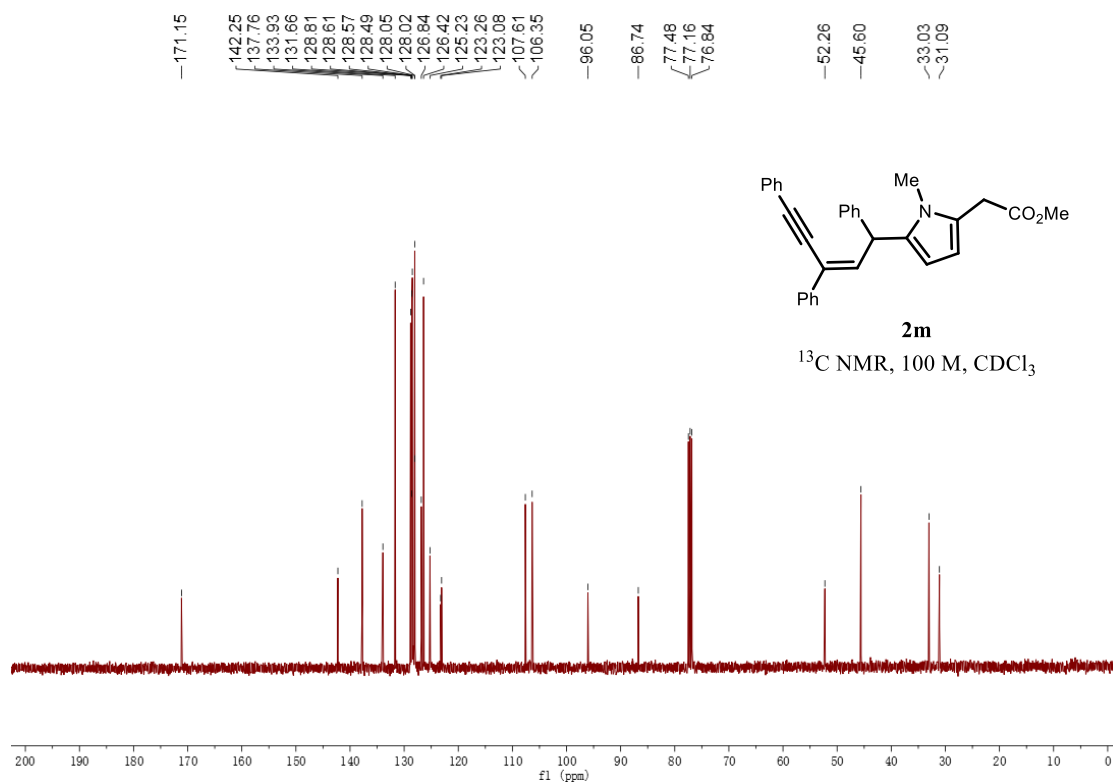
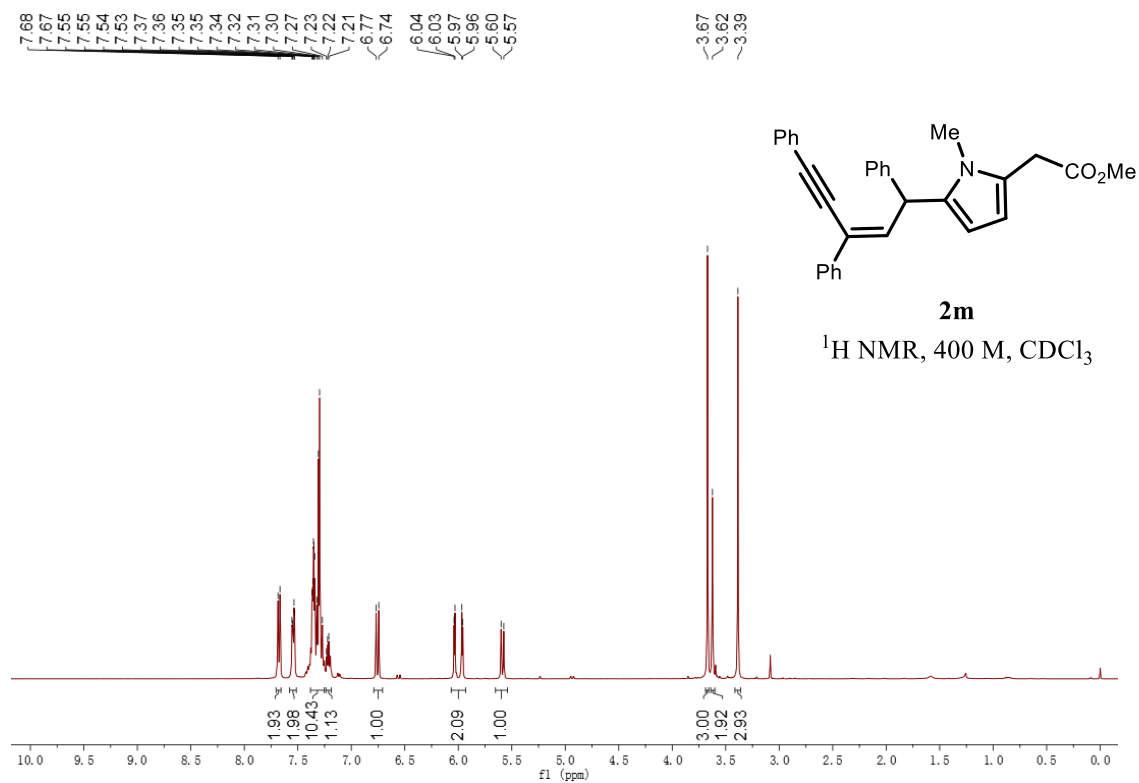
250109-11-723-2-5 36 (0.105)

1: TOF MS ES+
1.64e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
652.3004	652.3004	0.0	0.0	32.5	421.0	n/a	n/a	C ₅₀ H ₃₈ N



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1596 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

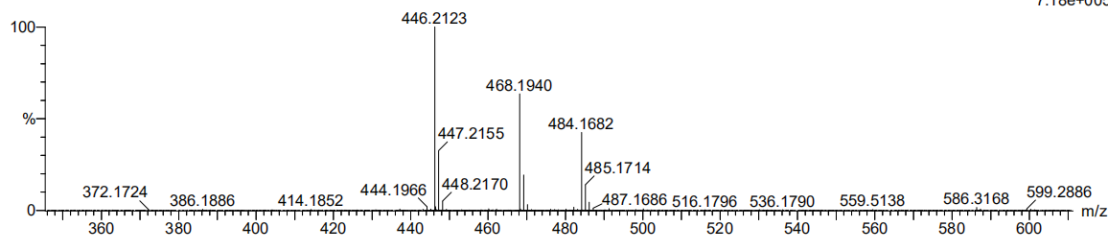
Elements Used:

C: 31-31 H: 28-28 N: 0-50 O: 0-50 Na: 0-3

32

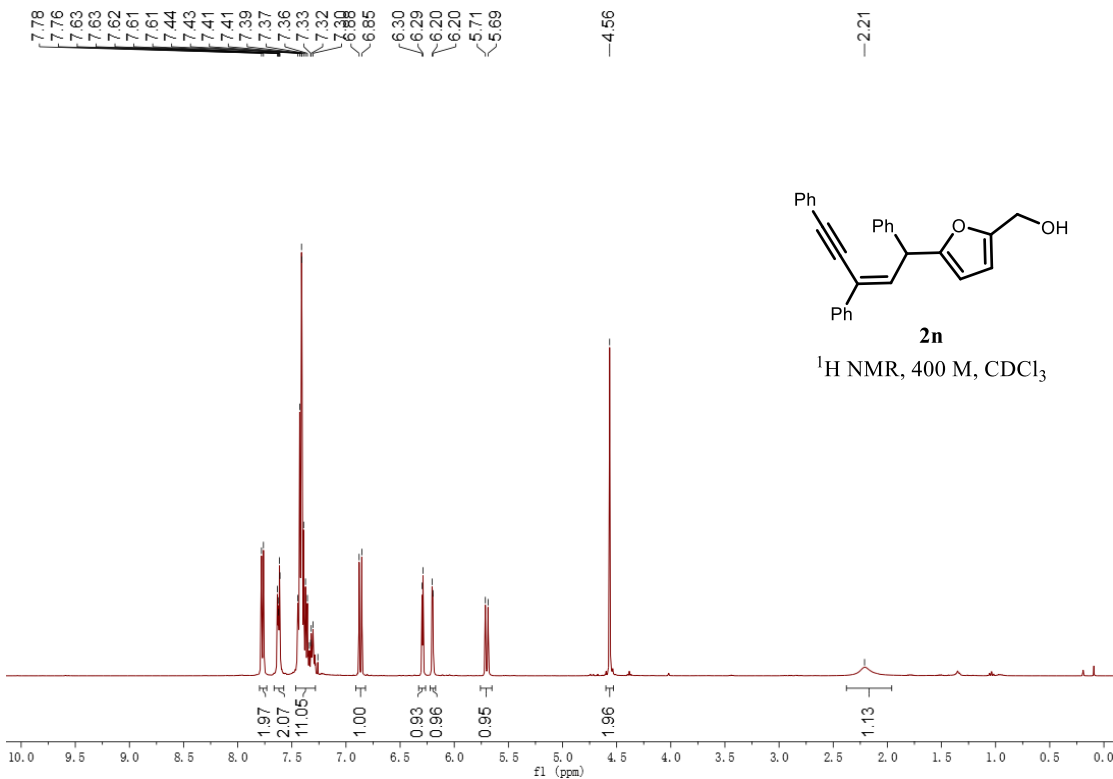
250109-11-723-2-7 36 (0.105)

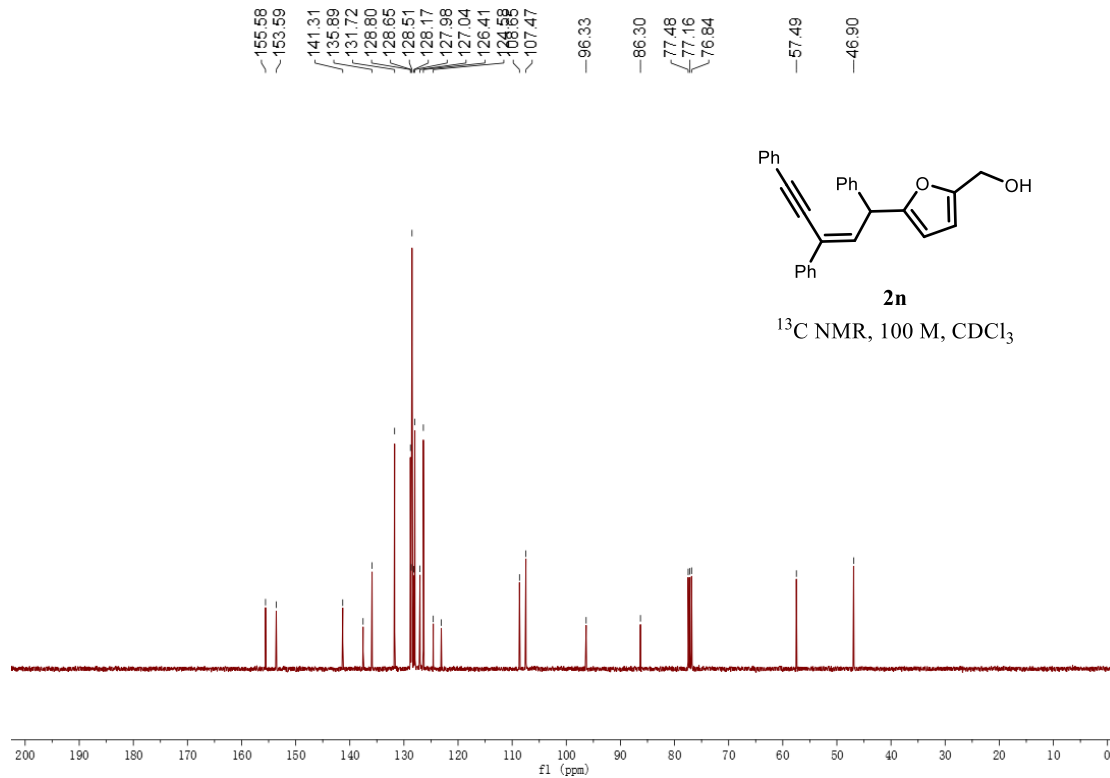
1: TOF MS ES+
7.18e+00e



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
446.2123	446.2120	0.3	0.7	18.5	642.9	n/a	n/a	C31 H28 N O2





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1350 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

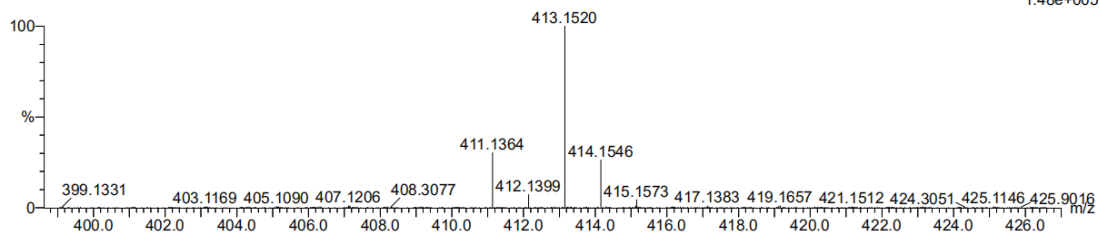
Elements Used:

C: 28-28 H: 22-22 N: 0-50 O: 0-50 Na: 0-3

25

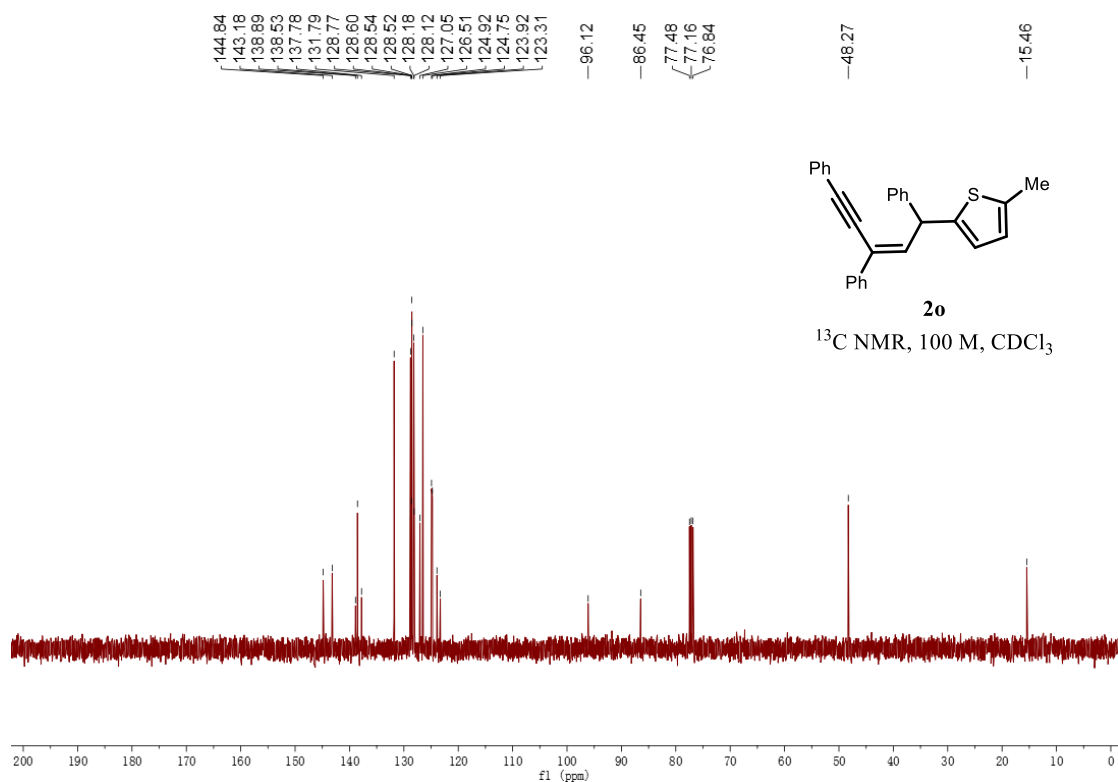
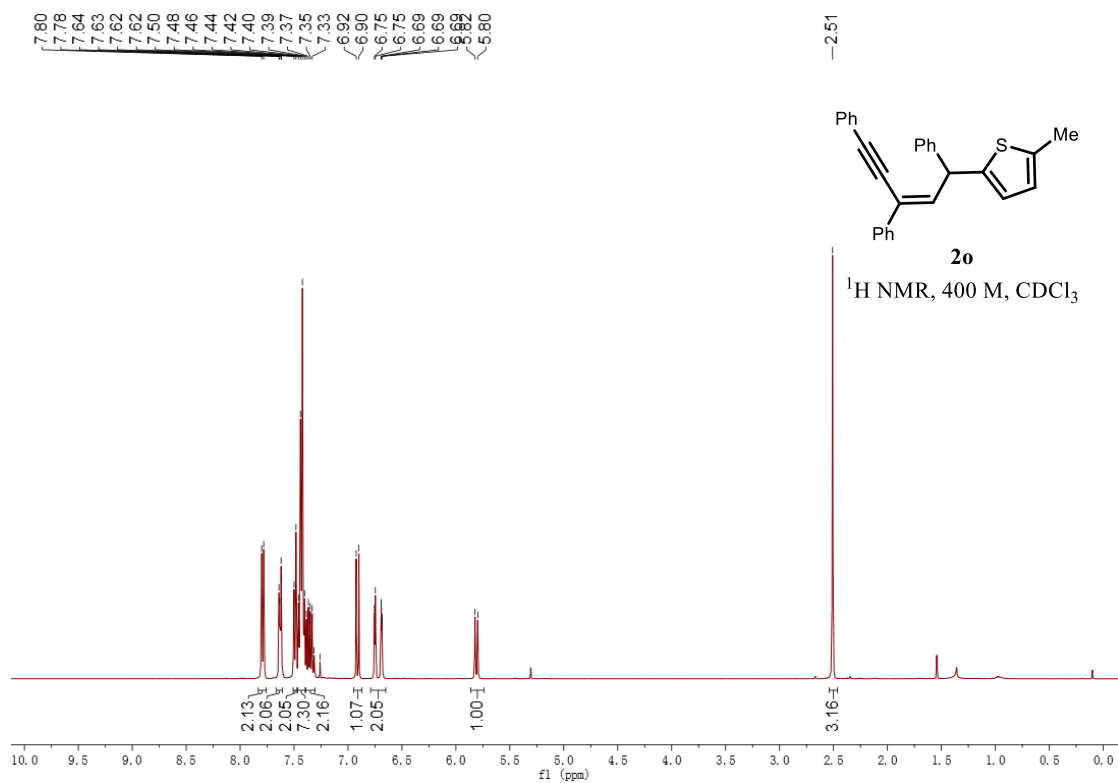
250109-11-723-2-2 25 (0.084)

1: TOF MS ES+
1.48e+005



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
413.1520	413.1517	0.3	0.7	17.5	482.7	n/a	n/a	C ₂₈ H ₂₂ O ₂ Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2933 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

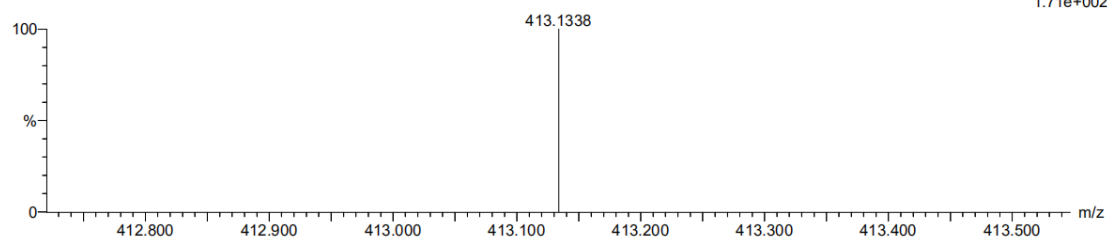
Elements Used:

C: 28-28 H: 22-22 N: 0-50 O: 0-50 Na: 0-3 S: 1-3

32

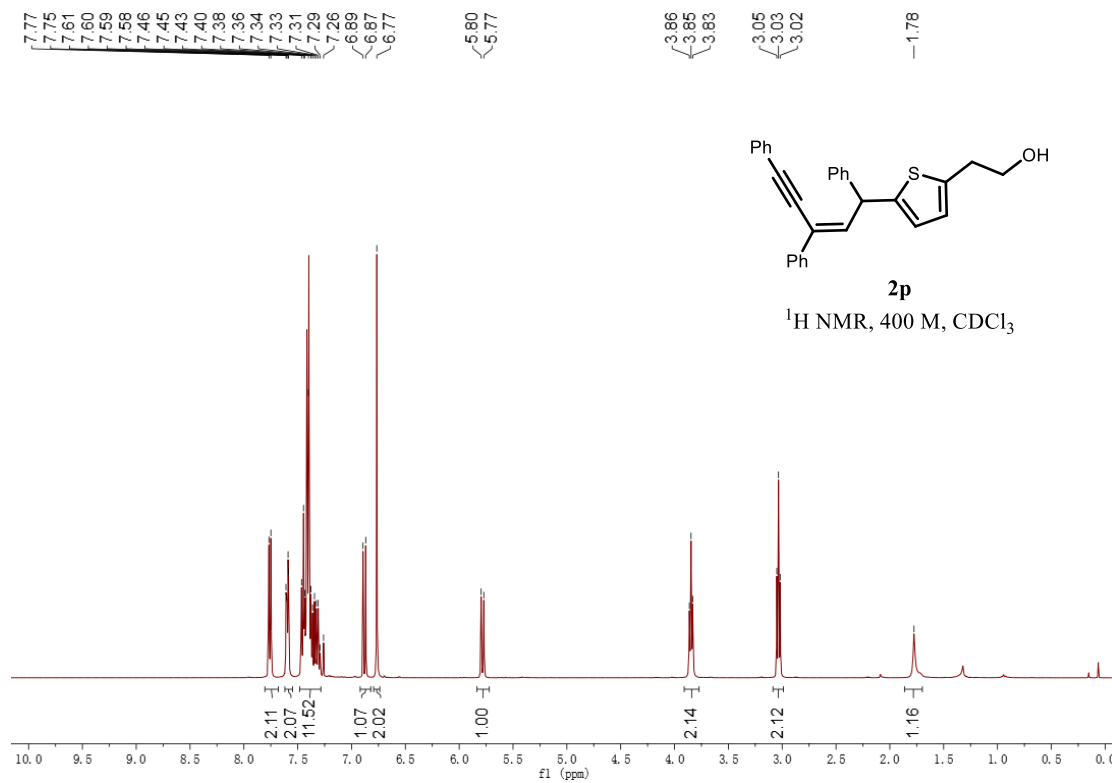
250109-11-723-2-3 54 (0.140)

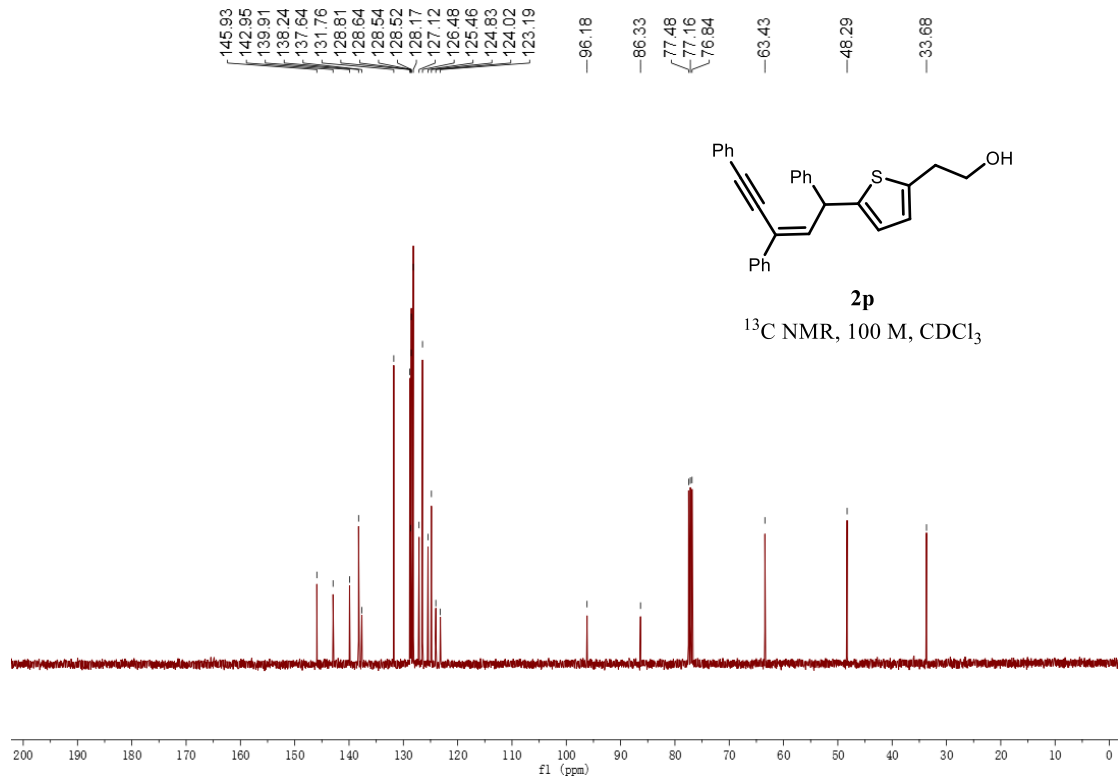
1: TOF MS ES+
1.71e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
413.1338	413.1340	-0.2	-0.5	17.5	19.6	n/a	n/a	C28 H22 Na S





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4255 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

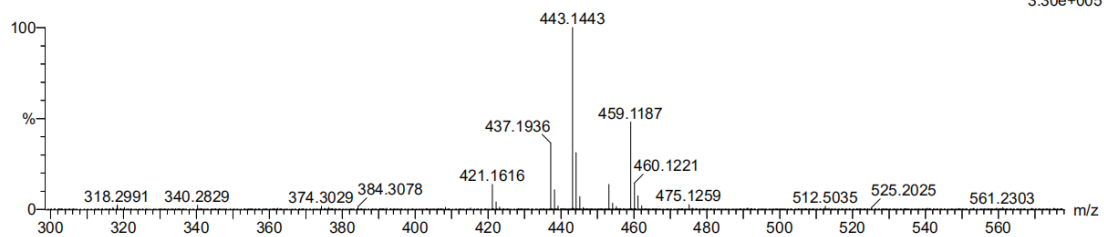
Elements Used:

C: 29-29 H: 24-24 N: 0-50 O: 0-50 Na: 0-3 S: 1-4

12

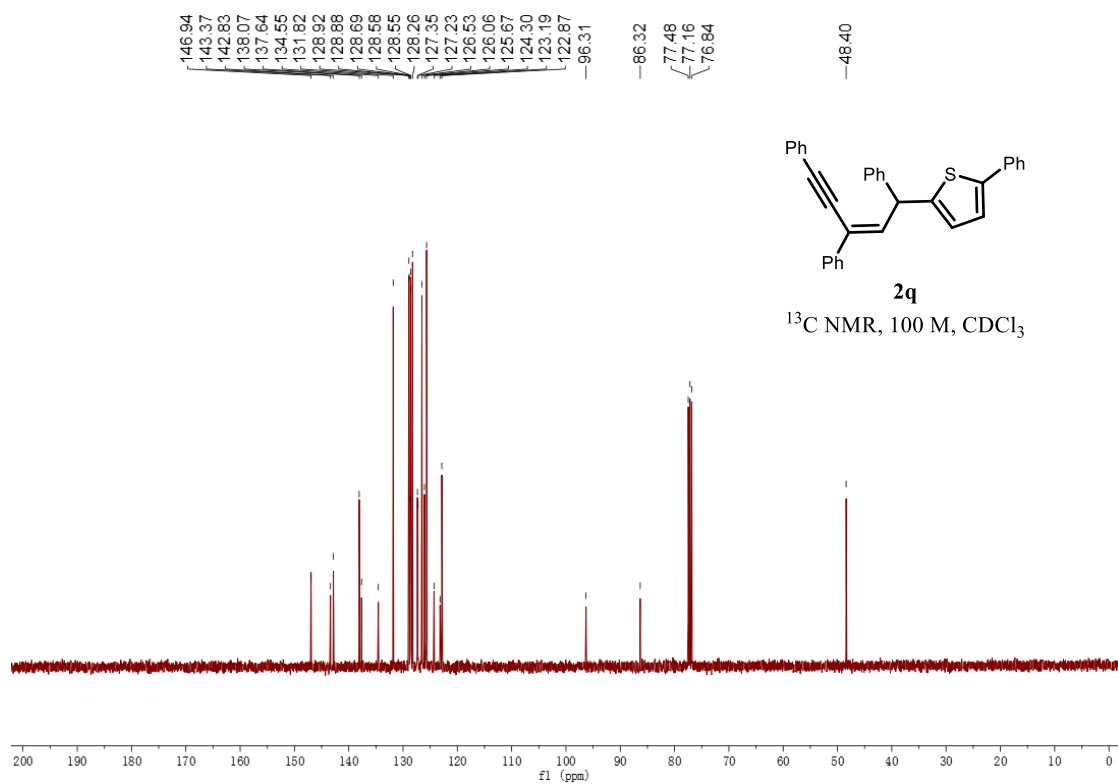
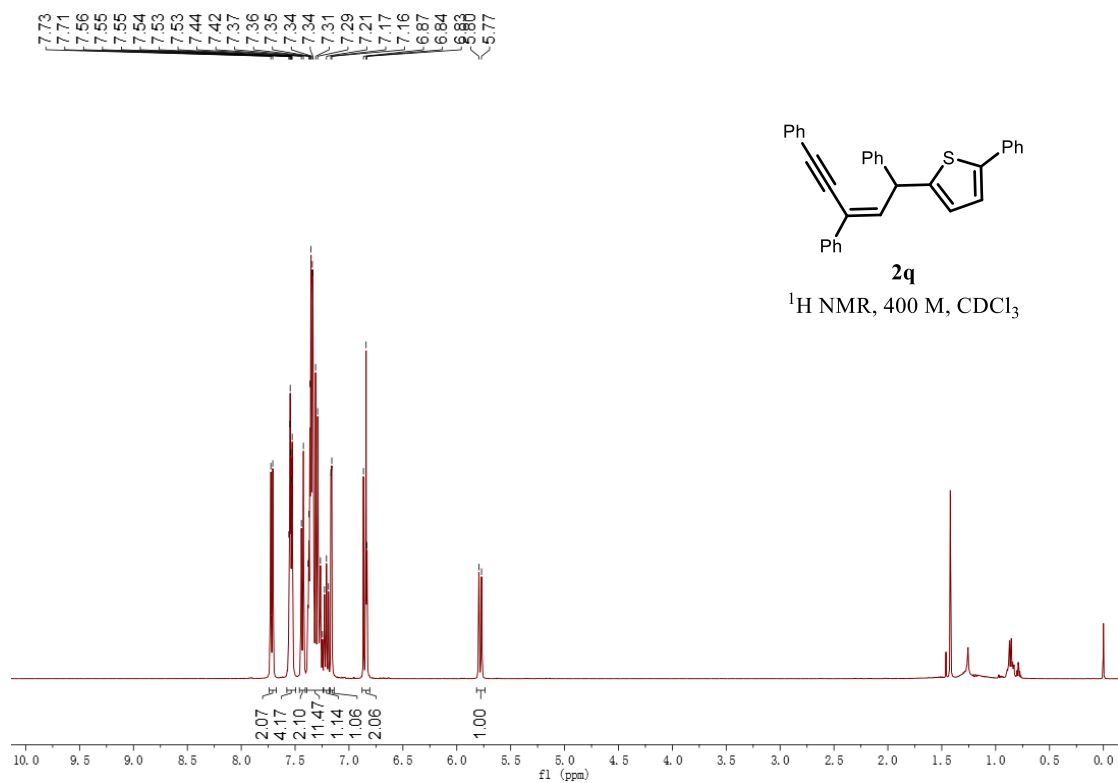
250115-20-728-3-YQZ-13 30 (0.082)

1: TOF MS ES+
3.30e+005



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
443.1443	443.1446	-0.3	-0.7	17.5	545.7	n/a	n/a	C ₂₉ H ₂₄ O Na S



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2117 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

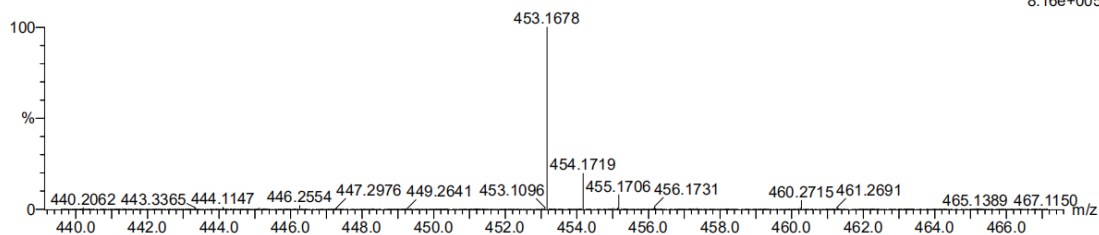
Elements Used:

C: 33-33 H: 25-25 N: 0-100 O: 0-100 Na: 0-2 S: 1-2

7

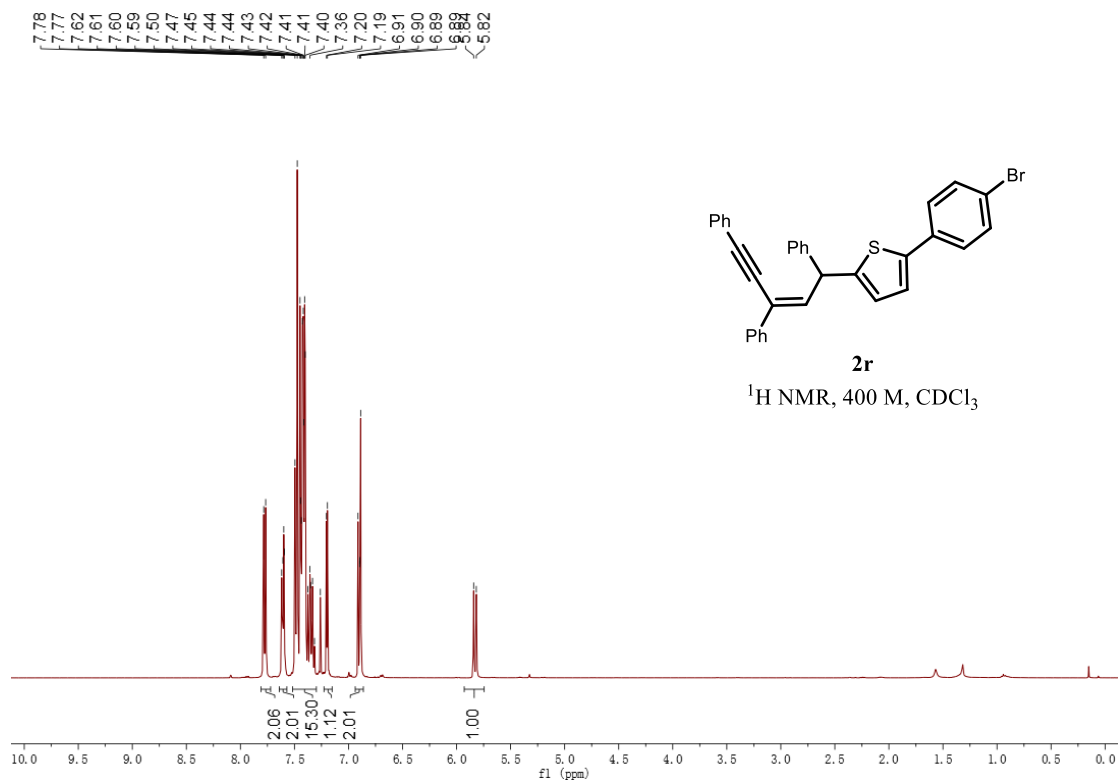
250403-12-761-2-YQZ-17 8 (0.092)

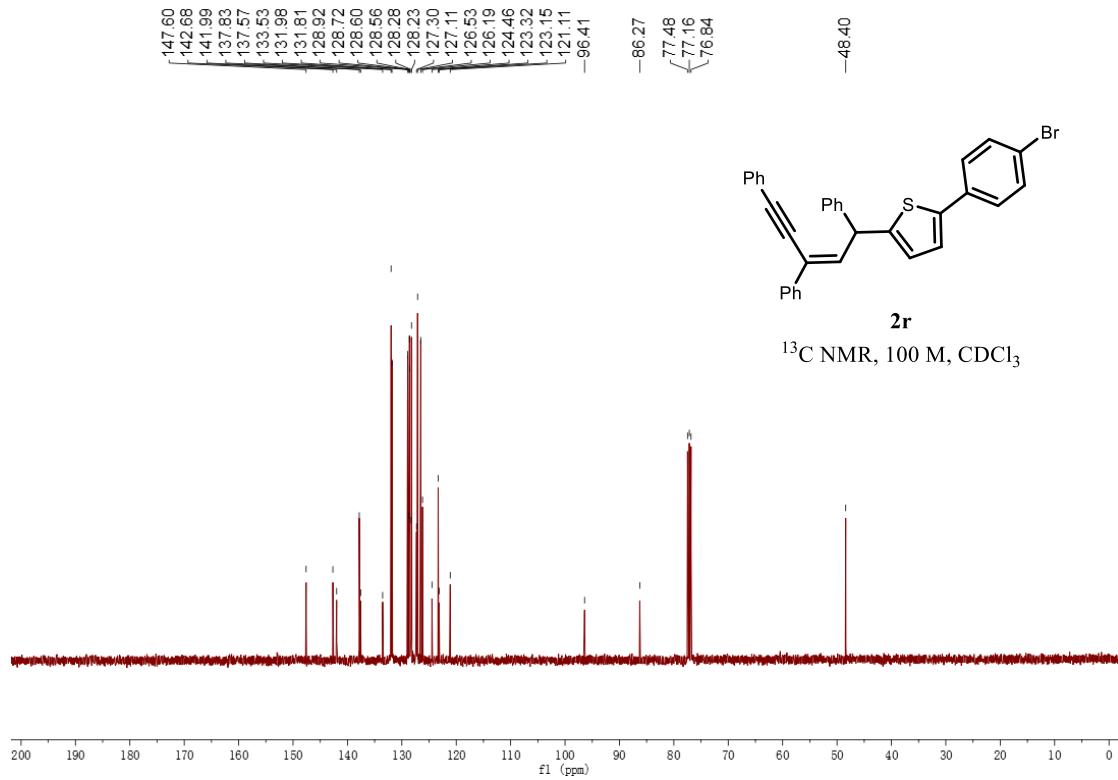
1: TOF MS ES+
8.16e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
453.1678	453.1677	0.1	0.2	21.5	934.0	n/a	n/a	C33 H25 S





