**Supporting Information**

# Gold(I) catalyzed cascade cyclization: intramolecular two-fold nucleophilic addition to vinylidenecyclopropanes (VDCPs)

*Wenqing Zang,*[†] *Yin Wei,*[†] *Min Shi*[†*]

[†]State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, University of Chinese Academy of Sciences, Chinese Academy of Sciences, 345 Ling-Ling Road, Shanghai, 200032, China.

*Mshi@mail.sioc.ac.cn. Fax* 86-21-64166128

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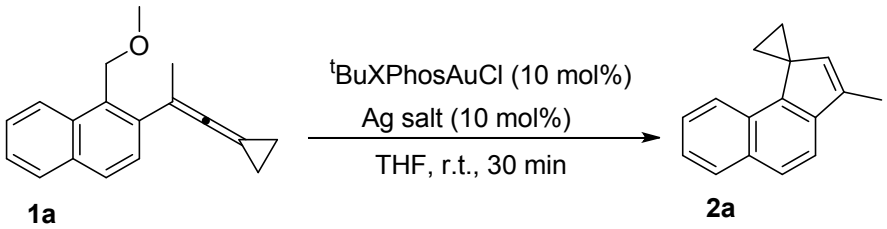
## 1. General Remarks

$^1$H NMR spectra were recorded on a Varian Mercury-300 and 400 spectrometer for solution in $CDCl_3$ with tetramethylsilane (TMS) as an internal standard; coupling constants J are given in Hz. 13C NMR spectra were recorded on a Varian Mercury-300 and 400 spectrophotometers (75 or 100 MHz) with complete proton decoupling spectrophotometers ($CDCl_3$: 77.0 ppm). Mass and HRMS spectra were recorded by EI or ESI method. GC-MS measurements were performed on a GCMS-QP2010ultra system. Organic solvents used were dried by standard methods when necessary. Infrared spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in $cm^{-1}$. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. UV-visible spectra were obtained on a Hitachi U-3900 Spectrophotometer. Fluorescence spectra for emission and excitation were obtained on a Hitachi F-2700 FL Spectrophotometer.Commercially obtained reagents were used without further purification. All these reactions were monitored by TLC with silica gel coated plates. Flash column chromatography was carried out using silica gel at increased pressure.

## 2. Identification of the Optimal Silver(I) Salt

To a flame dried, argon purged 25 mL Schlenk tube were added $^{t}$BuXPhosAuCl (0.01 mmoL) and Ag (I) (0.01 mmoL), and then 1.5 mL DCE was added. After stirring for 5 min at r.t. compound 1a (0.1 mmol) dissolved in 1.5 mL DCE was added to the reaction mixture dropwise via a syringe. The reaction mixture was stirred at room temperature for another 30 min. The yield was determined by $^{1}$H-NMR spectrum using 1,3,5-trimethoxybenzene as an internal standard. Yields are reported in Table S1.



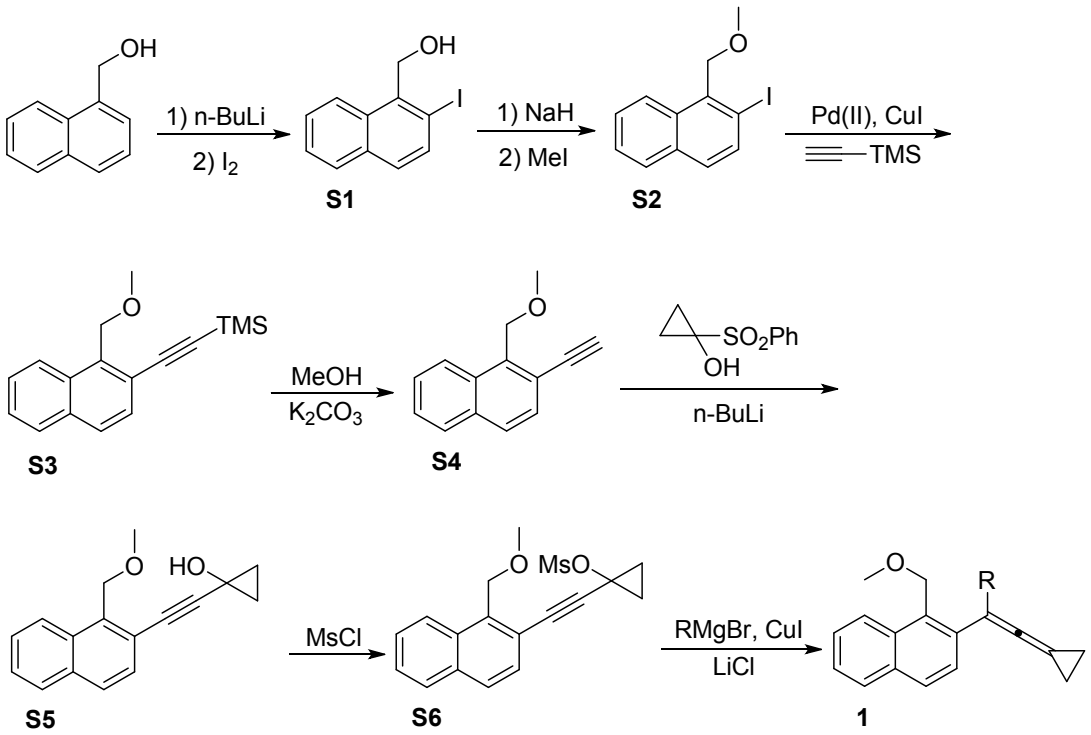

**1a** **2a**

**Table S1: Identification of the Optimal Silver(I) Salt**

| Silver salt | Yield [%][a] |
|---|---|
| $AgNTf_2$ | 13 |
| $AgSbF_6$ | N.R. |
| $AgPF_6$ | 7 |
| AgOTf | 13 |
| $AgBF_4$ | N.R. |
| AgOAc | N.R. |

[a] The yield was determined by $^{1}$H NMR spectrum using 1,3,5-trimethoxybenzene as an internal standard

**3. General Reaction Procedure.**




Representative procedure for the preparation of (2-iodonaphthalen-1-yl)methanol (S1): To a flame dried, argon purged 250 mL round-bottom flask was added $Et_2O$ (10 mL), then n-BuLi (45.8 mL, 110 mmol, 2.4 M in hexane) and TMEDA (16.5 mL, 110 mmol) was added at -78 °C. After stirring for 30 min, 1-naphthalenemethanol (7.9 g, 50 mmol) in 60 mL of $Et_2O$ was added during 40 min via a syringe at room temperature. The resulting mixture was stirred for 4 h and $I_2$ (15.2 g, 60 mmol) in 60 mL of diethyl ether was added quickly at 0 °C. Quenched by saturated aqueous $Na_2S_2O_3$, extracted by $Et_2O$ three-times (50 mL each), the combined the organic phase was dried over anhydrous $MgSO_4$. After filtration, the solution was concentrated under reduced pressure and the residue was purified by a silica gel flash column chromatography with petroleum ether-EtOAc as an eluent.

Representative procedure for the preparation of 2-iodo-1-(methoxymethyl)naphthalene (S2):

To a flame dried, argon purged round bottom flask was added 2-iodine-1-naphthalenemethanol (6 g, 21 mmol) dissolved in anhydrous THF (50 mL), and then NaH (1 g, 60 %, 25 mmol) was added in portions at 0 °C. After stirring for 1 h, MeI (1.56 mL, 25 mmol) was added slowly via a syringe. The reaction mixture was stirred at room temperature for 1 h. Quenched by water, extracted by $Et_2O$ three-times (20 mL each), the combined the organic phase was dried over anhydrous $MgSO_4$. After filtration, the solution

was concentrated under reduced pressure and the residue was purified by a silica gel flash column chromatography with petroleum ether-EtOAc as an eluent.

Representative procedure for the preparation of ((1-(methoxymethyl)naphthalen-2-yl)ethynyl) trimethylsilane (S3):

2-Iodine-1-naphthalenemethy ester (6.2 g, 21 mmol), $Pd(PPh_3)_2Cl_2$ (147 mg, 0.21 mmol) and CuI (65 mg, 0.35 mmol) were added to a flame dried, three-necked flask. Then $^{i}Pr_2NH$ (50 mL) was added to afford a yellow suspension. Ethynyltrimethylsilane (3.3 mL, 23 mmol) was added dropwise via a syringe and the resulting mixture was stirred for another 30 min at r.t. After filtration, the solution was concentrated under reduced pressure, which was directed used for the next reaction without further purification.

Representative procedure for the preparation of 2-ethynyl-1-(methoxymethyl)naphthalene (S4):

To a 250 mL round bottom flask was added **S3** in MeOH (50 mL), which was prepared by previous step. Then $K_2CO_3$ (5.5g, 40 mmol) was added and the resulting mixture was stirred for 2 h at r.t. After filtration, the solution was concentrated under reduced pressure and the residue was purified by a silica gel flash column chromatography with petroleum ether-EtOAc as an eluent.

Representative procedure for the preparation of 1-((1-(methoxymethyl)naphthalen-2-yl)ethynyl) cyclopropan-1-ol (S5):

To a flame dried, argon purged three-necked flask (marked as flask 1) was added **S4** (3.4 g, 17 mmol) dissolved in THF (50 mL). To another flame dried, argon purged three-necked flask (marked as flask 2) was added 1-(phenylsulfonyl)cyclopropanol (3.76 g, 19 mmol) dissolved in THF (50 mL). The two flasks were set in a dry ice-acetone bath and cooled down to -78 $^{o}$C. When the temperature reached, *n*-BuLi (7.9 mL, 2.4 M/L in hexane) was added dropwise to each of the flasks via syringes at the same temperature. The reaction mixtures were stirred at that temperature for 2 h. Then, the resulting mixture in flask 1 was transferred to flask 2 and the reaction vessel was removed from the bath and naturally warmed to room temperature. The reaction mixture was stirred at room temperature for 4 h. After that, the resulting dark mixture was quenched with water (20 mL) and extracted with ethyl acetate (45 mL) three times. The organic phase was concentrated under reduced pressure and the residue was purified by a silica gel flash column chromatography with petroleum ether-EtOAc as an eluent.

Representative procedure for the preparation of 1-((1-(methoxymethyl)naphthalen-2-yl)ethynyl) cyclopropyl methanesulfonate (S6):

To a flame dried, argon purged round bottom flask was added **S5** (3.68 g, 14.6 mmol), dissolved in dry dichloromethane (50 mL), then freshly redistilled triethylamine (3.1 mL, 22 mmol) was added. The reaction mixture was stirred and cooled down to 0 $^{o}$C with an ice-water bath. When the temperature reached, methanesulfonyl chloride (1.35 mL, 17.5 mmol) was added dropwise into the flask via a syringe. The reaction mixture was further stirred for 1 h. After that, the reaction was quenched by the addition of water (10 mL) and the organic mixture was extracted with dichloromethane (30 mL) three times. The organic phase was concentrated under reduced pressure and the residue was purified by a silica gel flash column chromatography with petroleum ether-EtOAc as an eluent.

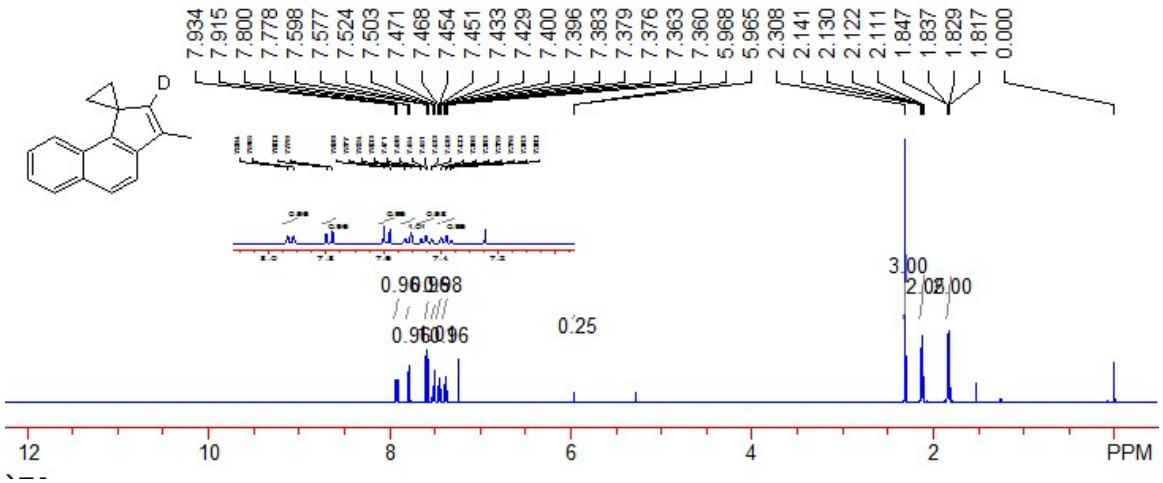
Representative procedure for the synthesis of substrates 1:

To a flame dried, argon purged Schlenk tube was added LiCl (126 mg, 3.0 mmol), heated vigorously, evacuated to dry, and purged with argon three times. Then CuI (570 g, 3.0 mmol) was added into the reaction vessel under argon. The reaction tube was set into a ice-water bath and was added with THF (8 mL) to generate a white suspension. Grignard reagent (3.0 mmol) was added and the reaction mixture was stirred for 30 min. After that, **S6** (1.0 mmol) dissolved in THF (10 mL) was added into the reaction tube. The reaction was carried out at 0 $^{o}$C for several hours. After that, the reaction mixture was concentrated under reduced pressure and the residue was purified by a silica gel flash column chromatography with petroleum ether-EtOAc as an eluent.

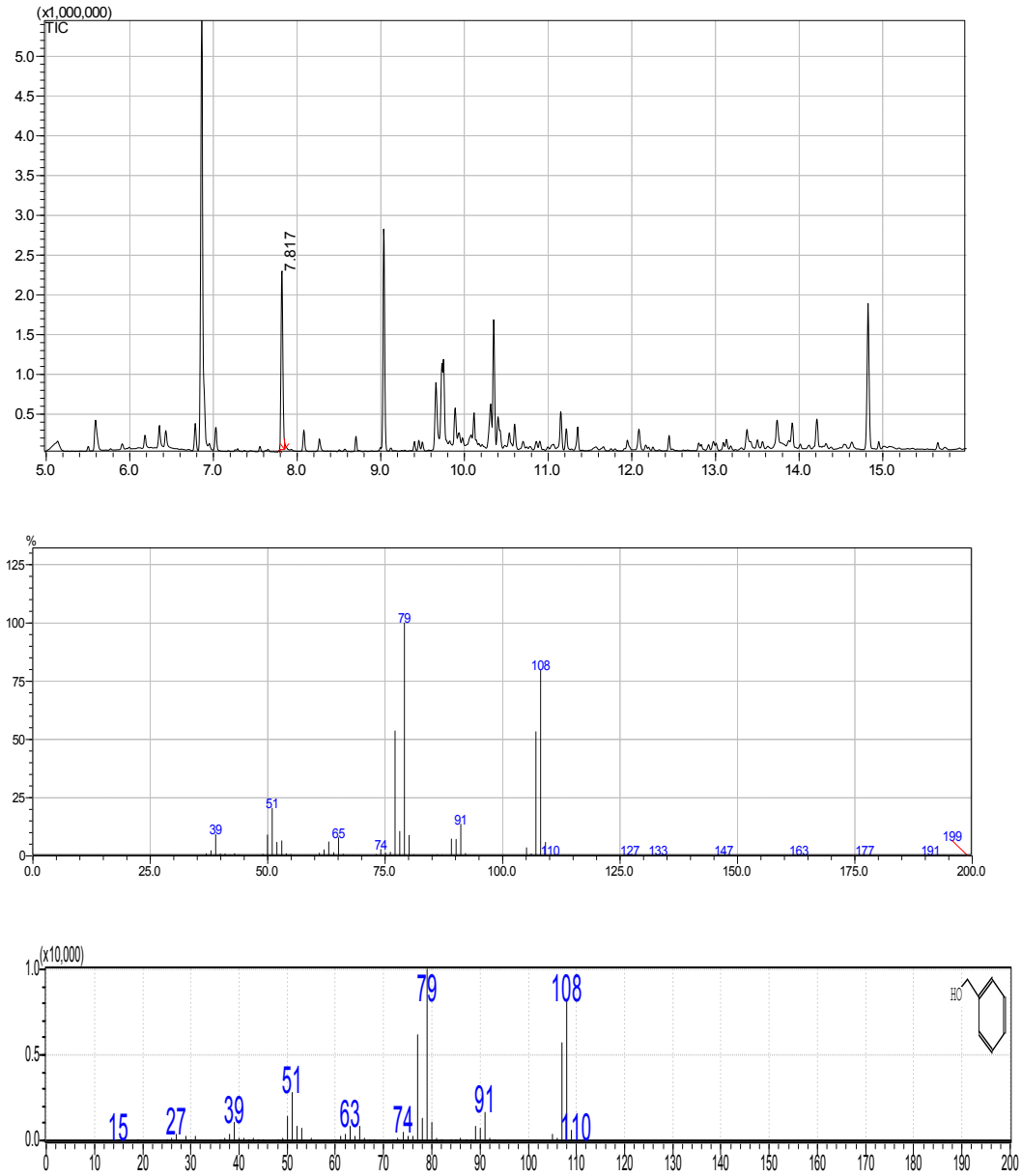
## 4. Mechanism Experiment

### 4.1 Deuterium Labeling Experiment

**Synthesis of product 2a-D:** To a 25 mL over-dried round-bottom flask were added IPrAuNTf$_2$ (0.02 mmol), 18 mg $D_2O$ under argon atmosphere, and then compound **1a** (0.2 mmol) dissolved in MTHF (6 mL) was added. The reaction mixture was stirred at room temperature for 6 hour. After that, the reaction mixture was concentrated under reduced pressure and the residue was purified by a silica gel flash column chromatography with petroleum ether as an eluent to afford the desired product in 41% yield (17 mg, D% = 75%).

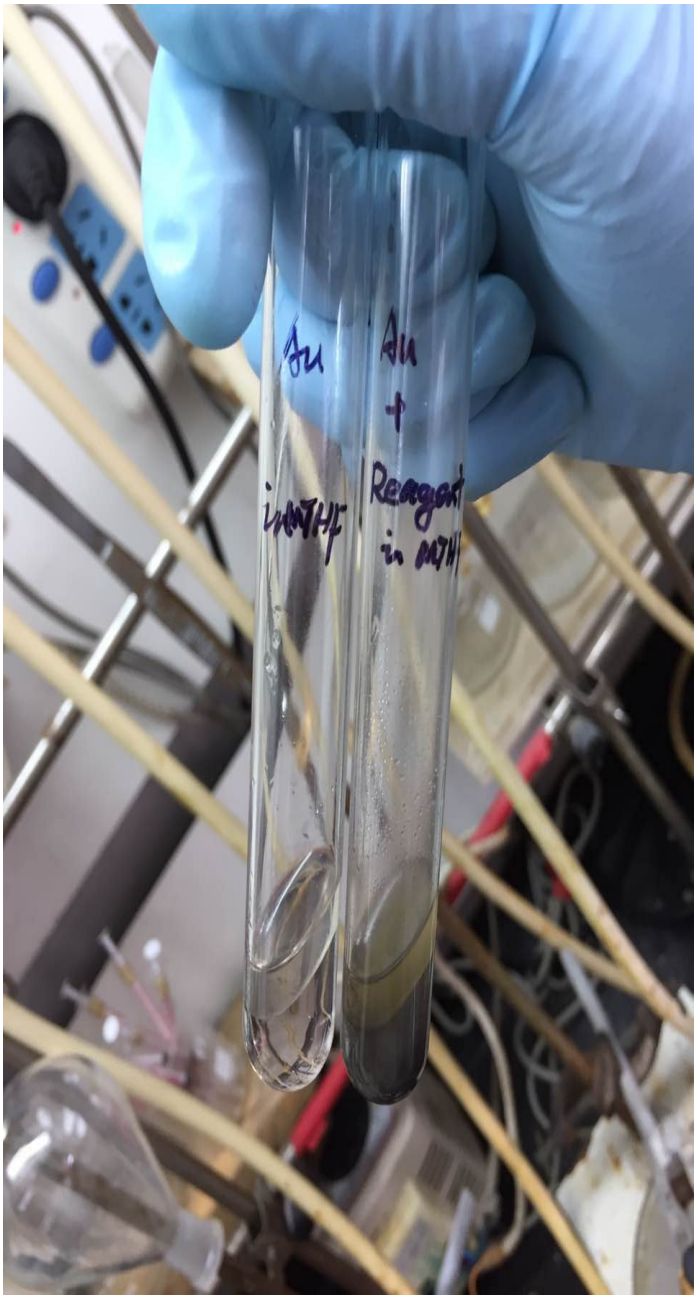


## 4.2 GC-MS Data of 1r in the Reaction Mixture




**Scheme S1.** The chromatogram of the reaction mixture of **1r** by GC-Mass (first), and the mass spectrum of the finding peak of **benzyl alcohol** in the sample (second) againt standard compound mass spectrum of **benzyl alcohol** (third)

### 4.3 Detection of HC(O)H



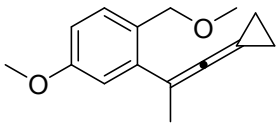
**Preparation of Tollens reagent**: To a clean 10 mL tube was added 2% $AgNO_3$ aq. solution (1.0 mL) followed by two drops of 10% NaOH aq., and then precipitates appeared. Then 2% $NH_3 \bullet H_2O$ was added dropwise while shaking the tube till the precipitates were dissolved. This reagent was prepared for the next testing.

**Procedure for the test of reaction mixture**: To a 8 mL glass vail with a septum cap were added $IPrAuNTf_2$ (0.02 mmol) and compound **1a** (0.2 mmol) dissolved in MTHF (4 mL). The reaction mixture was stirred at room temperature for 4 hour until all of the reagents were consumed completely (detected by TLC). Then, 1.0 mL of reaction mixture was sucked up and was added into the Tollens reagent dropwise. When the tube was put in a 40 $^oC$ oil bath for 5 min, **black suspension in water phase appeared (Right tube)**.

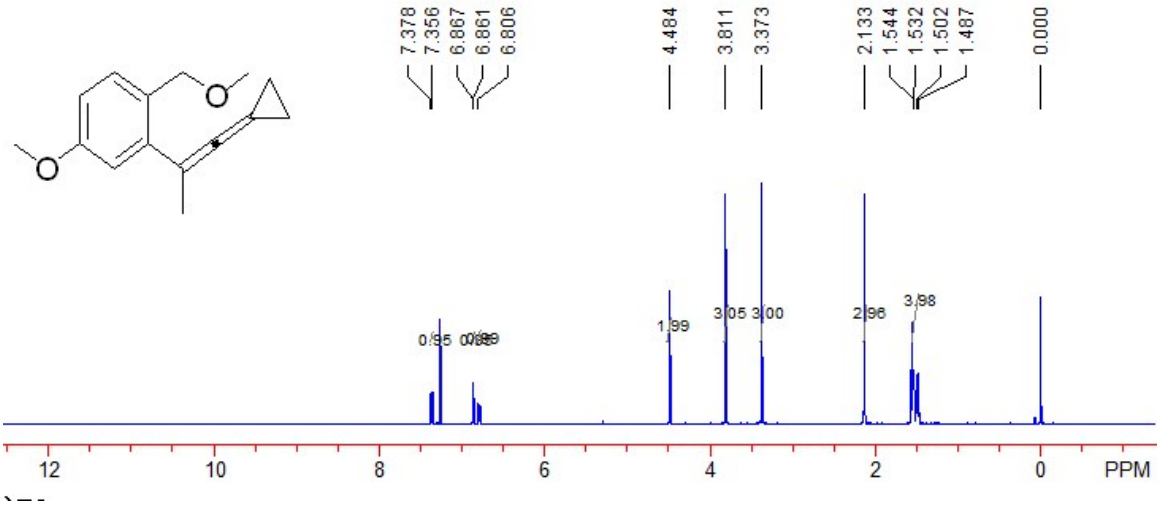
**Procedure for the test of the reaction mixture without 1a**: To a 8 mL vail with a septum cap was added $IPrAuNTf_2$ (0.02 mmoL) dissolved in MTHF (4 mL). The mixture was stirred at room temperature for 4 hour. Then, 1.0 mL mixture was sucked up and was added into the Tollens reagent dropwise. When the tube was put in 40 $^oC$ oil bath for 5 min, **no obvious phenomenon was observed (Left tube)**.

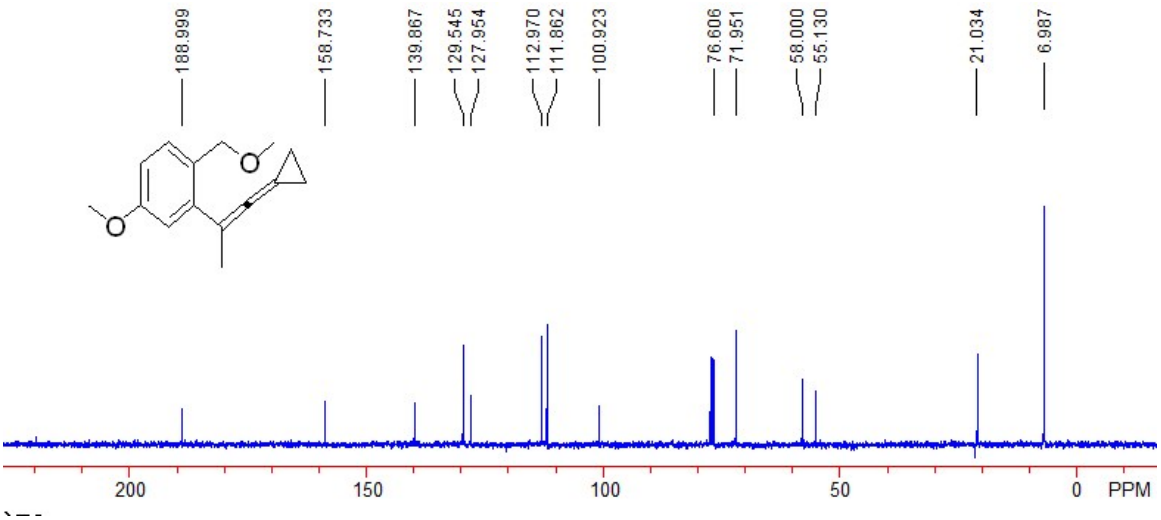
**Scheme S2. The reaction mixture for silver mirror reaction**

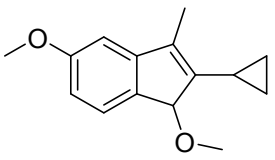
## 5. Spectroscopic Data



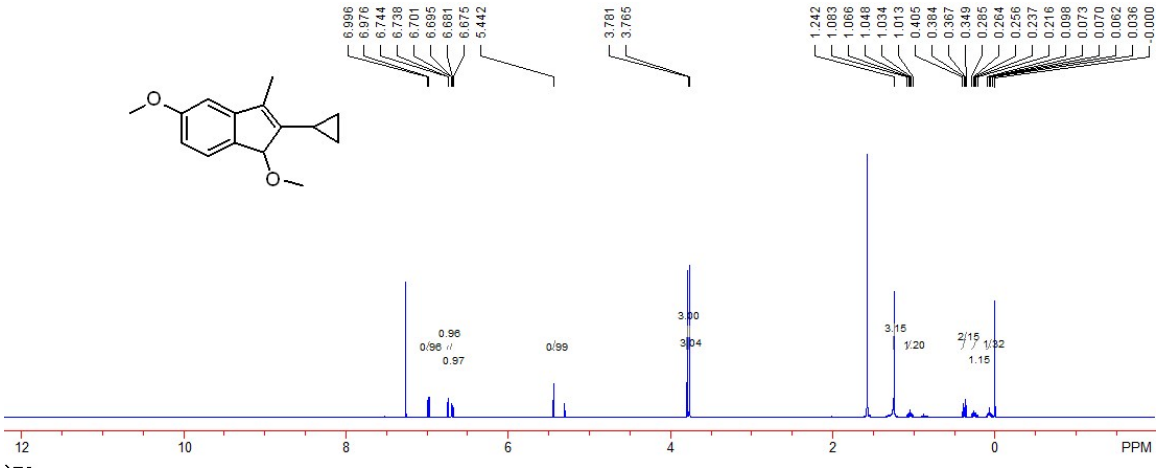
Compound **C**: 230 mg, yield: 99%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.48-1.55 (m, 4H, $2CH_2$), 2.13 (s, 3H, $CH_3$), 3.37 (s, 3H, $CH_3$), 3.81 (s, 3H, $CH_3$), 4.48 (s, 2H, $CH_2$), 6.77-6.81 (m, 2H, Ar), 6.86-6.87 (m, 1H, Ar), 7.37 (d, $J$ = 8.8 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.0, 21.0, 55.1, 58.0, 72.0, 76.6, 100.9, 111.9, 113.0, 128.0, 129.5, 139.9, 158.7, 189.0. IR (neat) ν 2982, 2912 2835, 2014, 1605, 1493, 1311, 1201, 1093, 729 cm$^{-1}$. MS (%) m/e 230 ($M^+$, 8.26), 215 (29.13), 202 (100.00), 185 (32.46), 159 (40.44), 153 (31.35), 141 (34.72), 128 (40.63), 115 (51.03). HRMS (EI) calcd. for $C_{15}H_{18}O$: 230.1307, Found: 230.1310.

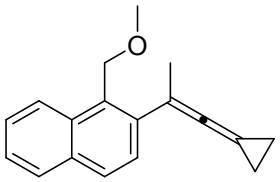


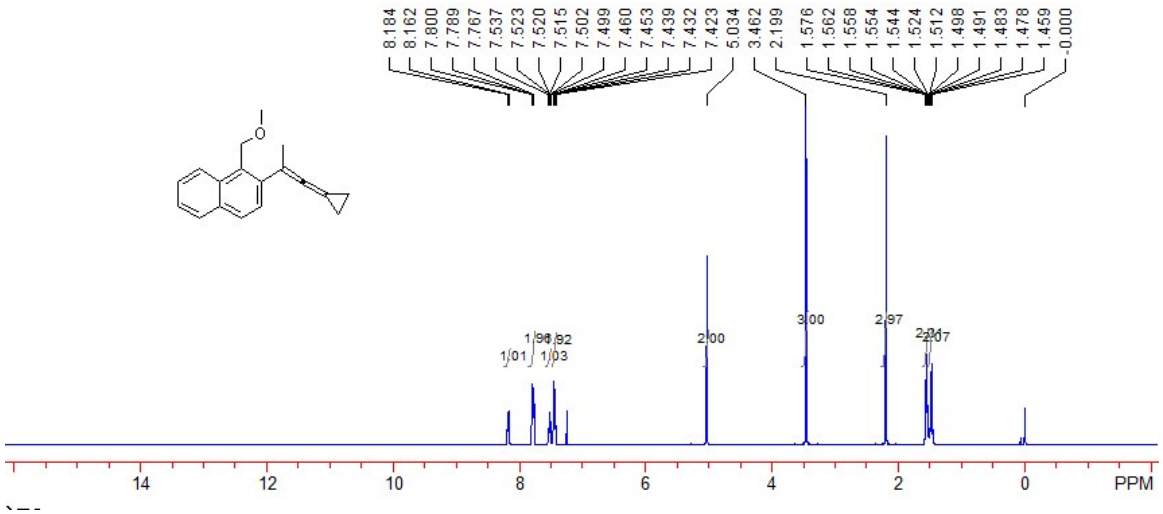



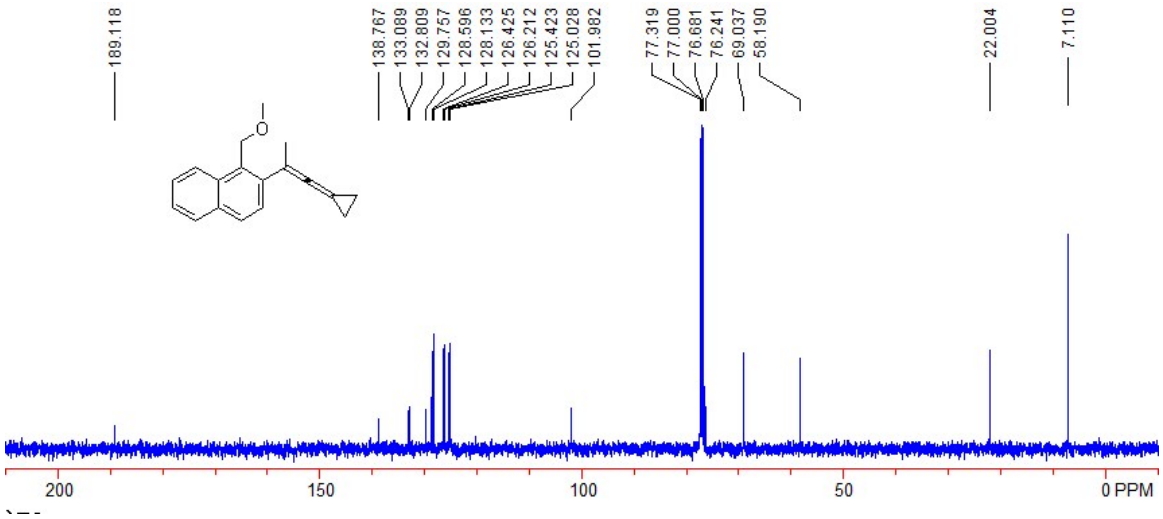
Compound **D**: 1.3 mg, yield:6%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.03-0.10 (m, 1H, $CH_2$), 0.21-0.29 (m, 1H, $CH_2$), 0.34-0.41 (m, 2H, $CH_2$), 1.01-1.09 (m, 1H, CH), 1.24 (s, 3H, $CH_3$), 3.77 (s, 3H, $CH_3$), 3.78 (s, 3H, $CH_3$), 5.44 (s, 1H, CH), 6.67-6.71 (m, 2H, Ar), 6.74 (d, *J* = 2.4 Hz, 1H, Ar), 6.99 (d, *J* = 8.0 Hz, 1H, Ar). IR (neat) ν 2953, 2922, 2852, 1605, 1462, 1377, 1153, 1025, 949, 811 cm$^{-1}$. MS (%) m/e 230 ($M^+$, 100.00), 231 (18.02), 215 (46.41), 202 (19.27), 191 (16.07), 189 (20.57), 187 (26.09), 159 (22.08). HRMS (EI) calcd. for $C_{15}H_{18}O_2$: 230.1307, Found: 230.1306.

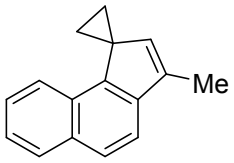


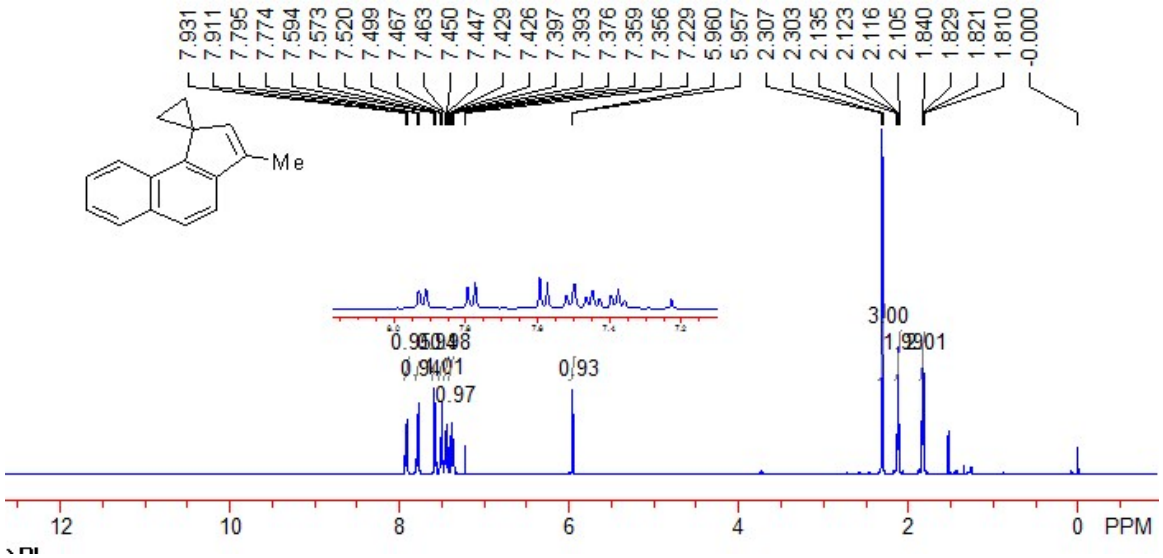
Compound **1a**. 250 mg, yield: 99%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.45-1.50 (m, 2H, $CH_2$), 1.52-1.58 (m, 2H, $CH_2$), 2.20 (s, 3H, $CH_3$), 3.46 (s, 3H, $CH_3$), 5.03 (s, 2H, $CH_2$), 7.42-7.46 (m, 2H, Ar), 7.49-7.53 (m, 1H, Ar), 7.76-7.80 (m, 2H, Ar), 8.17 (d, *J* = 8.8 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 22.0, 58.2, 69.0, 76.2, 102.0, 125.0, 125.4, 126.2, 126.4, 128.1, 128.6, 129.8, 132.8, 133.1, 138.8, 189.1. IR (neat) ν 3048, 2980, 2806, 2016, 1459, 1184, 1091, 953, 847, 746 cm$^{-1}$. MS (%) m/e 250 ($M^+$, 25.34), 235 (65.37), 222 (100.00), 207 (51.41), 203 (71.74), 202 (83.76), 191 (52.99), 189 (53.58), 178 (56.62). HRMS (EI) calcd. for $C_{18}H_{18}O$: 250.1358, Found: 250.1357.