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4583 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

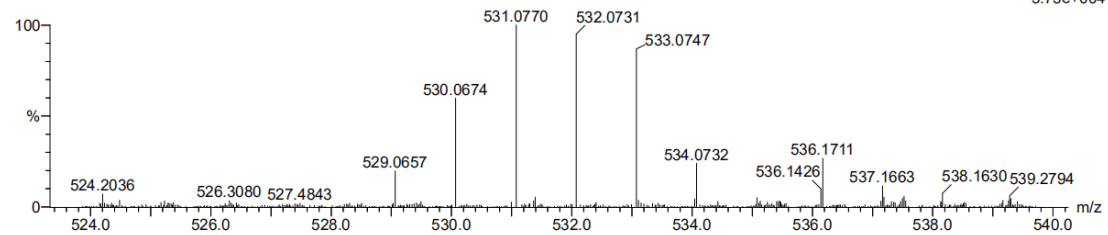
Elements Used:

C: 33-33 H: 24-24 N: 0-100 O: 0-100 Na: 0-2 S: 1-2 Br: 1-4

7

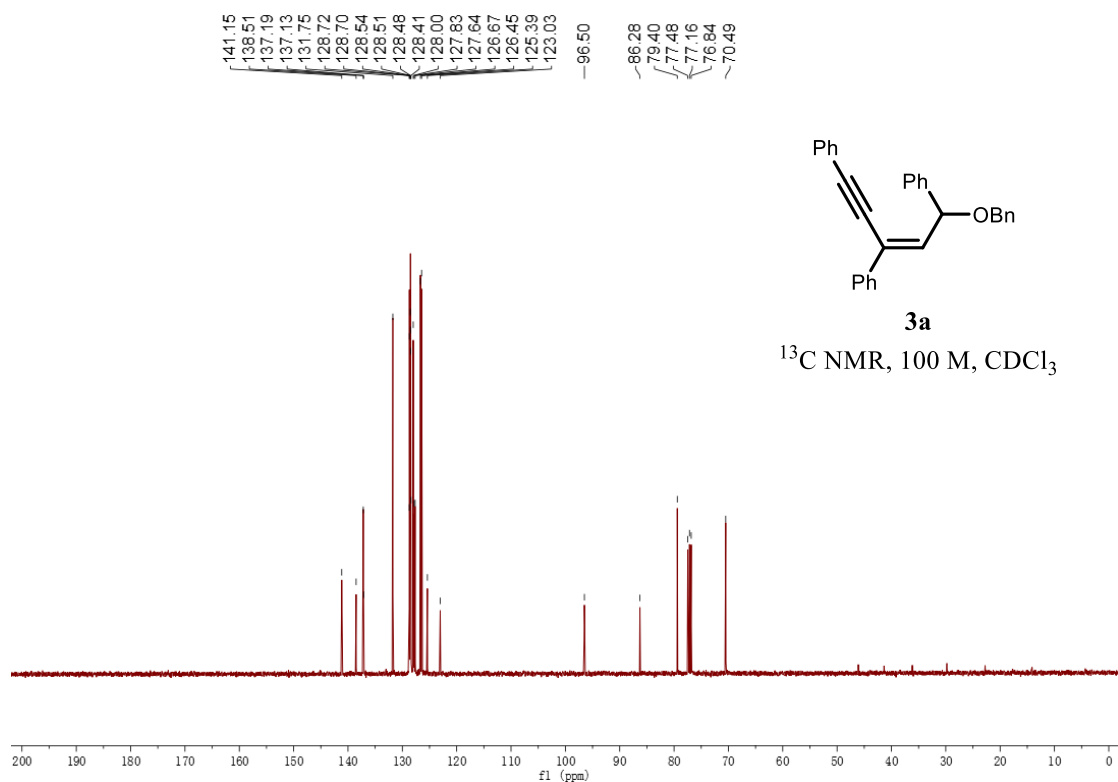
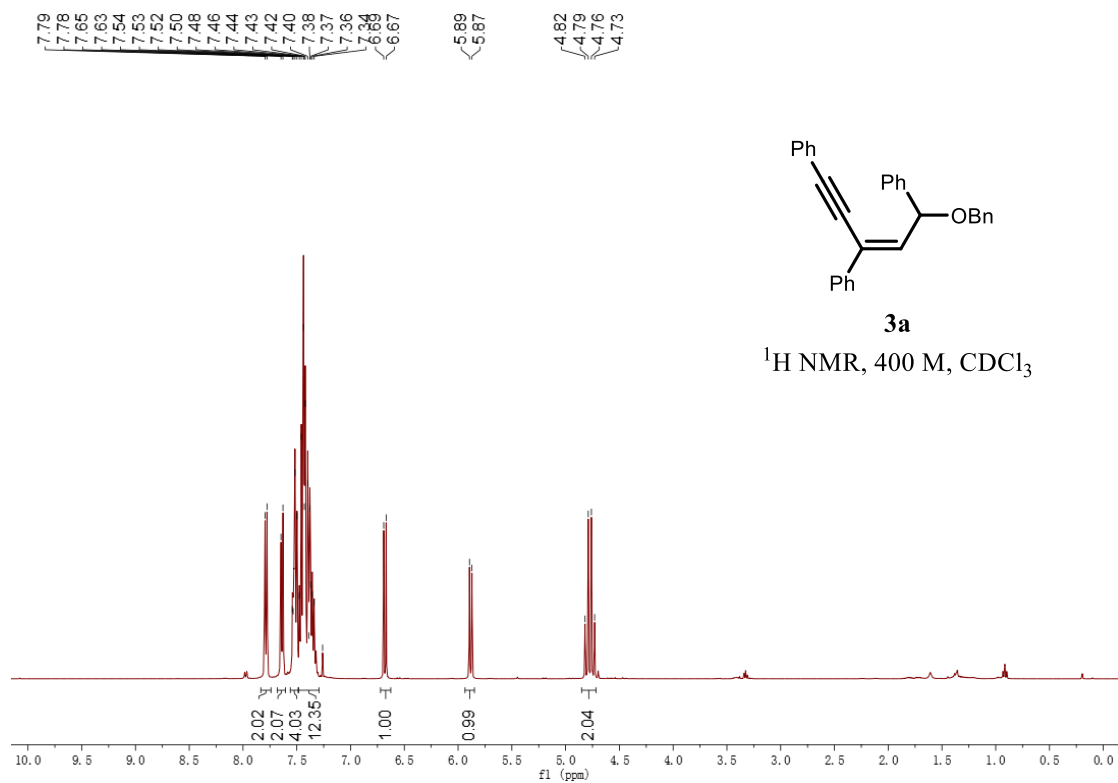
250403-12-761-2-YQZ-18 22 (0.218)

1: TOF MS ES+
3.73e+04



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
531.0770	531.0782	-1.2	-2.3	21.5	717.6	n/a	n/a	C ₃₃ H ₂₄ S Br



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1131 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

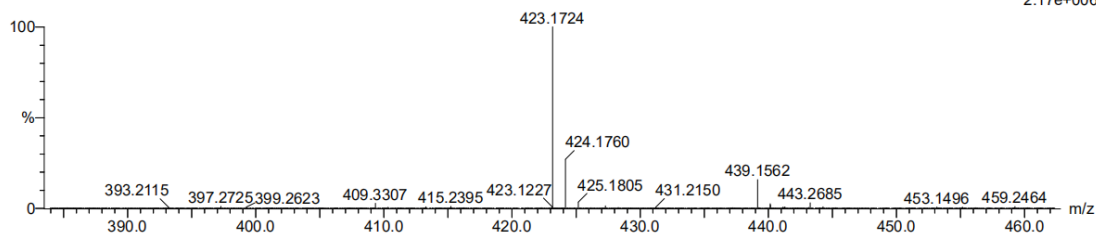
Elements Used:

C: 30-30 H: 24-24 N: 0-100 O: 0-100 Na: 0-2

7

250403-12-761-2-YQZ-19 21 (0.210)

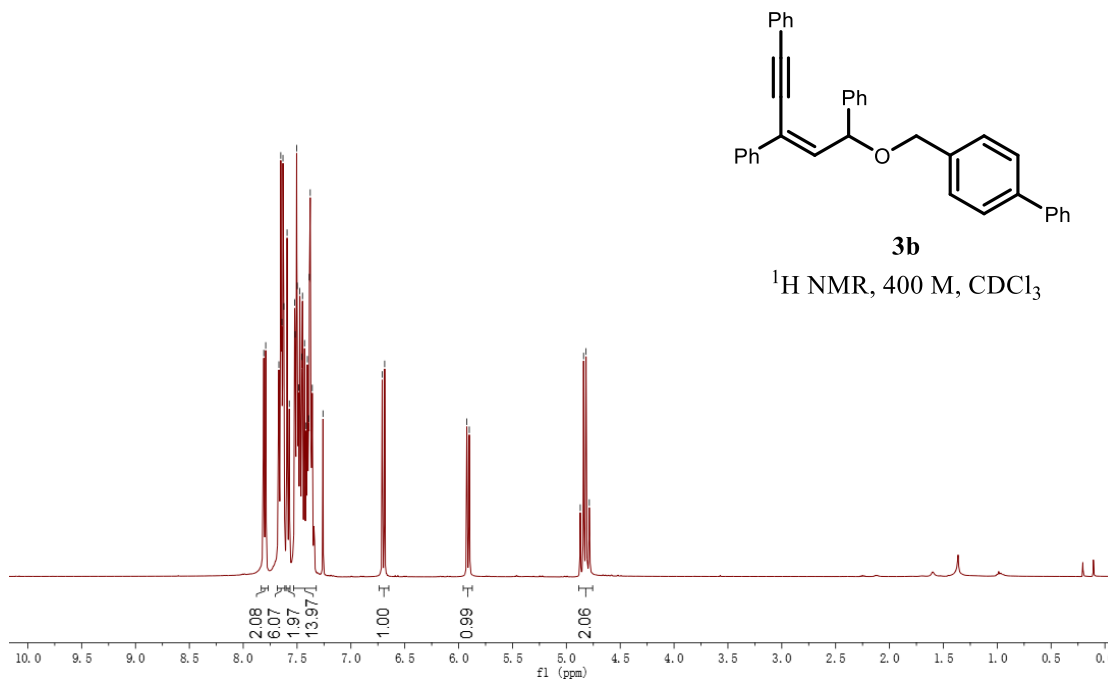
1: TOF MS ES+
2.17e+006

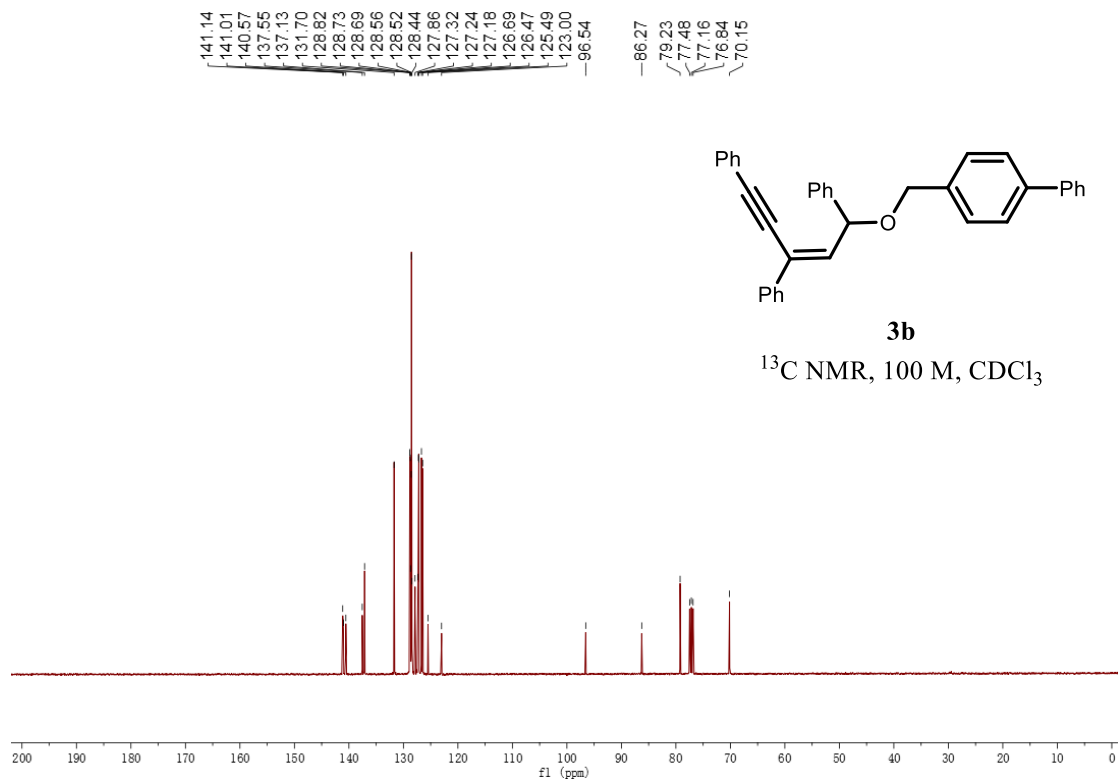


Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
423.1724	423.1725	-0.1	-0.2	18.5	981.1	n/a	n/a	C30 H24 O Na

7.81, 7.79, 7.76, 7.65, 7.64, 7.63, 7.62, 7.59, 7.56, 7.52, 7.50, 7.50, 7.47, 7.45, 7.45, 7.43, 7.40, 7.39, 6.98, 6.89, 5.92, 5.90, 4.87, 4.84, 4.82, 4.79





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1590 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

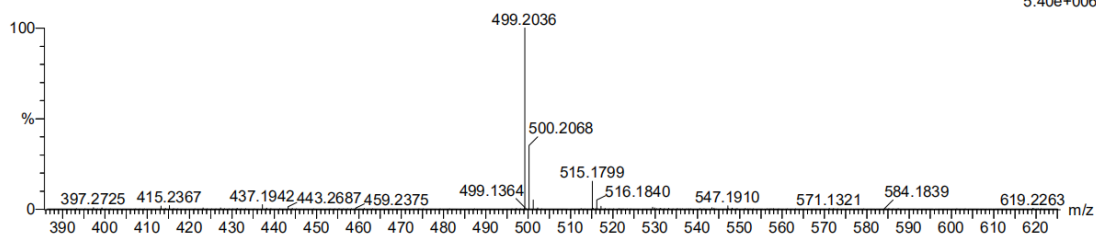
Elements Used:

C: 36-36 H: 28-28 N: 0-100 O: 0-100 Na: 0-2

7

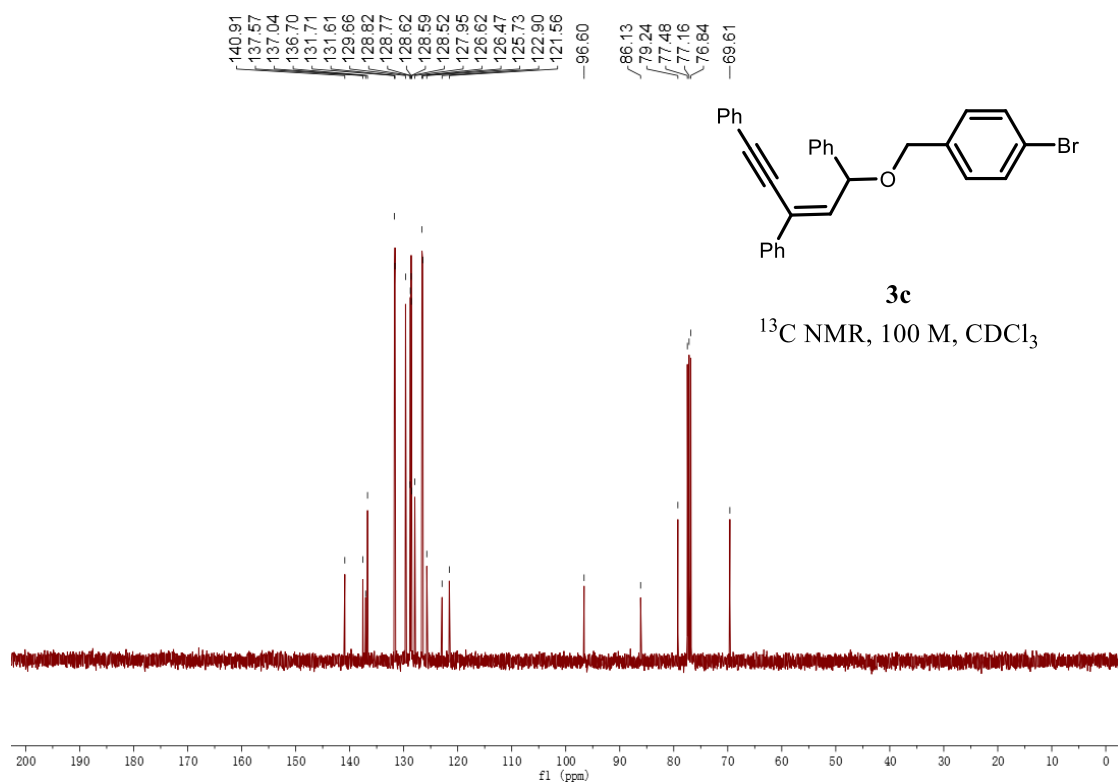
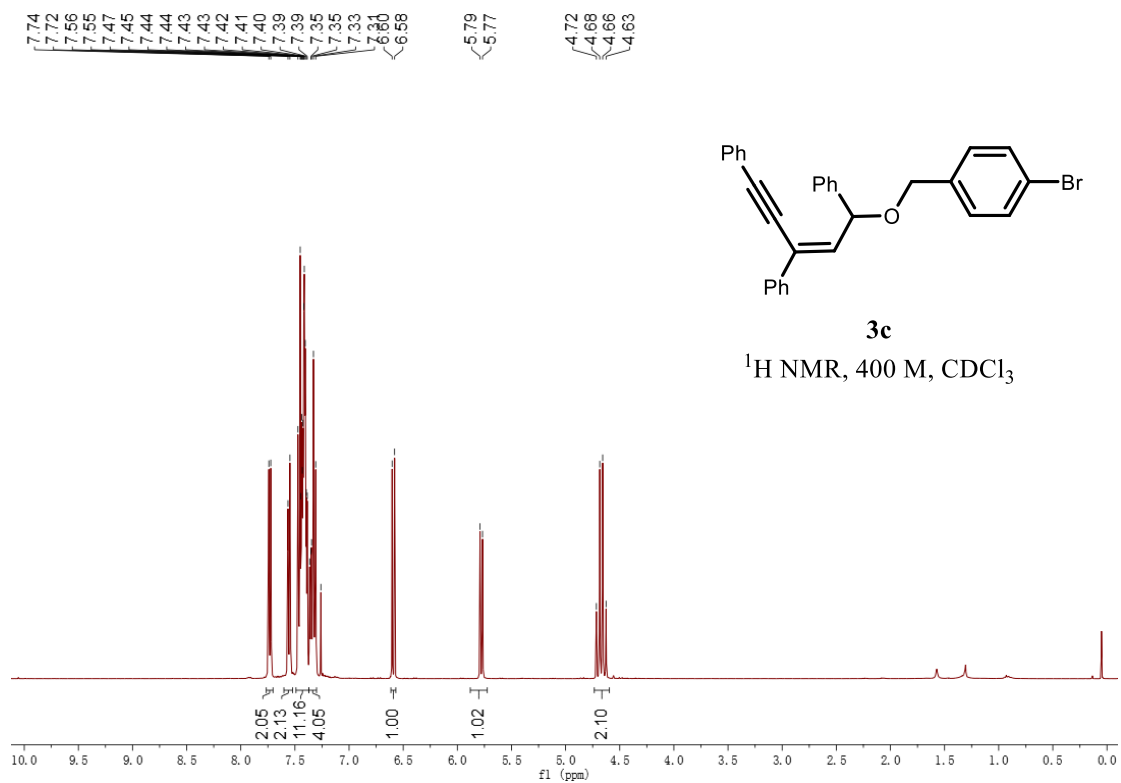
250403-12-761-2-YQZ-20 16 (0.161)

1: TOF MS ES+
5.40e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
499.2036	499.2038	-0.2	-0.4	22.5	1045.9	n/a	n/a	C ₃₆ H ₂₈ O Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

37 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

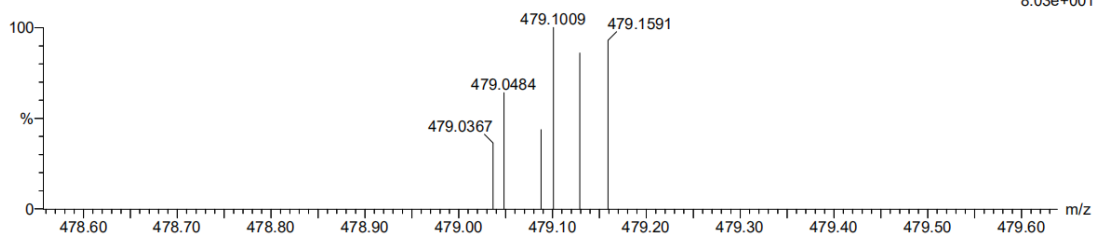
Elements Used:

C: 14-31 H: 1-60 O: 1-3 Br: 1-3

48

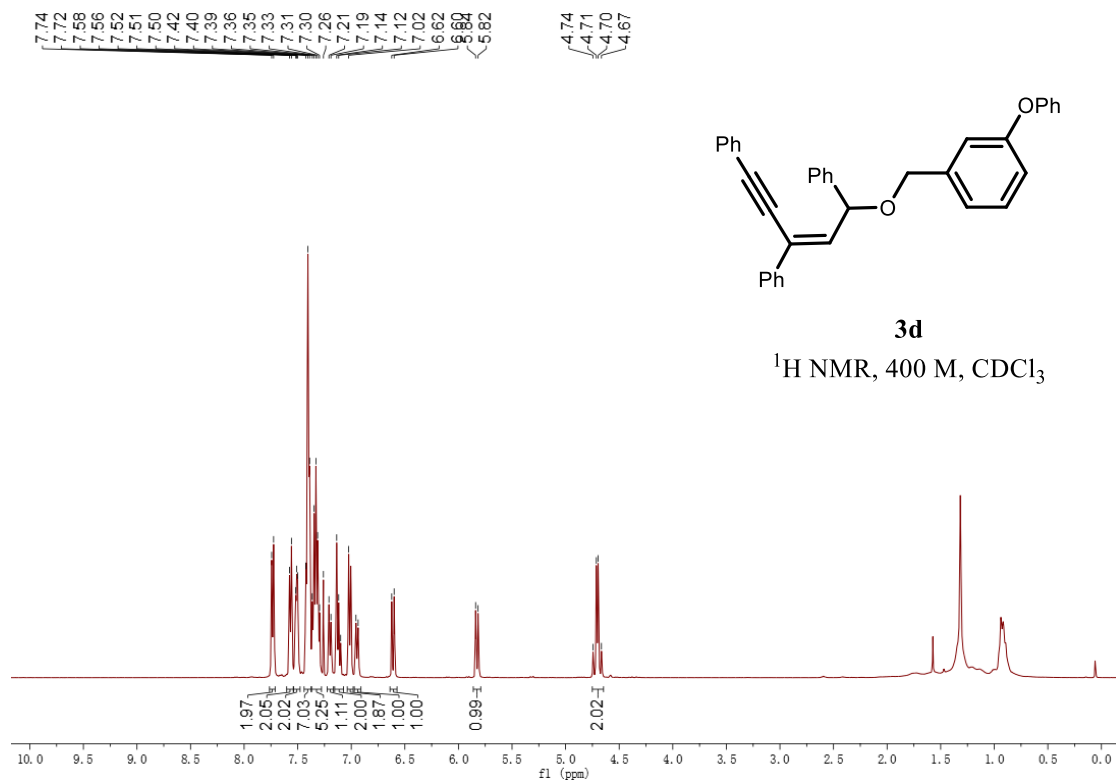
250511-2-57 34 (0.325)

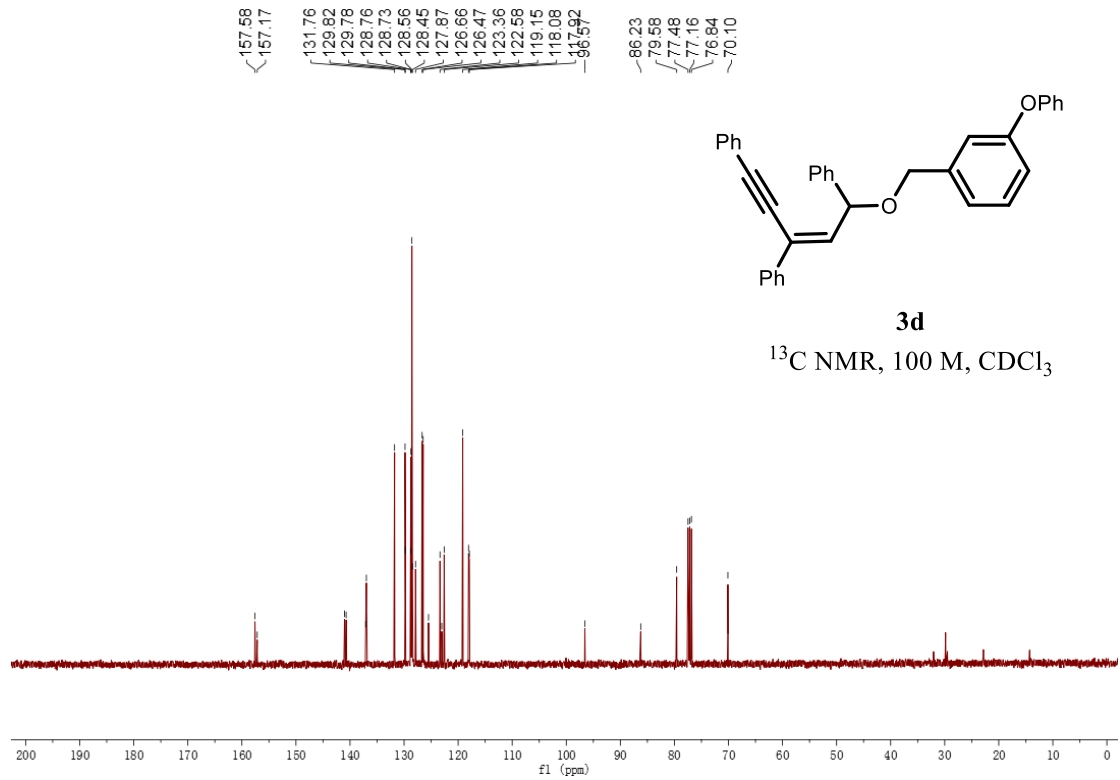
1: TOF MS ES+
8.03e+001



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
479.1009	479.1011	-0.2	-0.4	18.5	35.9	n/a	n/a	C30 H24 O Br





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1681 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

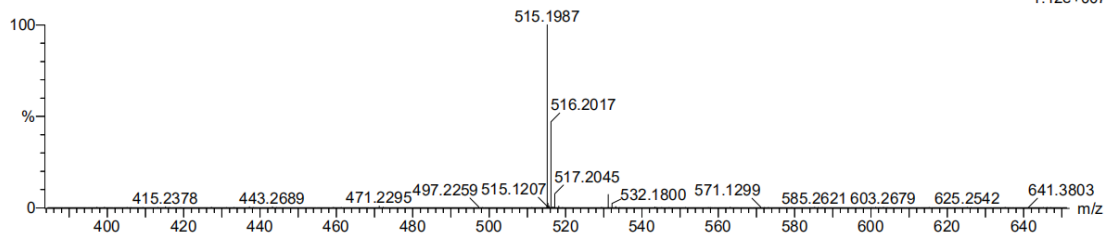
Elements Used:

C: 36-36 H: 28-28 N: 0-100 O: 0-100 Na: 0-2

7

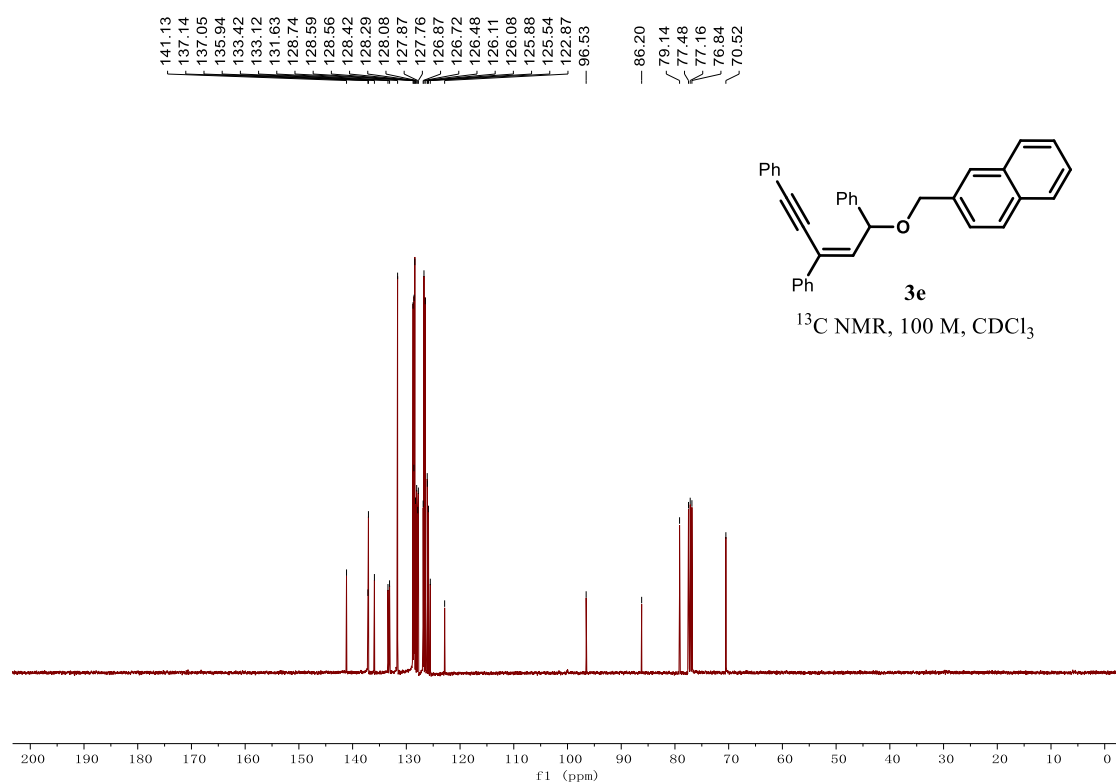
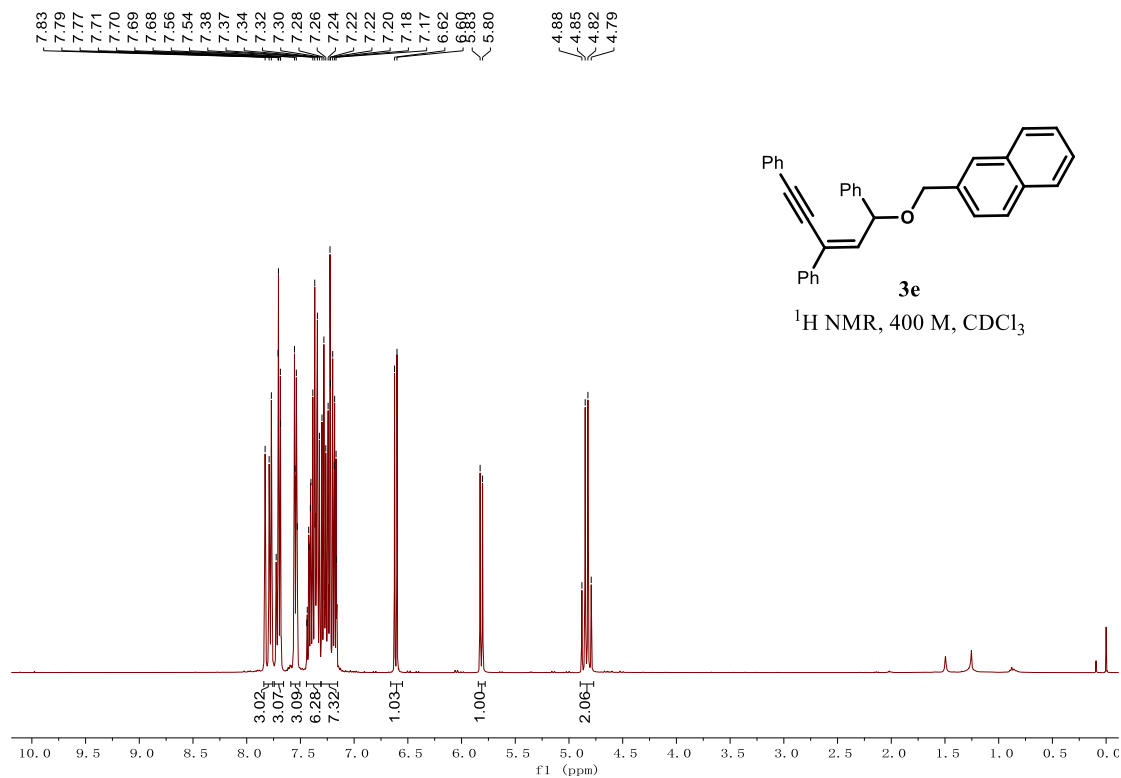
250403-12-761-2-YQZ-23 17 (0.169)

1: TOF MS ES+
1.12e+007



Minimum: -1.5
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
515.1987	515.1987	0.0	0.0	22.5	965.1	n/a	n/a	C ₃₆ H ₂₈ O ₂ Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1424 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

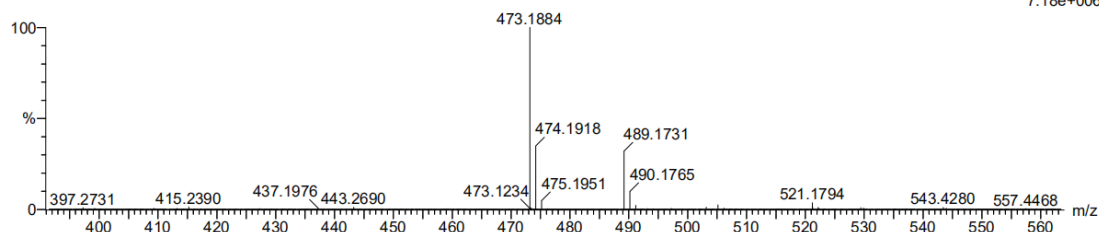
Elements Used:

C: 34-34 H: 26-26 N: 0-100 O: 0-100 Na: 0-2

7

250403-12-761-2-YQZ-21 17 (0.169)

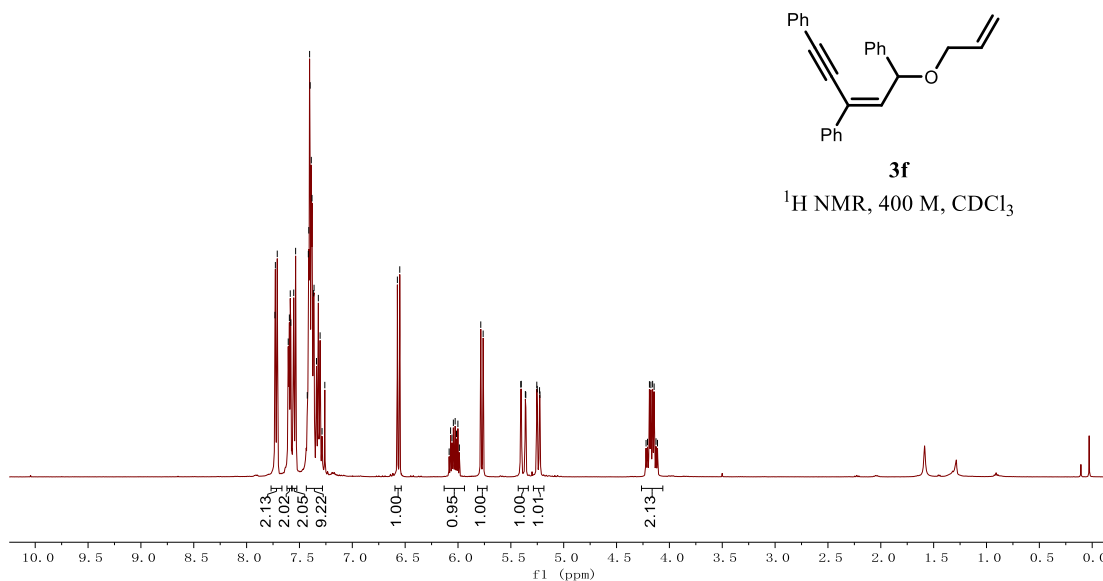
1: TOF MS ES+
7.18e+006

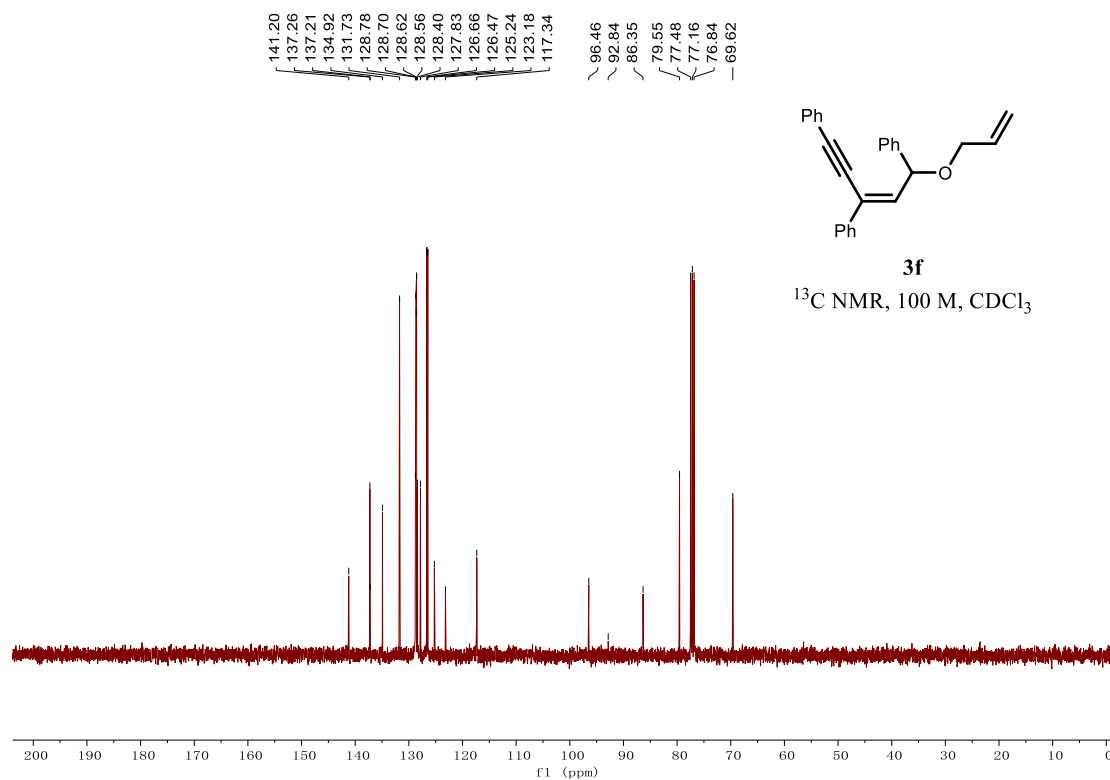


Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
473.1884	473.1881	0.3	0.6	21.5	1030.1	n/a	n/a	C34 H26 O Na