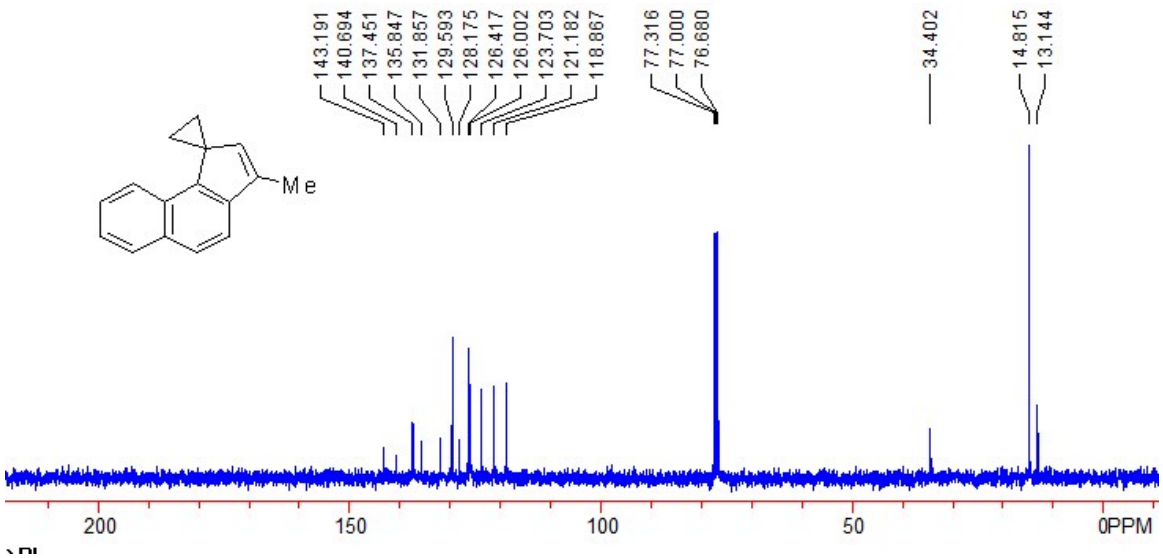


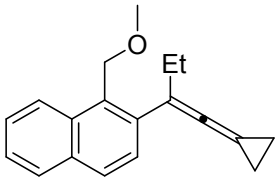



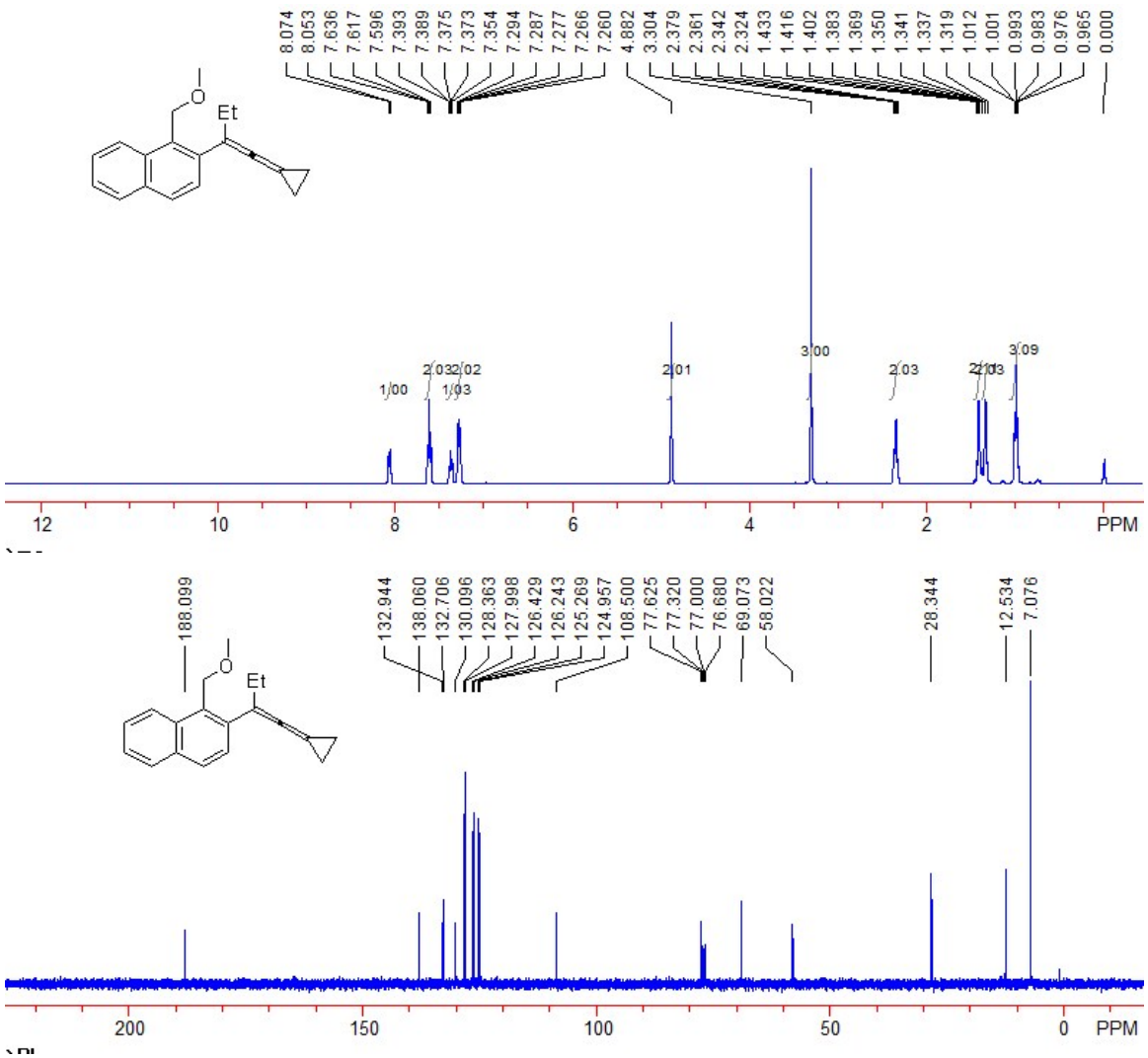

Compound **2a**. 26.4 mg, yield: 65%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.81-1.84 (m, 2H, $CH_2$), 2.10-2.14 (m, 2H, $CH_2$), 2.31 (d, $J$ = 1.6 Hz, 3H, $CH_3$), 5.96 (d, $J$ = 1.6 Hz, 1H, =CH), 7.35-7.40 (m, 1H, Ar), 7.42-7.47 (m, 1H, Ar), 7.51 (d, $J$ = 8.4 Hz, 1H, Ar), 7.59 (d, $J$ = 8.4 Hz, 1H, Ar), 7.79 (d, $J$ = 8.4 Hz, 1H, Ar), 7.93 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 13.1, 14.8, 34.4, 118.9, 121.2, 123.7, 126.0, 126.4, 128.2, 129.6, 131.9, 135.8, 137.5, 140.7, 143.2. IR (neat) ν 2953, 2922, 2868, 1713, 1460, 1377, 1161, 947, 816, 746 cm$^{-1}$. MS (%) m/e 206 ($M^+$, 78.28), 205 (36.30), 202 (18.57), 191 (100.00), 190 (42.21), 189 (46.04), 165 (30.22), 57 (18.93). HRMS (EI) calcd. for $C_{16}H_{14}$: 206.1096, Found: 206.1093.

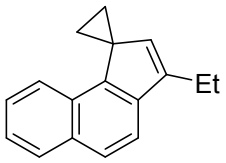


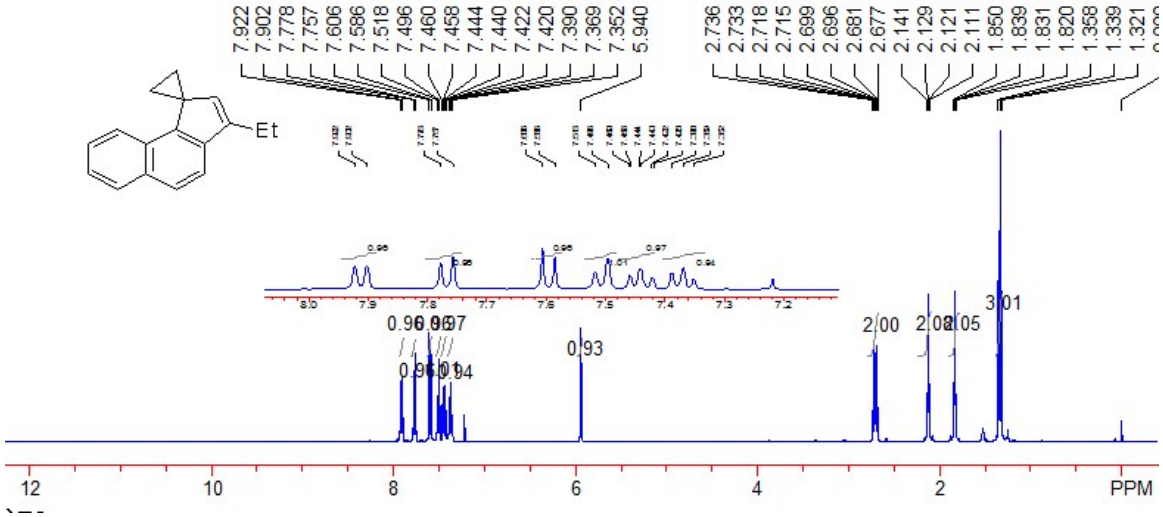



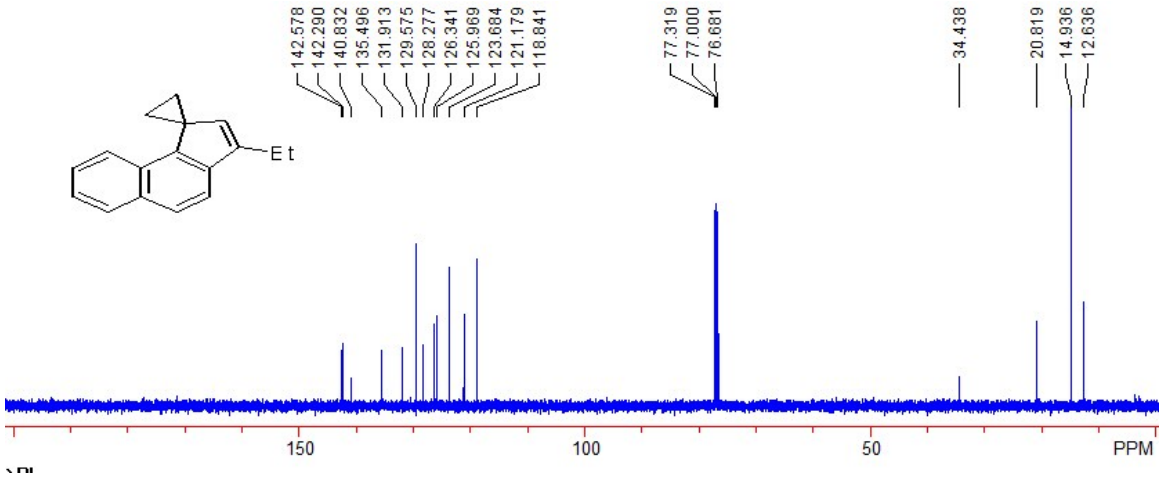

Compound **1b**. 260 mg, yield: 99%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.96-1.02 (m, 3H, $CH_3$), 1.31-1.37 (m, 2H, $CH_2$), 1.38-1.44 (m, 2H, $CH_2$), 2.32-2.38 (m, 2H, $CH_2$), 3.30 (s, 3H, $CH_3$), 4.88 (s, 2H, $CH_2$), 7.26-7.30 (m, 2H, Ar), 7.35-7.40 (m, 1H, Ar), 7.59-7.64 (m, 2H, Ar), 8.06 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 12.5, 28.3, 58.0, 69.1, 77.6, 108.5, 125.0, 125.3, 126.2, 126.4, 128.0, 128.4, 130.1, 132.7, 133.0, 138.1, 188.1. IR (neat) ν 3049, 2964, 2811, 2015, 1457, 1182, 1092, 840, 816, 745 cm$^{-1}$. MS (%) m/e 264 ($M^+$, 28.12), 249 (56.86), 236 (72.25), 235 (54.39), 221 (100), 204 (51.62), 203 (82.99), 202 (97.62), 191 (62.58). HRMS (EI) calcd. for $C_{19}H_{20}O$: 264.1514, Found: 264.1508.

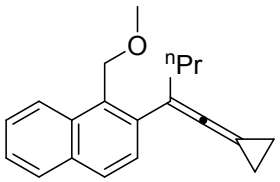


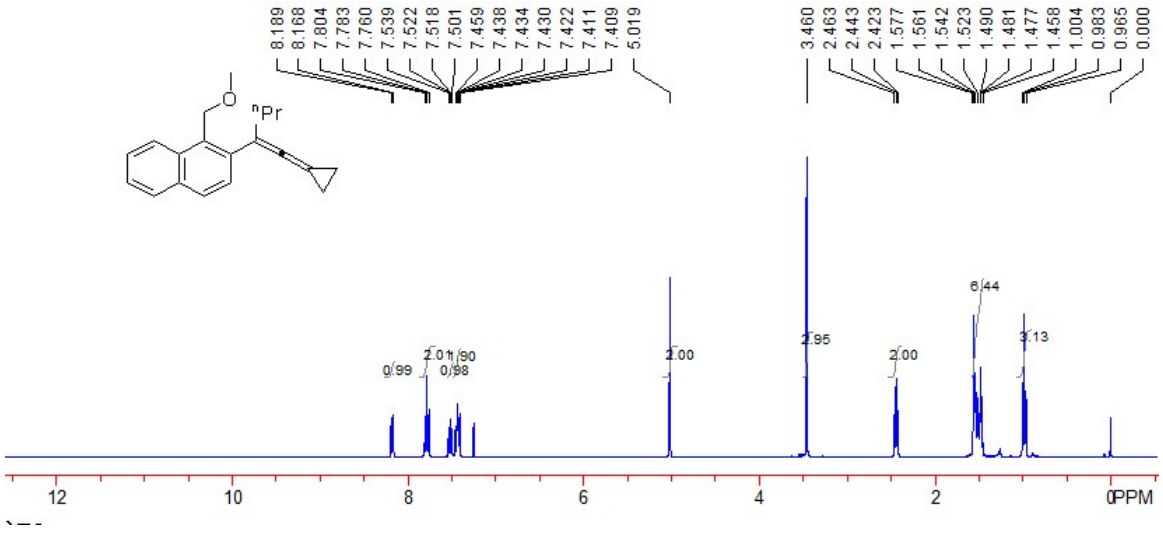

Compound **2b**. 26.4 mg, yield: 65%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.34 (t, $J$ = 7.2 Hz, 3H, $CH_3$), 1.84 (dd, $J_1$ = 4.2 Hz, $J_2$ = 7.8 Hz, 2H, $CH_2$), 2.13 (dd, $J_1$ = 4.2 Hz, $J_2$ = 7.8 Hz, 2H, $CH_2$), 2.67-2.74 (m, 2H, $CH_2$), 5.94 (s, 1H, =CH), 7.35-7.39 (m, 1H, Ar), 7.42-7.46 (m, 1H, Ar), 7.51 (d, $J$ = 8.8 Hz, 1H, Ar), 7.60 (d, $J$ = 8.0 Hz, 1H, Ar), 7.77 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 12.6, 14.9, 20.8, 34.4, 118.8, 121.2, 123.7, 126.0, 126.3, 128.3, 129.6, 131.9, 135.5, 140.8, 142.3, 142.6. IR (neat) ν 3051, 2964, 2931, 1732, 1696, 1519, 1459, 1409, 947, 786 cm$^{-1}$. MS (%) m/e 220 ($M^+$, 68.33), 205 (59.80), 203 (29.52), 202 (30.40), 192 (21.22), 191 (100.00), 190 (42.22), 189 (43.94). HRMS (EI) calcd. for $C_{17}H_{16}$: 220.1252, Found: 220.1262.

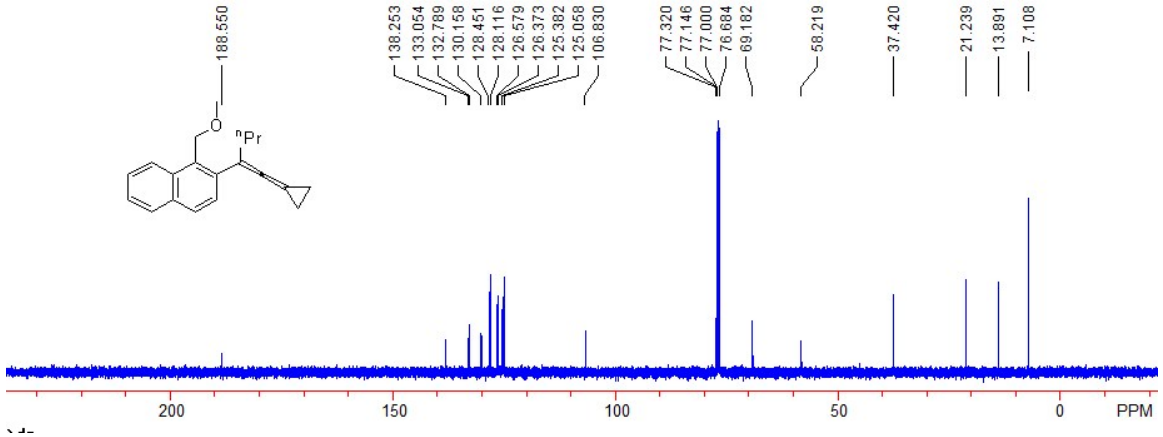


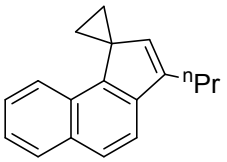



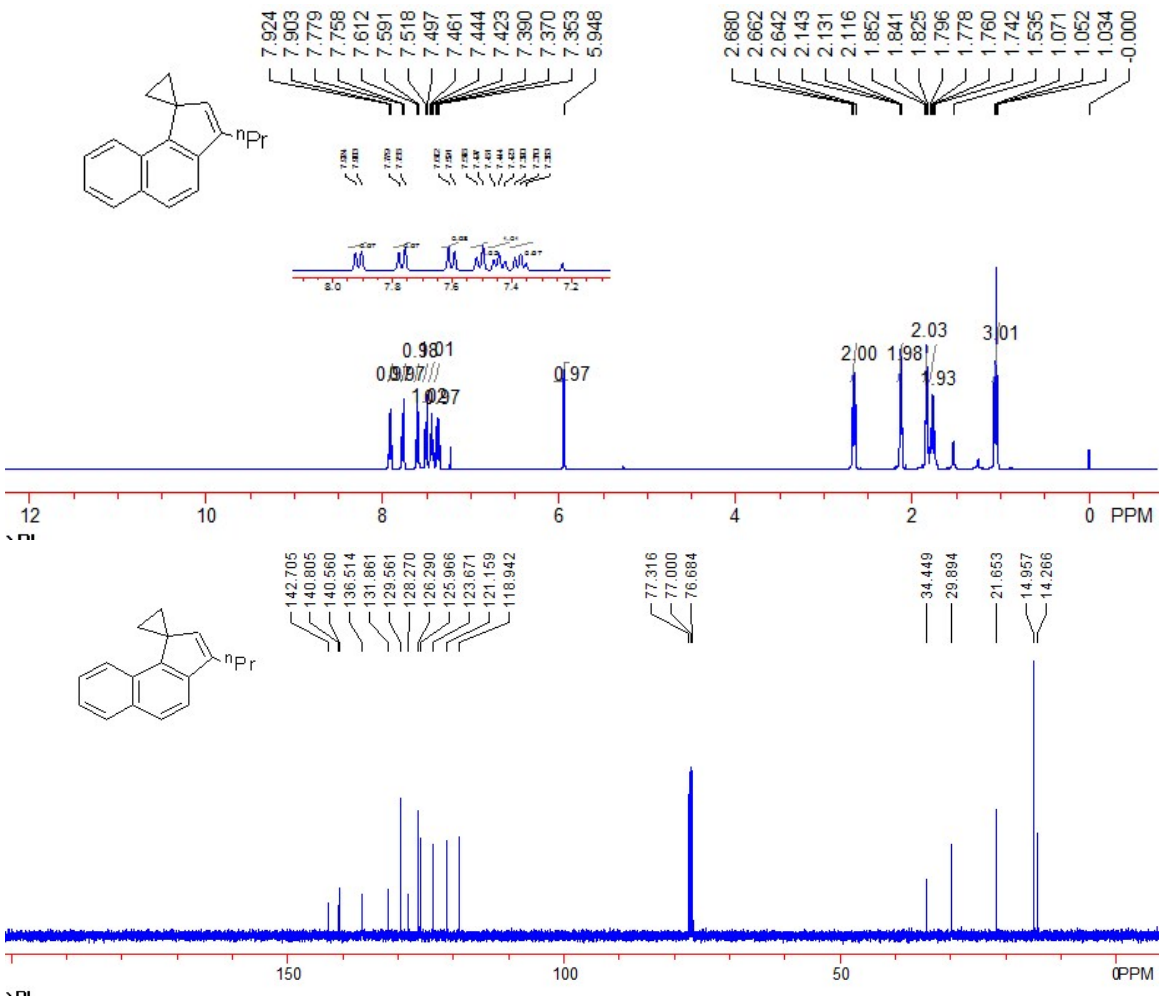

Compound **1c**. 215 mg, yield: 78%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.96-1.01 (m, 3H, $CH_3$), 1.45-1.58 (m, 6H, $3CH_2$), 2.42-2.47 (m, 2H, $CH_2$), 3.46 (s, 3H, $CH_3$), 5.02 (s, 2H, $CH_2$), 7.40-7.46 (m, 2H, Ar), 7.50-7.54 (m, 1H, Ar), 7.76-7.81 (m, 2H, Ar), 8.18 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 13.9, 21.2, 37.4, 58.2, 69.2, 77.1, 106.8, 125.1, 125.4, 126.4, 126.6, 128.1, 128.5, 130.2, 132.8, 133.1, 138.3, 188.6. IR (neat) ν 3051, 2956, 2924, 2870, 2016, 1410, 1376, 1094, 908, 792 cm$^{-1}$. MS (%) m/e 278 ($M^+$, 10.49), 250 (38.96), 249 (63.85), 221 (100.00), 217 (38.83), 215 (44.96), 203 (60.97), 202 (78.47), 191 (49.50). HRMS (EI) calcd. for $C_{20}H_{22}O$: 278.1671, Found: 278.1675.

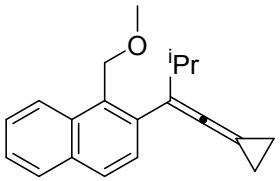


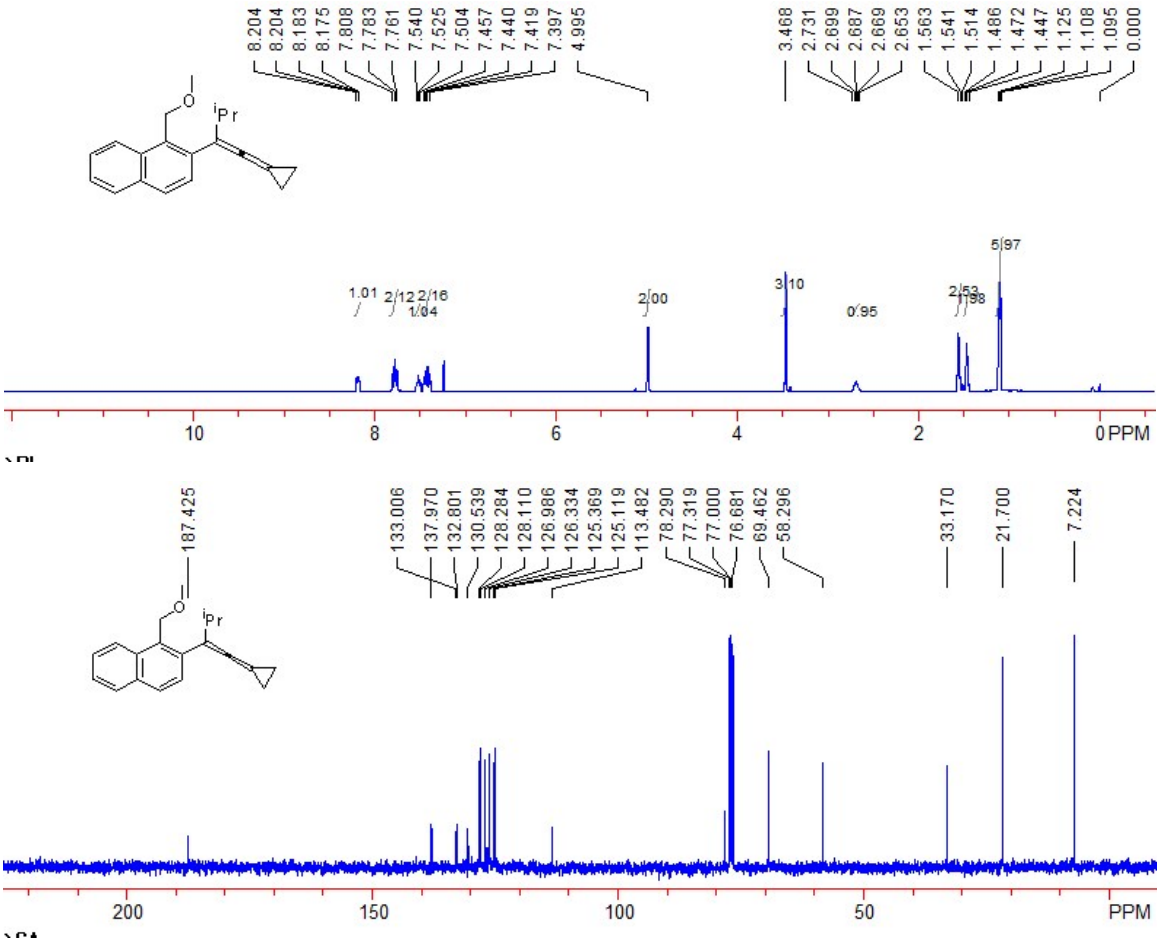



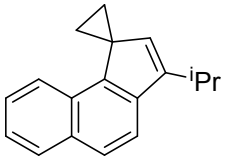

Compound **2c**. 32.9 mg, yield: 77%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.05 (t, $J$ = 7.2 Hz, 3H, $CH_3$), 1.74-1.80 (m, 2H, $CH_2$), 1.82-1.86 (m, 2H, $CH_2$), 2.11-2.15 (m, 2H, $CH_2$), 2.66 (t, $J$ = 8.0 Hz 2H, $CH_2$), 5.95 (s, 1H, =CH), 7.35-7.39 (m, 1H, Ar), 7.42-7.47 (m, 1H, Ar), 7.50 (d, $J$ = 8.4 Hz, 1H, Ar), 7.60 (d, $J$ = 8.4 Hz, 1H, Ar), 7.77 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 14.3, 15.0, 21.7, 29.9, 34.4, 118.9, 121.2, 123.7, 126.0, 126.3, 128.3, 129.6, 131.9, 136.5, 140.6, 140.8, 142.7. IR (neat) ν 3053, 2958, 2929, 2871, 1744, 1519, 1397, 833, 745, 685oll $cm^{-1}$. MS (%) m/e 234 ($M^+$, 60.65), 206 (34.51), 205 (54.87), 203 (32.48), 202 (35.58), 191 (100.00), 190 (38.28), 189 (38.27). HRMS (EI) calcd. for $C_{18}H_{18}$: 234.1409, Found: 234.1403.



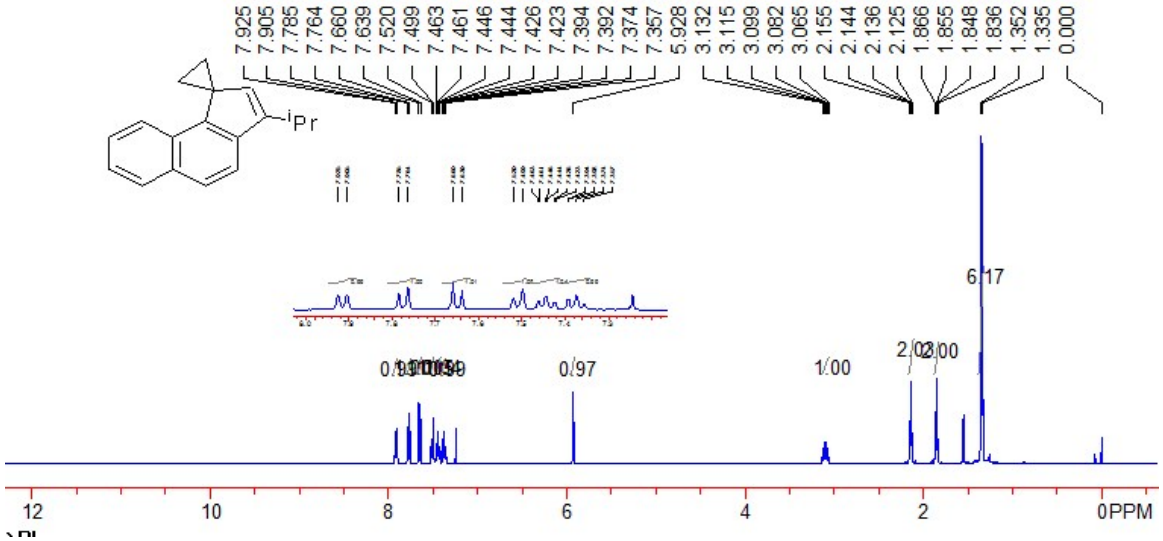



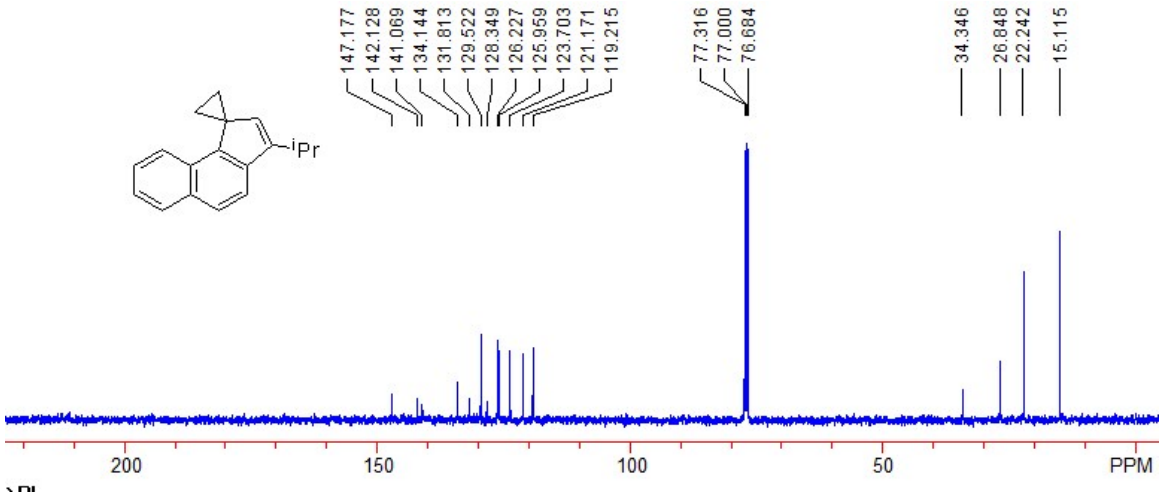

Compound **1d**. 212 mg, yield: 76%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.09-1.13 (m, 6H, $2CH_3$), 1.44-1.52 (m, 2H, $CH_2$), 1.54-1.57 (m, 2H, $CH_2$), 2.65-2.74 (m, 1H, CH), 3.47 (s, 3H, $CH_3$), 5.00 (s, 2H, $CH_2$), 7.39-7.46 (m, 2H, Ar), 7.50-7.54 (m, 1H, Ar), 7.76-7.81 (m, 2H, Ar), 8.17-8.21 (m, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.2, 21.7, 33.2, 58.3, 69.5, 78.3, 113.5, 125.1, 125.4, 126.3, 127.0, 128.1, 128.3, 130.5, 132.8, 133.0, 138.0, 187.4. IR (neat) ν 2958, 2923, 2868, 2016, 1458, 1095, 1066, 829, 810, 744 $cm^{-1}$. MS (%) m/e 278 ($M^+$, 12.37), 263 (52.69), 235 (100.00), 216 (62.69), 215 (69.22), 205 (46.51), 203 (68.84), 202 (71.26), 191 (44.90). HRMS (EI) calcd. for $C_{20}H_{22}O$: 278.1671, Found: 278.1669.

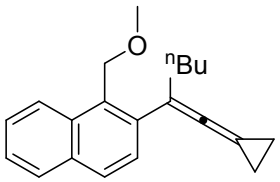


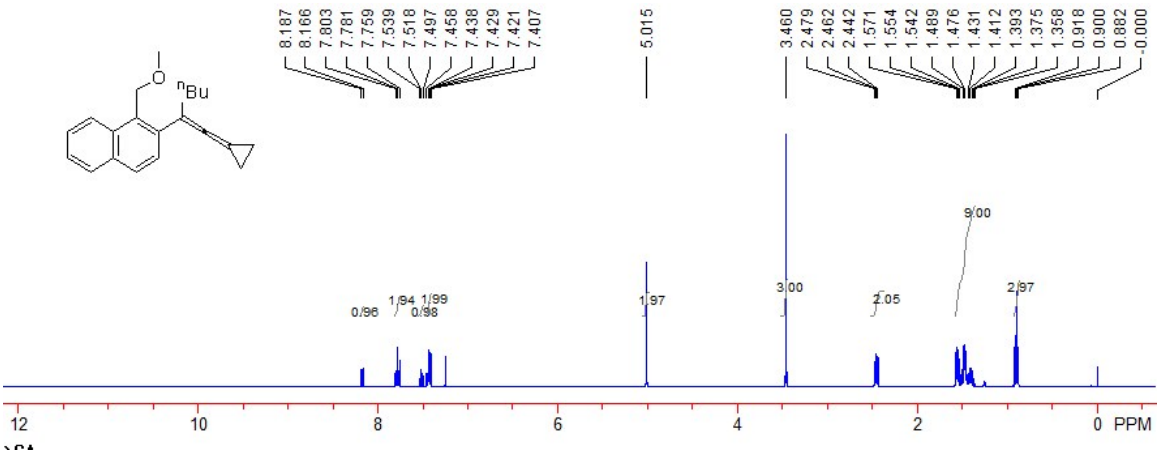

Compound **2d**. 32.9 mg, yield: 71%; white solid. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.34 (d, $J$ = 7.6 Hz, 6H, $CH_3$), 1.85 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.4 Hz, 2H, $CH_2$), 2.14 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.4 Hz, 2H, $CH_2$), 3.06-3.14 (m, 1H, CH), 5.93 (s, 1H, =CH), 7.35-7.40 (m, 1H, Ar), 7.42-7.47 (m, 1H, Ar), 7.51 (d, $J$ = 8.0 Hz, 1H, Ar), 7.50 (d, $J$ = 8.0 Hz, 1H, Ar), 7.77 (d, $J$ = 8.4 Hz, 1H, Ar), 7.92 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.1, 22.2, 26.8, 34.3, 119.2, 121.2, 123.7, 126.0, 126.3, 128.3, 129.5, 131.8, 134.1, 141.1, 142.1, 147.2. IR (neat) ν 2958, 2921, 2868, 2849, 1462, 1378, 1063, 832, 745, 743 $cm^{-1}$. MS (%) m/e 234 ($M^+$, 43.87), 219 (37.48), 203 (26.87), 202 (25.69), 192 (22.59), 191 (100.00), 190 (23.18), 189 (30.05). HRMS (EI) calcd. for $C_{18}H_{18}$: 234.1409, Found: 234.1403.

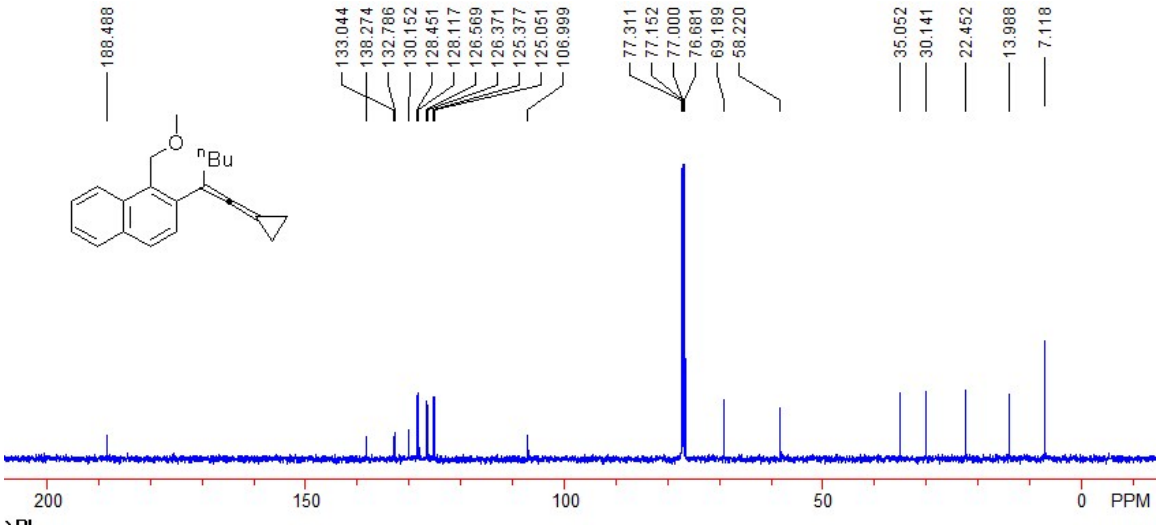


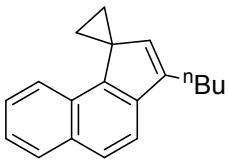



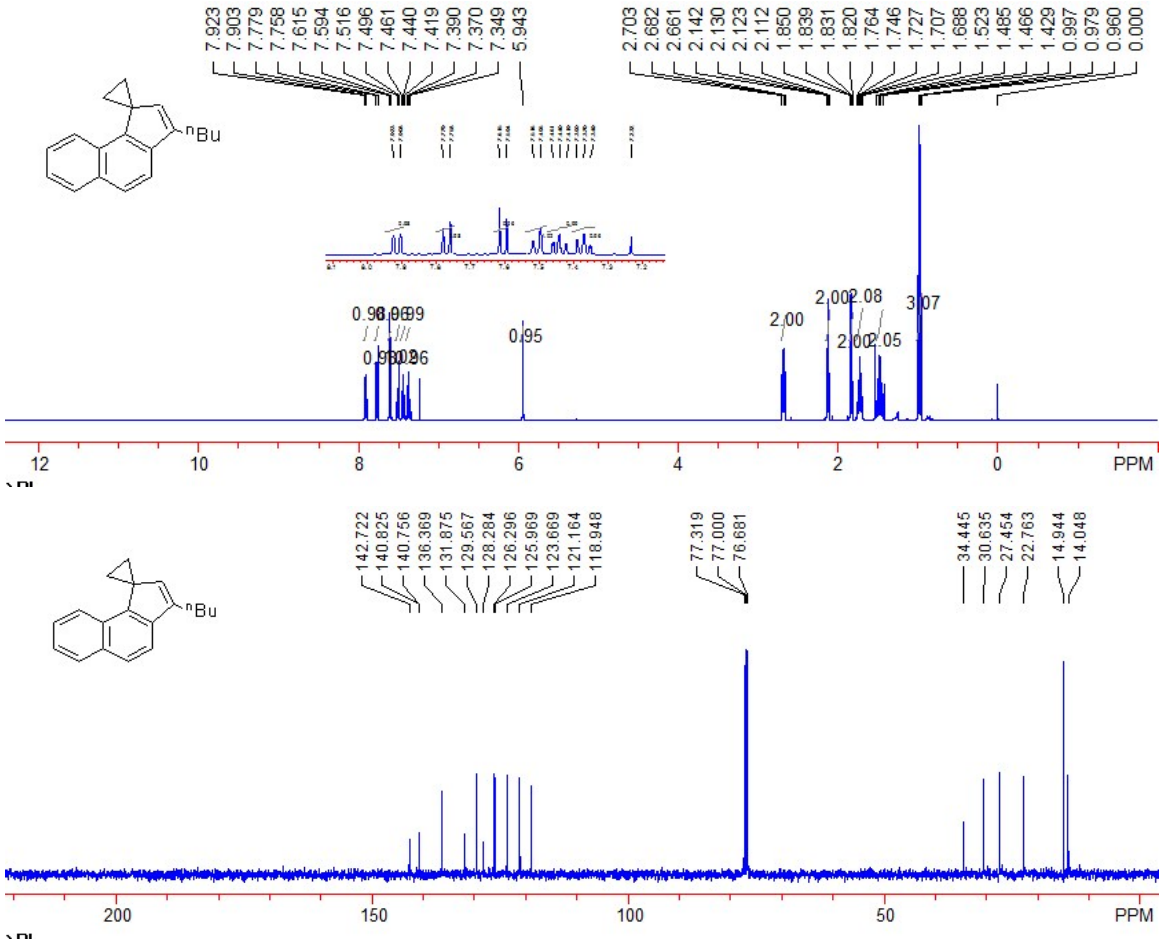

Compound **1e**. 200 mg, yield: 70%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.90 (t, $J$ = 7.2 Hz, 3H, $CH_3$), 1.35-1.58 (m, 8H, $4CH_2$), 2.46 (t, $J$ = 8.0 Hz, 2H, $CH_2$), 3.46 (s, 3H, $CH_3$), 5.02 (s, 2H, $CH_2$), 7.41-7.46 (m, 2H, Ar), 7.49-7.54 (m, 1H, Ar), 7.75-7.81 (m, 2H, Ar), 8.17 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 14.0, 22.5, 30.1, 35.1, 58.2, 69.2, 77.2, 107.0, 125.1, 125.4, 126.4, 126.6, 128.1, 128.5, 130.2, 132.8, 133.0, 138.3, 188.5. IR (neat) ν 3058, 2982, 2016, 1507, 1493, 1185, 953, 907, 817, 699 cm$^{-1}$. MS (%) m/e 292 ($M^+$, 10.95), 249 (47.35), 221 (100.00), 217 (35.96), 215 (44.45), 203 (55.25), 202 (68.45), 191 (46.44), 189 (35.33). HRMS (EI) calcd. for $C_{21}H_{24}O$: 292.1827, Found: 292.1833.