7.73
7.73
7.71
7.61
7.60
7.59
7.58
7.55
7.54
7.42
7.41
7.40
7.39
7.39
7.38
7.37
7.36
7.34
7.32
7.30
6.89
6.85
6.08
6.07
6.06
6.04
6.03
6.01
6.00
5.99
5.78
5.76
5.41
5.40
5.36
5.36
5.25
5.25
5.23
5.22
4.22
4.21
4.19
4.18
4.16
4.14
4.13
4.11





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

871 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

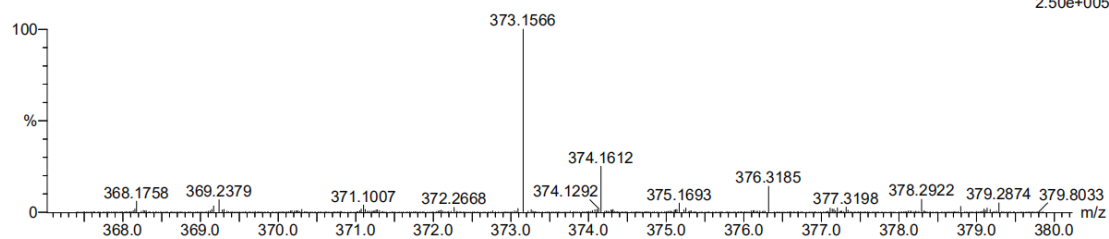
Elements Used:

C: 26-26 H: 22-22 N: 0-100 O: 0-100 Na: 0-2

7

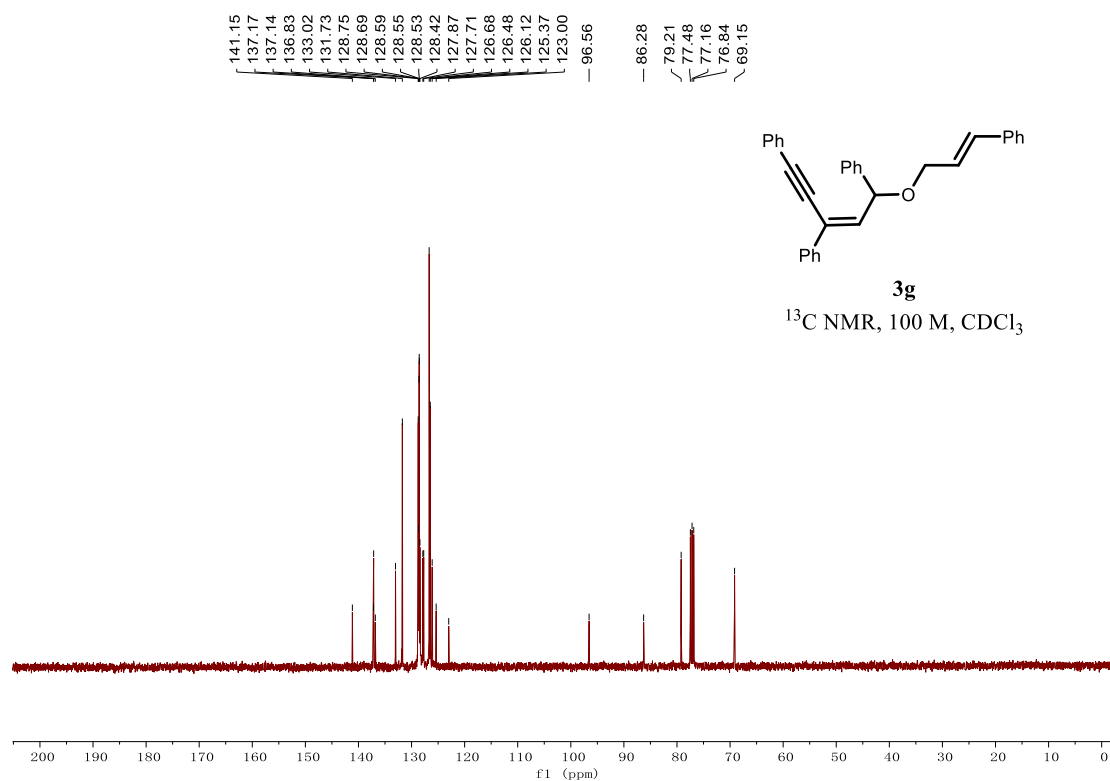
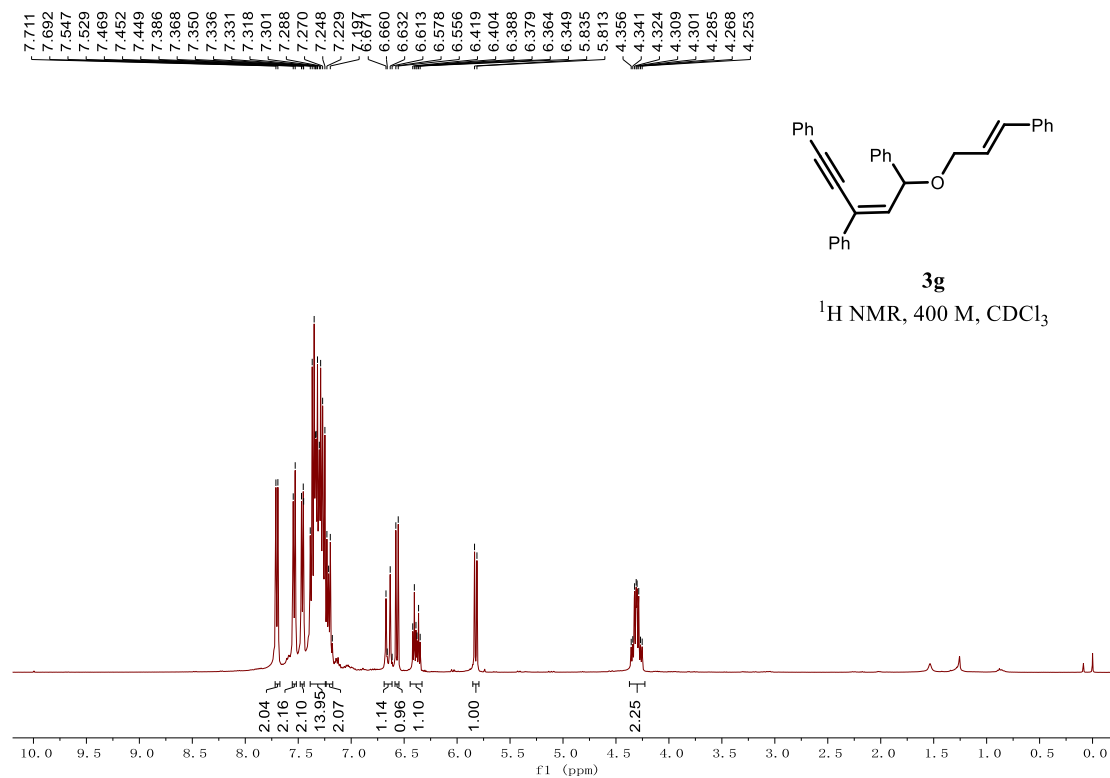
250403-12-761-2-YQZ-26 15 (0.152)

1: TOF MS ES+
2.50e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
373.1566	373.1568	-0.2	-0.5	15.5	1228.4	n/a	n/a	C ₂₆ H ₂₂ O Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1279 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

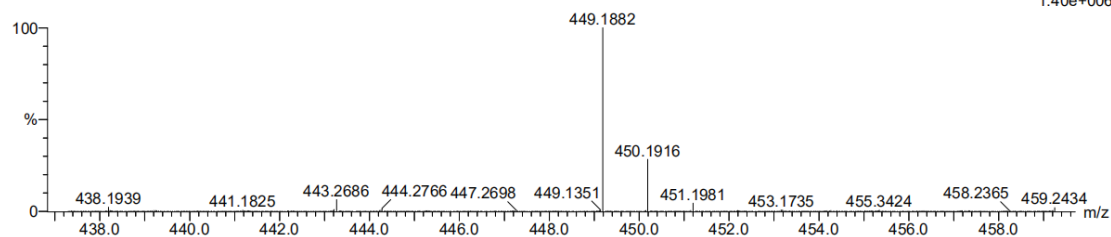
Elements Used:

C: 32-32 H: 26-26 N: 0-100 O: 0-100 Na: 0-2

7

250403-12-761-2-YQZ-15 17 (0.169)

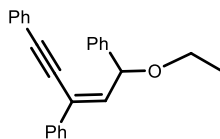
1: TOF MS ES+
1.40e+006



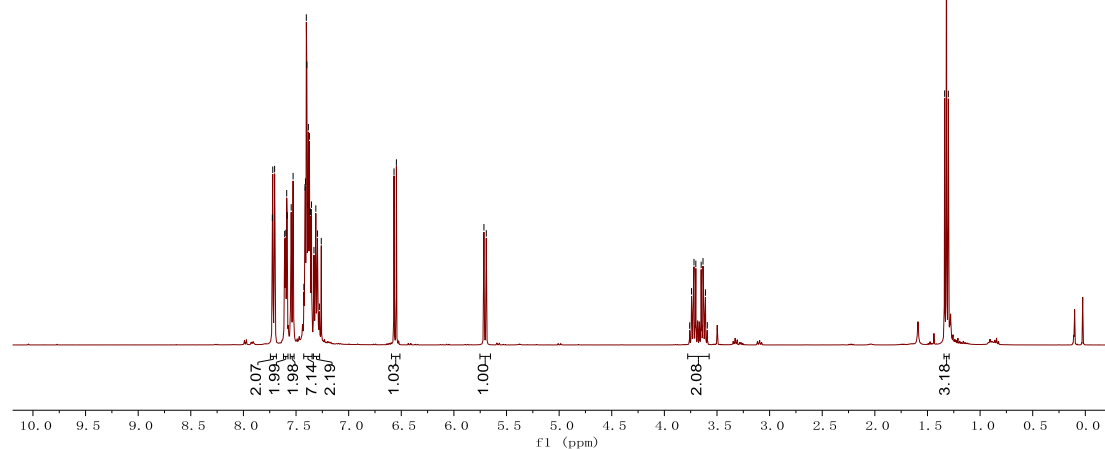
Minimum: -1.5
Maximum: 5.0 10.0 50.0

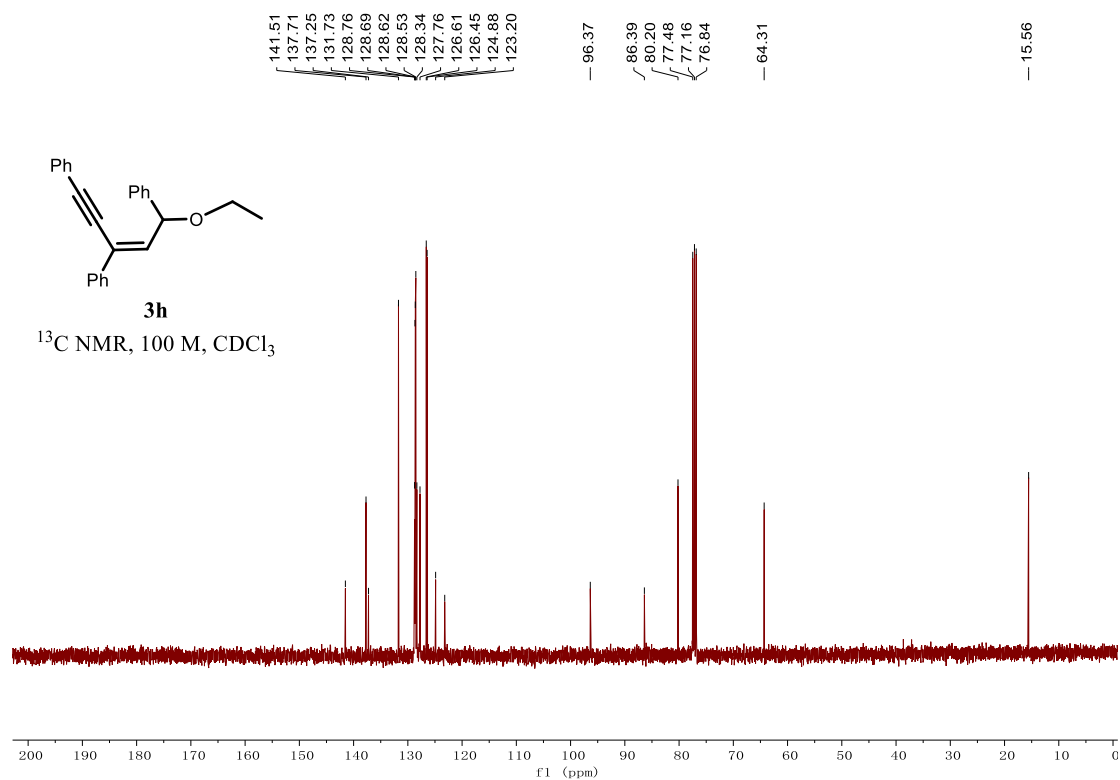
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
449.1882	449.1881	0.1	0.2	19.5	963.7	n/a	n/a	C32 H26 O Na

7.72 7.70 7.60 7.59 7.58 7.55 7.53 7.42 7.41 7.40 7.39 7.38 7.37 7.36 7.35 7.31 6.55 5.71 5.69 3.76 3.74 3.72 3.70 3.65 3.63 3.61 3.59 1.34 1.32 1.30



¹H NMR, 400 M, CDCl₃





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

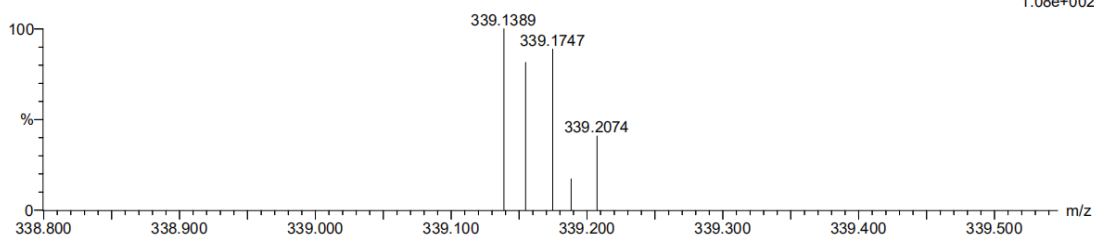
Elements Used:

C: 25-31 H: 1-60 O: 1-12

48

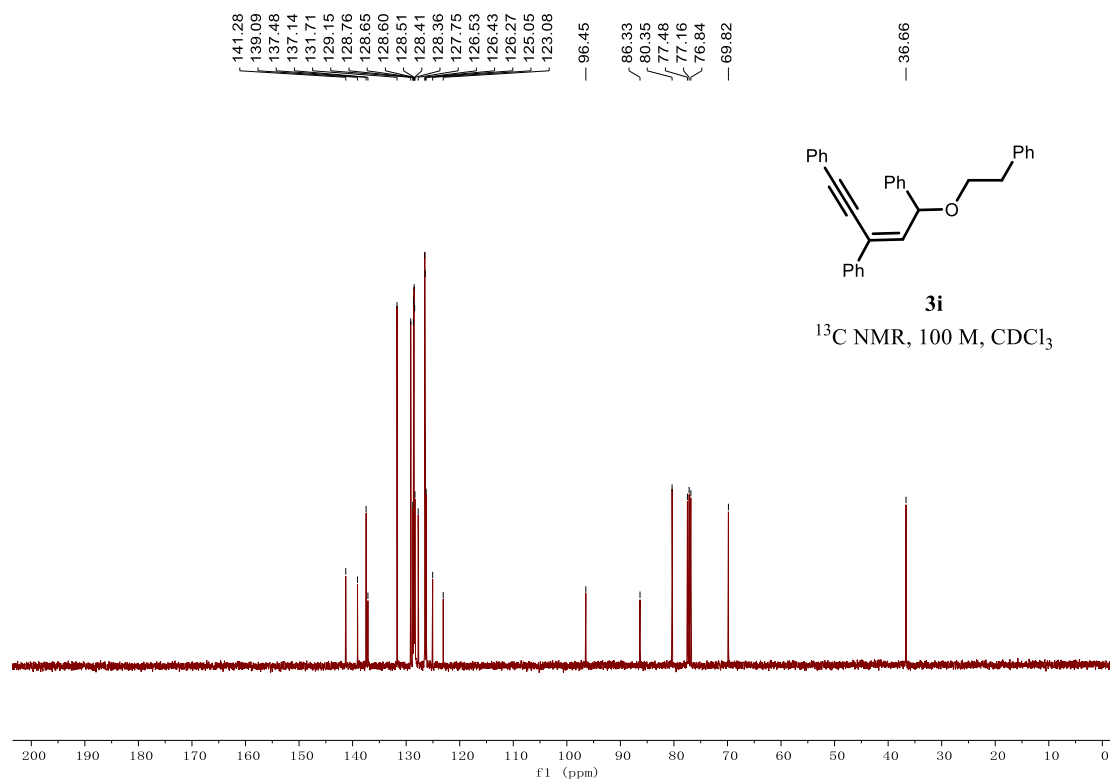
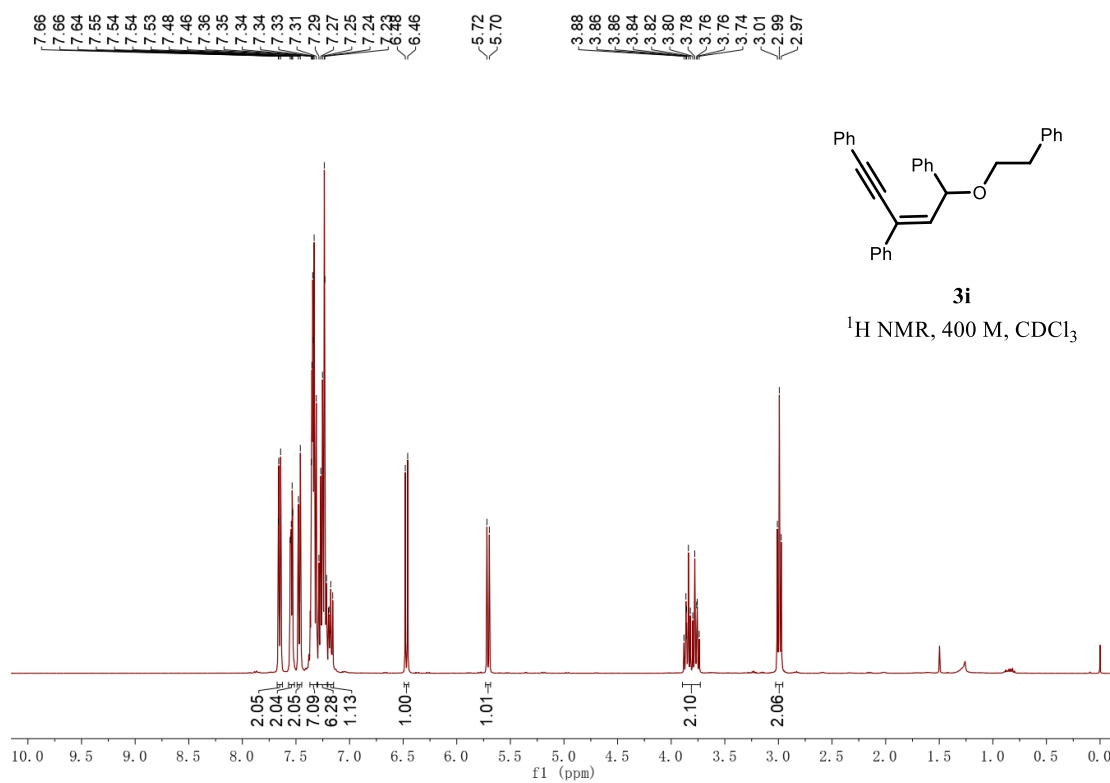
250511-2-55 52 (0.487)

1: TOF MS ES+
1.08e+002



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
339.1747	339.1749	-0.2	-0.6	14.5	31.4	n/a	n/a	C ₂₅ H ₂₃ O



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1208 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

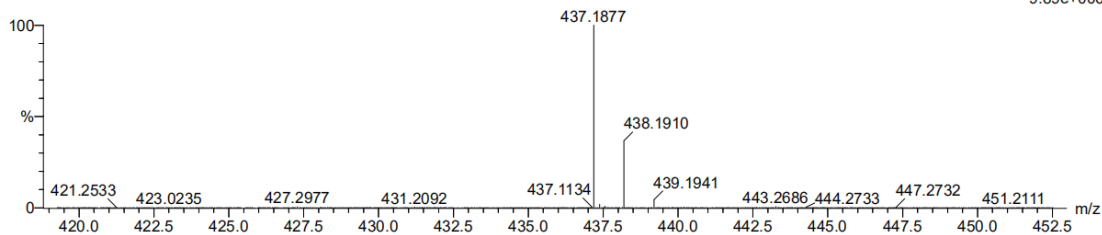
Elements Used:

C: 31-31 H: 26-26 N: 0-100 O: 0-100 Na: 0-2

7

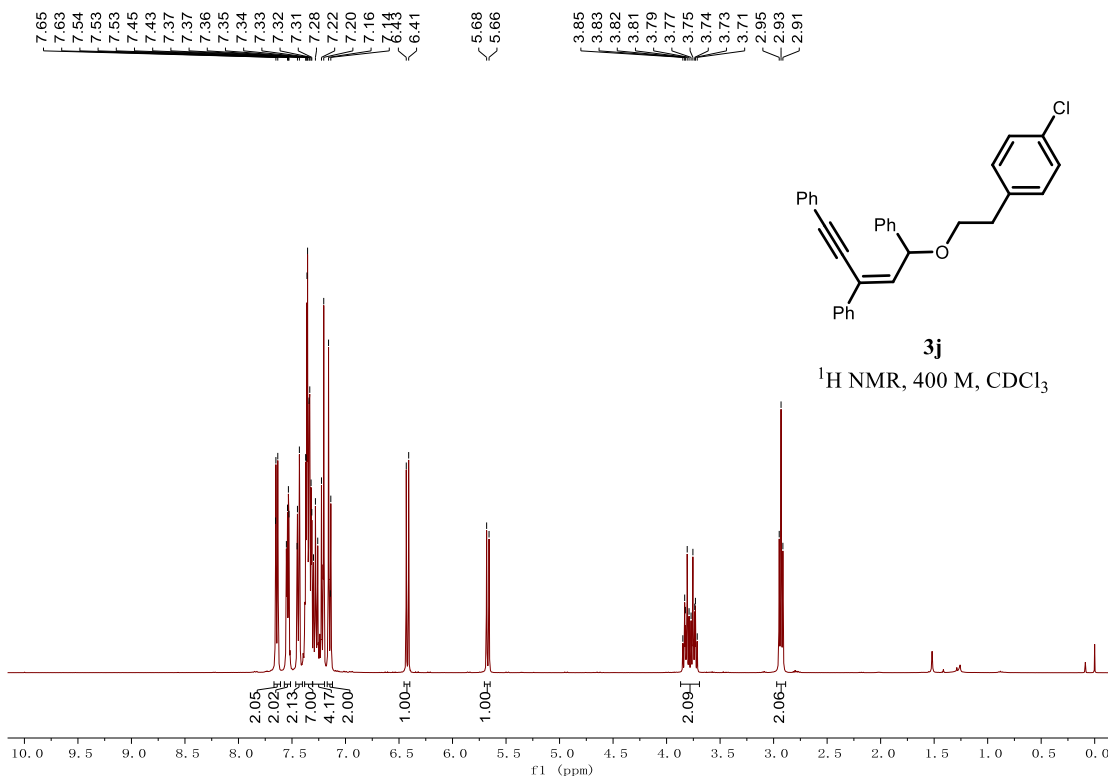
250403-12-761-2-YQZ-14 15 (0.152)

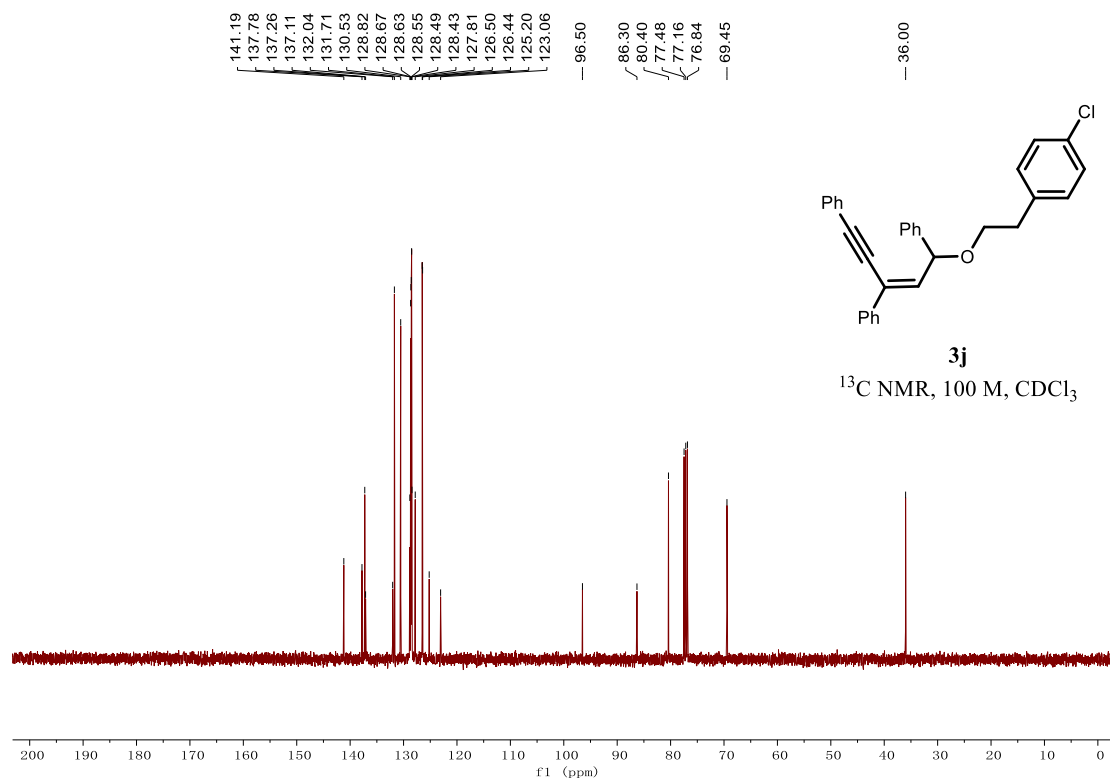
1: TOF MS ES+
9.89e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
437.1877	437.1881	-0.4	-0.9	18.5	1058.8	n/a	n/a	C31 H26 O Na





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

3802 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

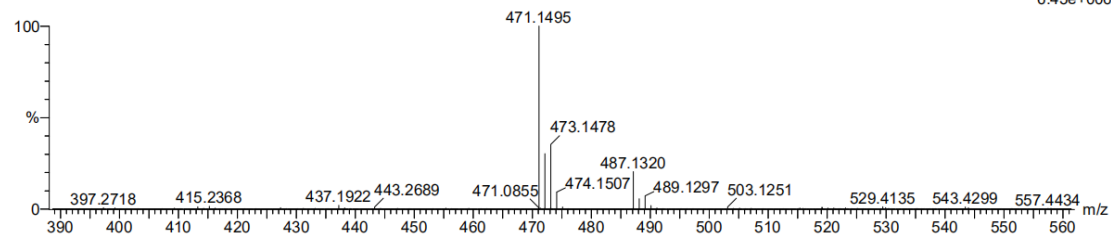
Elements Used:

C: 31-31 H: 25-25 N: 0-100 O: 0-100 Na: 0-2 Cl: 1-4

7

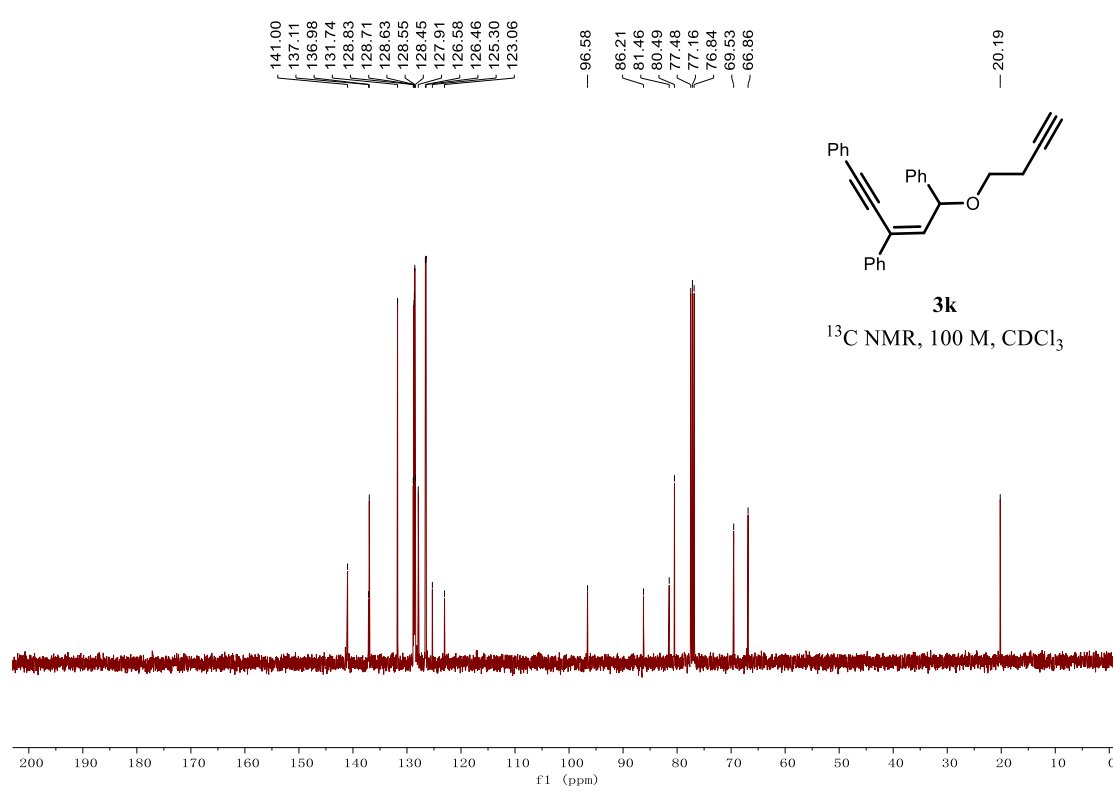
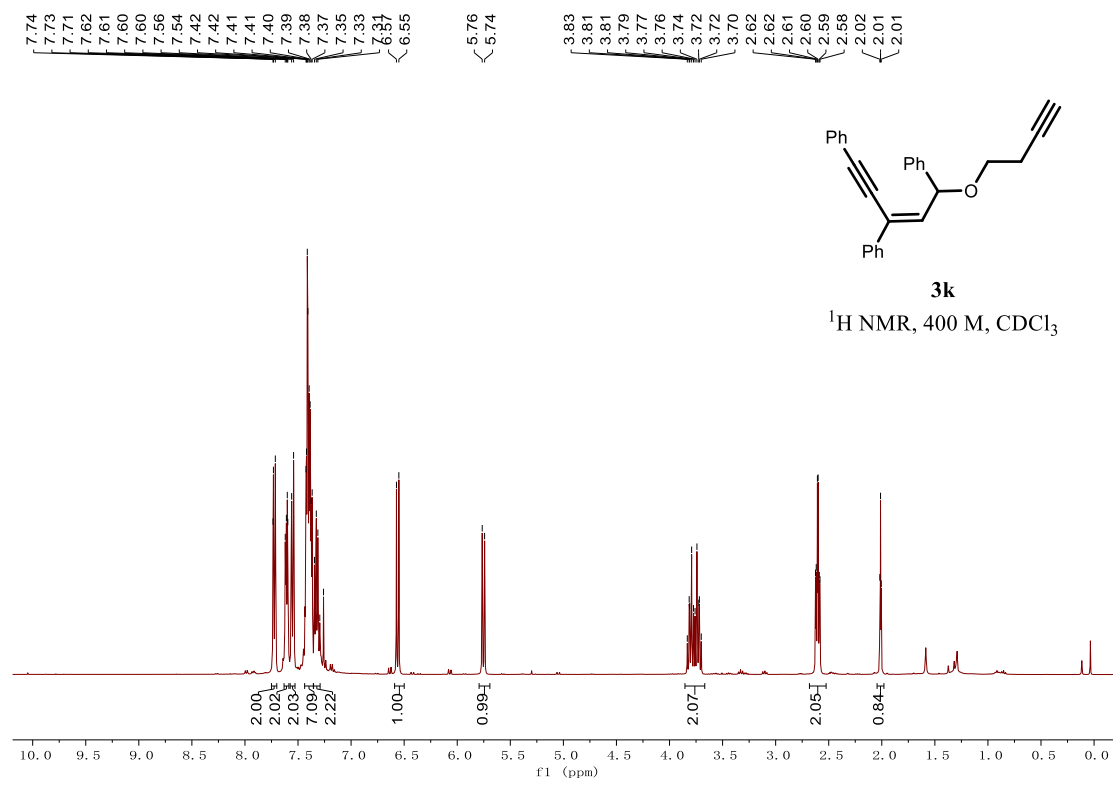
250403-12-761-2-YQZ-28 16 (0.161)

1: TOF MS ES+
6.45e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
471.1495	471.1492	0.3	0.6	18.5	1027.5	n/a	n/a	C31 H25 O Na Cl



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

14 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

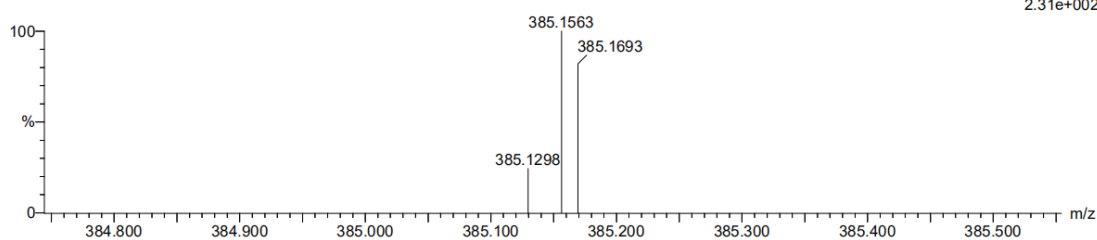
Elements Used:

C: 14-27 H: 1-60 O: 1-3 Na: 1-1

48

250511-2-53 4 (0.059)

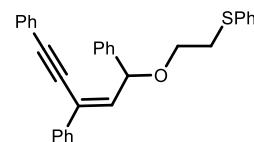
1: TOF MS ES+
2.31e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

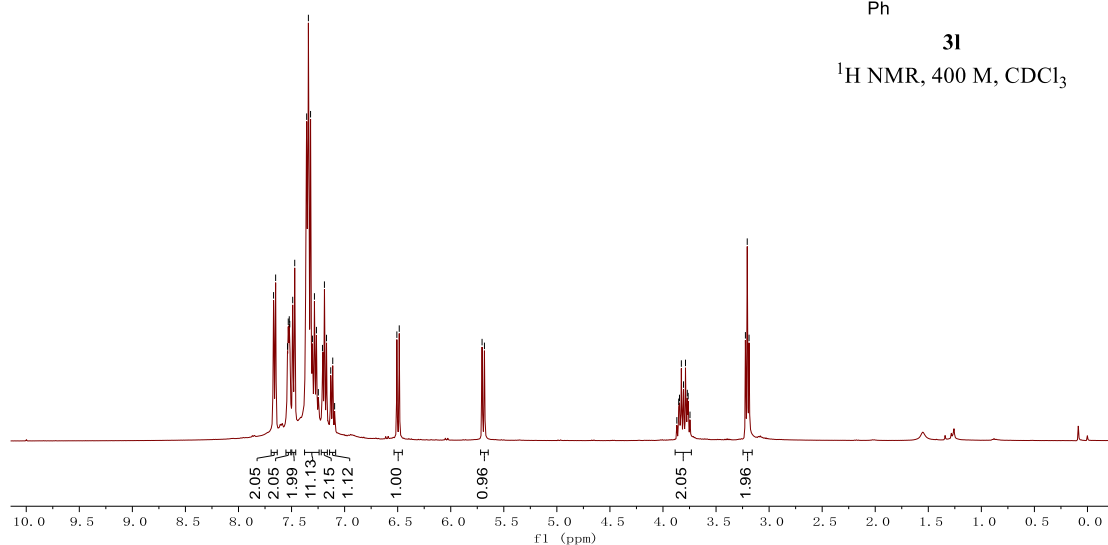
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
385.1563	385.1568	-0.5	-1.3	16.5	30.9	n/a	n/a	C27 H22 O Na