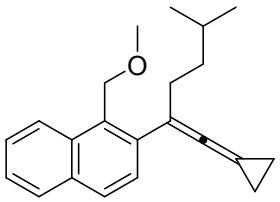


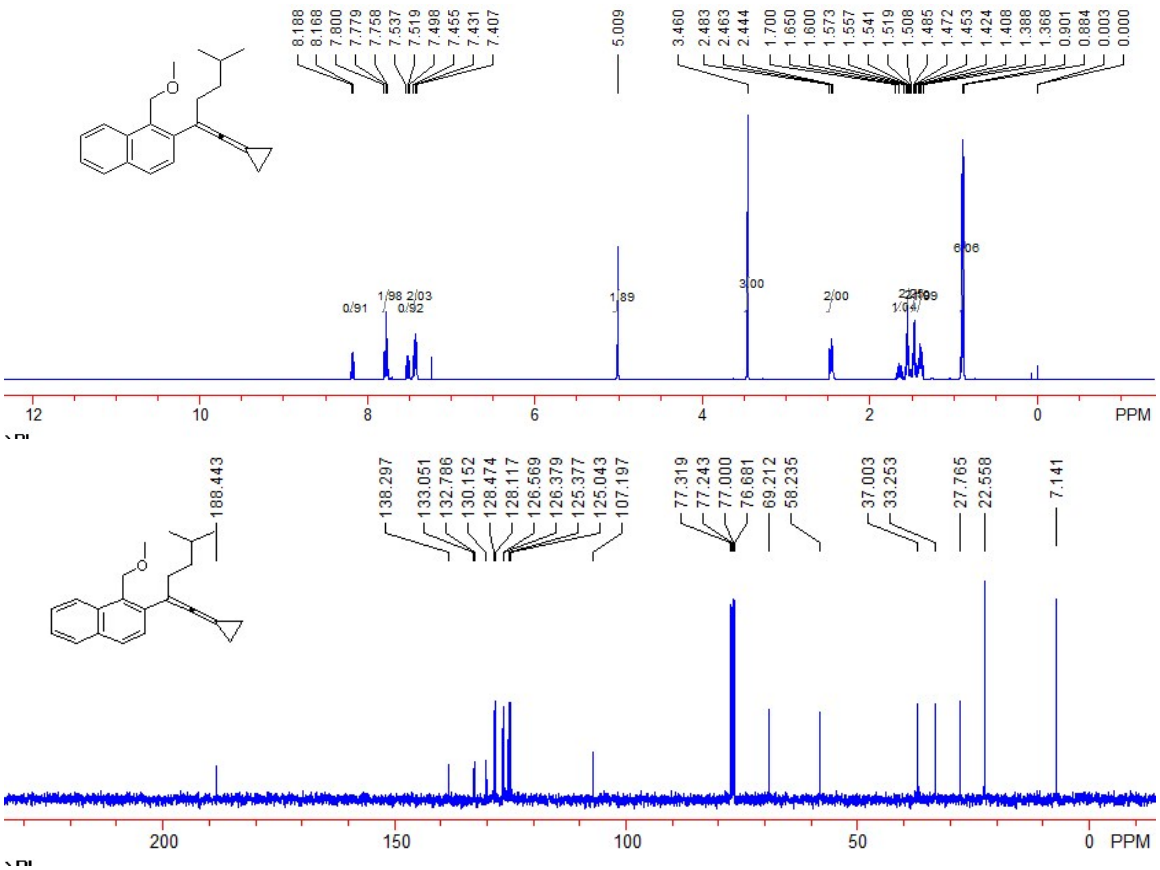




Compound **2e**. 34.9 mg, yield: 71%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.98 (t, $J$ = 7.6 Hz, 3H, $CH_3$), 1.42-1.53 (m, 2H, $CH_2$), 1.68-1.77 (m, 2H, $CH_2$), 1.84 (dd, $J_1$ = 4.4 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 2.14 (dd, $J_1$ = 4.4 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 2.66-2.71 (m, 2H, $CH_2$), 5.94 (s, 1H, =CH), 7.34-7.39 (m, 1H, Ar), 7.41-7.47 (m, 1H, Ar), 7.51 (d, $J$ = 8.0 Hz, 1H, Ar), 7.60 (d, $J$ = 8.4 Hz, 1H, Ar), 7.70 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 14.0, 15.0, 22.8, 27.5, 30.6, 34.4, 118.9, 121.2, 123.7, 126.0, 126.3, 128.3, 129.6, 131.9, 136.4, 140.76, 140.83, 142.7. IR (neat) ν 3048, 2955, 2927, 2870, 1746, 1519, 1048, 947, 832, 744 cm$^{-1}$. MS (%) m/e 248 ($M^+$, 53.11), 206 (64.37), 205 (56.96), 203 (27.29), 202 (33.46), 191 (100.00), 190 (34.01), 189 (35.20). HRMS (EI) calcd. for $C_{19}H_{20}$: 248.1565, Found: 248.1560.

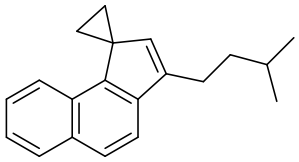


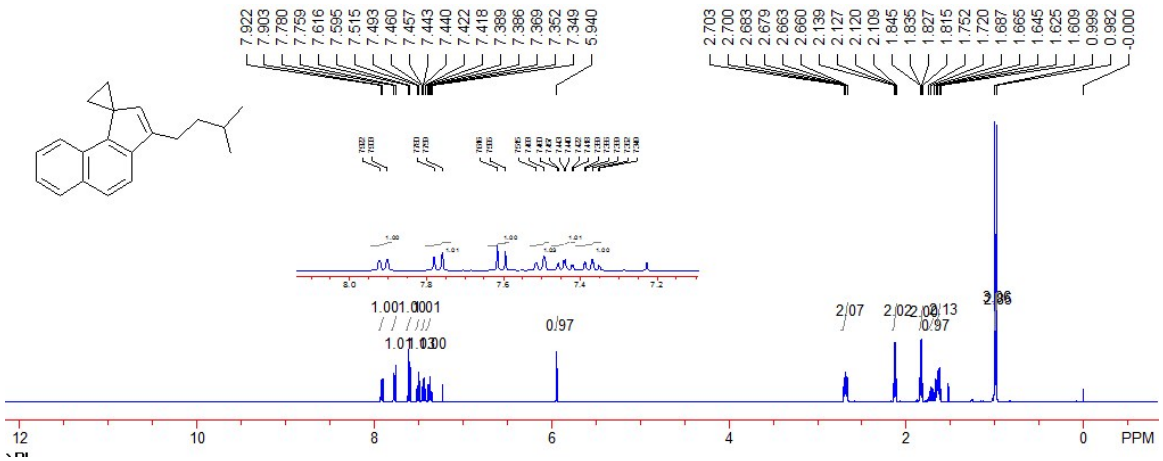

Compound **1f**. 290 mg, yield: 90%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.89 (d, $J$ = 6.8 Hz, 6H, $CH_3$), 1.36-1.43 (m, 2H, $CH_2$), 1.45-1.51 (m, 2H, $CH_2$), 1.51-1.58 (m, 2H, $CH_2$), 1.60-1.70 (m, 2H, $CH_2$), 2.44-2.49 (m, 2H, $CH_2$), 3.46 (s, 3H, $CH_3$), 5.01 (s, 2H, $CH_2$), 7.40-7.46 (m, 2H, Ar), 7.49-7.54 (m, 1H, Ar), 7.75-7.80 (m, 2H, Ar), 8.17 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 22.6, 27.8, 33.3, 37.0, 58.2, 69.2, 77.2, 107.2, 125.0, 125.4, 126.4, 126.6, 128.1, 128.5, 130.2, 132.8, 133.1, 138.3, 188.4. IR (neat) ν 3045, 2953, 2923, 2016, 1507, 1383, 1095, 907, 774, 746 cm$^{-1}$. MS (%) m/e 306 ($M^+$, 14.31), 249 (42.67), 235 (38.98), 221 (100.00), 217 (40.28), 215 (44.31), 203 (63.24), 202 (69.79), 191 (41.60). HRMS (EI) calcd. for $C_{22}H_{26}O$: 306.1984, Found: 306.1989.

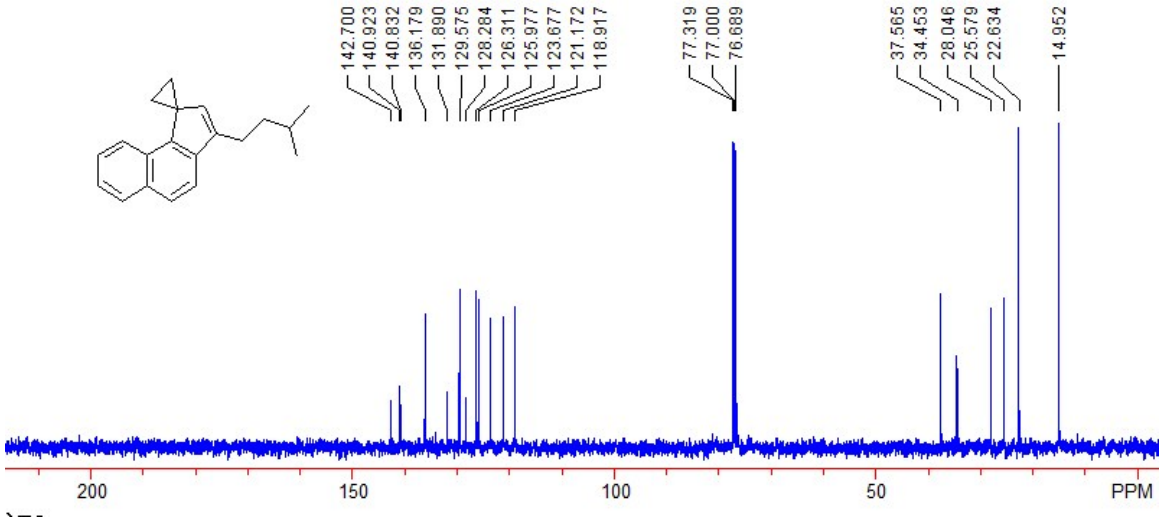


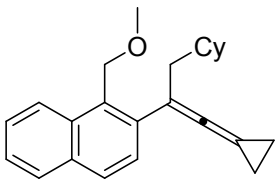




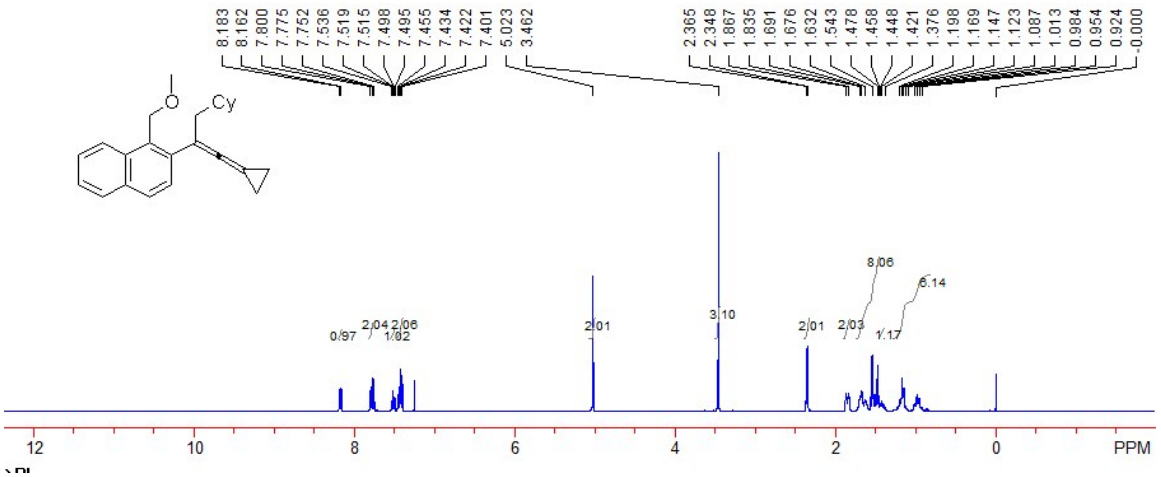
Compound **2f**. 39.7 mg, yield: 76%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.99 (d, $J$ = 6.8 Hz, 6H, $CH_3$), 1.61-1.67 (m, 2H, $CH_2$), 1.68-1.76 (m, 1H, CH), 1.83 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 2.13 (dd, $J_1$ = 4.4 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 2.66-2.71 (m, 2H, $CH_2$), 5.94 (s, 1H, =CH), 7.34-7.39 (m, 1H, Ar), 7.41-7.46 (m, 1H, Ar), 7.50 (d, $J$ = 8.8 Hz, 1H, Ar), 7.61 (d, $J$ = 8.4 Hz, 1H, Ar), 7.77 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 7.2 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.0, 22.6, 25.6, 28.0, 34.5, 37.6, 118.9, 121.2, 123.7, 126.0, 126.3, 128.3, 129.6, 131.9, 136.2, 140.8, 140.9, 142.7. IR (neat) ν 3051, 2953, 2924, 2867, 1466, 1384, 946, 831, 742, 685 cm$^{-1}$. MS (%) m/e 262 ($M^+$, 33.90), 206 (100.00), 205 (44.08), 203 (24.46), 202 (29.39), 191 (60.06), 190 (24.17), 189 (29.27). HRMS (EI) calcd. for $C_{20}H_{22}$: 262.1722, Found: 262.1716.

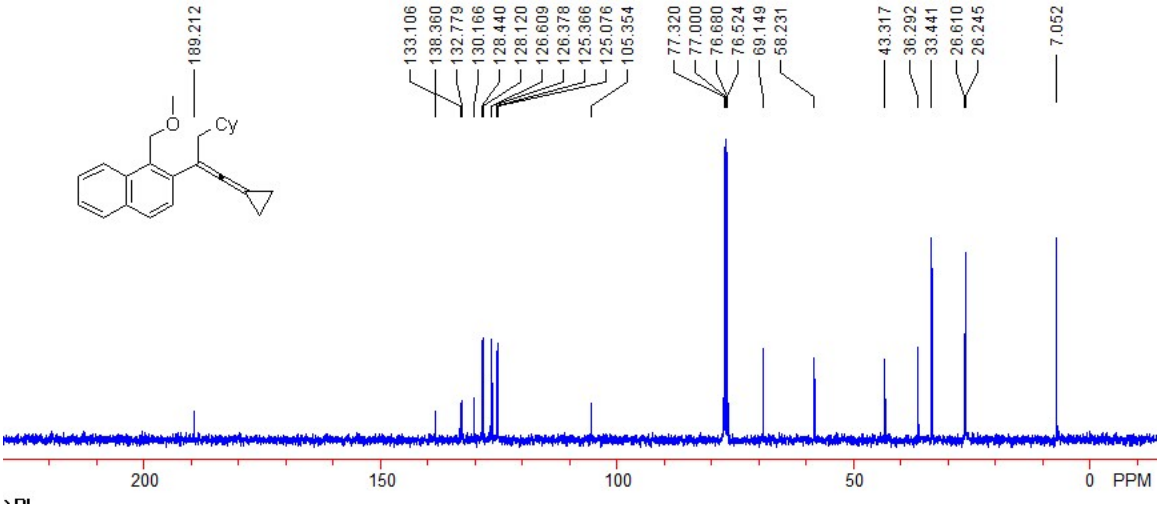


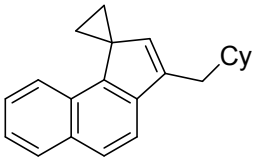




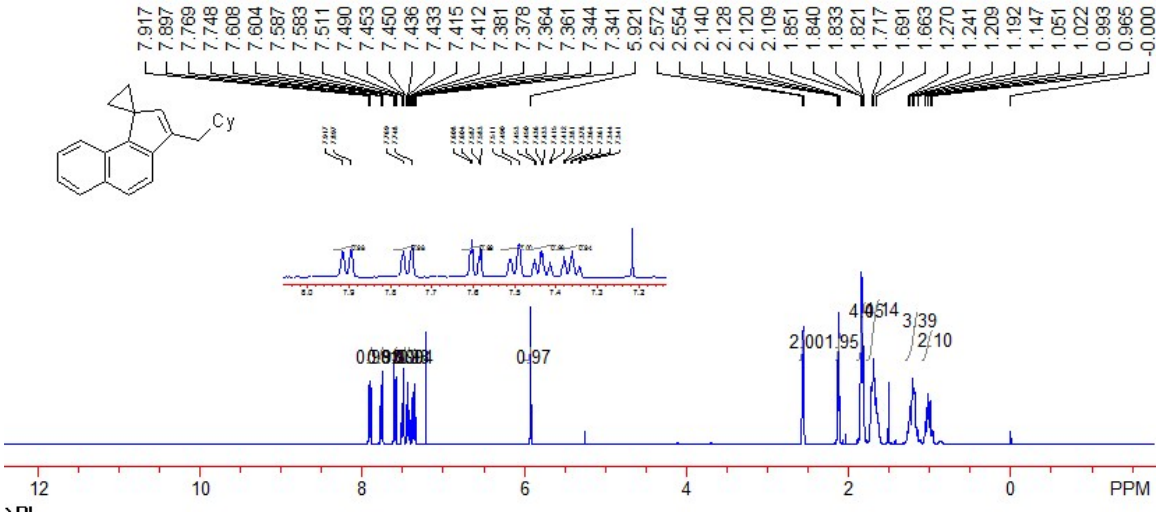

Compound **1g**. 290 mg, yield: 90%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.92-1.20 (m, 6H, $3CH_2$), 1.37-1.45 (m, 1H, CH), 1.45-1.70 (m, 8H, $4CH_2$), 1.85 (d, $J$ = 12.8 Hz, 2H, $CH_2$), 2.36 (d, 2H, $J$ = 6.8 Hz, $CH_2$), 3.46 (s, 3H, $CH_3$), 5.02 (s, 2H, $CH_2$), 7.40-7.46 (m, 2H, Ar), 7.49-7.54 (m, 1H, Ar), 7.75-7.80 (m, 2H, Ar), 8.17 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 26.2, 26.6, 33.4, 36.3, 43.3, 58.2, 69.1, 76.5, 105.4, 125.1, 125.4, 126.4, 126.6, 128.1, 128.4, 130.2, 132.8, 133.1, 138.4, 189.2. IR (neat) ν 3042, 2919, 2848, 2015, 1447, 1183, 1094, 975, 818, 747 cm$^{-1}$. MS (%) m/e 332 ($M^+$, 15.01), 249 (56.03), 221 (100.00), 219 (28.17), 217 (33.09), 215 (25.67), 203 (35.15), 202 (46.86), 191 (27.92). HRMS (EI) calcd. for $C_{24}H_{28}O$: 332.2140, Found: 332.2148.

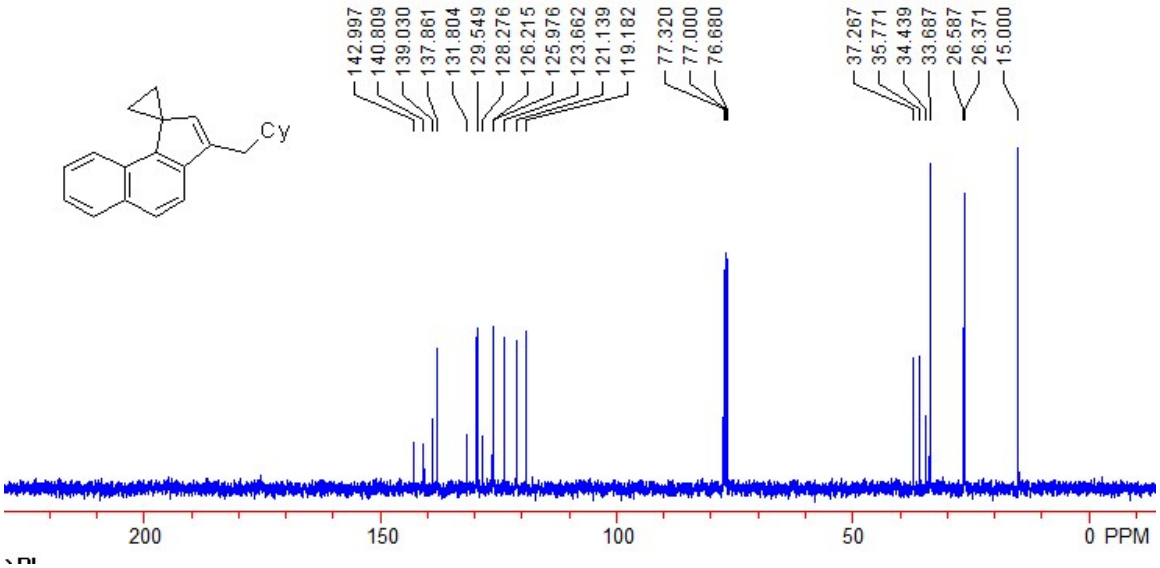


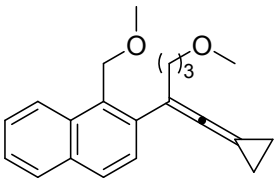



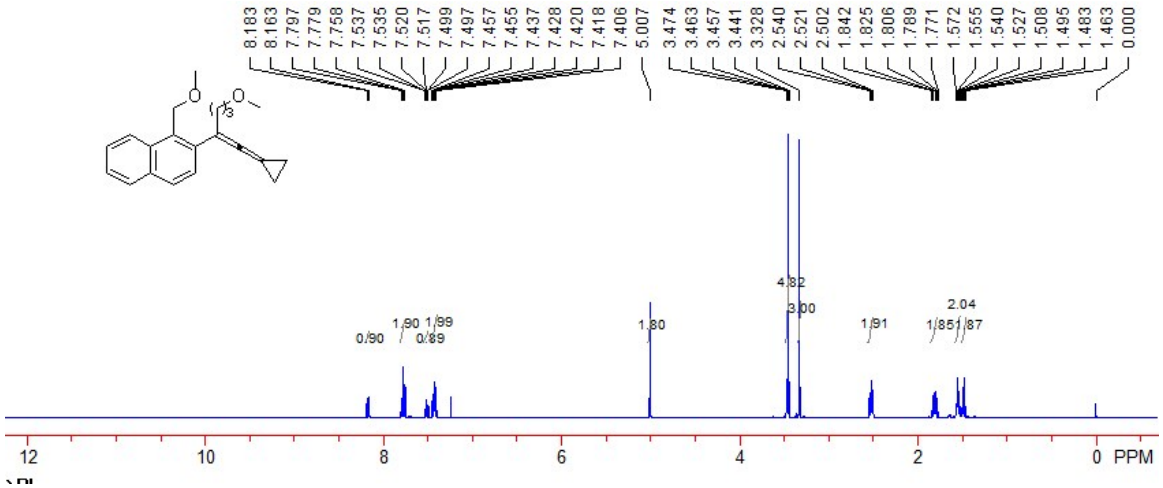

Compound **2g**. 53.0 mg, yield: 92%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 0.96-1.06 (m, 2H, $CH_2$), 1.14-1.27 (m, 3H, CH, $CH_2$), 1.66-1.72 (m, 4H, $2CH_2$), 1.82-1.86 (m, 4H, $2CH_2$), 2.10-2.14 (m, 2H, $CH_2$), 2.56 (d, $J$ = 7.2 Hz, 2H, $CH_2$), 5.92 (s, 1H, =CH), 7.34-7.39 (m, 2H, Ar), 7.41-7.46 (m, 1H, Ar), 7.50 (d, $J$ = 8.4 Hz, 1H, Ar), 7.58-7.61 (m, 1H, Ar), 7.76 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.0, 26.4, 26.6, 33.7, 34.4, 35.8, 37.3, 119.2, 121.1, 123.7, 126.0, 126.2, 128.3, 129.5, 131.8, 137.9, 139.0, 140.8, 143.0. IR (neat) ν 3040, 2919, 2848, 1447, 1398, 1020, 947, 889, 832, 743 cm$^{-1}$. MS (%) m/e 288 ($M^+$, 49.94), 206 (100.00), 205 (49.44), 203 (24.55), 202 (26.25), 191 (69.39), 190 (25.39), 189 (27.55). HRMS (EI) calcd. for $C_{22}H_{24}$: 288.1878, Found: 288.1877.

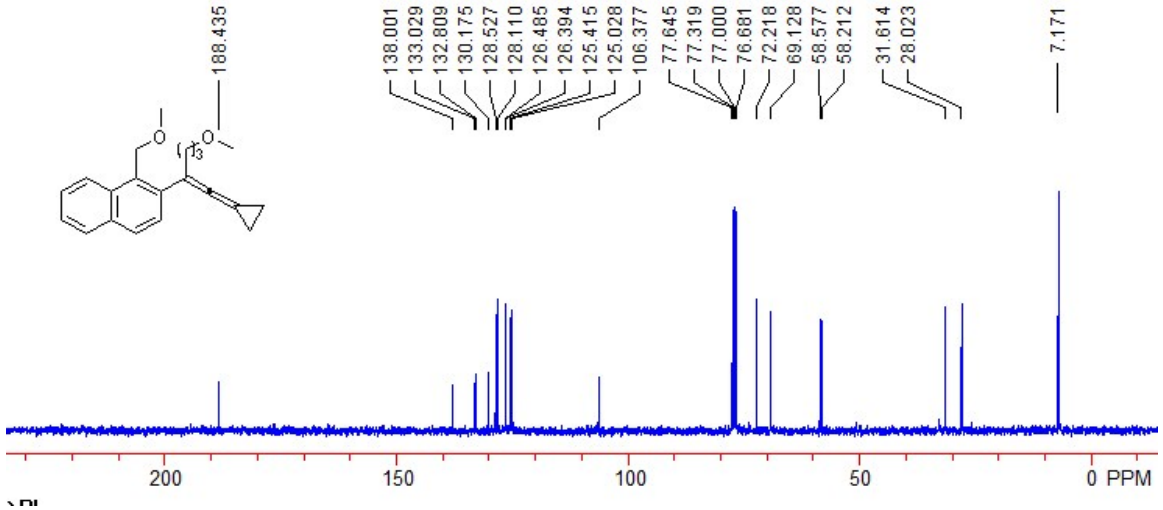


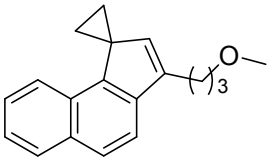



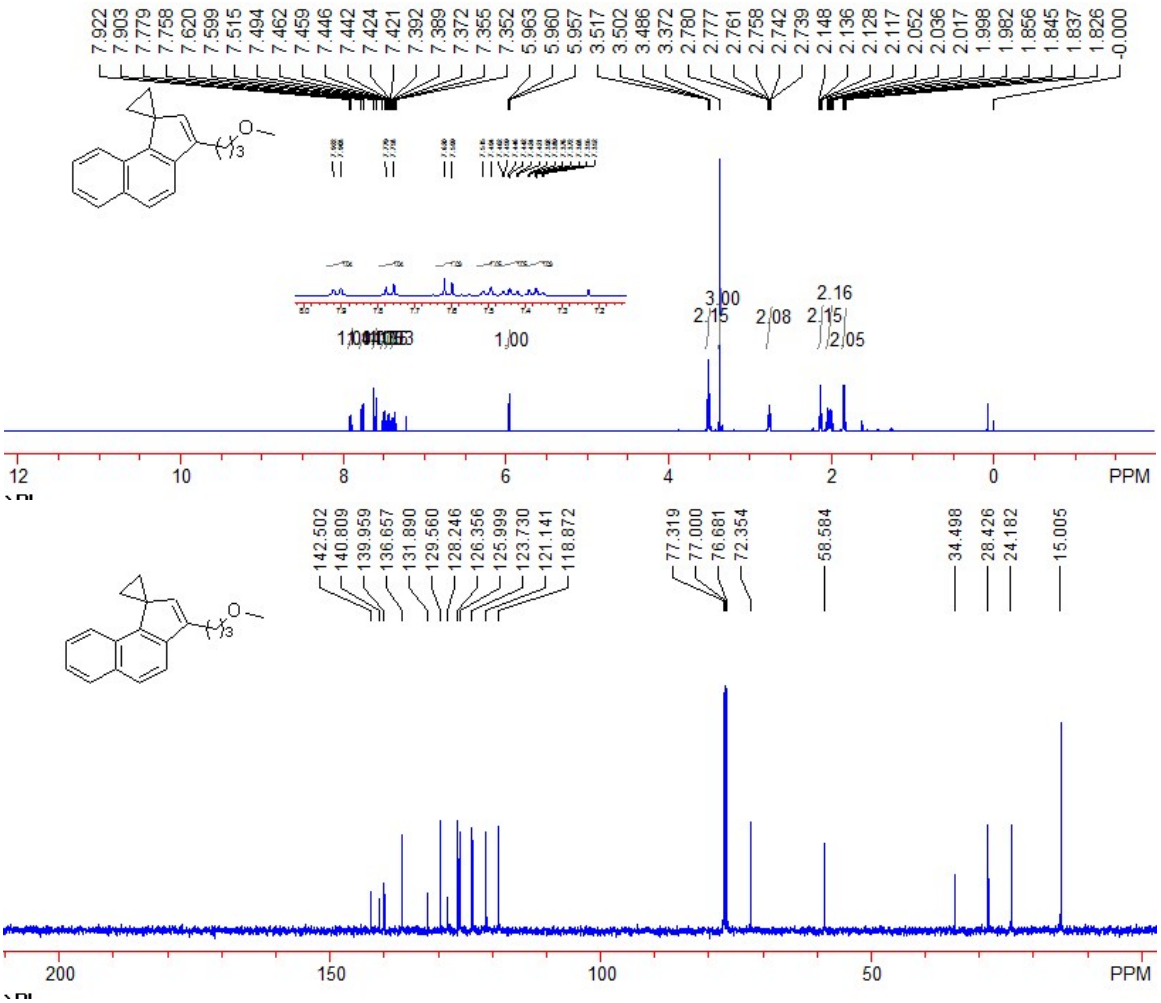

Compound **1h**. 220 mg, yield: 72%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.46-1.51 (m, 2H, $CH_2$), 1.52-1.58 (m, 2H, $CH_2$), 1.77-1.85 (m, 2H, $CH_2$), 2.52 (t, $J$ = 7.6 Hz, 2H, $CH_2$), 3.33 (s, 3H, $CH_3$), 3.44-3.48 (m, 5H, $CH_2$, $CH_3$), 5.01 (s, 2H, $CH_2$), 7.40-7.46 (m, 2H, Ar), 7.49-7.54 (m, 1H, Ar), 7.75-7.80 (m, 2H, Ar), 8.17 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.2, 28.0, 31.6, 58.2, 58.6, 69.1, 72.2, 77.6, 106.4, 125.0, 125.4, 126.4, 126.5, 128.1, 128.5, 130.2, 132.8, 133.0, 138.0, 188.4. IR (neat) ν 3047, 2922, 2869, 2016, 1385, 1116, 1093, 954, 819, 774 cm$^{-1}$. MS (%) m/e 308 ($M^+$, 12.43), 235 (59.76), 221 (79.47), 217 (70.22), 216 (52.88), 215 (83.96), 203 (77.06), 202 (100.00), 191 (49.56). HRMS (EI) calcd. for $C_{21}H_{24}O_2$: 308.1776, Found: 308.1772.

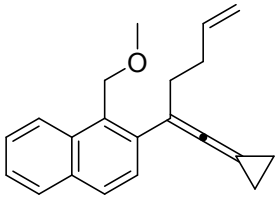


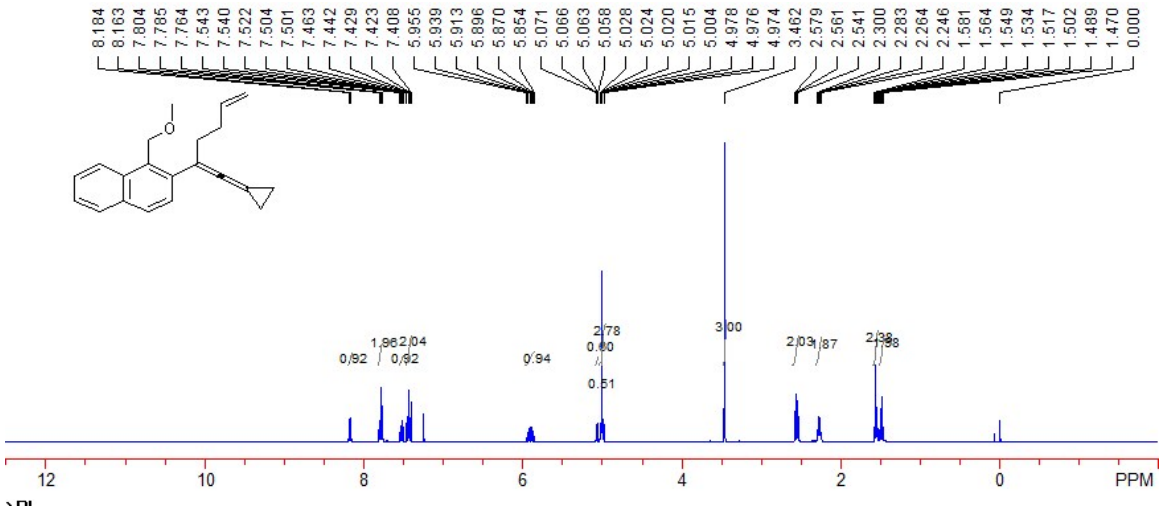



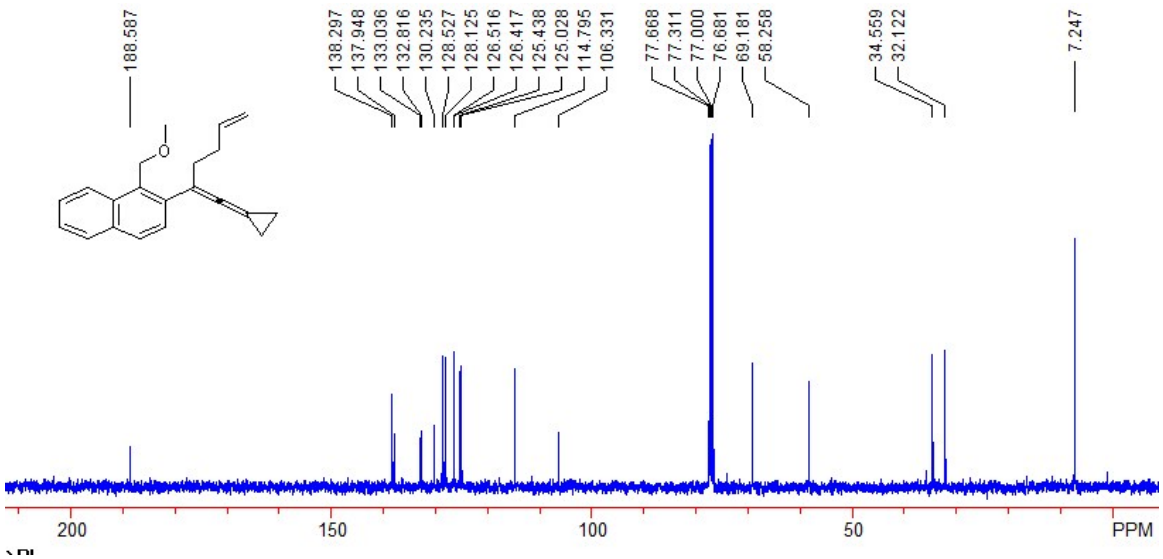

Compound **2h**. 40.0 mg, yield: 76%; white solid. Mp: 145-150 $^{o}$C $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.84 (dd, $J_1$ = 4.4 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 1.98-2.06 (m, 2H, $CH_2$), 2.13 (dd, $J_1$ = 4.4 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 2.73-2.78 (m, 2H, $CH_2$), 3.37 (s, 3H, $CH_3$), 3.50 (t, $J$ = 6.2 Hz, 1H, $CH_2$), 5.95-6.00 (m, 1H, =CH), 7.35-7.40 (m, 1H, Ar), 7.42-7.47 (m, 1H, Ar), 7.50 (d, $J$ = 8.4 Hz, 1H, Ar), 7.61 (d, $J$ = 8.0 Hz, 1H, Ar), 7.70 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.0, 24.2, 28.4, 34.5, 58.6, 72.4, 118.9, 121.1, 123.7, 126.0, 126.4, 128.2, 129.6, 131.9, 136.7, 140.0, 140.8, 142.5. IR (neat) ν 2976, 2928, 2869, 1736, 1518, 1239, 1118, 1046, 955, 784 cm$^{-1}$. MS (%) m/e 264 ($M^+$, 33.89), 206 (100.00), 205 (40.32), 203 (33.15), 202 (35.67), 191 (46.11), 190 (22.59), 189 (27.38). HRMS (EI) calcd. for $C_{19}H_{20}O$: 264.1514, Found: 264.1511.

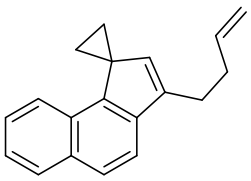




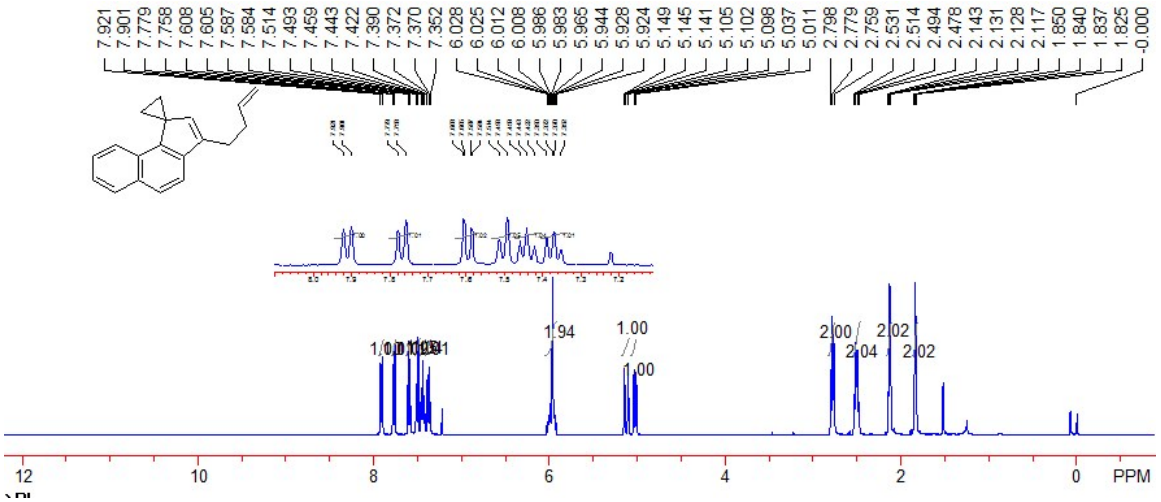
Compound **1i**. 281 mg, yield: 99%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.47-1.52 (m, 2H, $CH_2$), 1.53-1.59 (m, 2H, $CH_2$), 2.24-2.30 (m, 2H, $CH_2$), 2.54-2.58 (m, 2H, $CH_2$), 3.46 (s, 3H, $CH_3$), 5.00 (s, $CH_2$, 2H), 4.97-5.01 (m, 1H, =$CH_2$), 5.01-5.08 (m, 1H, =$CH_2$), 5.85-6.00 (m, 1H, =CH), 7.40-7.47 (m, 2H, Ar), 7.50-7.55 (m, 1H, Ar), 7.76-7.81 (m, 2H, Ar), 8.17 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.2, 32.1, 34.6, 58.3, 69.2, 77.7, 106.3, 114.8, 125.0, 125.4, 126.4, 126.5, 128.1, 128.5, 130.2, 132.8, 133.0, 138.0, 138.3, 188.6. IR (neat) ν 3062, 2980, 2922, 2016, 1639, 1507, 1411, 1094, 1044, 747 cm$^{-1}$. MS (%) m/e 290 ($M^+$, 2.23), 249 (66.51), 221 (100.00), 217 (51.81), 215 (54.79), 203 (59.67), 202 (85.78), 191 (49.08), 189 (37.72). HRMS (EI) calcd. for $C_{21}H_{22}O$: 290.1671, Found: 290.1670.