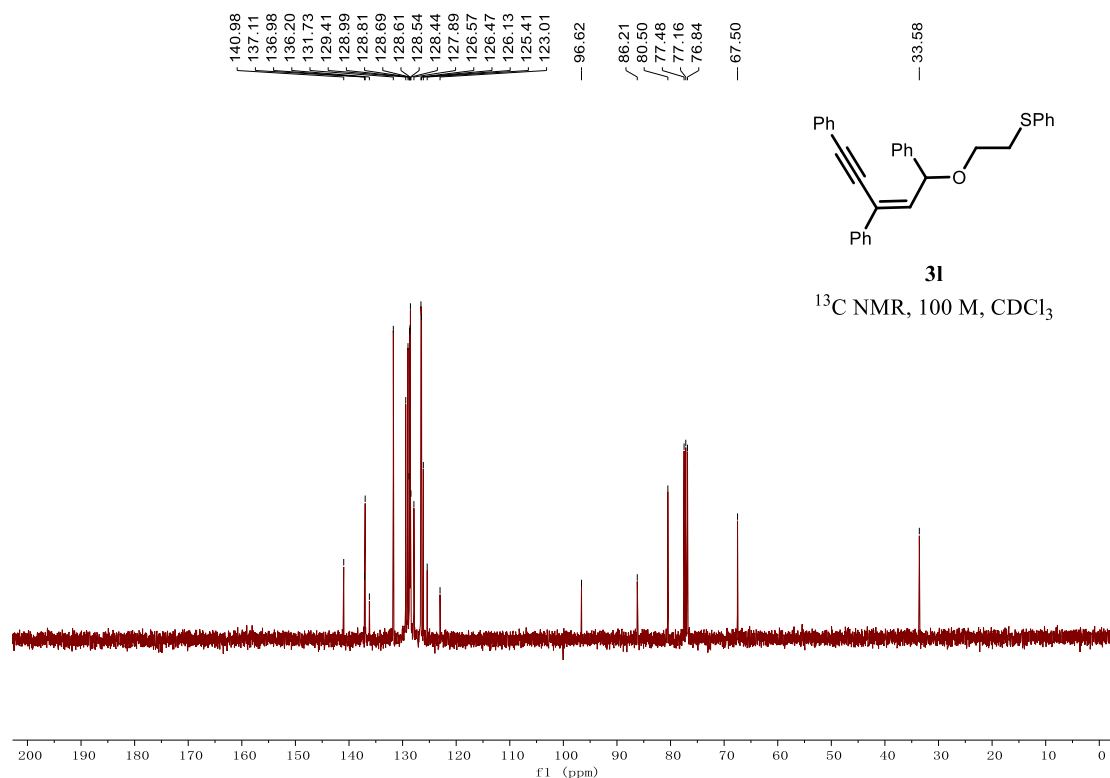
7.67, 7.65, 7.54, 7.53, 7.52, 7.49, 7.47, 7.36, 7.34, 7.32, 7.30, 7.28, 7.27, 7.25, 7.21, 7.19, 7.17, 7.13, 6.41, 6.49, 5.70, 5.68, 3.87, 3.85, 3.84, 3.83, 3.81, 3.79, 3.77, 3.76, 3.75, 3.22, 3.21, 3.19



31

¹H NMR, 400 M, CDCl₃





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

22 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

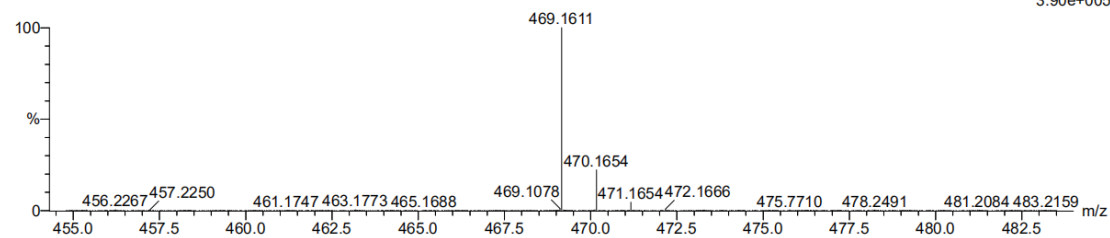
Elements Used:

C: 31-31 H: 1-60 O: 1-12 S: 1-2 Na: 1-1

48

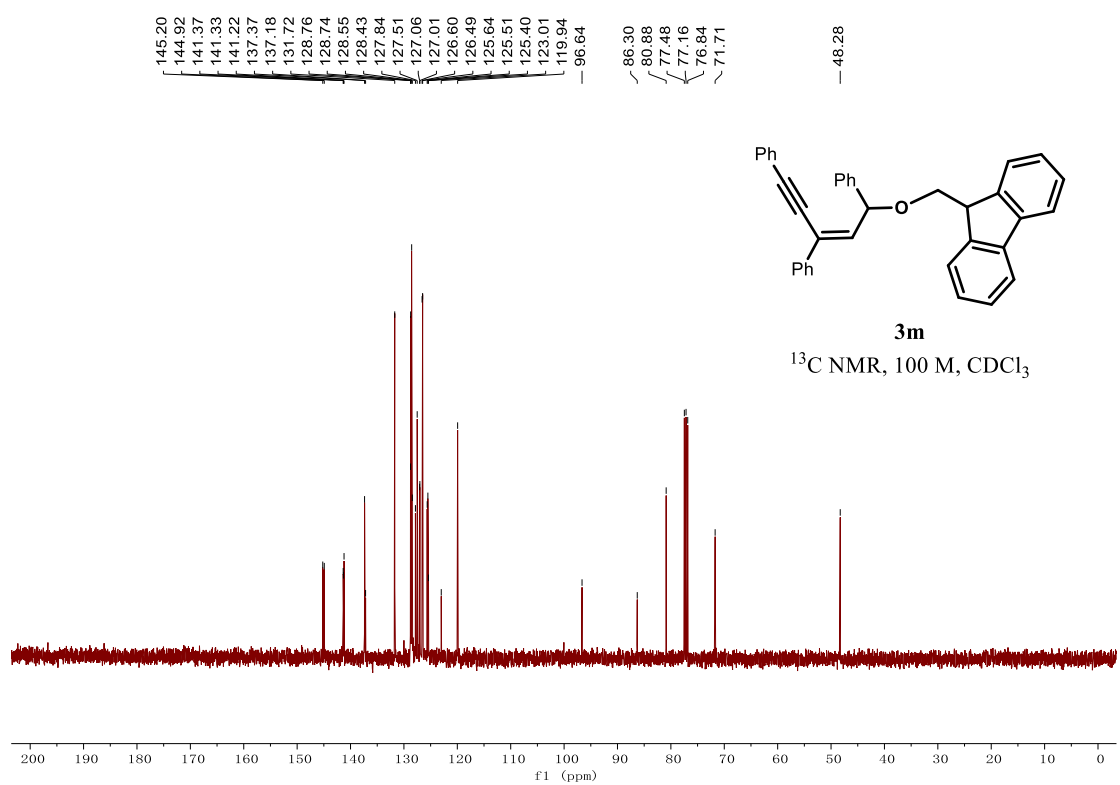
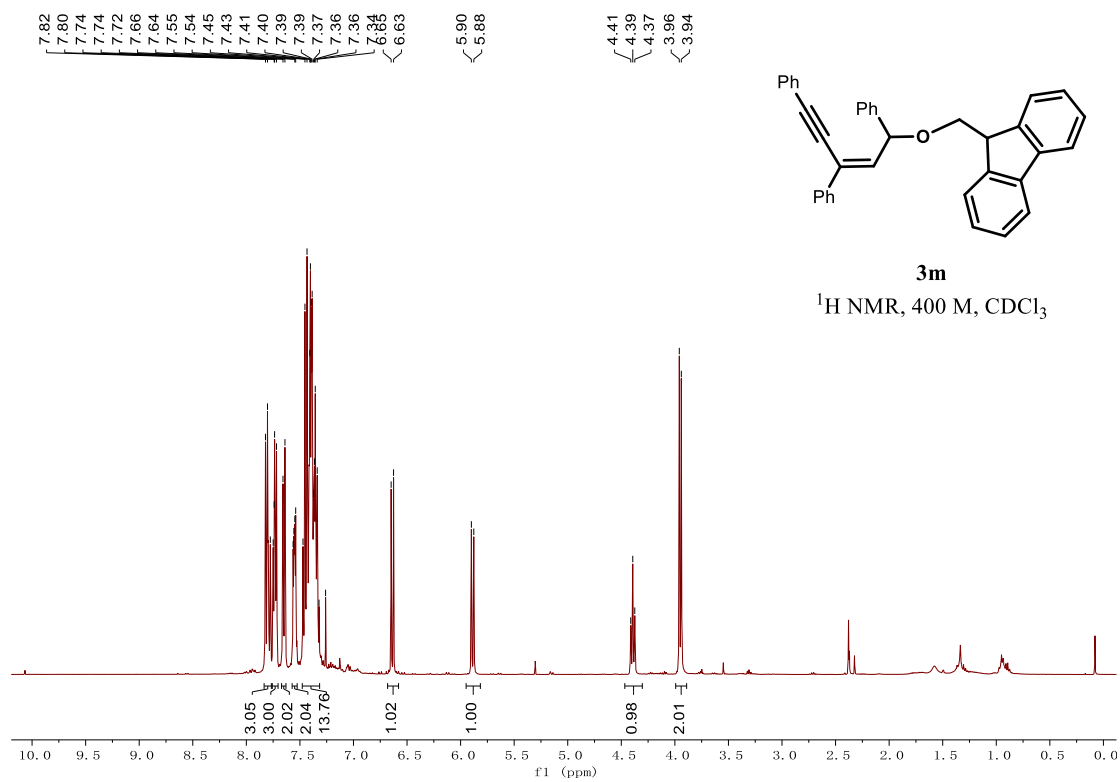
250511-2-59 16 (0.162)

1: TOF MS ES+
3.90e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
469.1611	469.1602	0.9	1.9	18.5	768.5	n/a	n/a	C ₃₁ H ₂₆ O ₁ S ₁ Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

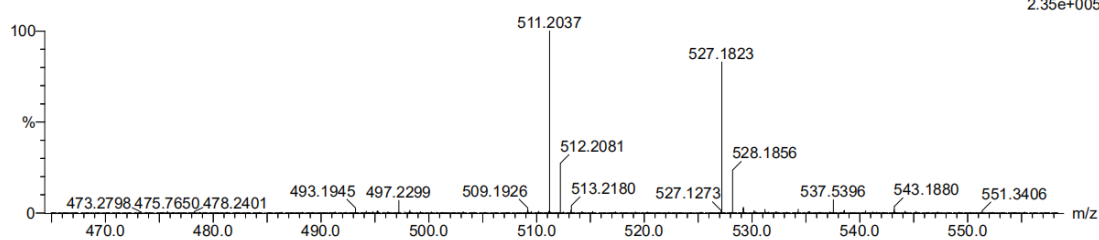
Elements Used:

C: 14-37 H: 1-60 O: 1-3 Na: 1-1

48

250511-2-62 16 (0.162)

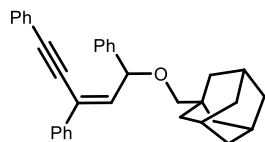
1: TOF MS ES+
2.35e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

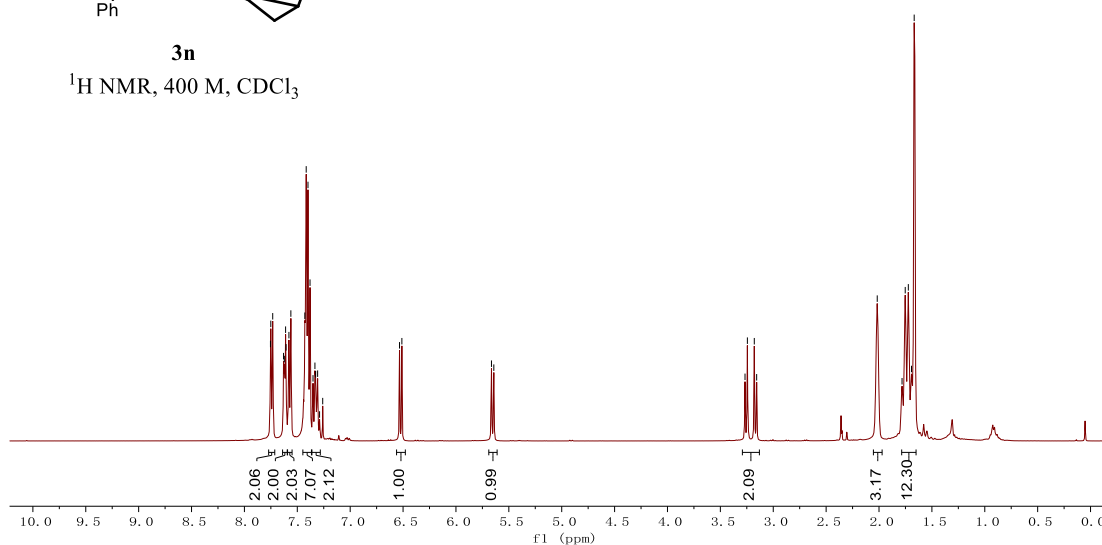
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
511.2037	511.2038	-0.1	-0.2	23.5	663.7	n/a	n/a	C37 H28 O Na

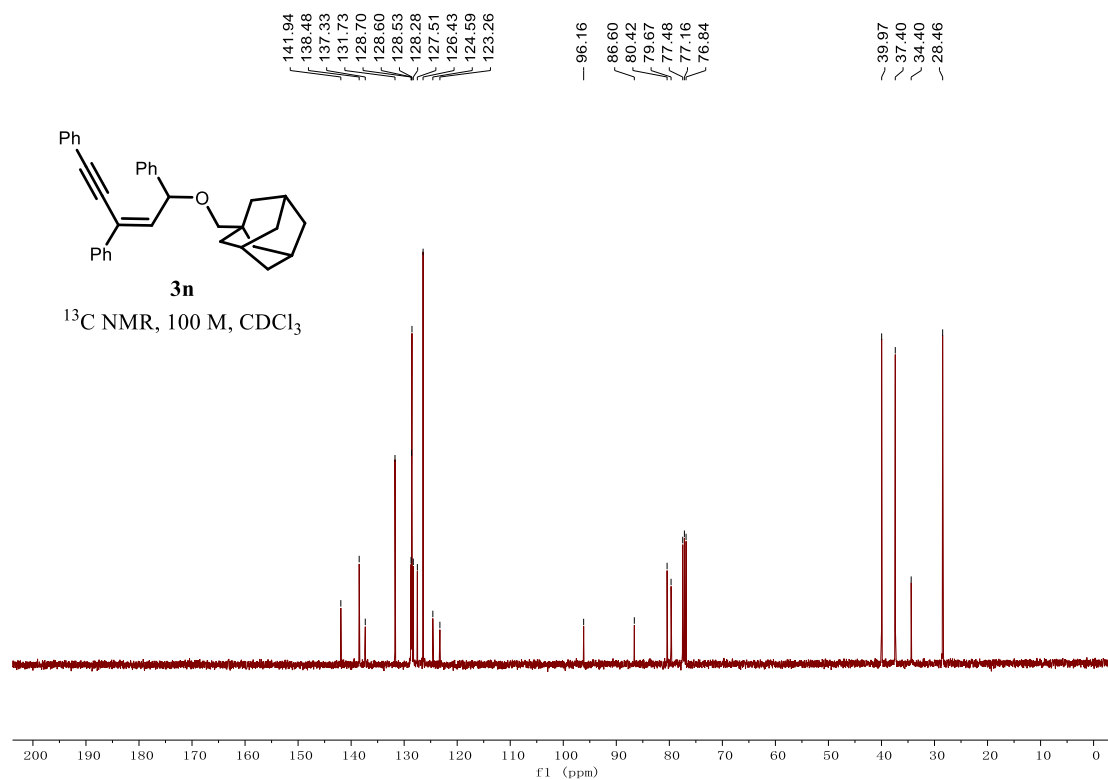
7.75
7.73
7.63
7.62
7.61
7.58
7.56
7.43
7.42
7.40
7.38
7.35
7.33
7.33
7.31
7.29
7.26
6.53
6.51
5.66
5.64
3.27
3.24
3.18
3.16
2.02
1.78
1.75
1.72
1.69
1.67



3n

¹H NMR, 400 M, CDCl₃





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

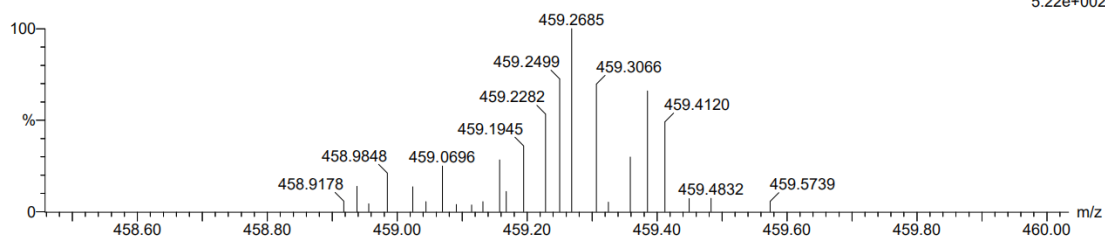
Elements Used:

C: 34-34 H: 1-60 O: 1-12

48

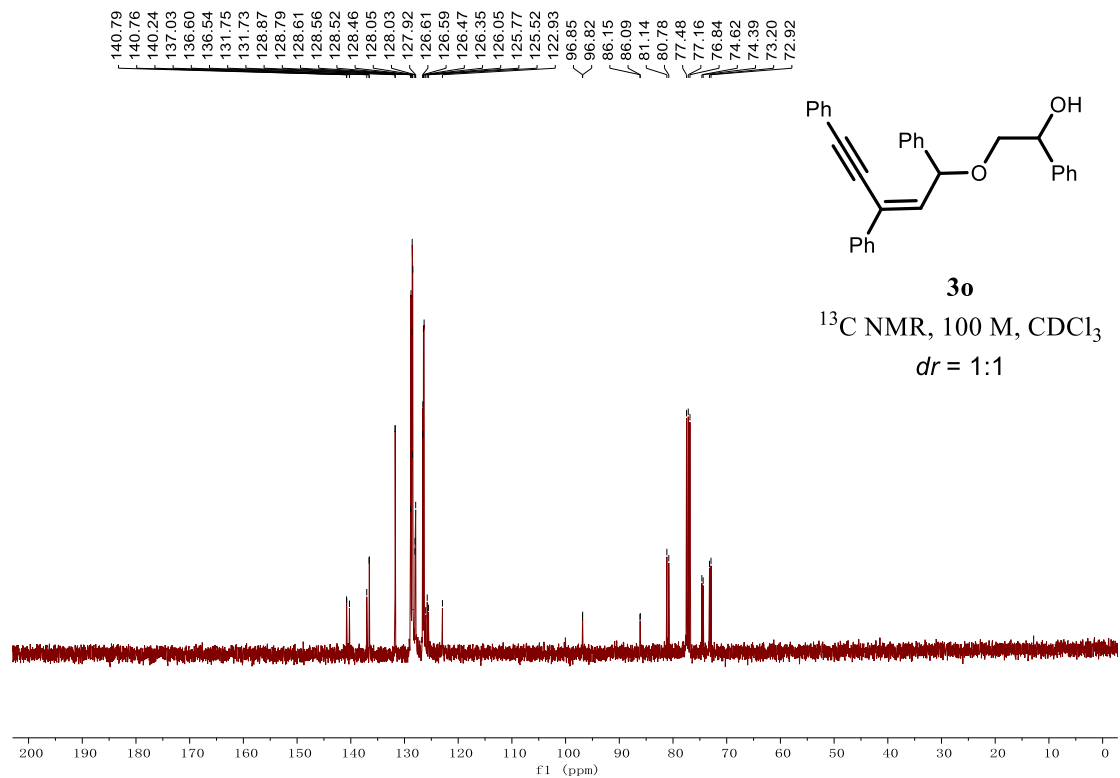
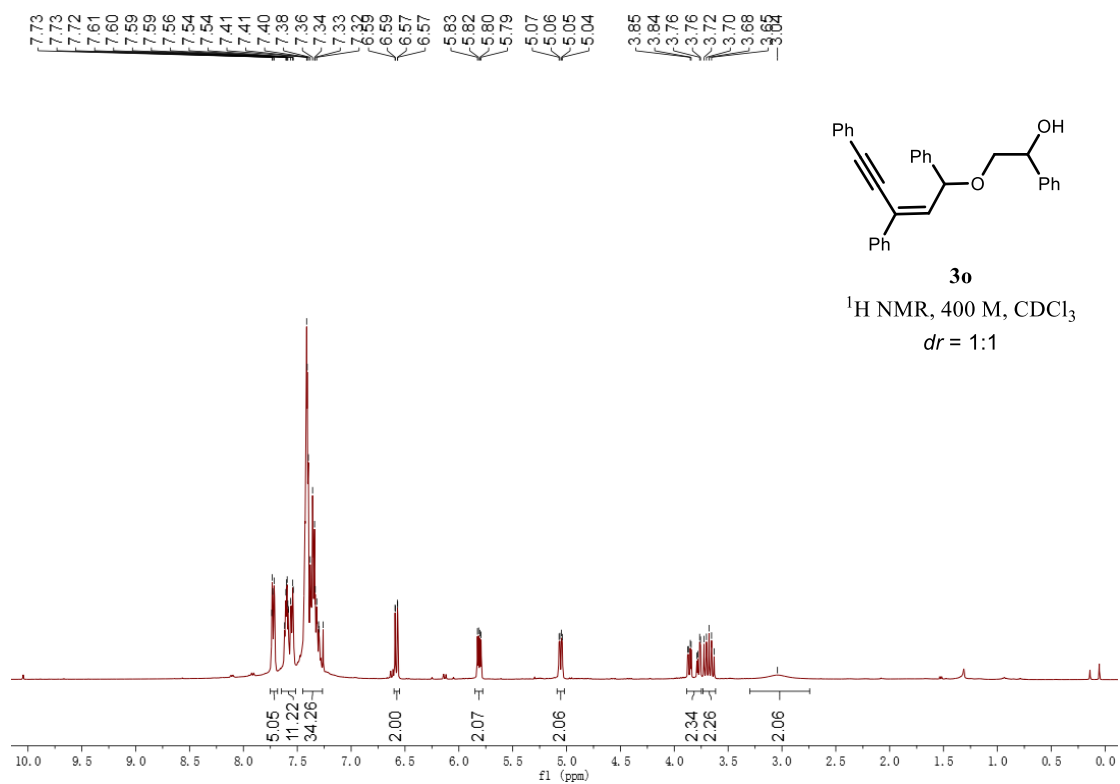
250511-2-56 23 (0.230)

1: TOF MS ES+
5.22e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
459.2685	459.2688	-0.3	-0.7	17.5	95.4	n/a	n/a	C34 H35 O



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1287 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

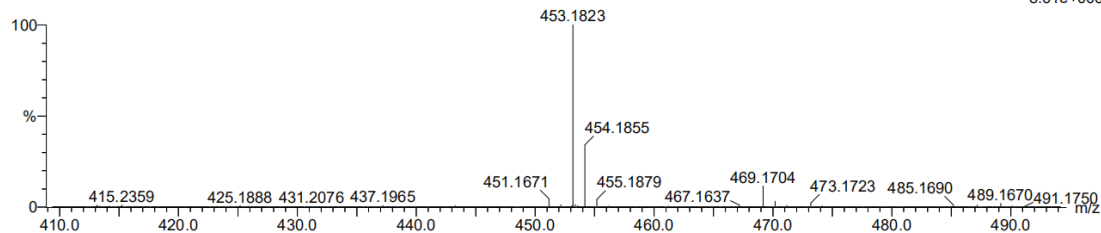
Elements Used:

C: 31-31 H: 26-26 N: 0-100 O: 0-100 Na: 0-2

7

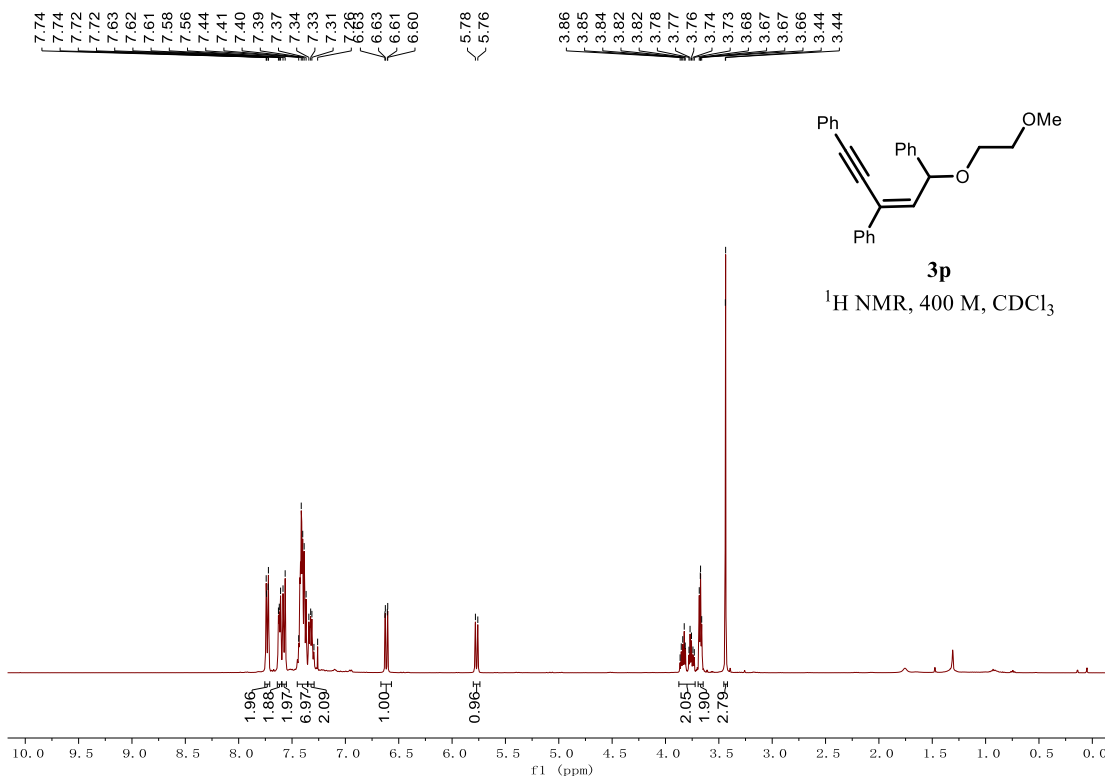
250403-12-761-2-YQZ-31 16 (0.161)

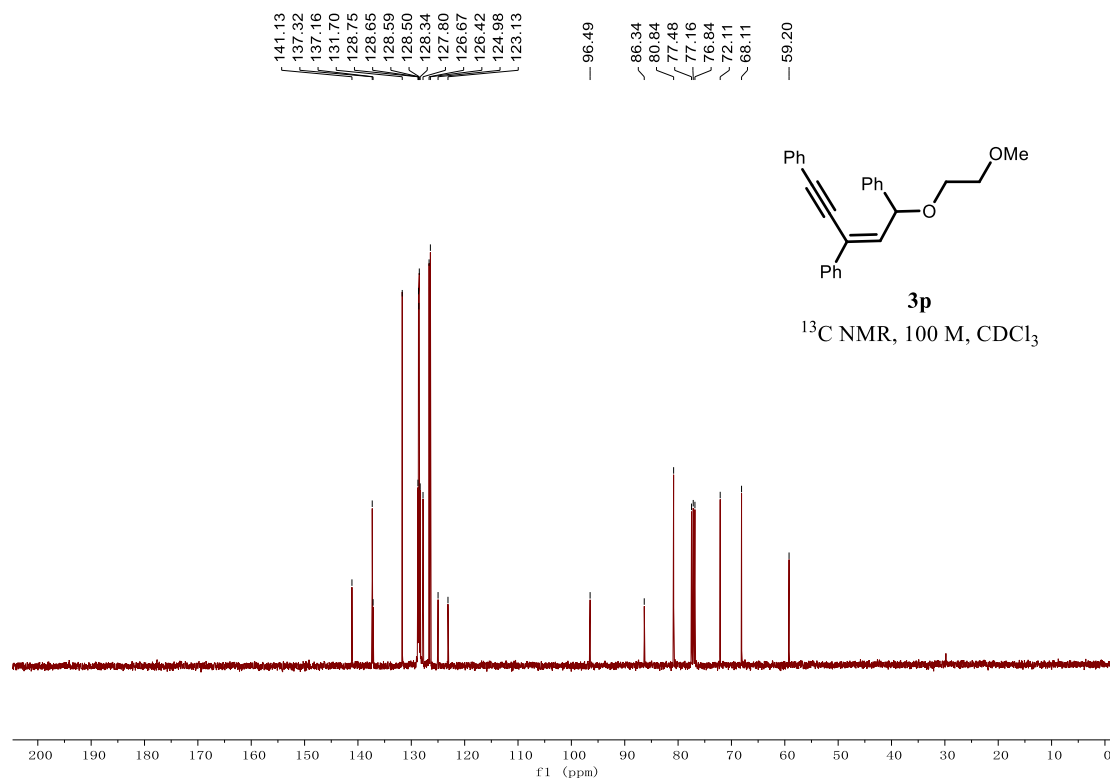
1: TOF MS ES+
8.61e+006



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
453.1823	453.1830	-0.7	-1.5	18.5	1112.4	n/a	n/a	C31 H26 O2 Na





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

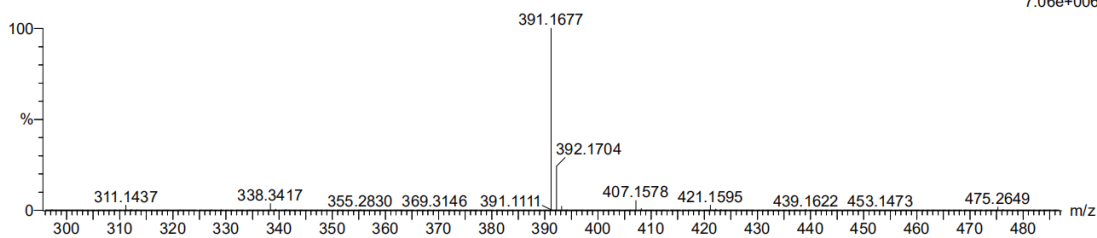
Elements Used:

C: 14-37 H: 1-60 O: 1-3 Na: 1-1

48

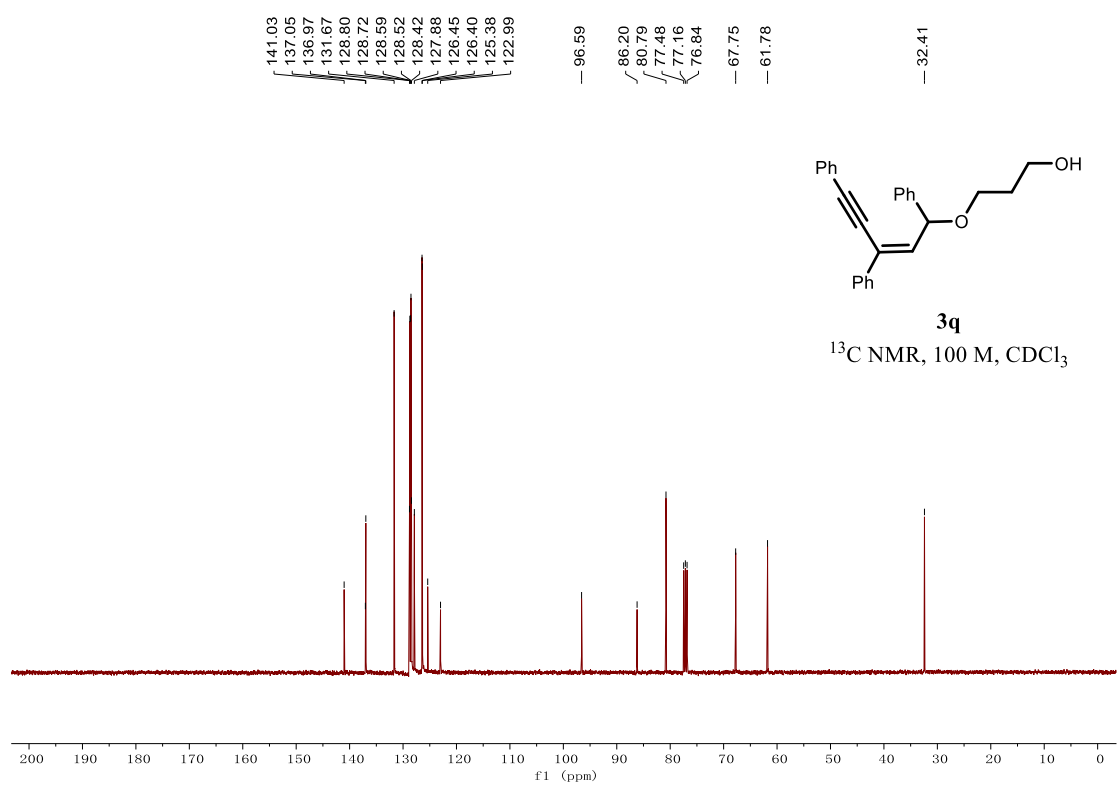
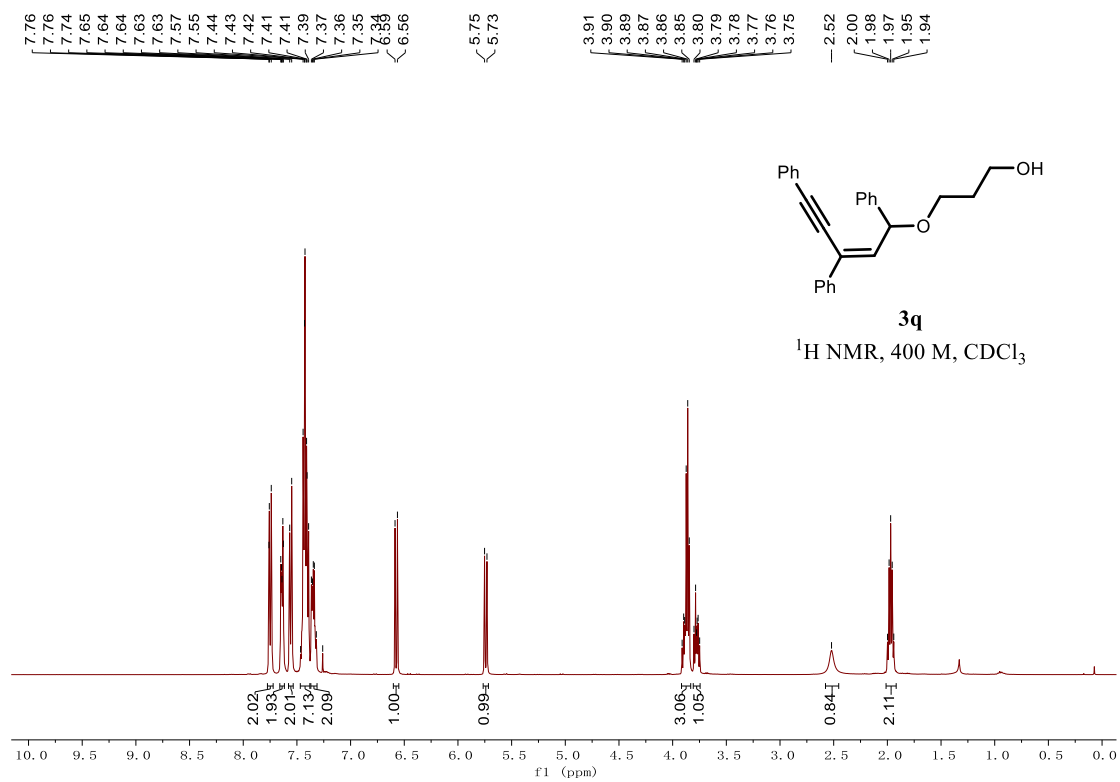
250511-2-67 13 (0.137)

1: TOF MS ES+
7.06e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
391.1677	391.1674	0.3	0.8	14.5	1045.4	n/a	n/a	C ₂₆ H ₂₄ O ₂ Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

16 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

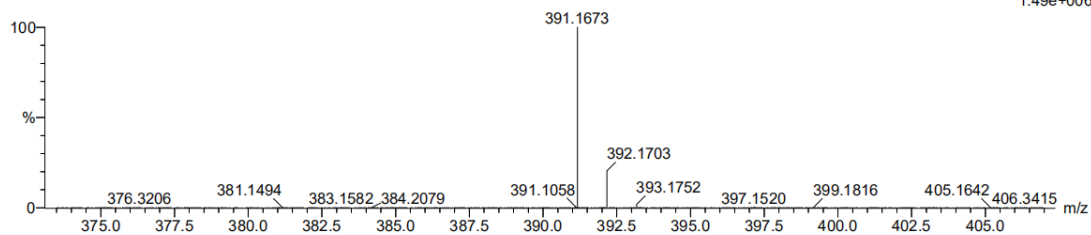
Elements Used:

C: 26-34 H: 1-60 O: 1-12 Na: 1-1

48

250511-2-66 12 (0.128)

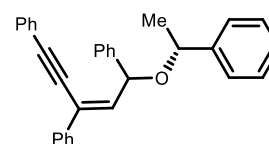
1: TOF MS ES+
1.49e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
391.1673	391.1674	-0.1	-0.3	14.5	902.8	n/a	n/a	C26 H24 O2 Na