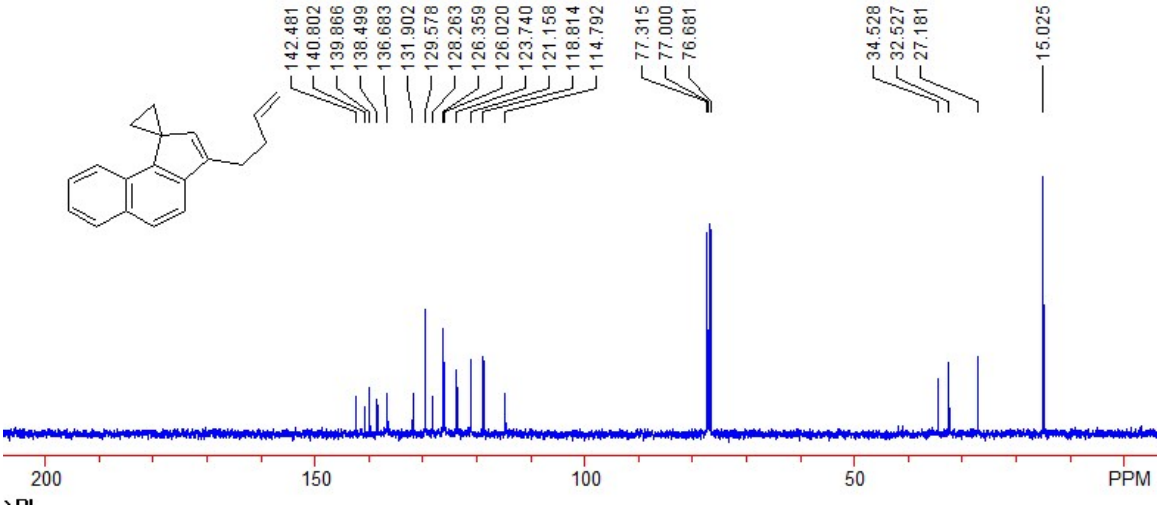


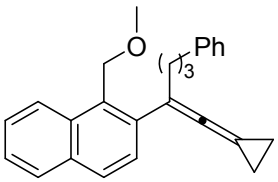



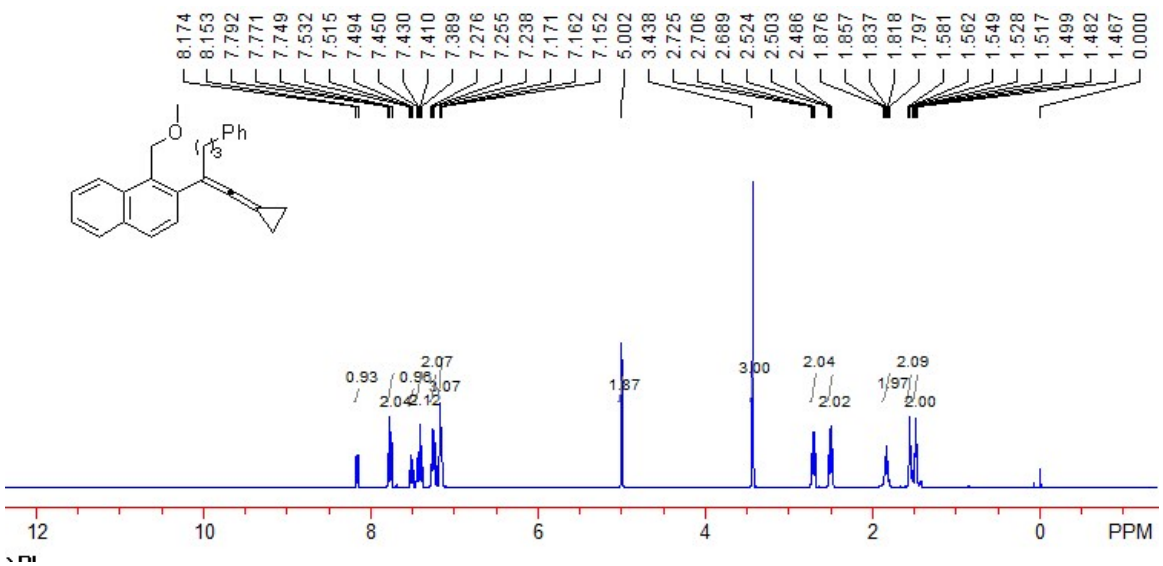
Compound **2i**. 37.8 mg, yield: 77%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.82-1.85 (m, 2H, $CH_2$), 2.11-2.15 (m, 2H, $CH_2$), 2.47-2.54 (m, 2H, $CH_2$), 2.78 (t, $J$ = 8.0 Hz, 2H, $CH_2$), 5.02 (dd, 1H, $J_1$ = 1.6 Hz, $J_2$ = 10.8 Hz, =$CH_2$), 5.13 (dd, $J_1$ = 1.6 Hz, $J_2$ = 17.6 Hz, 1H, =$CH_2$), 5.92-6.03 (m, 2H, =CH), 7.35-7.39 (m, 1H, Ar), 7.42-7.46 (m, 1H, Ar), 7.50 (d, $J$ = 8.4 Hz, 1H, Ar), 7.58-7.61 (m, 1H, Ar), 7.77 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.0, 27.2, 32.5, 34.5, 114.8, 118.8, 121.2, 123.7, 126.0, 126.4, 128.3, 129.6, 131.9, 136.7, 138.5, 139.9, 140.8, 142.5. IR (neat) ν 3051, 2922, 1640, 1519, 1366, 1011, 946, 906, 832, 743 cm$^{-1}$. MS (%) m/e 246 ($M^+$, 78.54), 205 (100.00), 204 (40.36), 203 (58.32), 202 (60.87), 191 (59.65), 190 (60.37), 189 (54.86). HRMS (EI) calcd. for $C_{19}H_{18}$: 246.1409, Found: 246.1417.

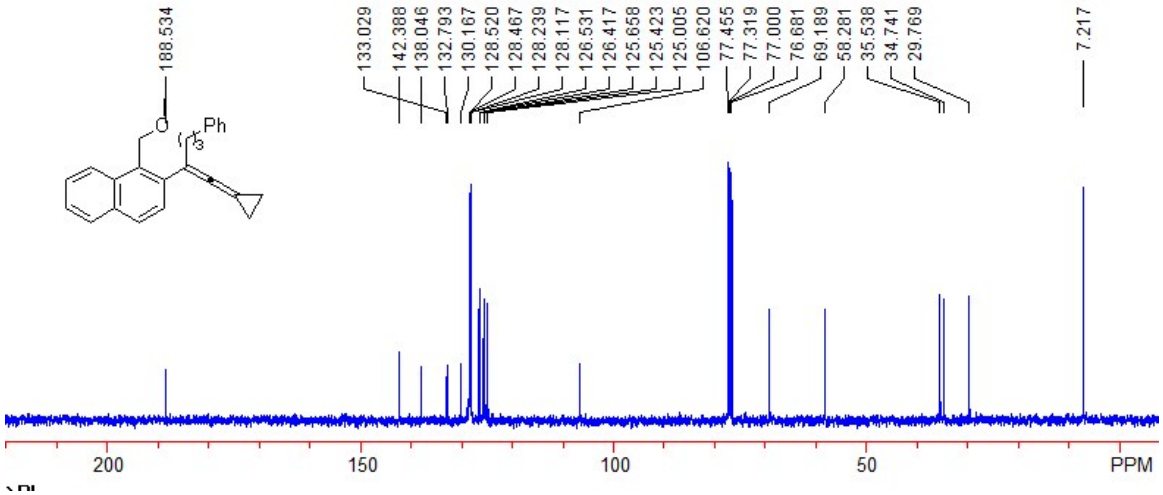


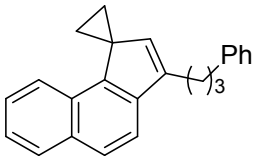



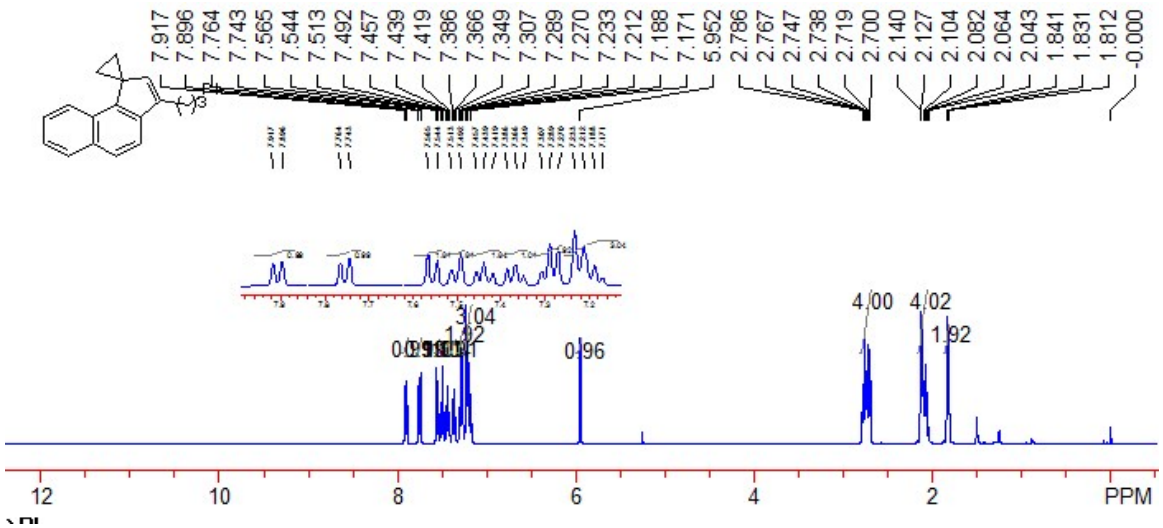

Compound **1j**. 348 mg, yield: 98%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.46-1.52 (m, 2H, $CH_2$), 1.52-1.59 (m, 2H, $CH_2$), 1.79-1.88 (m, 2H, $CH_2$), 2.48-2.53 (m, 2H, $CH_2$), 2.68-2.73 (m, 2H, $CH_2$), 3.44 (s, 3H, $CH_3$), 5.00 (s, 2H, $CH_2$), 7.15-7.18 (m, 3H, Ar), 7.23-7.28 (m, 2H, Ar), 7.38-7.45 (m, 2H, Ar), 7.49-7.54 (m, 1H, Ar), 7.74-7.80 (m, 2H, Ar), 8.16 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.2, 29.8, 34.7, 35.5, 58.3, 69.2, 77.5, 106.6, 125.0, 125.4, 125.7, 126.4, 126.5, 128.1, 128.2, 128.47, 128.52, 130.2, 132.8, 133.0, 138.0, 142.4, 188.5. IR (neat) ν 3051, 2978, 2924, 2016, 1495, 1093, 907, 819, 729, 698 cm$^{-1}$. MS (%) m/e 354 ($M^+$, 15.07), 235 (54.72), 221 (100.00), 217 (42.96), 215 (54.88), 203 (63.14), 202 (78.01), 191 (43.90), 91 (48.04). HRMS (EI) calcd. for $C_{26}H_{26}O$: 354.1984, Found: 354.1982.

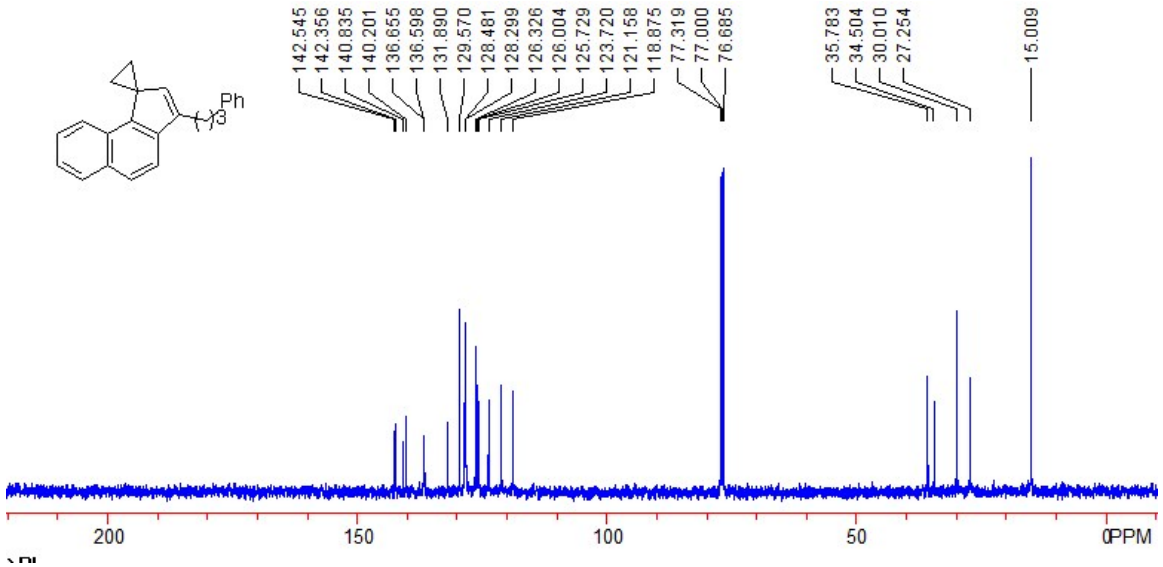


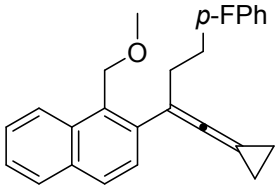



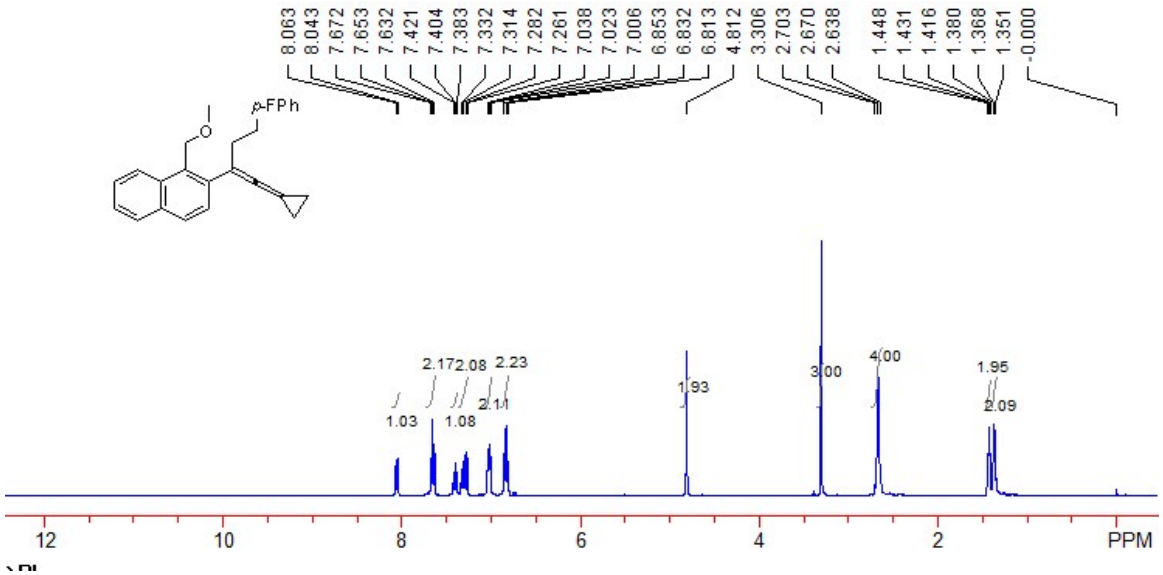

Compound **2j**. 52.4 mg, yield: 85%; white solid, Mp: 93-95 $^{o}$C. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.81-1.85 (m, 2H, $CH_2$), 2.04-2.14 (m, 4H, $2CH_2$), 2.70-2.79 (m, 4H, $2CH_2$), 5.95 (s, 1H, =CH), 7.17-7.24 (m, 3H, Ar), 7.27-7.31 (m, 2H, Ar), 7.34-7.39 (m, 1H, Ar), 7.41-7.46 (m, 1H, Ar), 7.50 (d, $J$ = 8.4 Hz, 1H, Ar), 7.55 (d, $J$ = 8.4 Hz, 1H, Ar), 7.75 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.0, 27.3, 30.0, 34.5, 35.8, 118.9, 121.2, 123.7, 125.7, 126.0, 126.3, 128.3, 128.5, 129.6, 131.9, 136.6, 136.7, 140.2, 140.8, 142.4, 142.5. IR (neat) ν 3052, 2928, 2847, 1519, 1453, 1049, 947, 832, 731, 698 cm$^{-1}$. MS (%) m/e 310 ($M^+$, 22.39), 207 (19.59), 206 (100.00), 205 (34.55), 203 (16.26), 202 (17.18), 191 (39.77), 189 (16.28). HRMS (EI) calcd. for $C_{24}H_{22}$: 310.1722, Found: 310.1733.

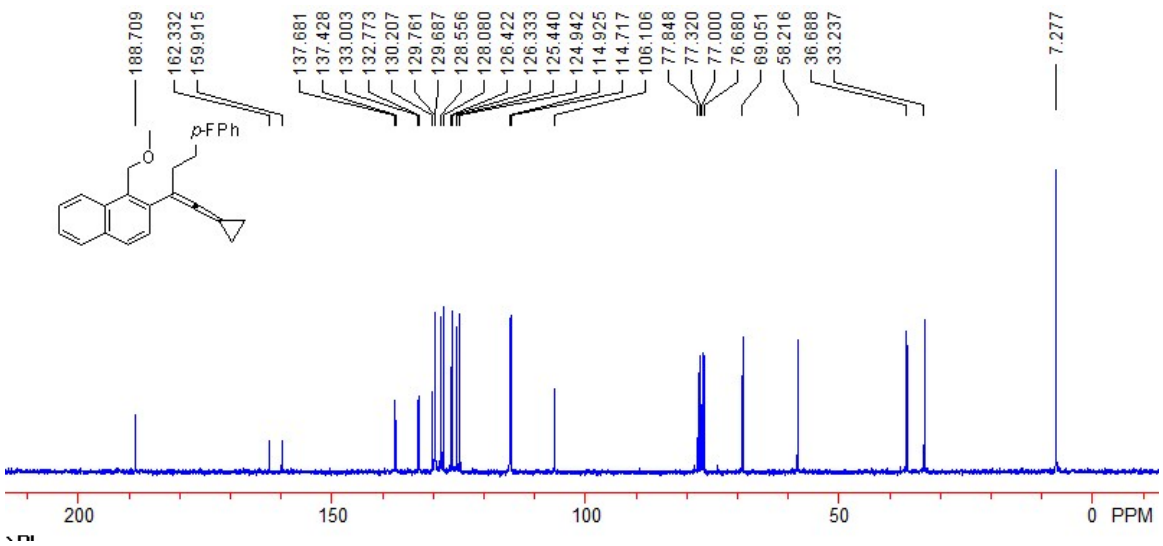


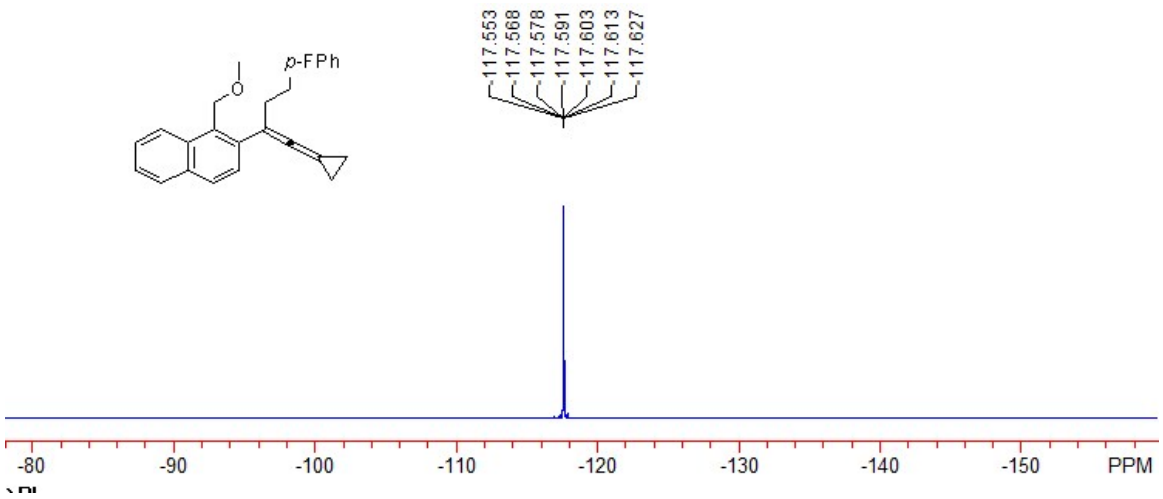



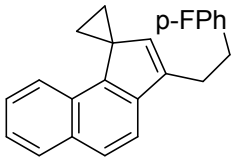




Compound **1k**. 200 mg, yield: 98%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.35-1.38 (m, 2H, $CH_2$), 1.41-1.45 (m, 2H, $CH_2$), 2.63-2.71 (m, 4H, $2CH_2$), 3.31 (s, 3H, $CH_3$), 4.81 (s, 2H, $CH_2$), 6.81-6.85 (m, 2H, Ar), 7.01-7.04 (m, 2H, Ar), 7.26-7.34 (m, 2H, Ar), 7.38-7.42 (m, 1H, Ar), 7.63-7.68 (m, 2H, Ar), 8.15 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.3, 33.2, 36.7, 58.2, 69.1, 77.8, 106.1, 114.8 (d, $J_{C\text{-}F}$ = 20.8 Hz), 125.0, 125.4, 126.4 (d, $J_{C\text{-}F}$ = 8.9 Hz), 128.1, 128.6, 129.7 (d, $J_{C\text{-}F}$ = 7.4 Hz), 130.2, 132.8, 133.0, 137.4, 137.7, 161.1 (d, $J_{C\text{-}F}$ = 241.7 Hz), 188.7. $^{19}$F NMR (376 MHz, $CDCl_3$, $CFCl_3$): δ -117.63 ~ -117.55 (m, 1F). IR (neat) ν 2990, 2870, 2801, 2016, 1508, 1219, 1093, 820, 771, 746 cm$^{-1}$. MS (%) m/e 358 ($M^+$, 5.69), 249 (83.75), 221 (96.16), 217 (41.17), 215 (31.54), 203 (42.05), 202 (75.65), 191 (35.16), 109 (100.00). HRMS (EI) calcd. for $C_{25}H_{23}OF$: 358.1733, Found: 358.1731.