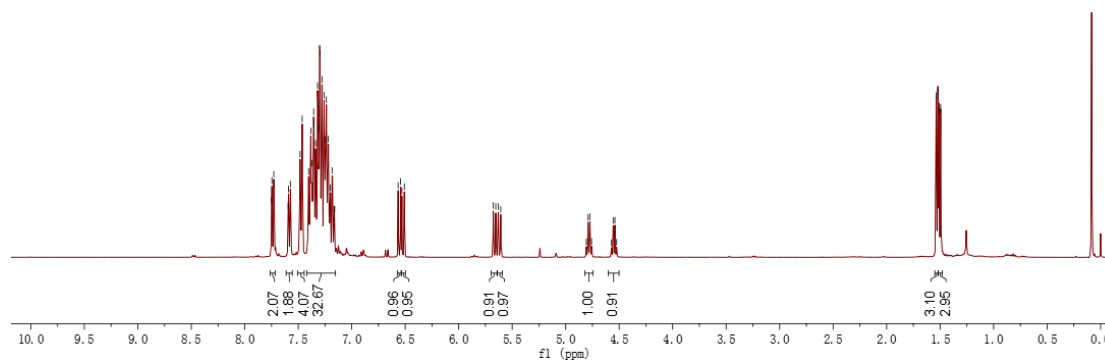
7.75
7.74
7.73
7.69
7.67
7.67
7.46
7.40
7.38
7.37
7.36
7.35
7.34
7.32
7.31
7.30
7.28
7.25
7.24
7.22
7.20
7.19
6.84
6.84
6.51
5.88
5.85
5.83
5.61
4.81
4.79
4.77
4.76
4.57
4.56
4.54
4.54
4.52
1.54
1.52
1.51
1.49

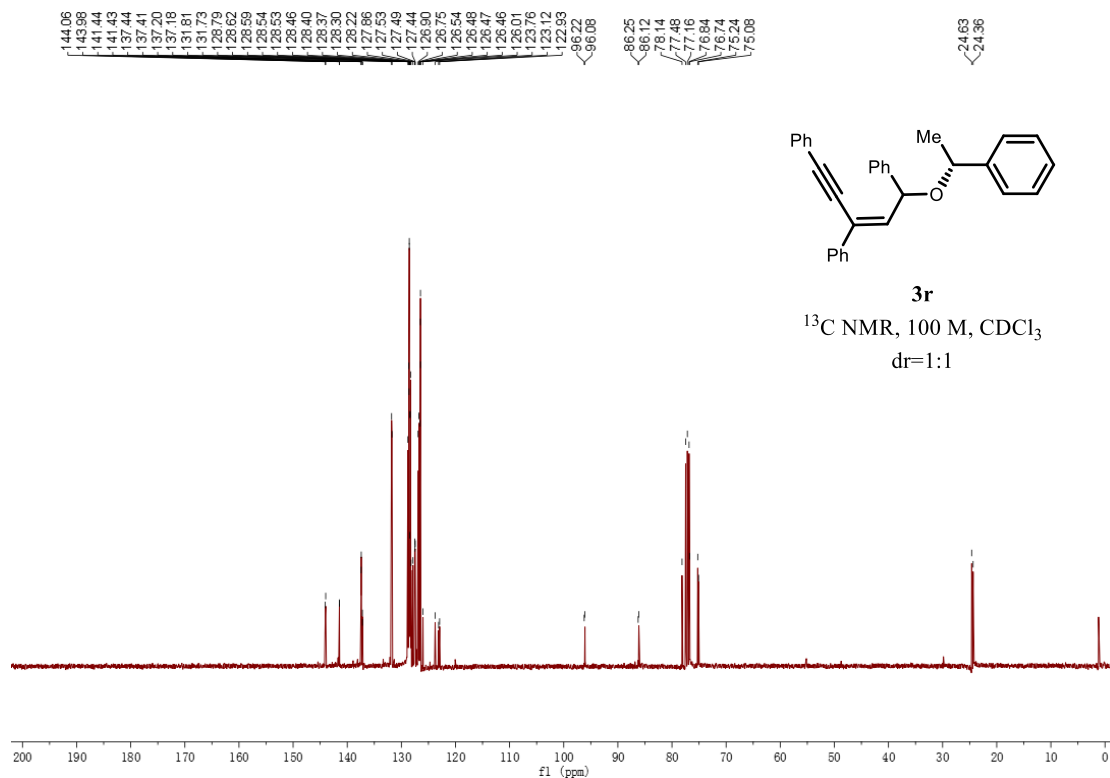


3r

¹H NMR, 400 M, CDCl₃

dr=1:1





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1208 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

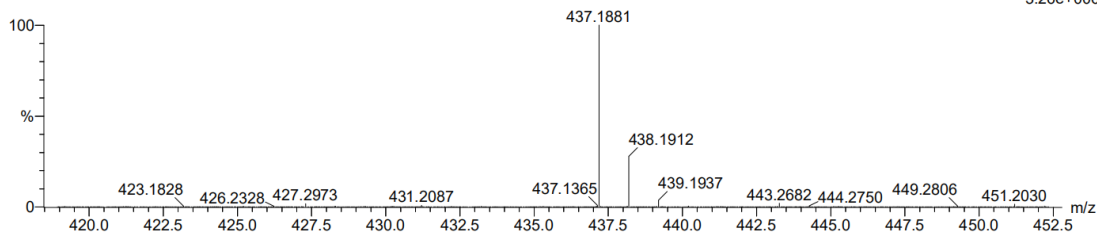
Elements Used:

C: 31-31 H: 26-26 N: 0-100 O: 0-100 Na: 0-2

7

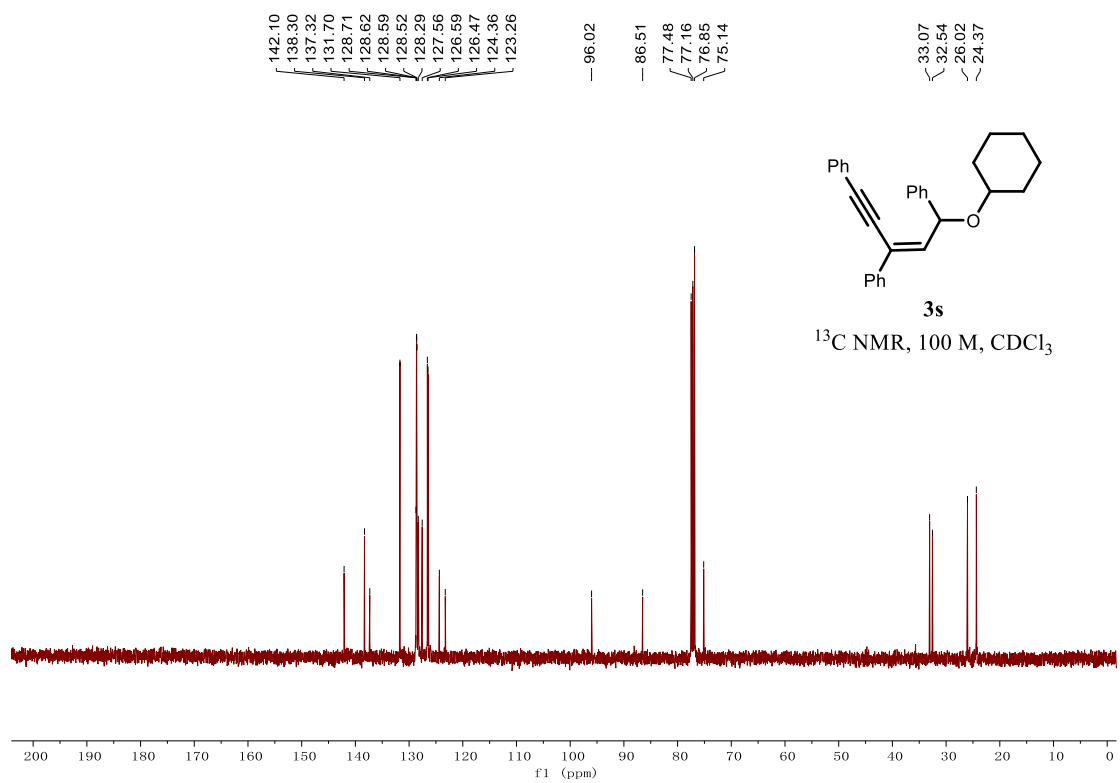
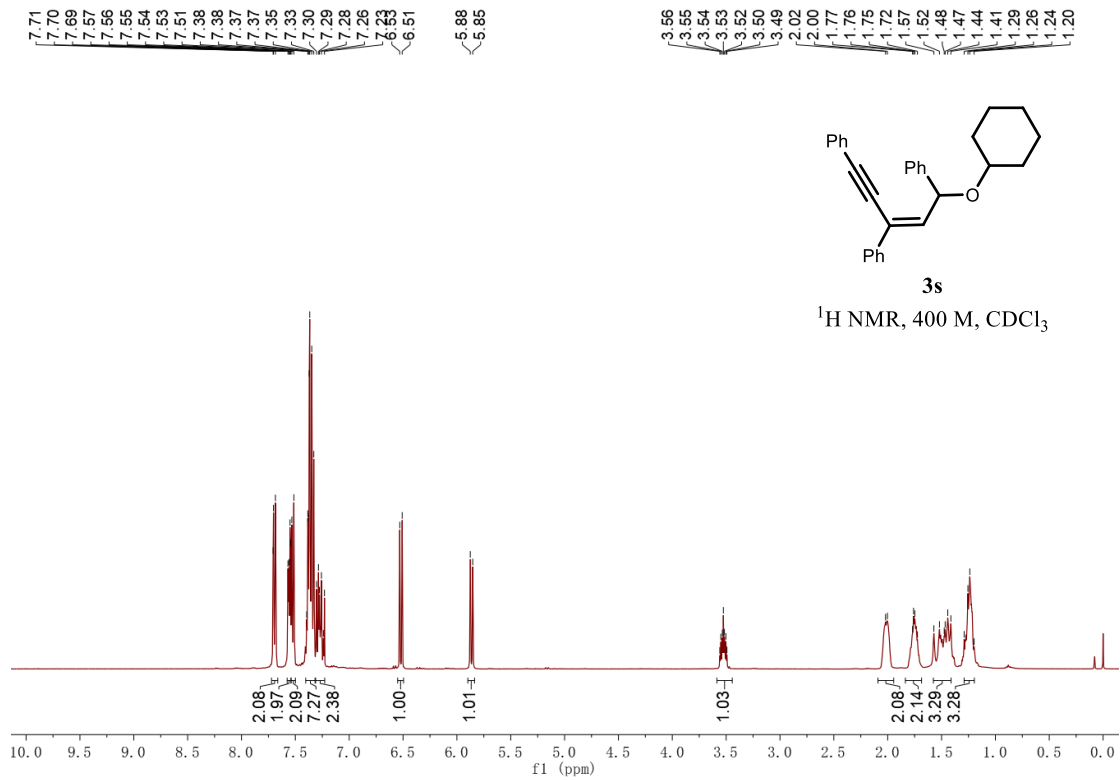
250403-12-761-2-YQZ-29 16 (0.161)

1: TOF MS ES+
3.26e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PIM	DBE	i-FIT	Norm	Conf (%)	Formula
437.1881	437.1881	0.0	0.0	18.5	1040.1	n/a	n/a	C ₃₁ H ₂₆ O



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

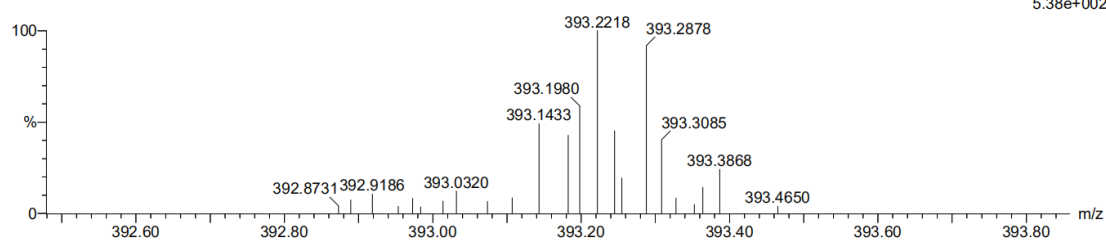
Elements Used:

C: 14-37 H: 1-60 O: 1-1

48

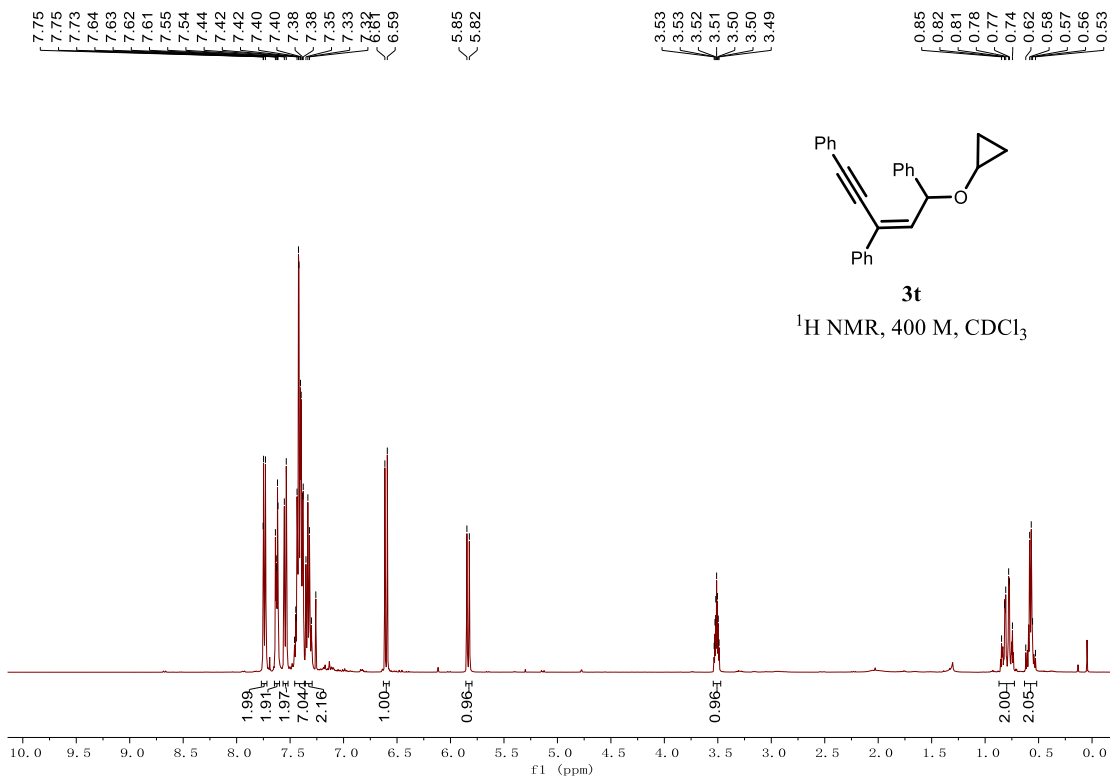
250511-2-69 4 (0.059)

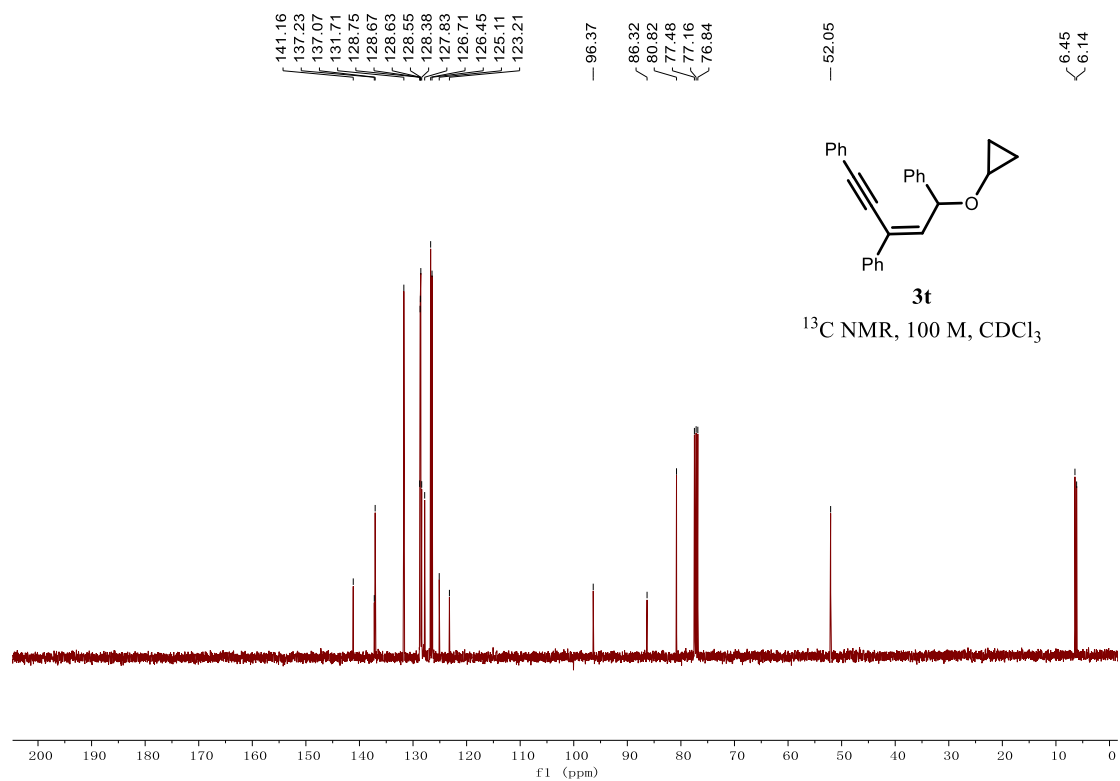
1: TOF MS ES+
5.38e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
393.2218	393.2218	0.0	0.0	15.5	104.7	n/a	n/a	C29 H29 O





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

14 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

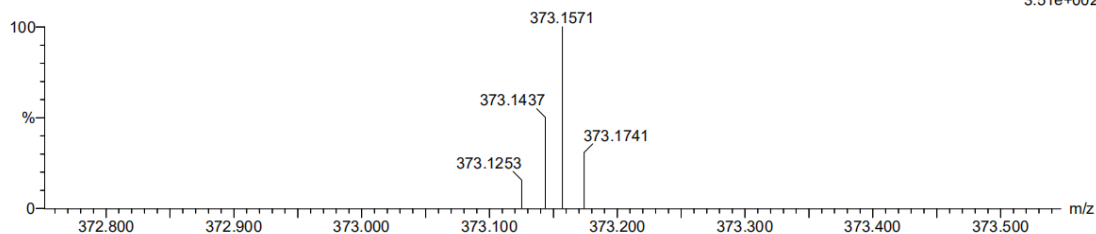
Elements Used:

C: 14-31 H: 1-60 O: 1-3 Na: 1-1

48

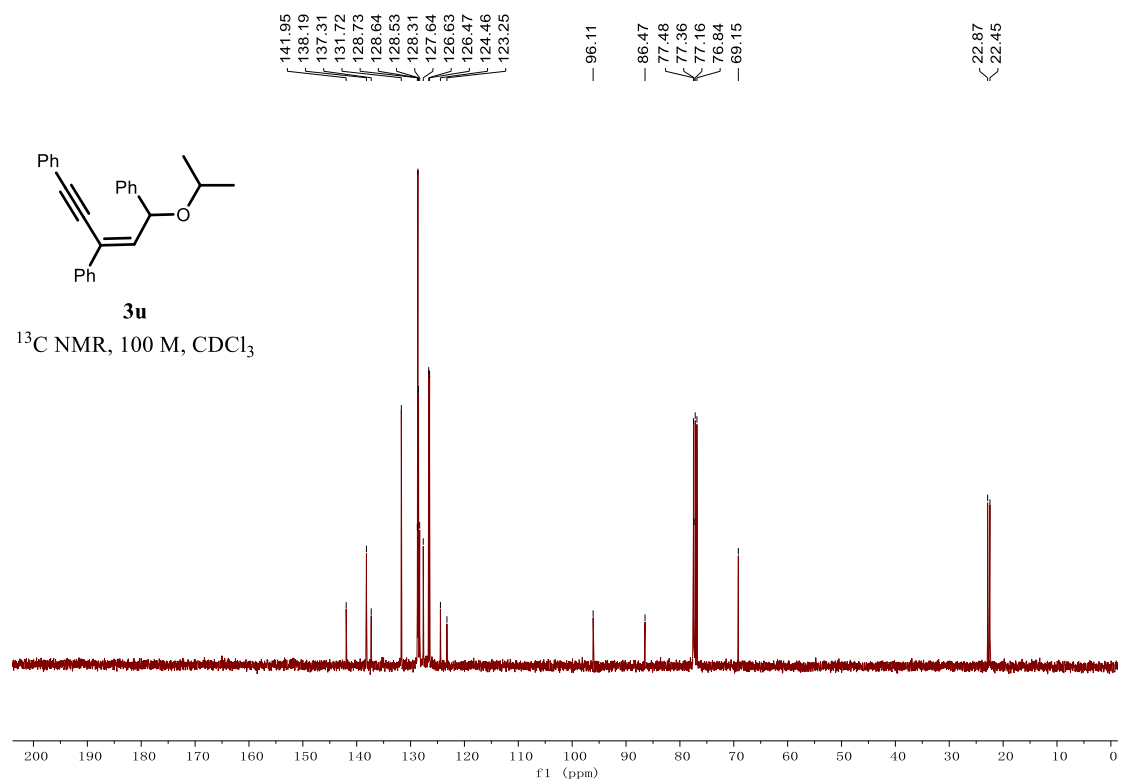
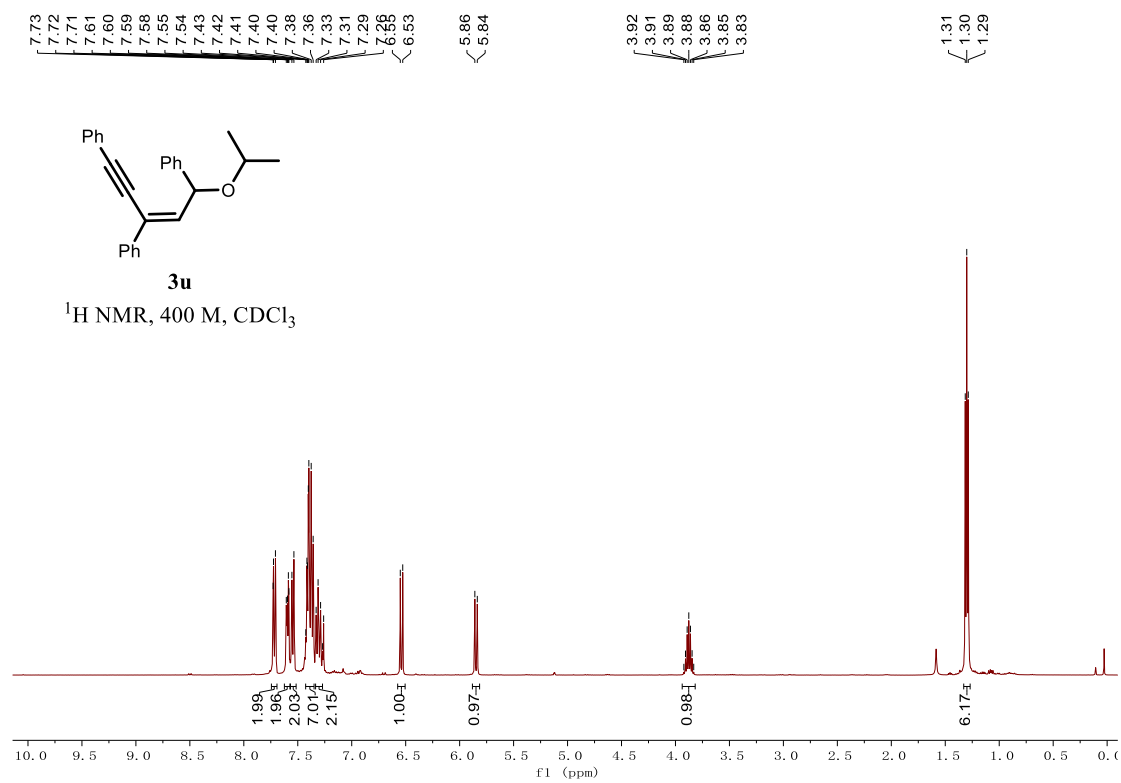
250511-2-58 50 (0.470)

1: TOF MS ES+
3.51e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
373.1571	373.1568	0.3	0.8	15.5	30.7	n/a	n/a	C ₂₆ H ₂₂ O Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

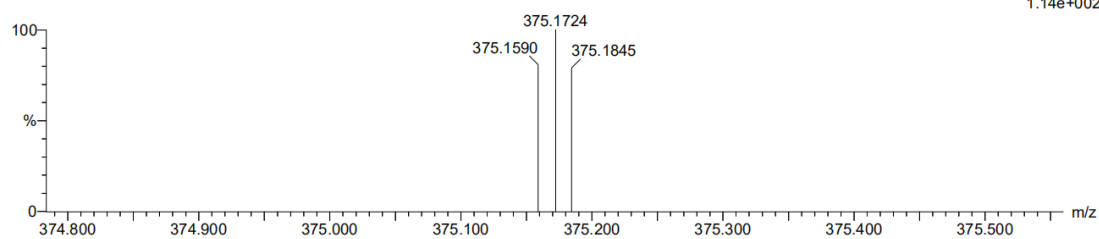
Elements Used:

C: 14-31 H: 1-60 O: 1-3 Na: 1-1

48

250511-2-60 51 (0.479)

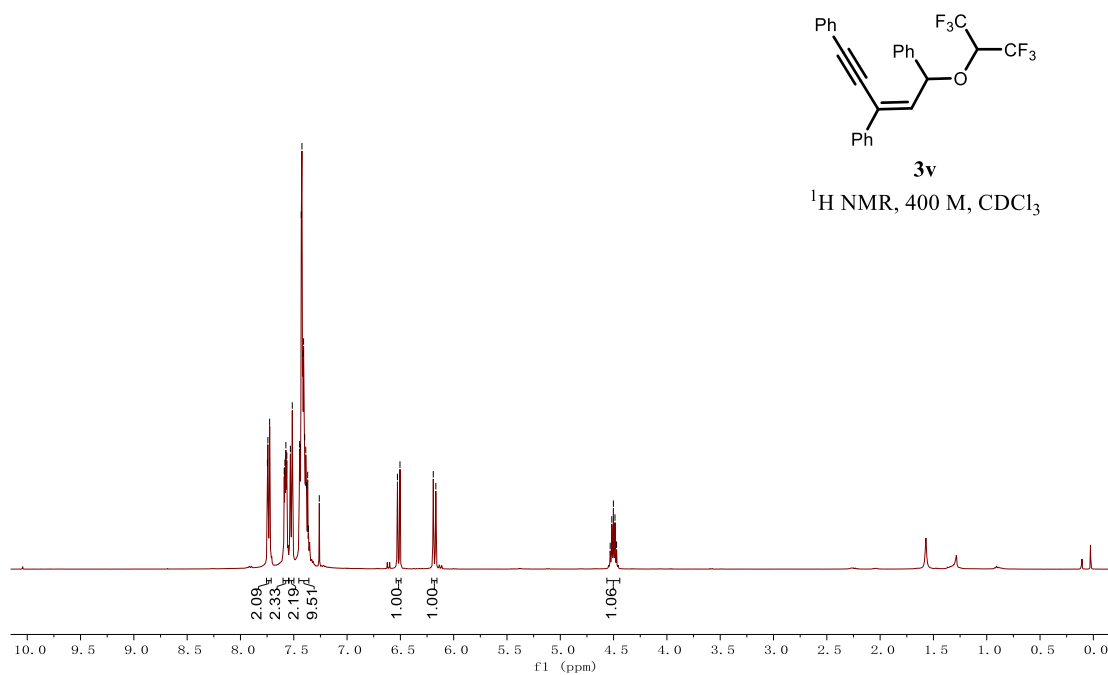
1: TOF MS ES+
1.14e+002

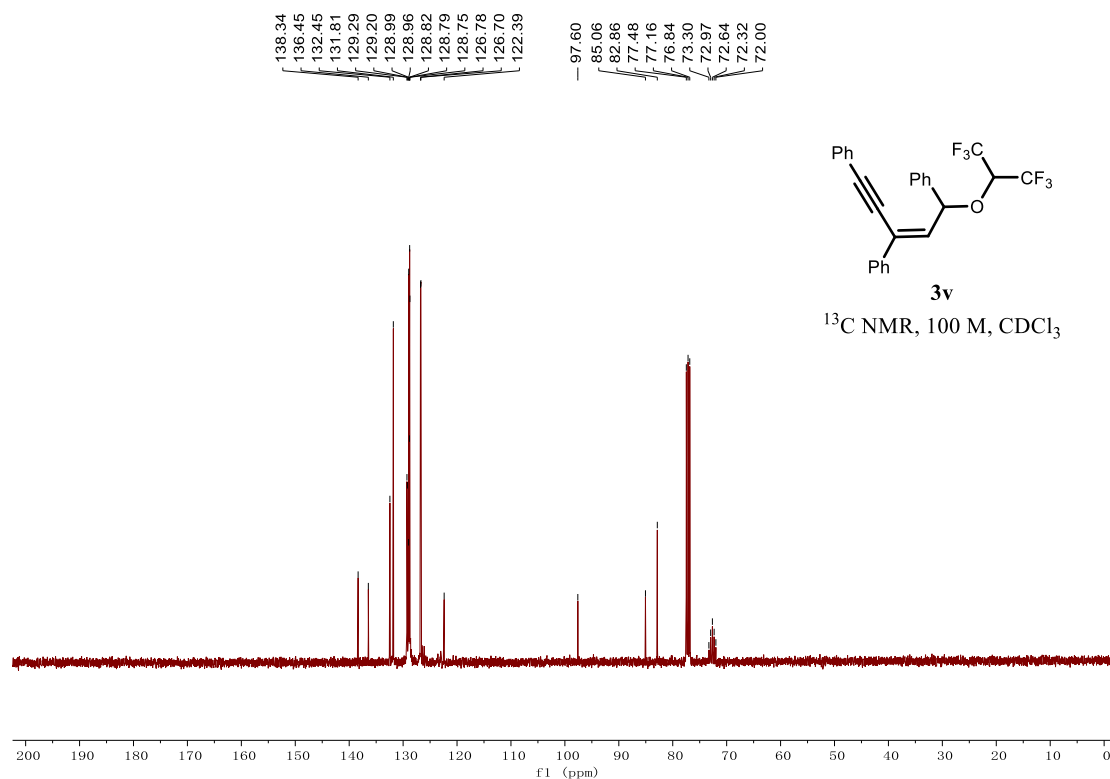


Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
375.1724	375.1725	-0.1	-0.3	14.5	27.4	n/a	n/a	C ₂₆ H ₂₄ O Na

7.75
7.74
7.73
7.59
7.58
7.57
7.57
7.53
7.51
7.44
7.44
7.43
7.42
7.41
7.41
7.40
7.39
7.38
7.37
6.50
6.50
6.19
6.17
4.53
4.52
4.50
4.49
4.47





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

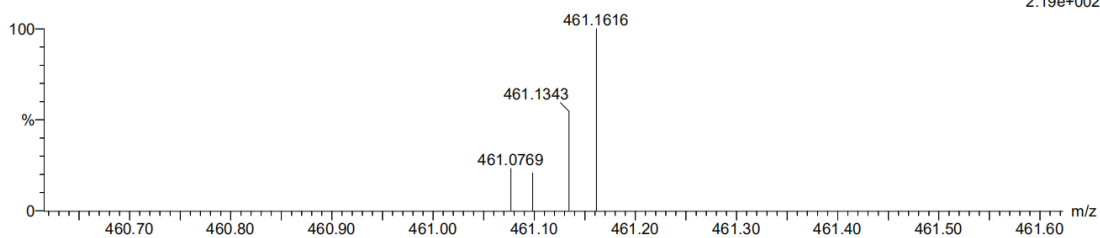
Elements Used:

C: 14-37 H: 1-60 O: 1-1 F: 6-6

48

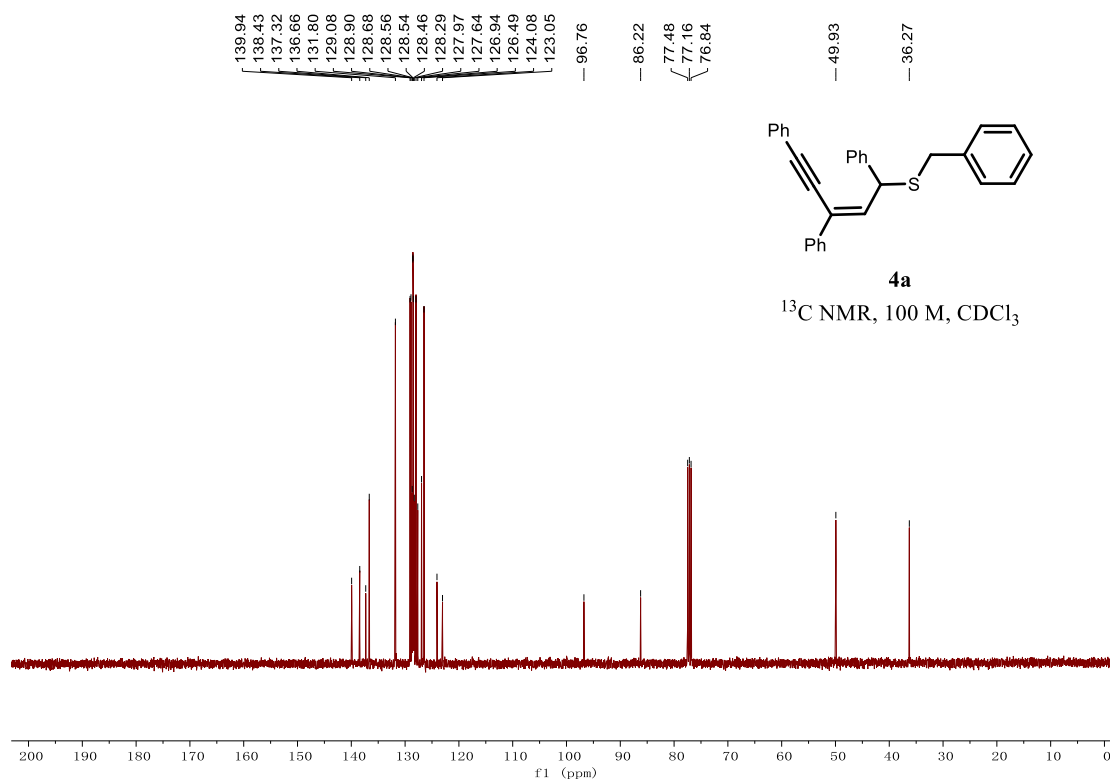
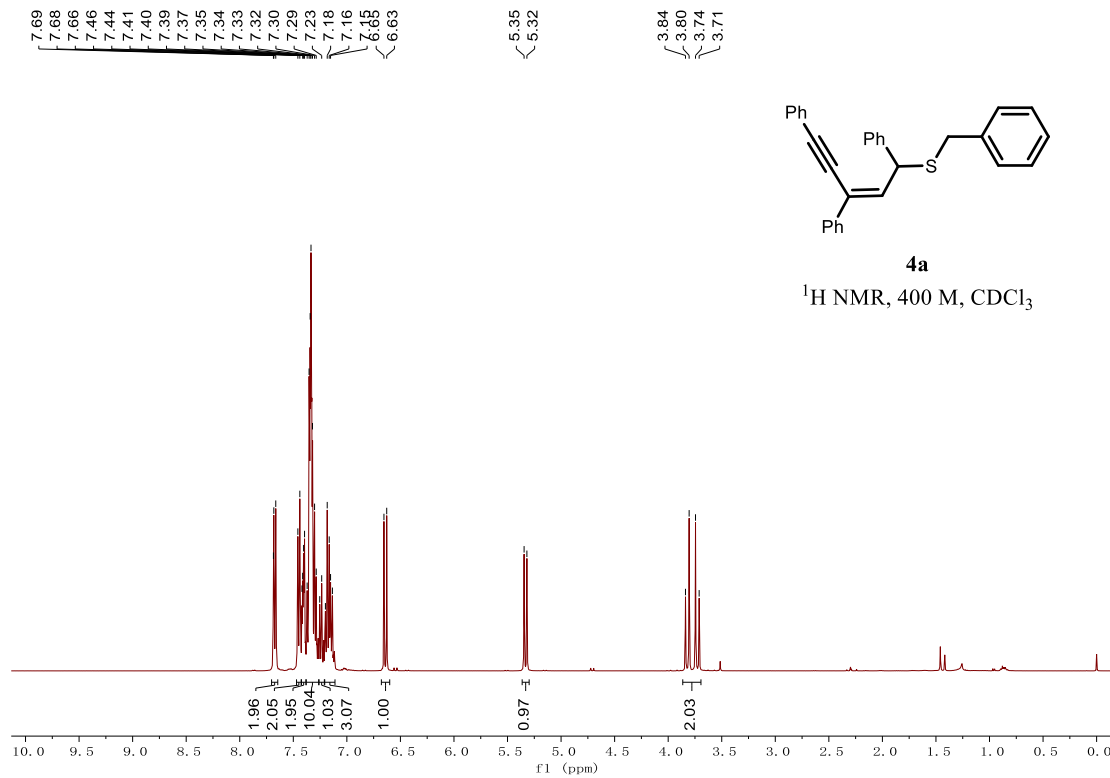
250511-2-68 19 (0.196)

1: TOF MS ES+
2.19e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
461.1343	461.1340	0.3	0.7	14.5	29.5	n/a	n/a	C ₂₆ H ₁₉ O F ₆



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

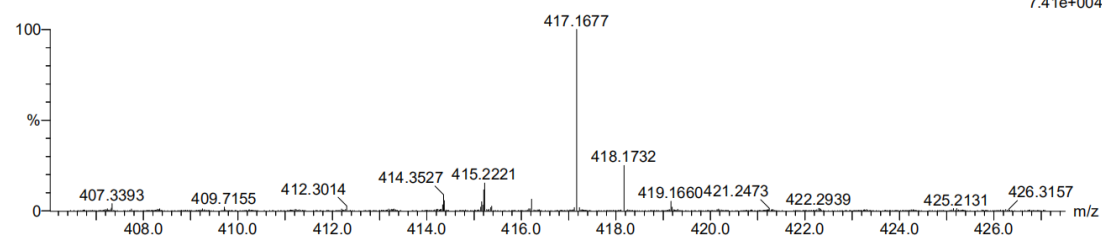
Elements Used:

C: 14-37 H: 1-60 S: 1-1

48

250511-2-63 9 (0.102)

1: TOF MS ES+
7.41e+004



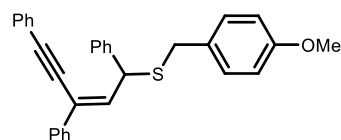
Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
417.1677	417.1677	0.0	0.0	18.5	775.3	n/a	n/a	C30 H25 S

7.79
7.78
7.76
7.55
7.53
7.50
7.49
7.49
7.47
7.45
7.43
7.42
7.41
7.39
7.38
7.36
7.34
7.32
6.81
6.80
6.79
6.75
6.72

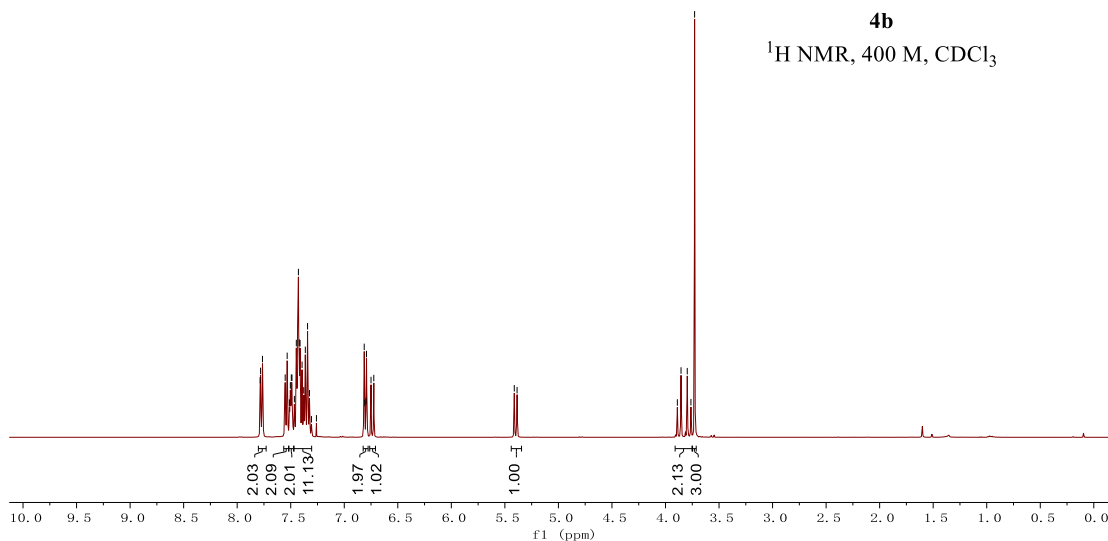
5.41
5.39

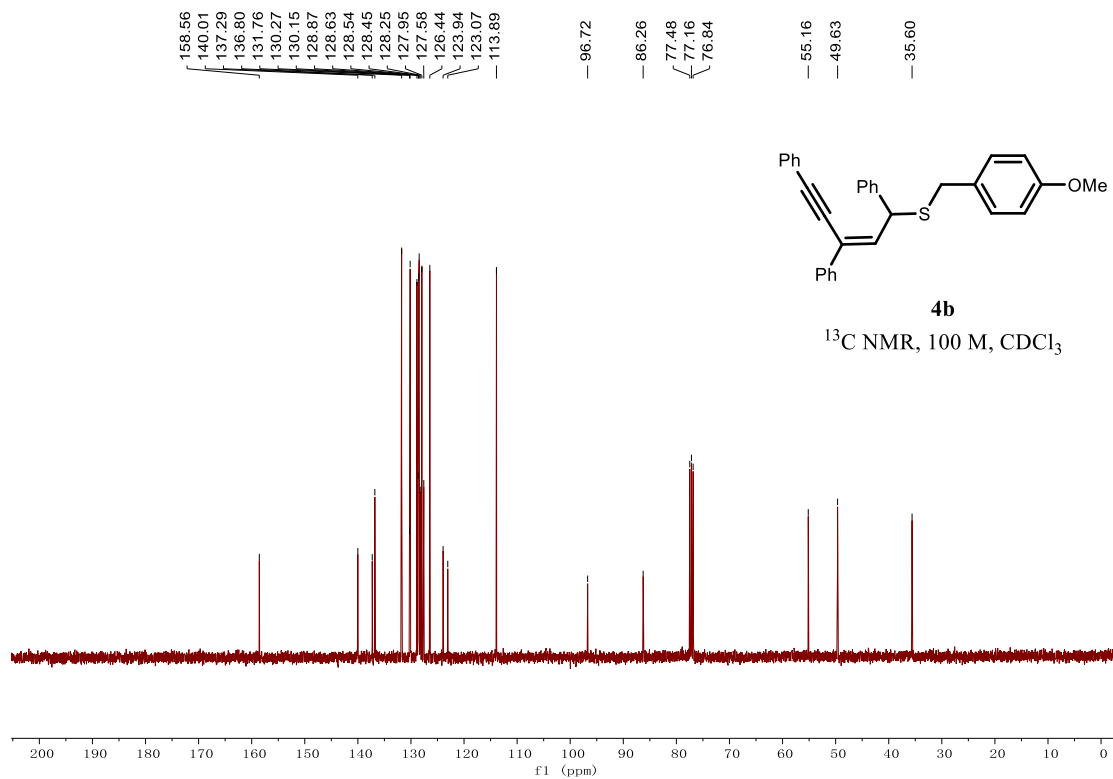
3.89
3.85
3.80
3.76
3.73



4b

¹H NMR, 400 M, CDCl₃





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

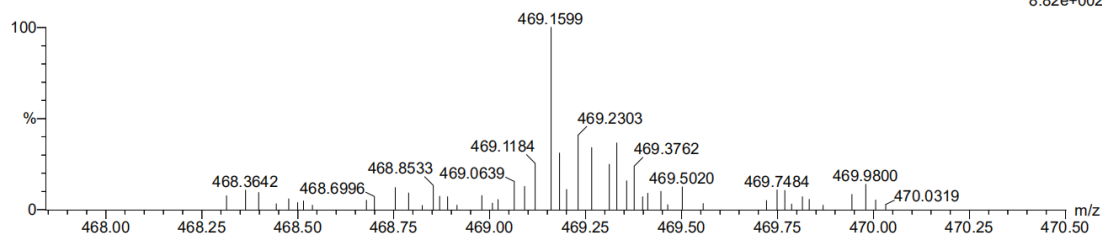
Elements Used:

C: 14-37 H: 1-60 O: 1-3 Na: 1-1 S: 1-1

48

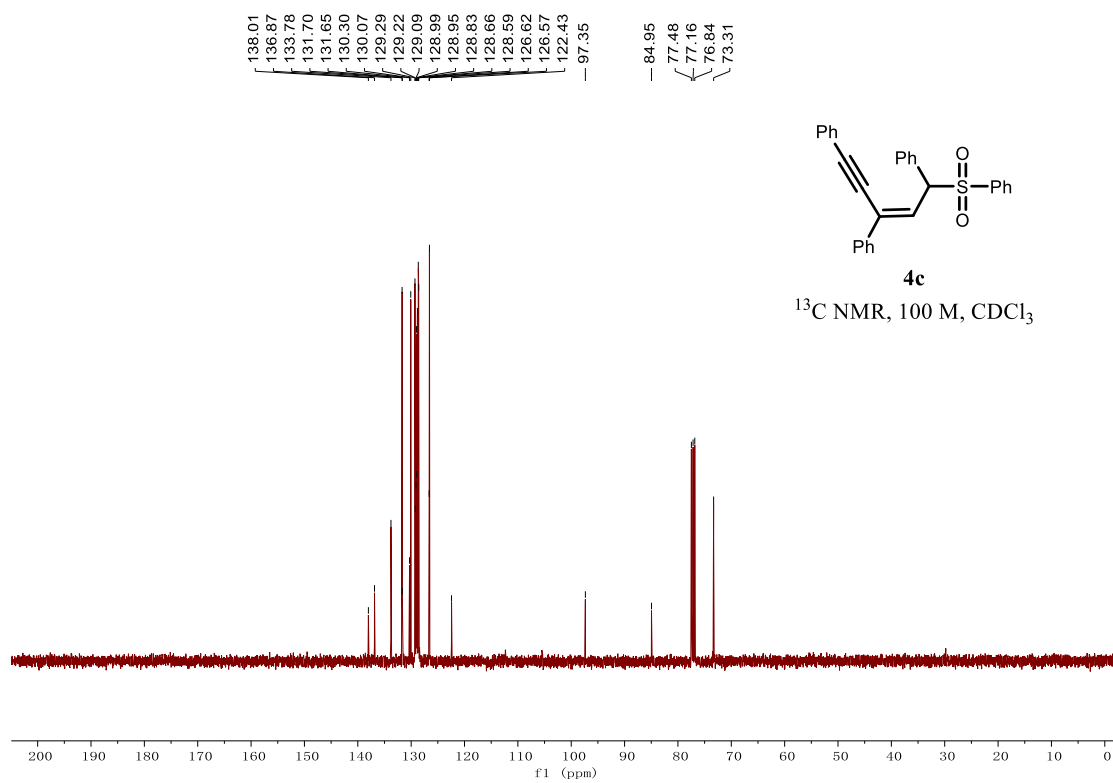
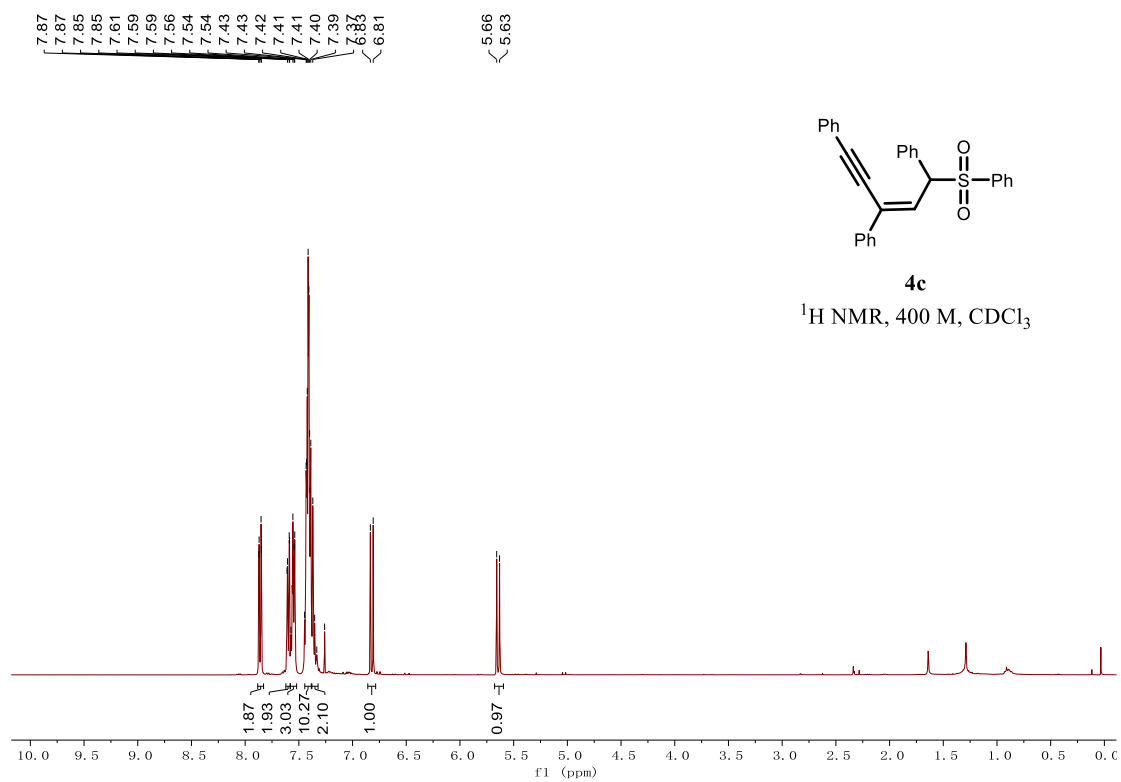
250511-2-65 10 (0.111)

1: TOF MS ES+
8.82e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
469.1599	469.1602	-0.3	-0.6	18.5	245.8	n/a	n/a	C31 H26 O Na S



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

15 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

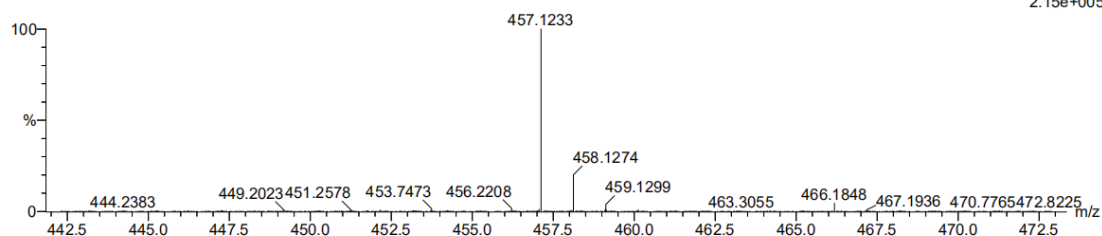
Elements Used:

C: 14-37 H: 1-60 O: 1-3 S: 1-1 Na: 1-1

48

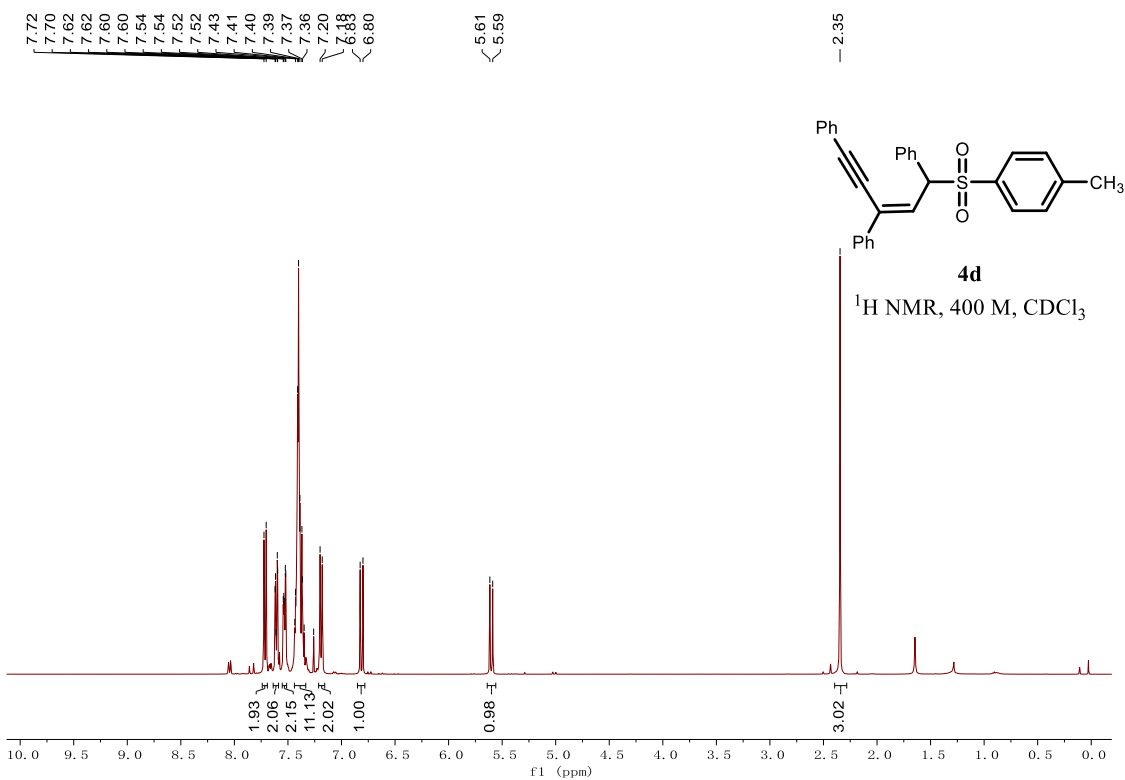
250511-2-64 13 (0.137)

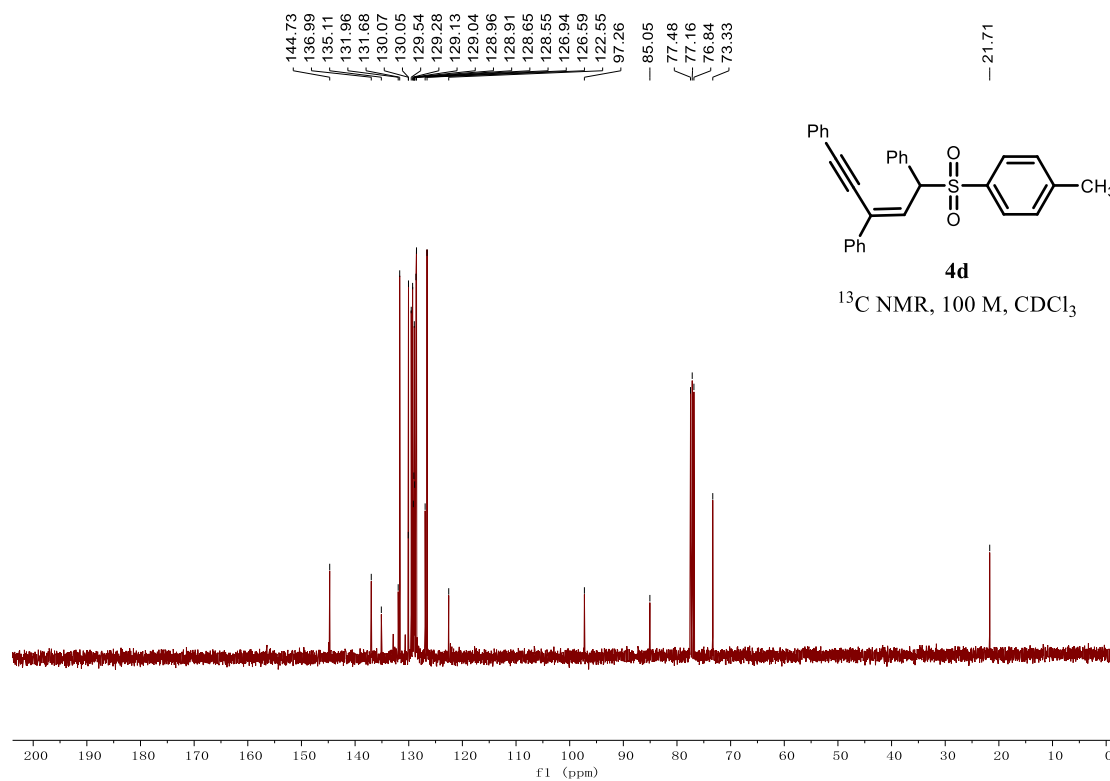
1: TOF MS ES+
2.15e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
457.1233	457.1238	-0.5	-1.1	18.5	755.4	n/a	n/a	C ₂₉ H ₂₂ O ₂ S Na





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

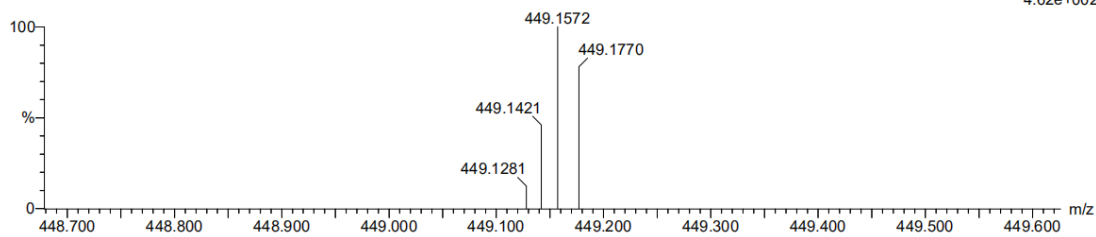
Elements Used:

C: 14-31 H: 1-60 O: 1-3 S: 1-1

48

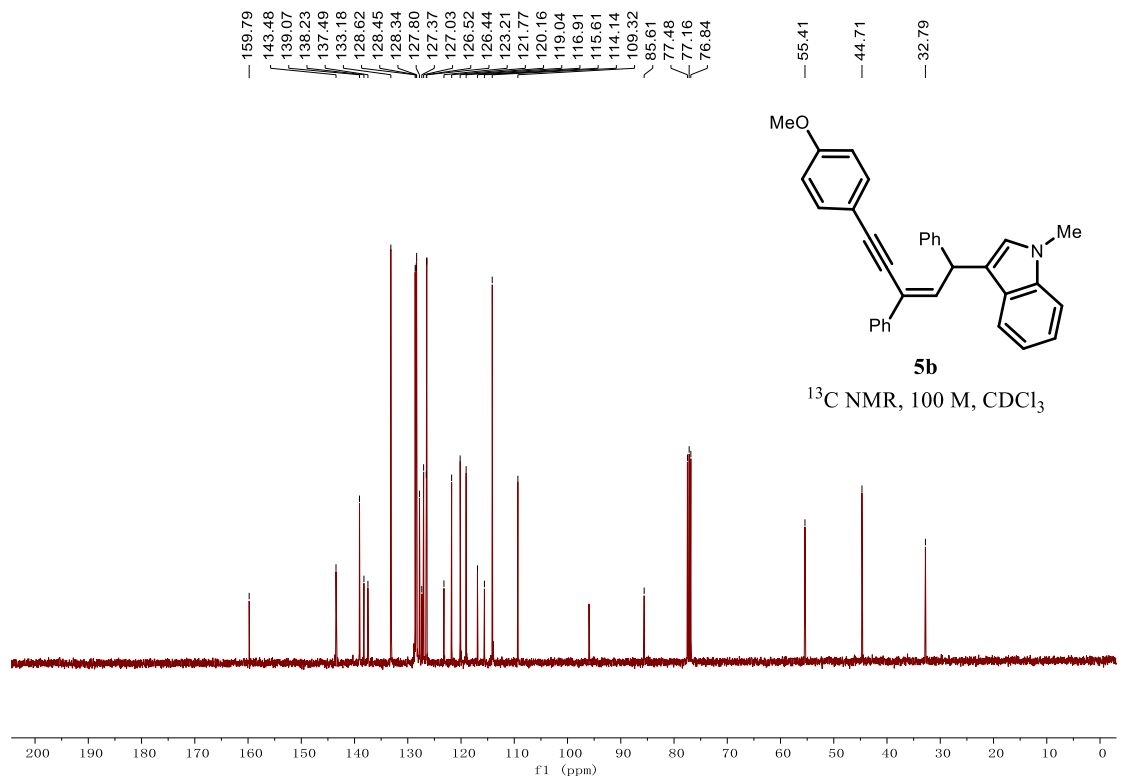
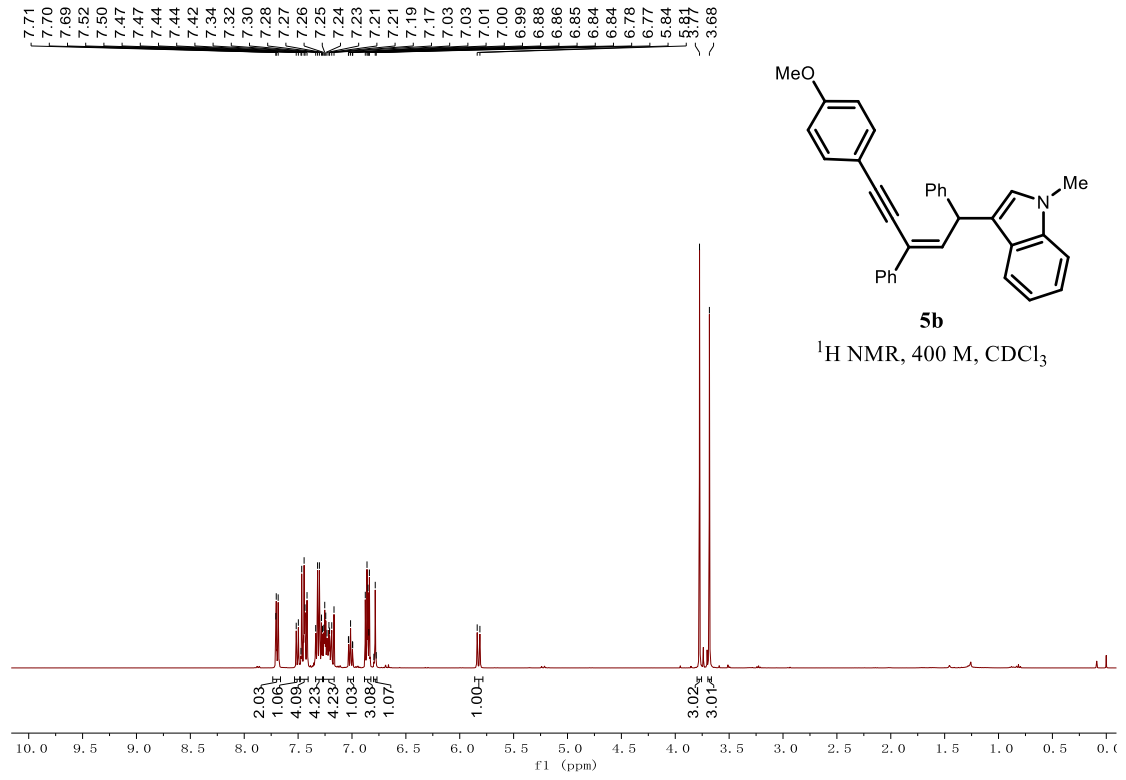
250511-2-61 29 (0.282)

1: TOF MS ES+
4.62e+002



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
449.1572	449.1575	-0.3	-0.7	18.5	34.1	n/a	n/a	C ₃₀ H ₂₅ O ₂ S



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1431 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

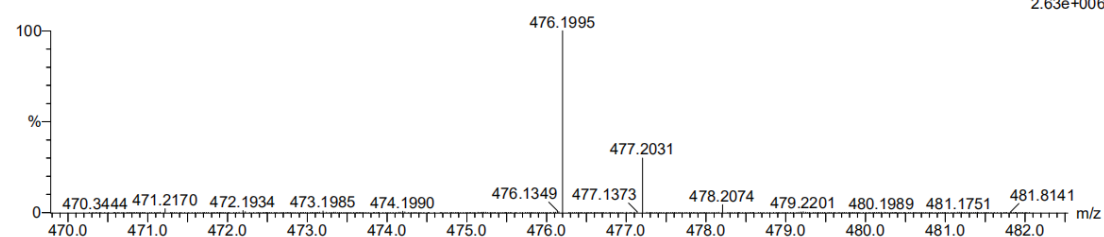
Elements Used:

C: 33-33 H: 27-27 N: 0-100 O: 0-100 Na: 0-2

7

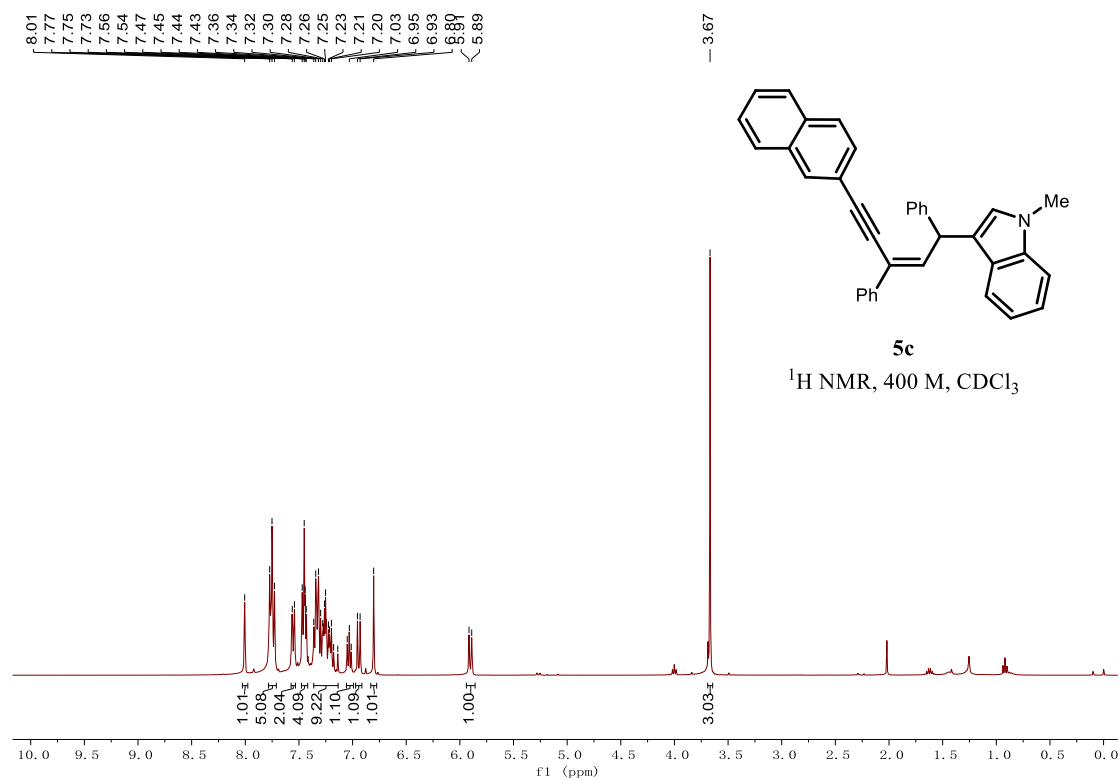
250403-12-761-2-YQZ-16 14 (0.143)

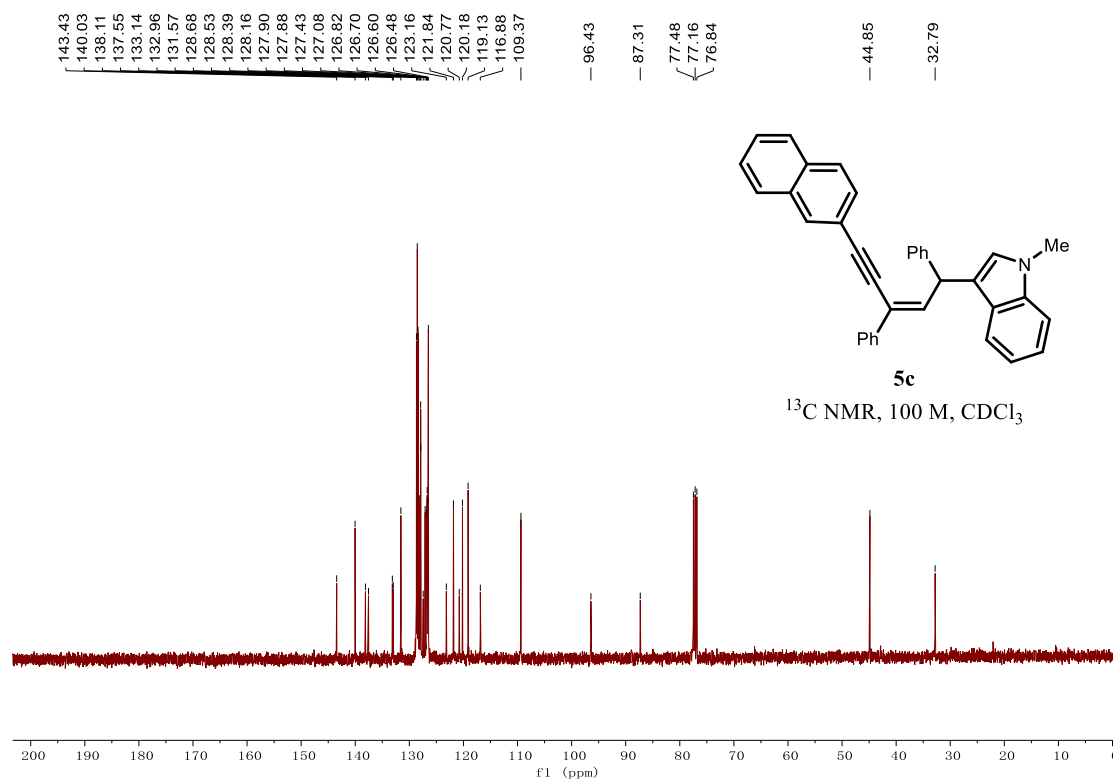
1: TOF MS ES+
2.63e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
476.1995	476.1990	0.5	1.0	20.5	992.0	n/a	n/a	C33 H27 N 0 Na





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1447 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

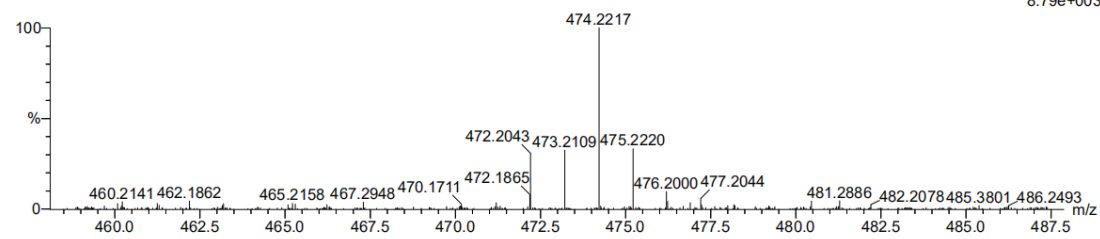
Elements Used:

C: 36-36 H: 28-28 N: 0-100 O: 0-100 Na: 0-2

46

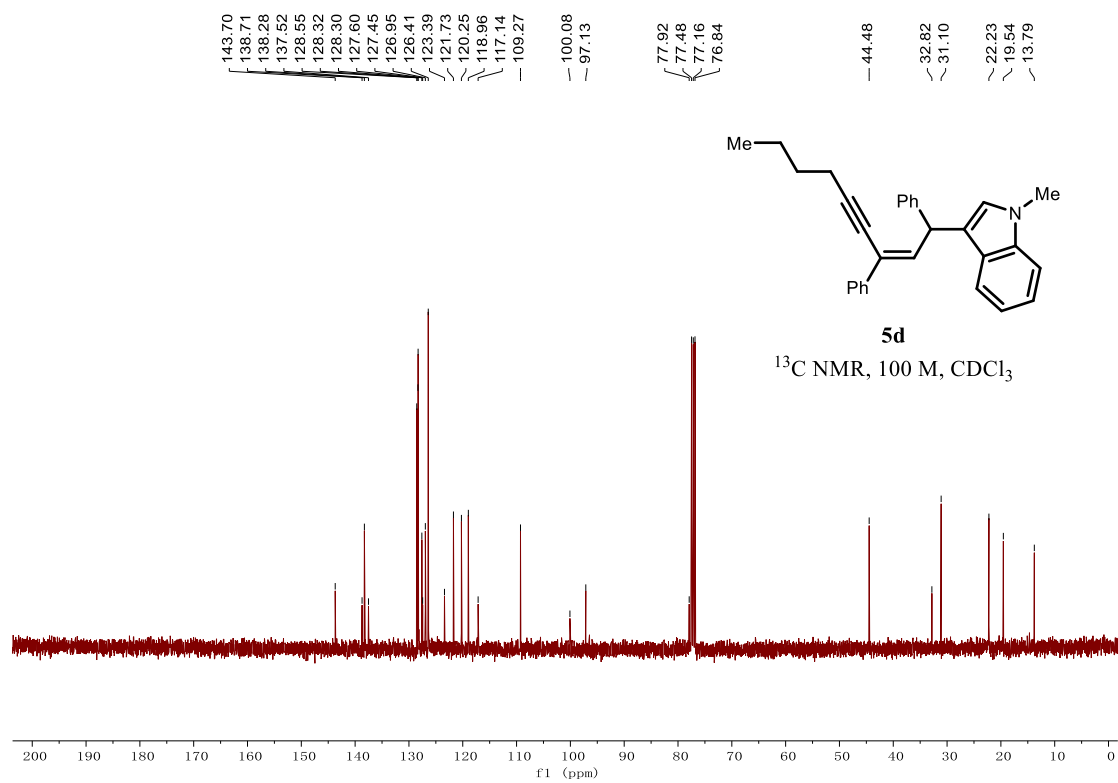
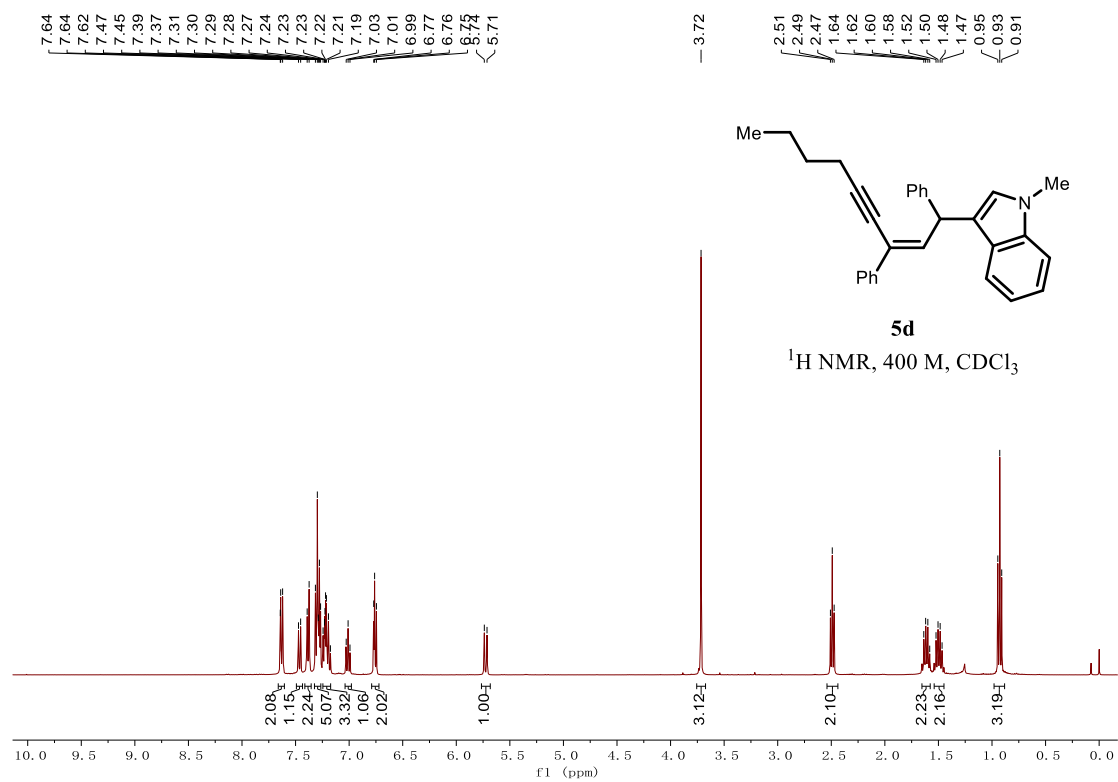
250809-1-12 16 (0.109)

1: TOF MS ES+
8.79e+003



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
474.2217	474.2222	-0.5	-1.1	23.5	233.8	n/a	n/a	C ₃₆ H ₂₈ N



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1147 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

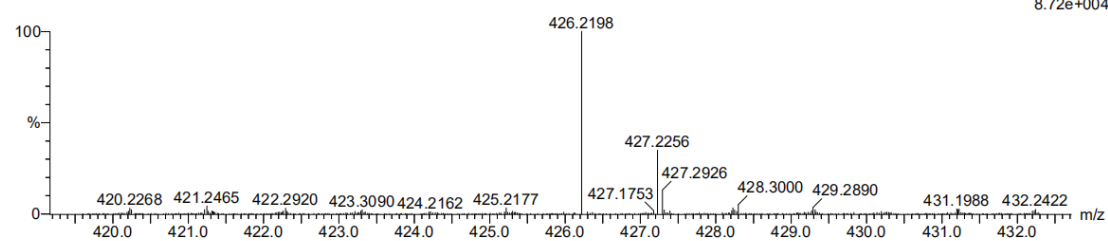
Elements Used:

C: 30-30 H: 29-29 N: 0-100 O: 0-100 Na: 0-2

7

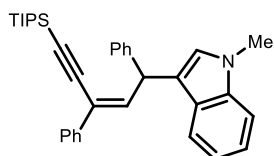
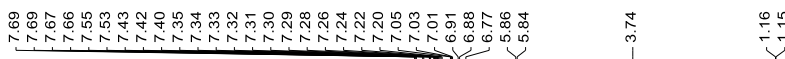
250403-12-761-2-YQZ-30 23 (0.227)

1: TOF MS ES+
8.72e+004



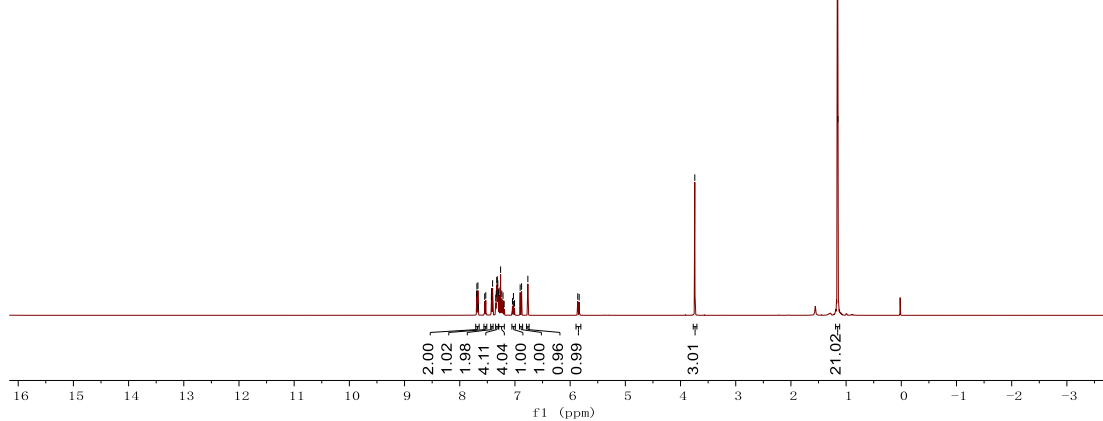
Minimum: -1.5
Maximum: 5.0 10.0 50.0

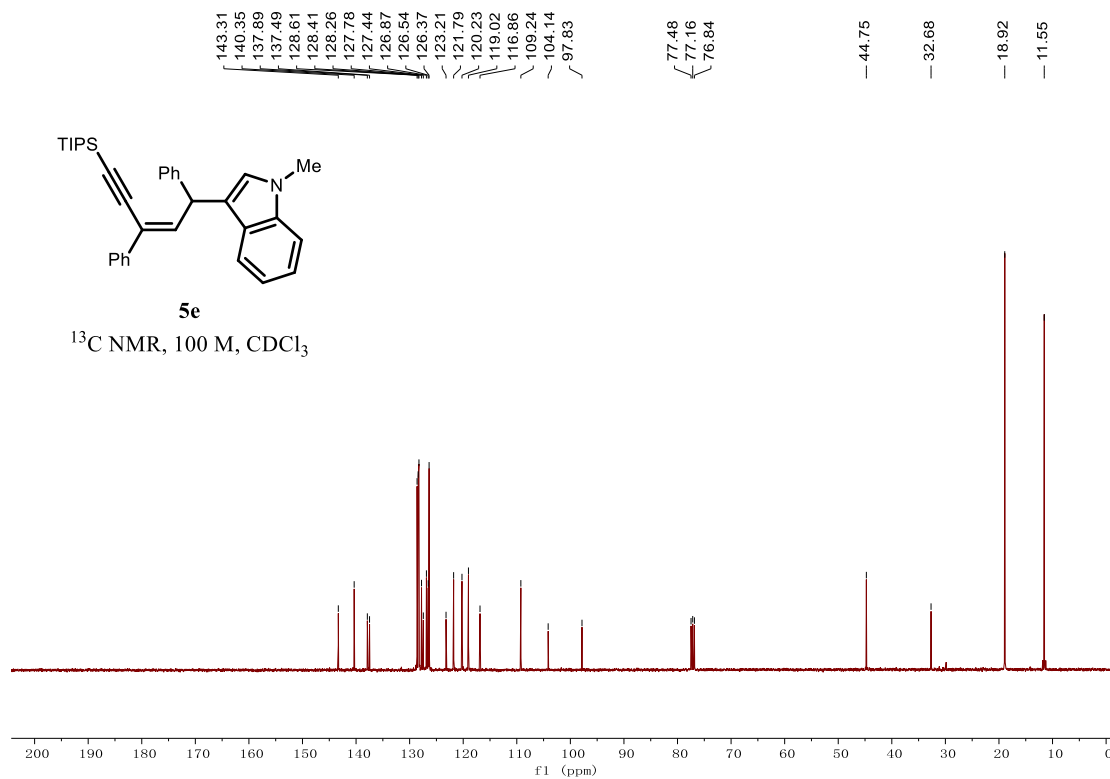
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
426.2198	426.2198	0.0	0.0	16.5	738.8	n/a	n/a	C30 H29 N Na



5e

¹H NMR, 400 M, CDCl₃





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1425 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

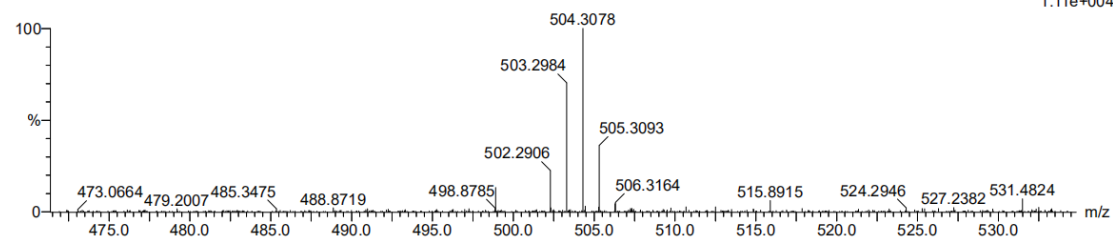
Elements Used:

C: 35-35 H: 42-42 N: 0-100 O: 0-100 Si: 1-3

46

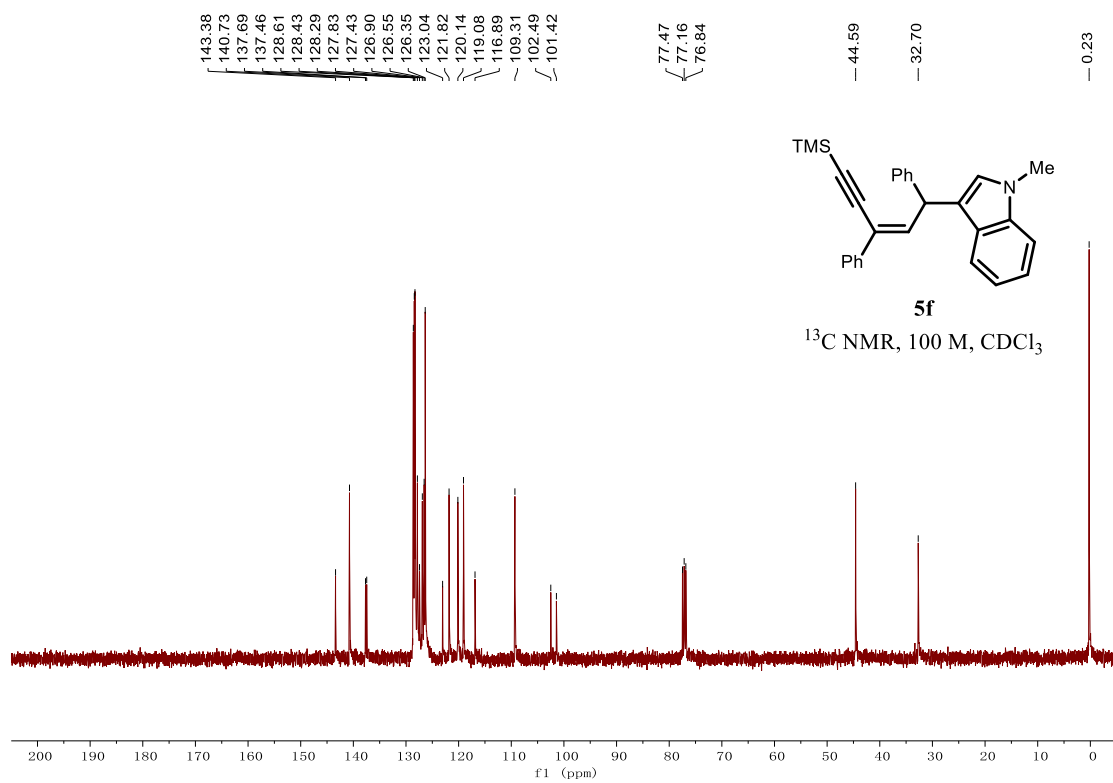
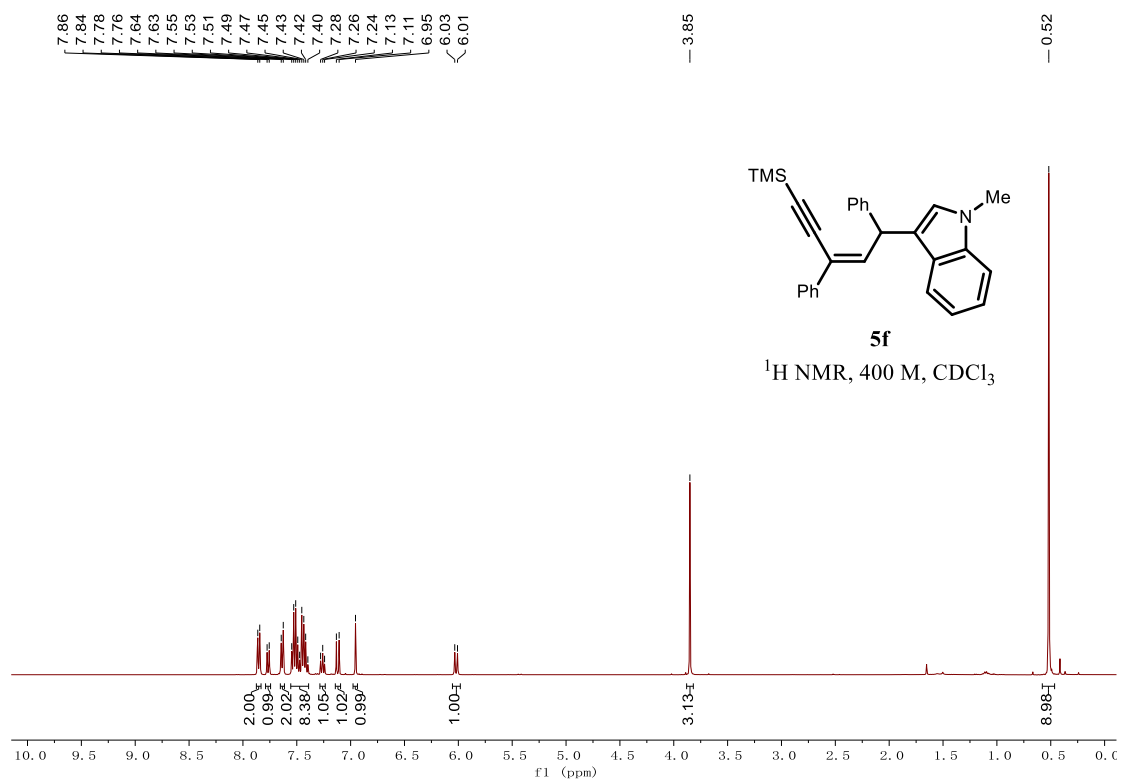
250809-1-13 26 (0.161)

1: TOF MS ES+
1.11e+004



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
504.3078	504.3087	-0.9	-1.8	16.5	208.3	n/a	n/a	C ₃₅ H ₄₂ N Si



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

20 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

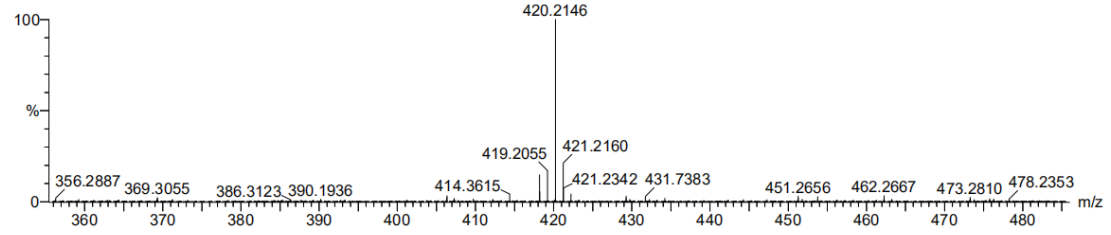
Elements Used:

C: 29-29 H: 1-60 N: 1-10 Si: 1-2

48

250511-2-71 19 (0.196)

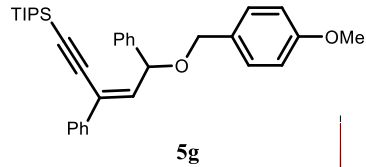
1: TOF MS ES+
9.11e+004



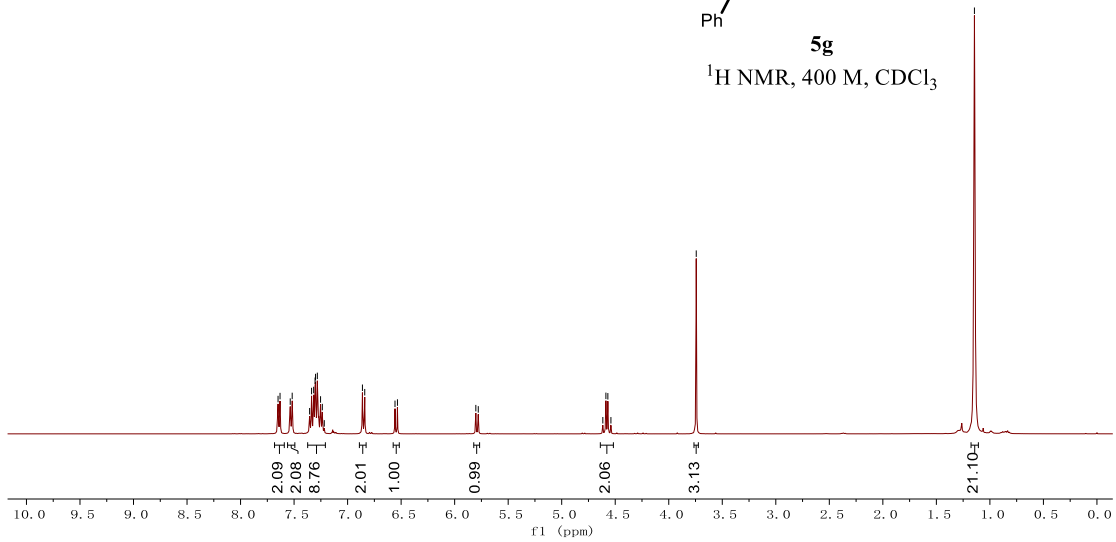
Minimum: -1.5
Maximum: 5.0 10.0 50.0

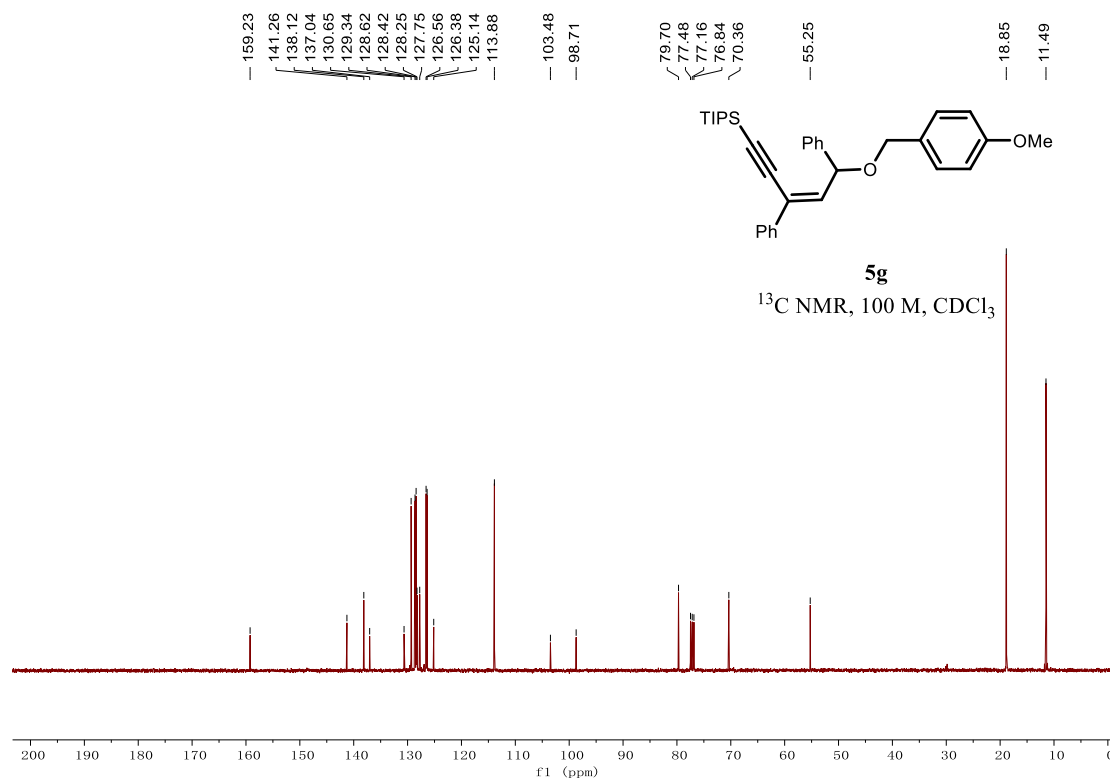
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
420.2146	420.2148	-0.2	-0.5	16.5	554.2	n/a	n/a	C29 H30 N Si

7.65, 7.63, 7.54, 7.52, 7.35, 7.34, 7.32, 7.30, 7.28, 7.25, 7.24, 7.22, 6.86, 6.84, 6.56, 6.53, 5.80, 5.78, 4.62, 4.59, 4.57, 4.54, 3.74, 1.14



¹H NMR, 400 M, CDCl₃





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4335 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

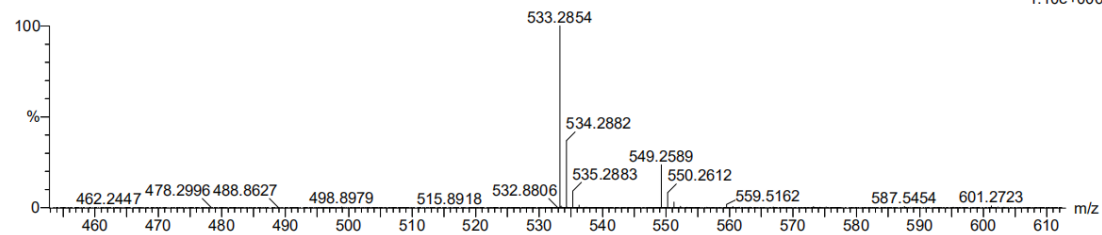
Elements Used:

C: 34-34 H: 42-42 N: 0-100 O: 0-100 Na: 0-2 Si: 1-3

46

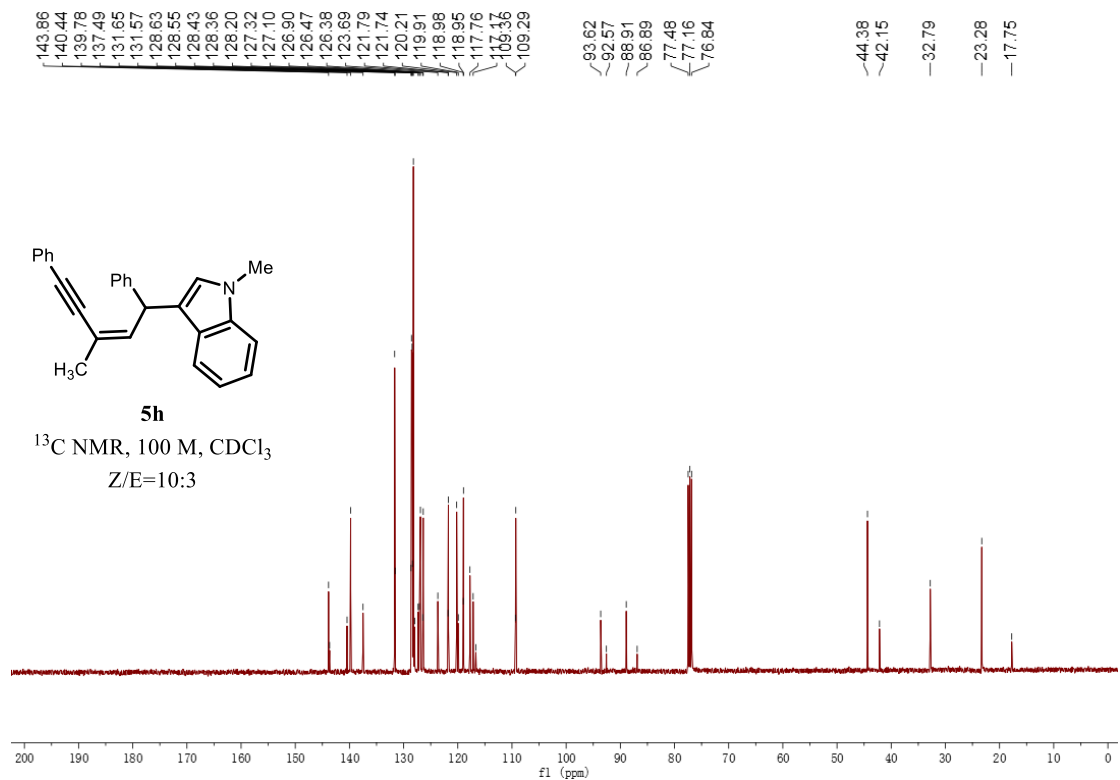
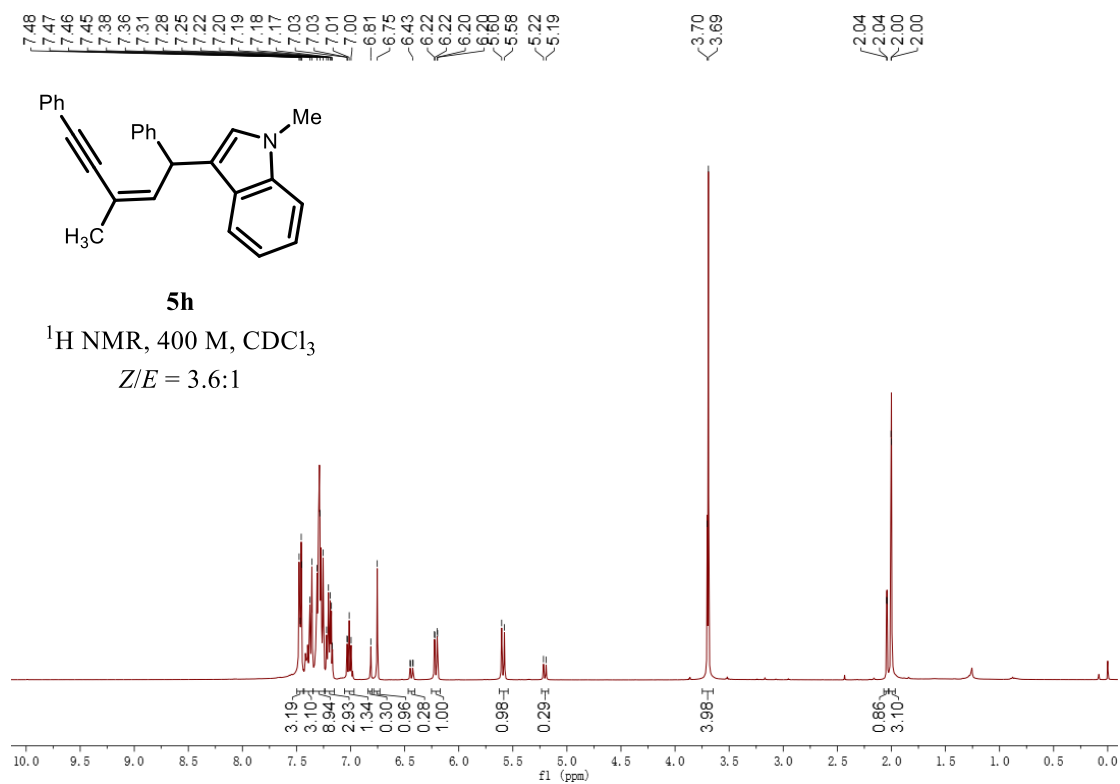
250809-1-16 28 (0.172)

1: TOF MS ES+
1.10e+006



Minimum: -1.5
 Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
533.2854	533.2852	0.2	0.4	14.5	749.3	n/a	n/a	C34 H42 O2 Na Si



HRMS spectrum

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

929 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

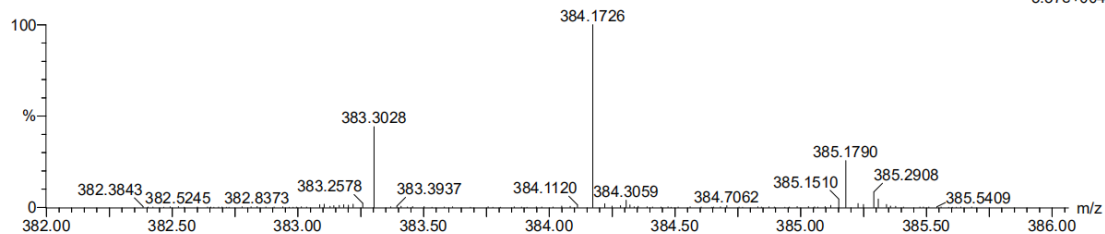
Elements Used:

C: 27-27 H: 23-23 N: 0-100 O: 0-100 Na: 0-2

7

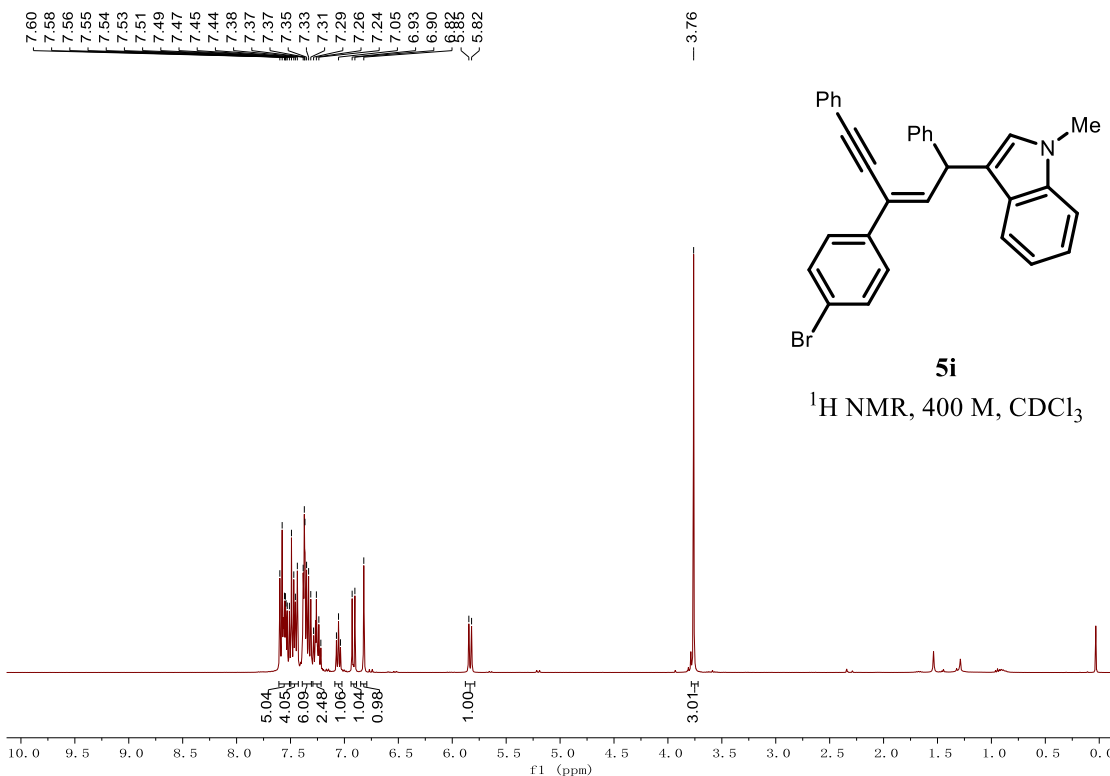
250403-12-761-2-YQZ-22 23 (0.227)

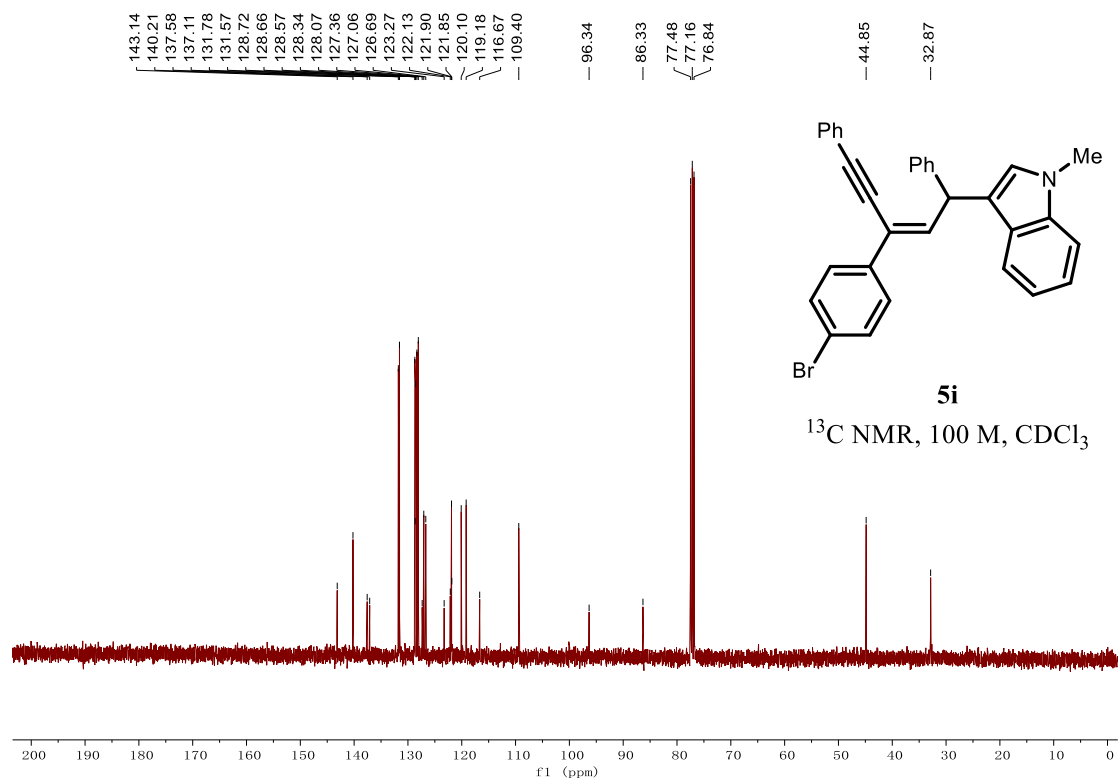
1: TOF MS ES+
5.37e+004



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
384.1726	384.1728	-0.2	-0.5	16.5	560.3	n/a	n/a	C27 H23 N Na





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

28 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

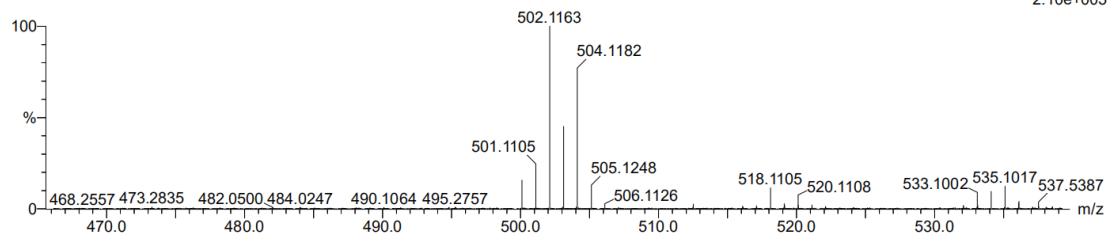
Elements Used:

C: 29-32 H: 1-60 N: 1-10 Br: 1-2

48

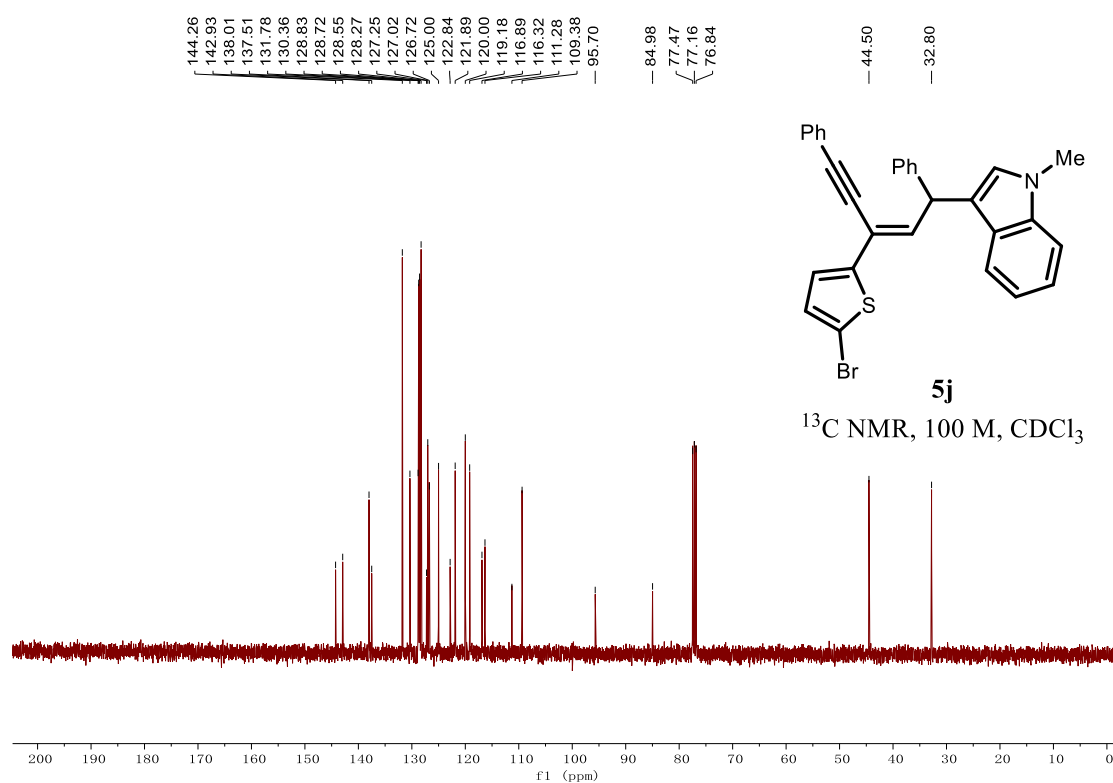
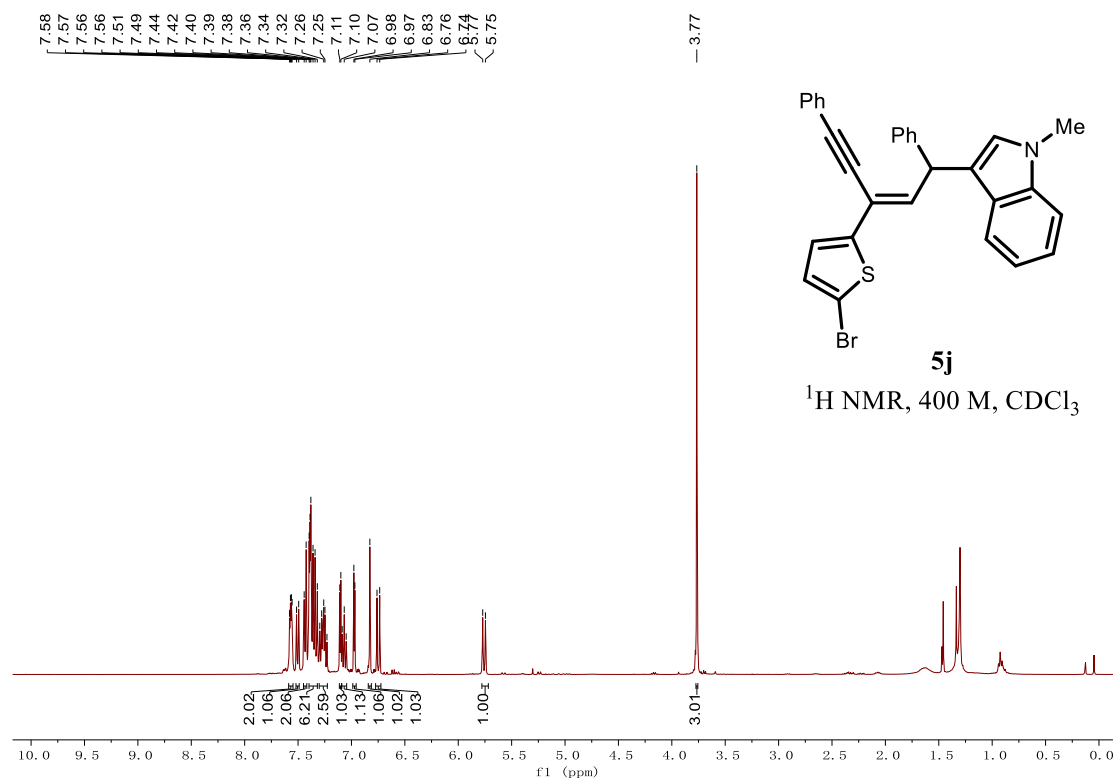
250511-2-72 10 (0.111)

1: TOF MS ES+
2.10e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
502.1163	502.1170	-0.7	-1.4	20.5	764.7	n/a	n/a	C32 H25 N Br



HRMS spectrum

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

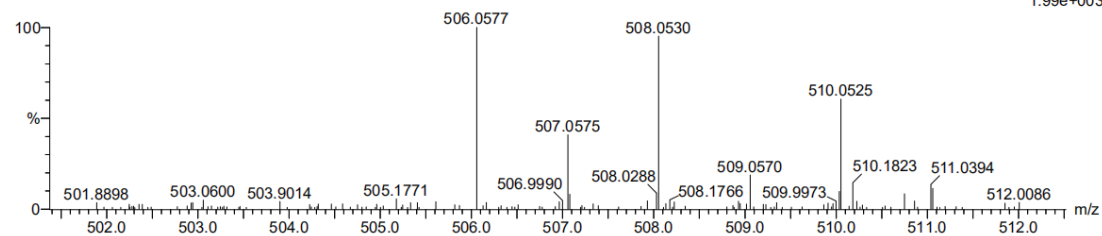
1905 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 30-30 H: 21-21 N: 0-100 O: 0-100 S: 1-4 Br: 1-2

46

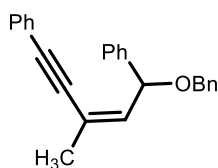
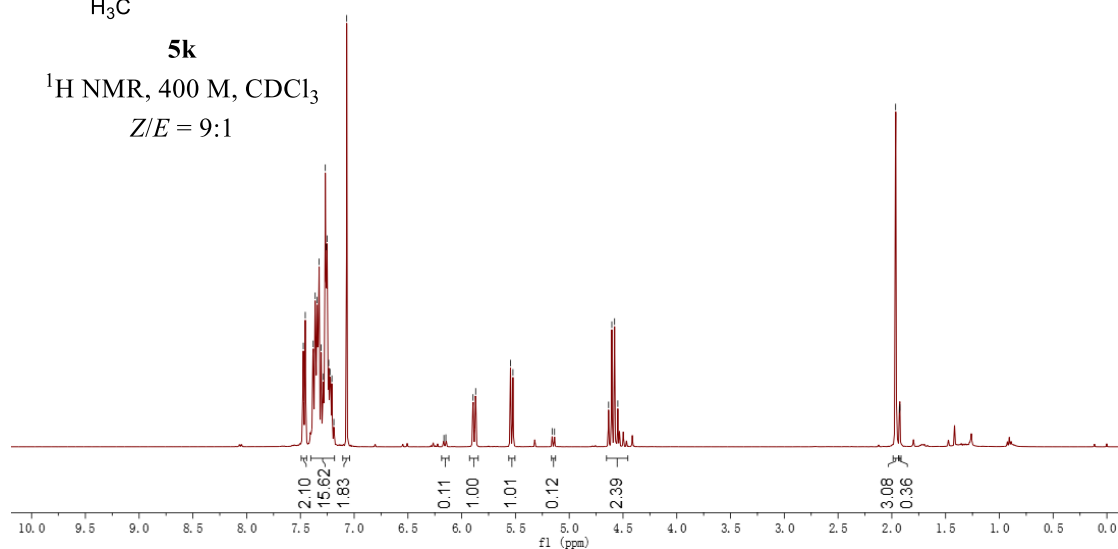
250809-1-14 7 (0.062)

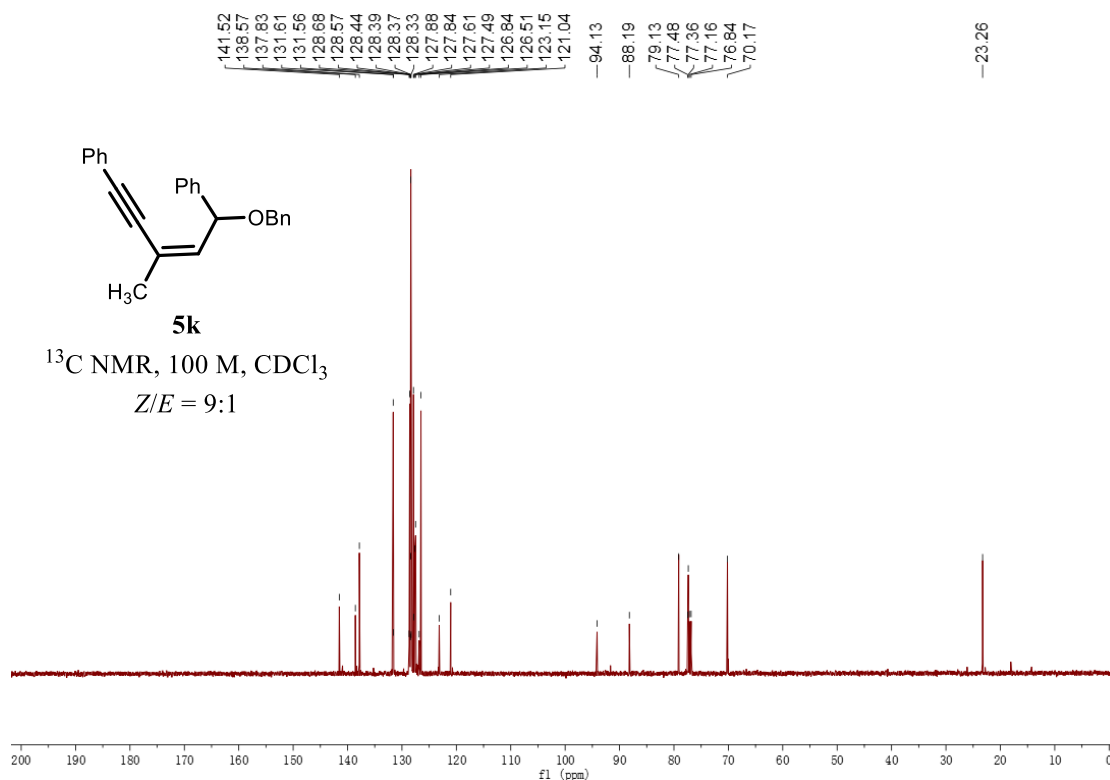
1: TOF MS ES+
1.99e+003

Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula	N	S	Br
506.0577	506.0578	-0.1	-0.2	20.5	230.5	n/a	n/a	C30 H21 N S Br			

7.47
7.45
7.38
7.36
7.34
7.33
7.31
7.29
7.27
7.26
7.25
7.24
7.22
7.21
7.19
7.07
6.17
6.15
5.89
5.87
5.55
5.52
5.16
5.14
4.63
4.60
4.58
4.55
1.96
1.93
1.92

**5k**¹H NMR, 400 M, CDCl₃*Z/E* = 9:1



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

813 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

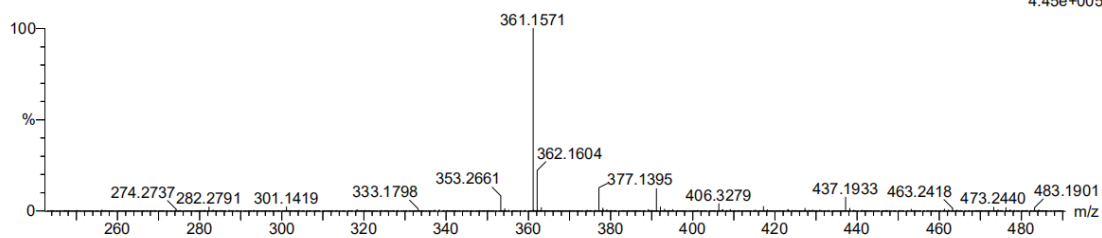
Elements Used:

C: 25-25 H: 22-22 N: 0-100 O: 0-100 Na: 0-2

46

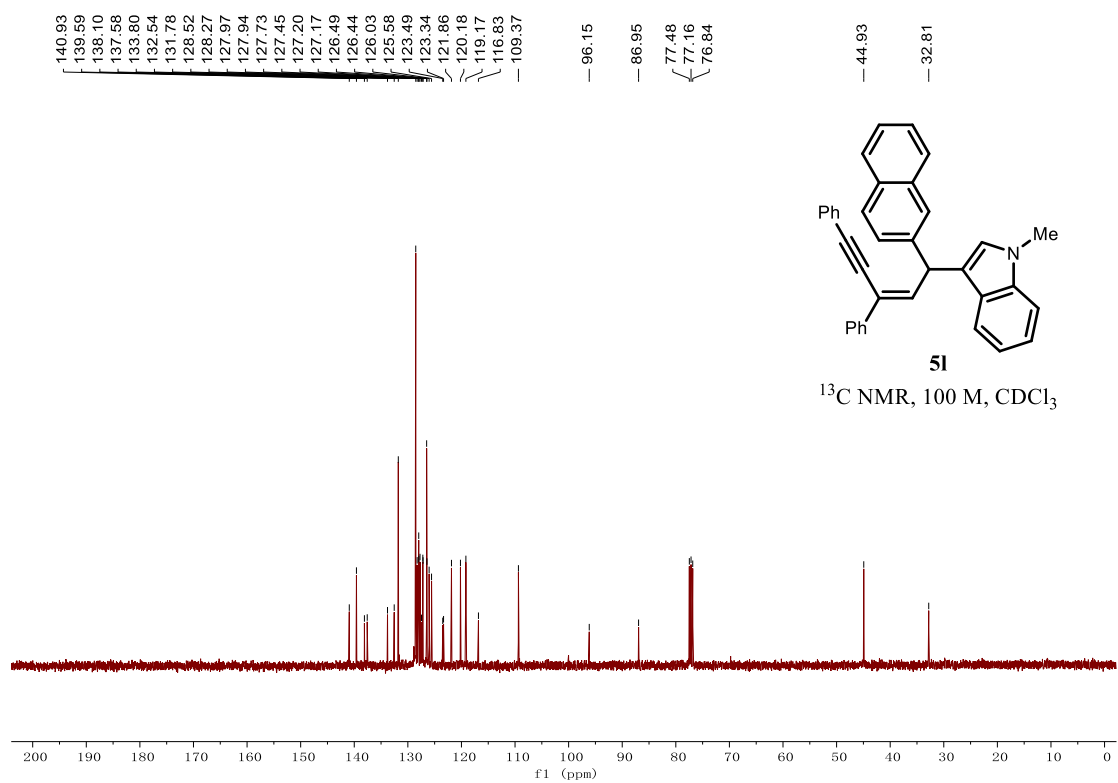
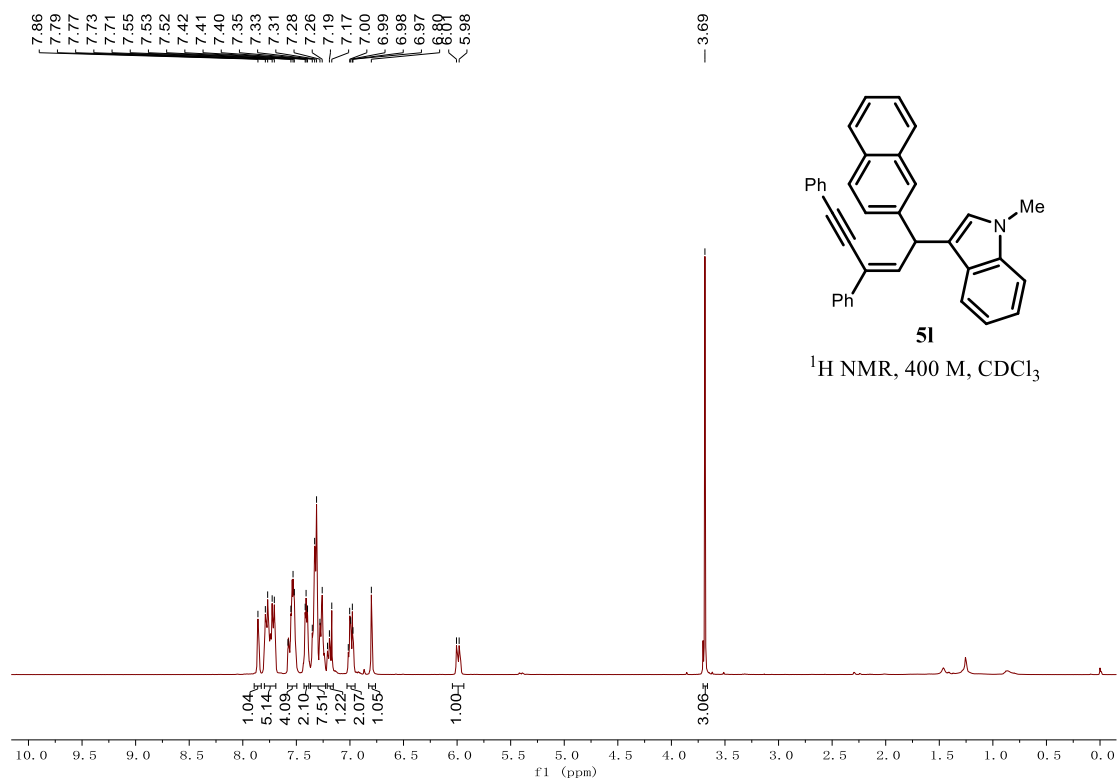
250809-1-20 13 (0.093)

1: TOF MS ES+
4.45e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
361.1571	361.1568	0.3	0.8	14.5	600.0	n/a	n/a	C ₂₅ H ₂₂ O Na



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

42 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

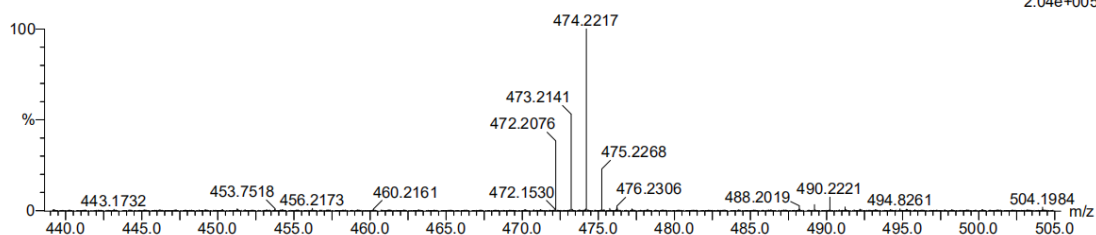
Elements Used:

C: 26-36 H: 1-60 N: 1-10

48

250511-2-70 13 (0.137)

1: TOF MS ES+
2.04e+005



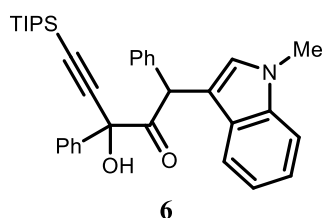
Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
474.2217	474.2222	-0.5	-1.1	23.5	714.2	n/a	n/a	C36 H28 N

7.91
7.90
7.89
7.88
7.87
7.86
7.85
7.84
7.83
7.82
7.81
7.80
7.79
7.78
7.77
7.76
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7.01
7.00
6.99
6.98
6.97
6.96
6.95
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6.93
6.92
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6.89
6.88
6.87
6.86
6.85
6.84
6.83
6.82
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6.05
6.04
6.03
6.02
6.01
6.00
5.99
5.98
5.97
5.96
5.95
5.94
5.93
5.92
5.91
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5.03
5.02
5.01
5.00

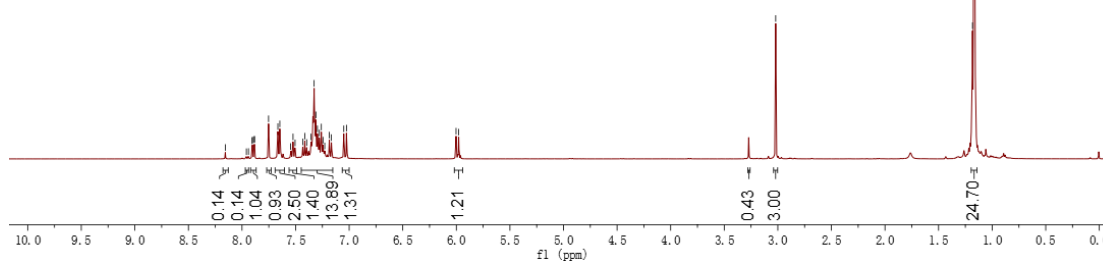
-3.02

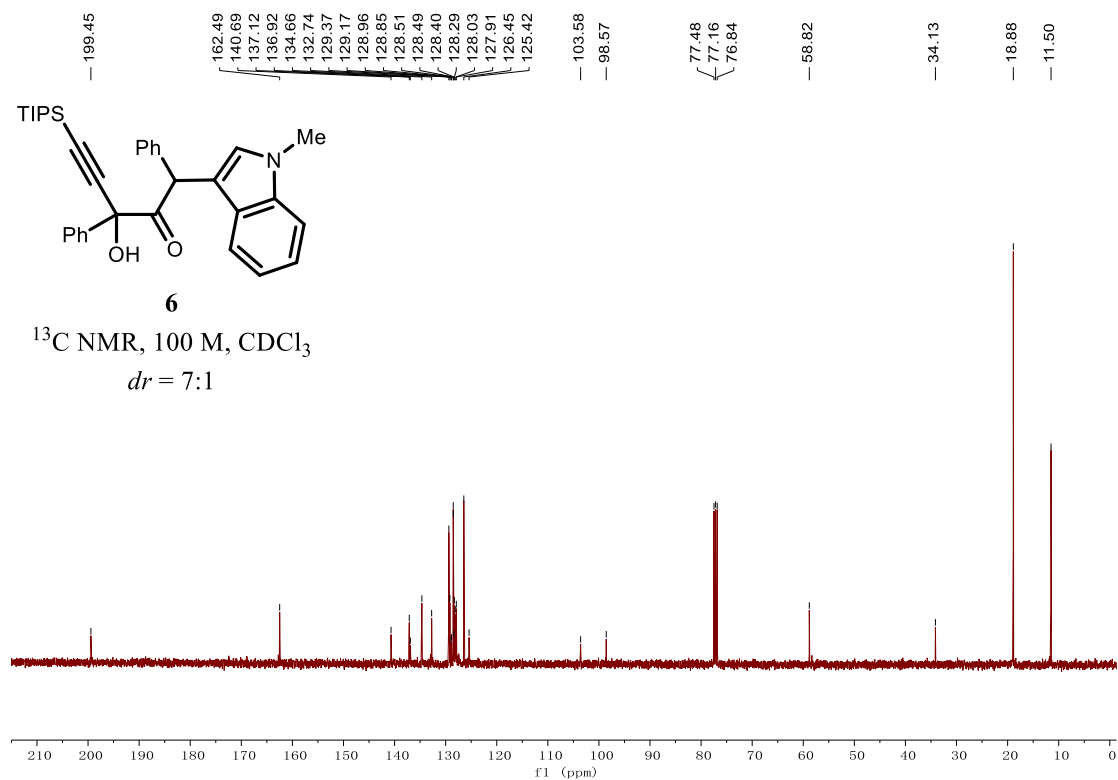
1.18
1.17
1.16



¹H NMR, 400 M, CDCl₃

dr = 7:1





HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4784 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

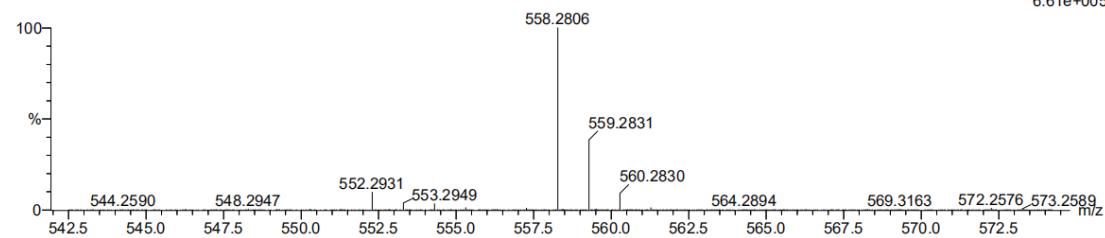
Elements Used:

C: 35-35 H: 41-41 N: 0-100 O: 0-100 Si: 1-3 Na: 0-2

46

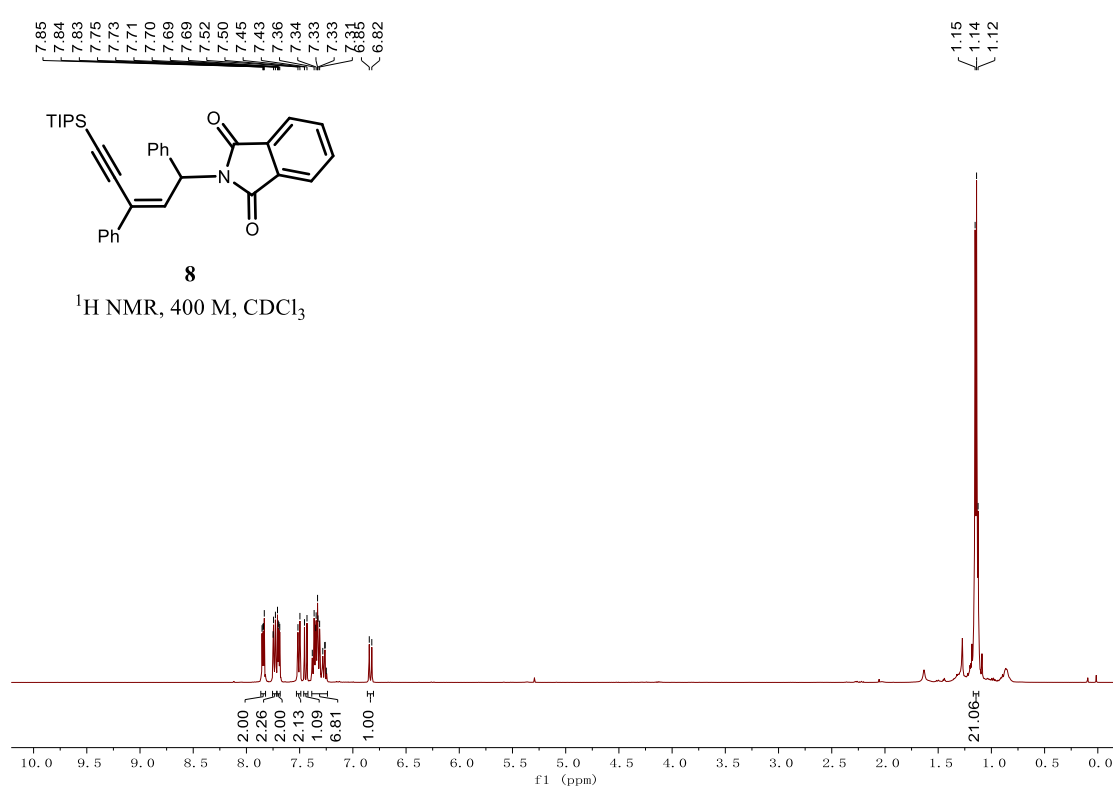
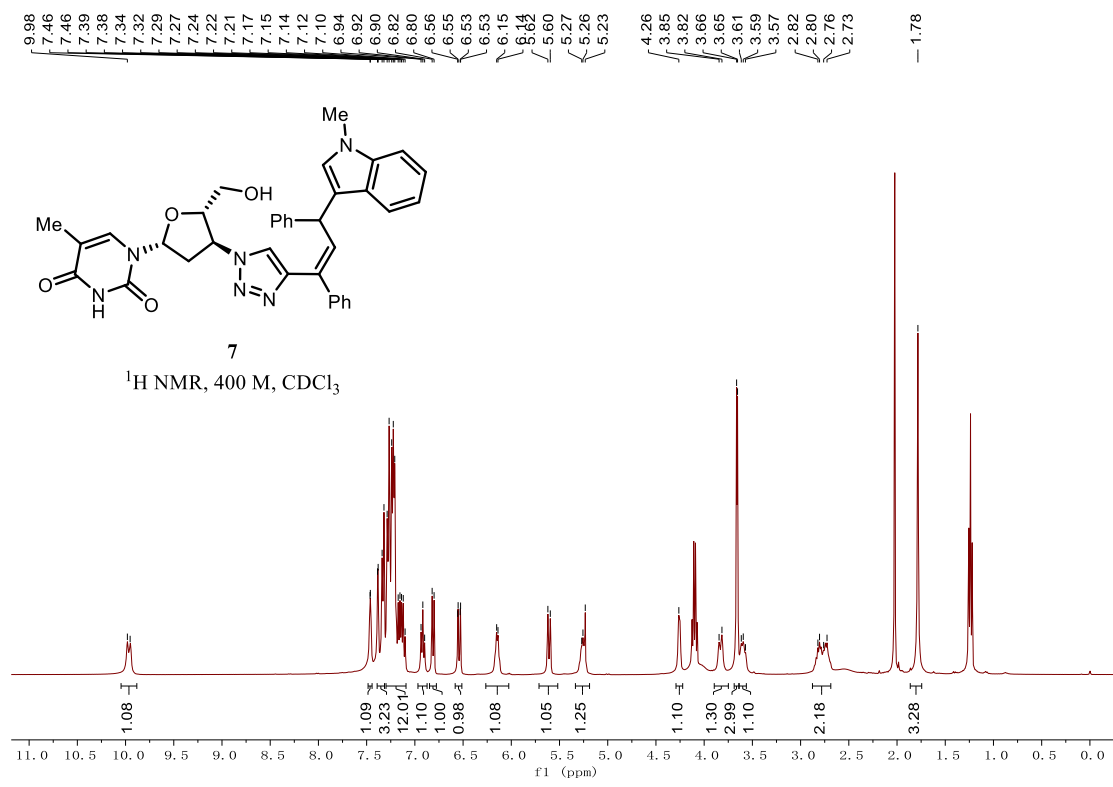
250809-1-15 16 (0.109)

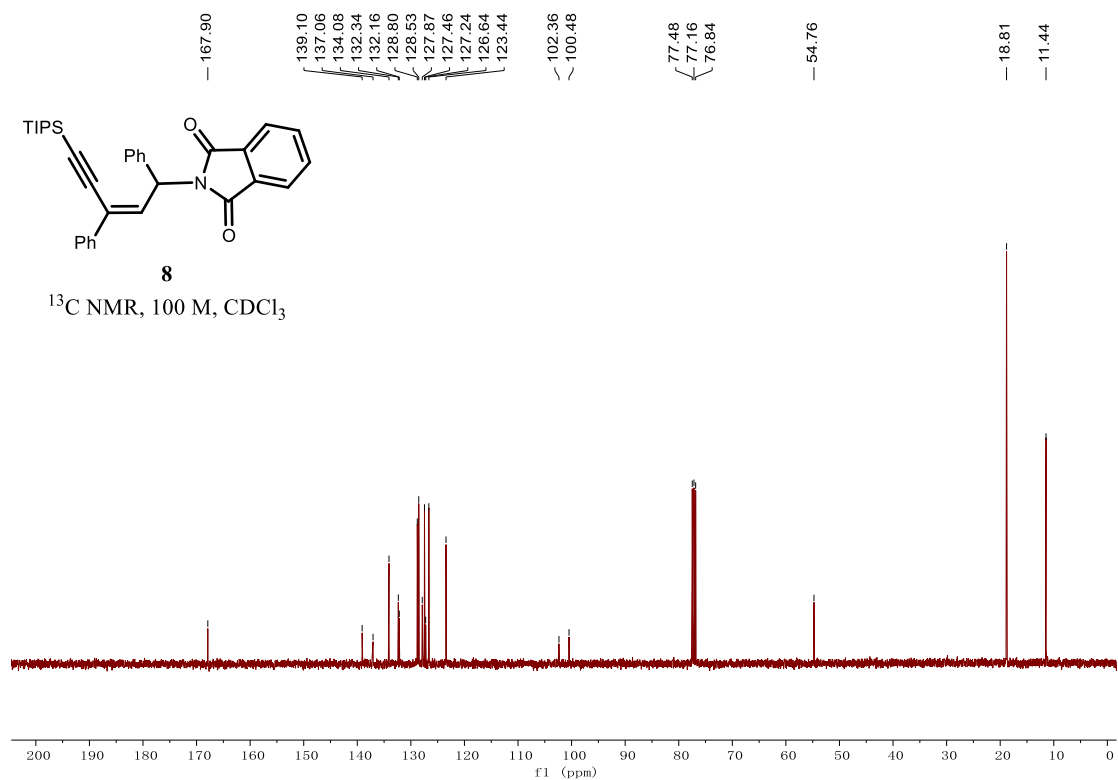
1: TOF MS ES+
6.61e+005



Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
558.2806	558.2804	0.2	0.4	16.5	741.4	n/a	n/a	C35 H41 N O2 Si Na





HRMS spectrum

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

4485 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

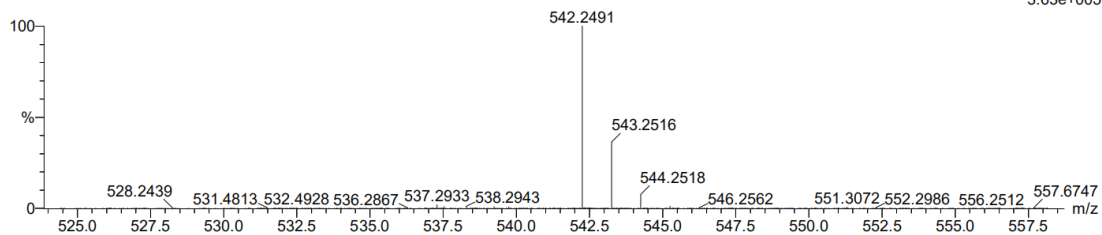
Elements Used:

C: 34-34 H: 37-37 N: 0-100 O: 0-100 Na: 0-2 Si: 1-3

46

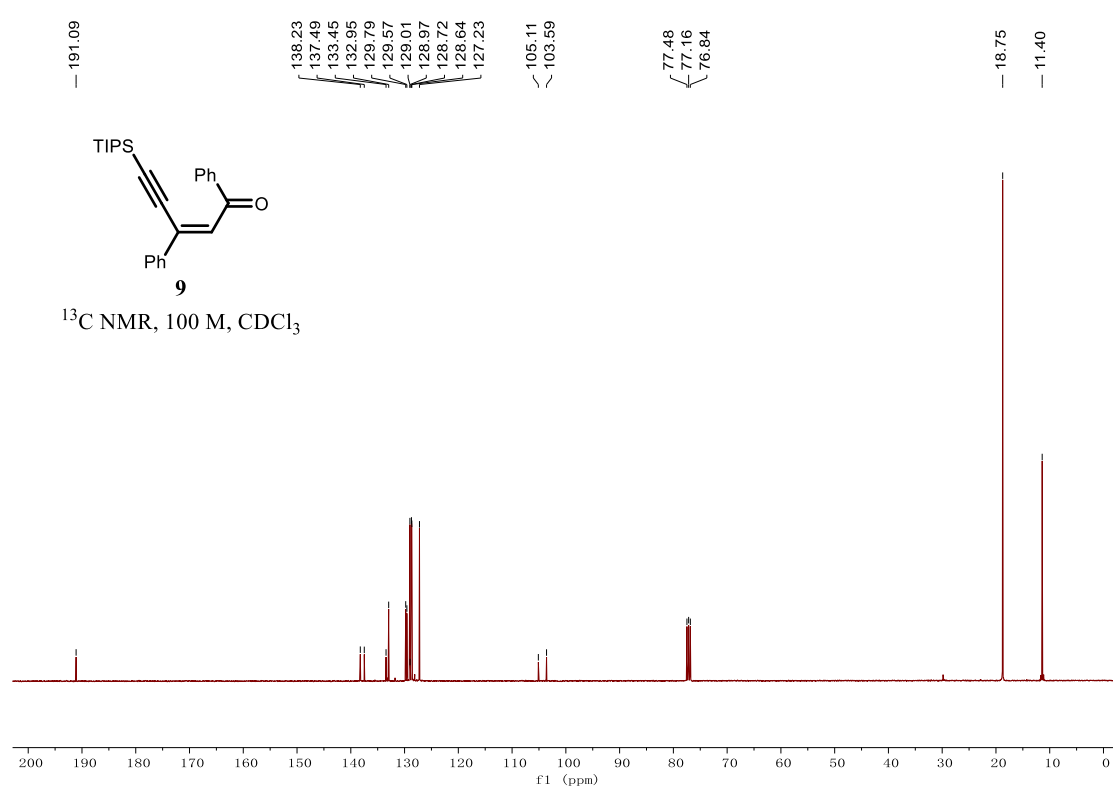
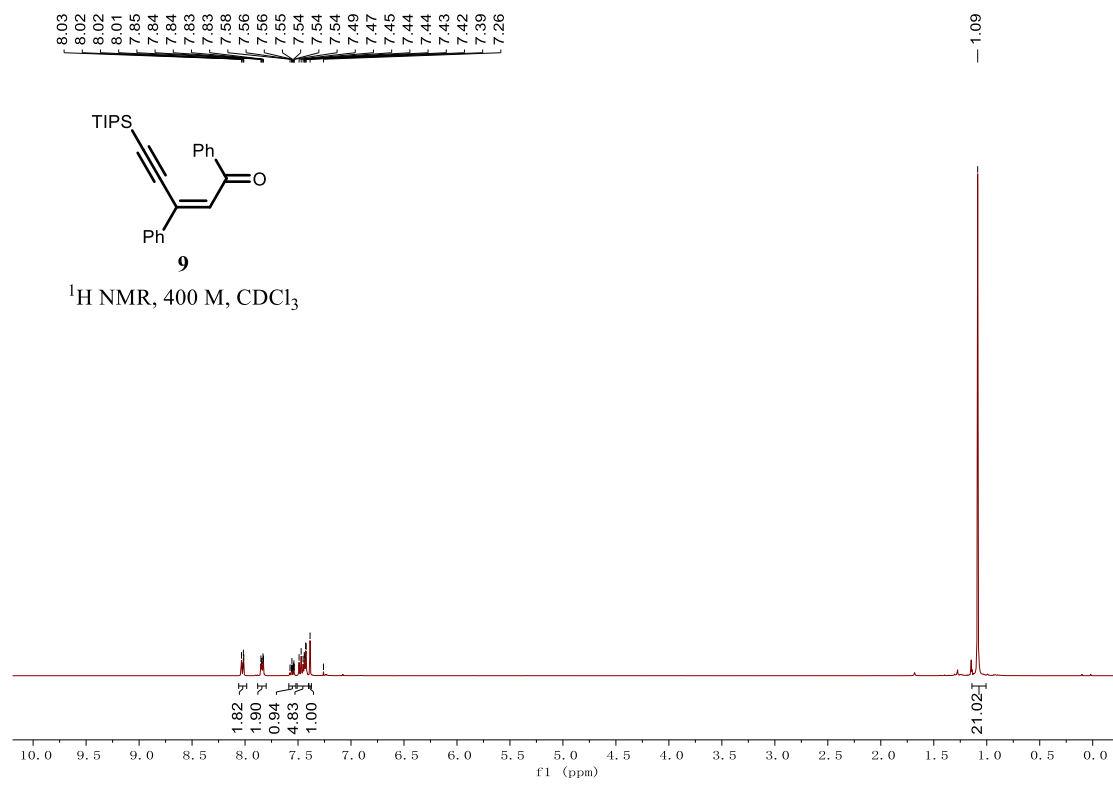
250809-1-19 24 (0.151)

1: TOF MS ES+
3.63e+005



Minimum: -1.5
Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
542.2491	542.2491	0.0	0.0	17.5	567.6	n/a	n/a	C ₃₄ H ₃₇ N ₀ O ₂ Na ₁ Si ₁



HRMS spectrum

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2124 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

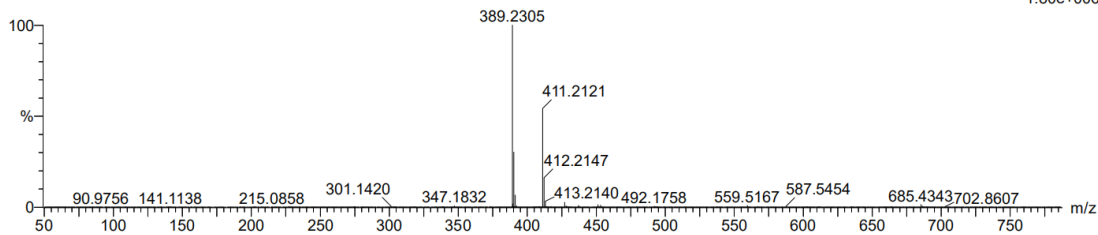
Elements Used:

C: 26-26 H: 33-33 N: 0-100 O: 0-100 Na: 0-2 Si: 1-3

46

250809-1-17 22 (0.140)

1: TOF MS ES+
1.80e+006



Minimum: -1.5

Maximum: 5.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
389.2305	389.2301	0.4	1.0	11.5	890.9	n/a	n/a	C ₂₆ H ₃₃ O Si

9 References

D. Luo, S. Niu, F. Gong, C. Xu, S. Lan, J. Liu, S. Yang, X. Fang, *ACS Catal.* 2024, **14**, 2746–2757.