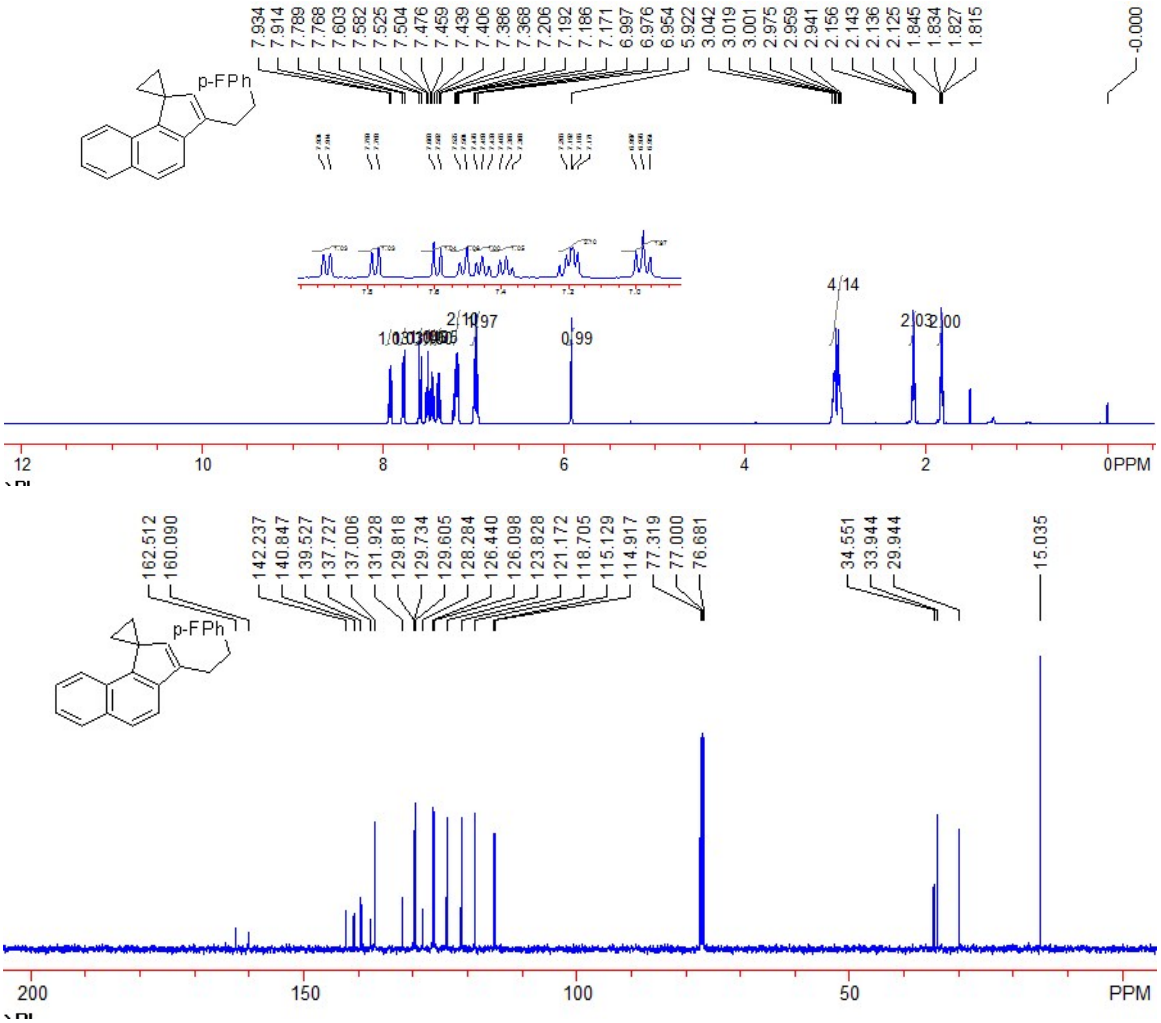



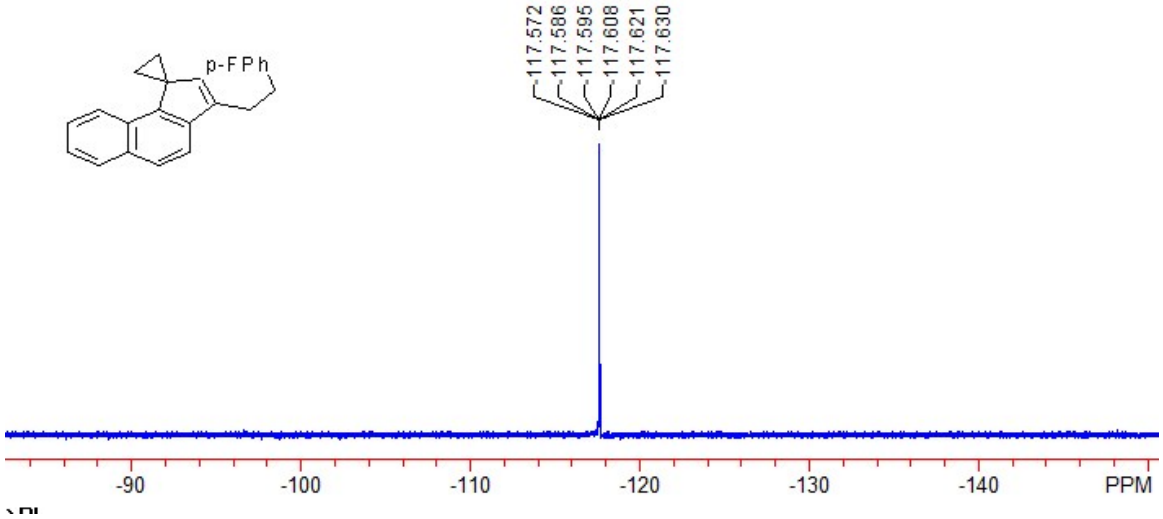



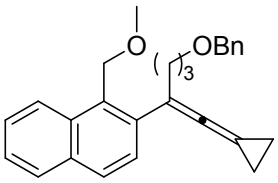




Compound **2k**. 44.0 mg, yield: 70%; pale yellow oil. $^1$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.81-1.85 (m, 2H, $CH_2$), 2.12-2.16 (m, 2H, $CH_2$), 2.94-3.05 (m,

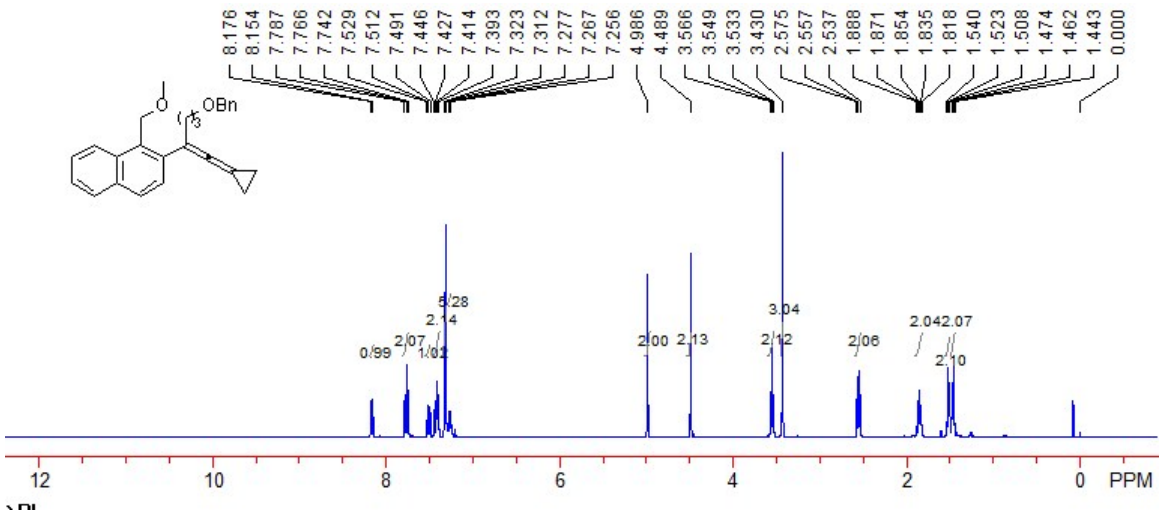
4H, 2$CH_2$), 5.92 (s, 1H, =CH), 6.95-7.00 (m, 2H, Ar), 7.17-7.21 (m, 2H, Ar), 7.36-7.41 (m, 1H, Ar), 7.43-7.53 (m, 2H, Ar), 7.59 (d, $J$ = 8.4 Hz, 1H, Ar), 7.78 (d, $J$ = 8.0 Hz, 1H, Ar), 7.92 (d, $J$ = 8.0 Hz, 1H, Ar), $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.0, 29.9, 33.9, 34.6, 115.0 (d, $J_{C\text{-}F}$ = 21.2 Hz), 118.7, 121.2, 123.8, 126.3 (d, $J_{C\text{-}F}$ = 34.2 Hz), 128.3, 129.6, 129.8 (d, $J_{C\text{-}F}$ = 8.4 Hz), 131.9, 137.0, 137.7, 139.5, 140.8, 142.2, 161.3 (d, $J_{C\text{-}F}$ = 242.2 Hz). $^{19}$F NMR (376 MHz, $CDCl_3$, $CFCl_3$): δ -117.63 ~ -117.57 (m, 1F). IR (neat) ν 3051, 1600, 1508, 1365, 1219, 1156, 946, 832, 744, 672 cm$^{-1}$. MS (%) m/e 314 ($M^+$, 88.64), 205 (100.00), 204 (25.32), 203 (38.68), 202 (41.11), 191 (62.94), 190 (45.97), 189 (36.37). HRMS (EI) calcd. for $C_{23}H_{19}F$: 314.1471, Found: 314.1467.

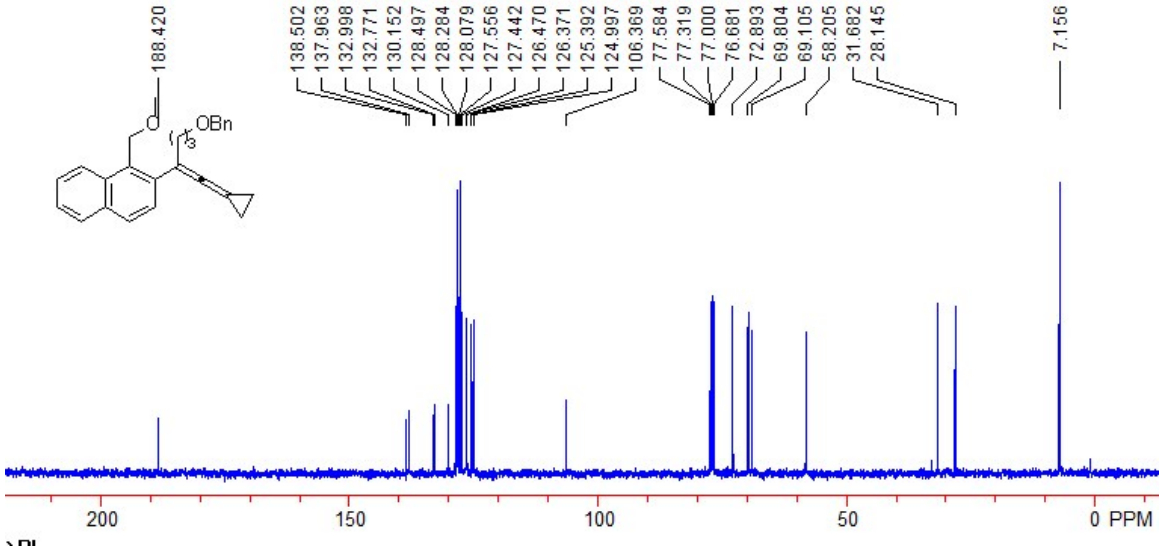


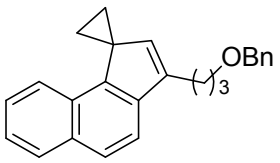


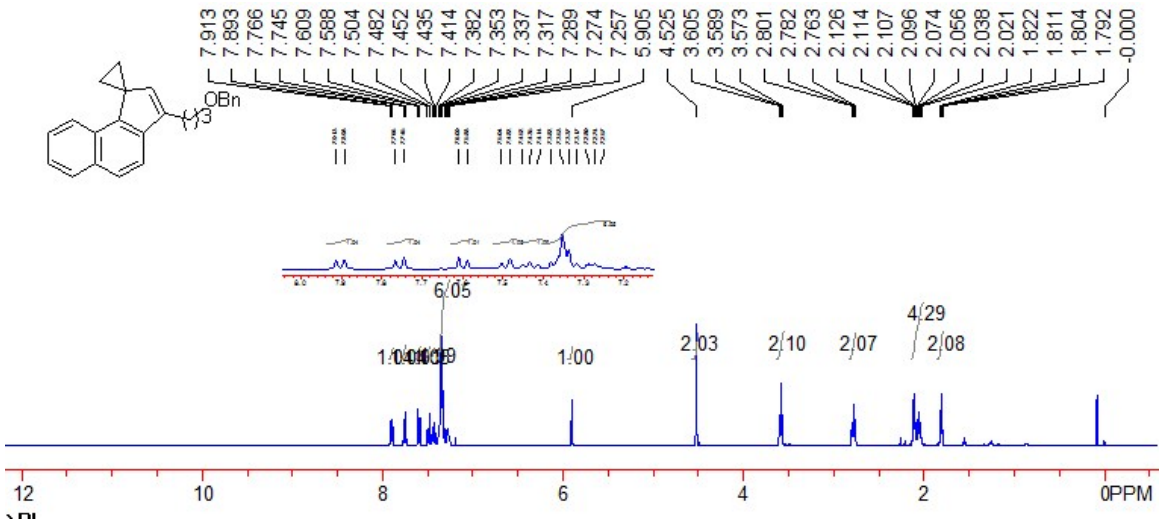

Compound **1l**. 160 mg, yield: 42%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.44-1.48 (m, 2H, $CH_2$), 1.50-1.54 (m, 2H, $CH_2$), 1.81-1.89 (m, 2H, $CH_2$), 2.56 (t, *J* = 8.0 Hz, 2H, $CH_2$), 3.43 (s, 3H, $CH_3$), 3.55 (t, *J* = 6.4 Hz, 2H, $CH_2$), 4.49 (s, 2H, $CH_2$), 4.99 (s, 2H, $CH_2$), 7.25-7.33 (m, 5H, Ar), 7.39-7.45 (m, 2H, Ar), 7.49-7.53 (m, 1H, Ar), 7.74-7.79 (m, 1H, Ar), 8.17 (d, *J* = 8.8 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.2, 28.1, 31.7, 58.2, 69.1, 69.8, 72.9, 77.6, 106.4, 125.0, 125.4, 126.4, 126.5, 127.4, 127.6, 128.1, 128.3, 128.5, 130.2, 132.8, 133.0, 138.0, 138.5, 188.4. IR (neat) ν 3065, 2984, 2860, 2015, 1495, 1093, 907, 818, 732, 697 cm$^{-1}$. MS (%) m/e 384 ($M^+$, 13.11), 235 (53.32), 221 (88.42), 219 (49.55), 217 (67.42), 215 (76.59), 203 (68.75), 202 (89.16), 91 (100.00). HRMS (EI) calcd. for $C_{27}H_{28}O_2$: 384.2089, Found: 384.2102.

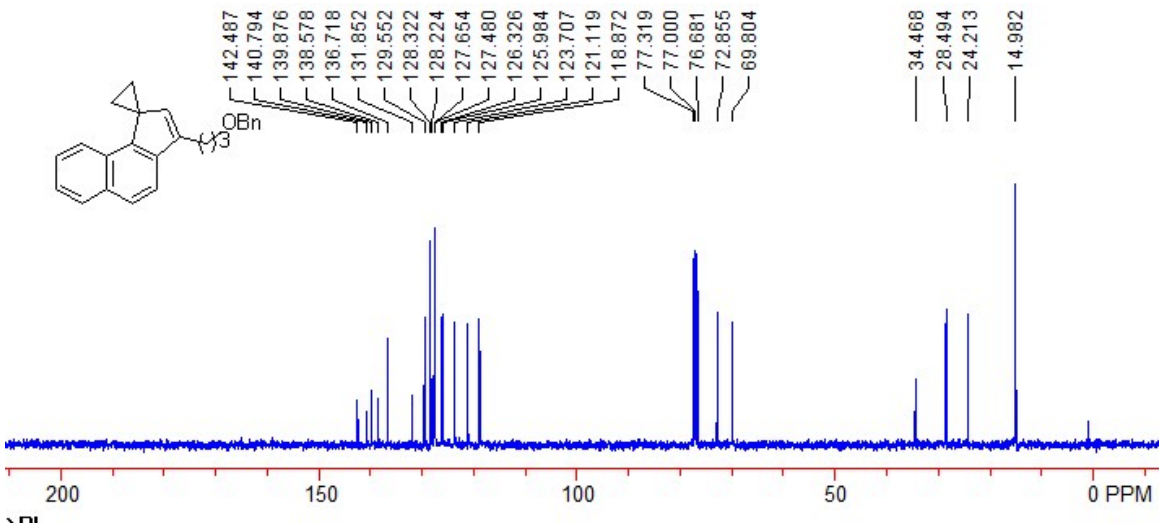


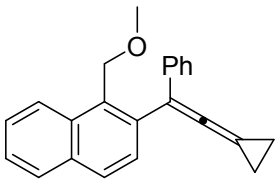


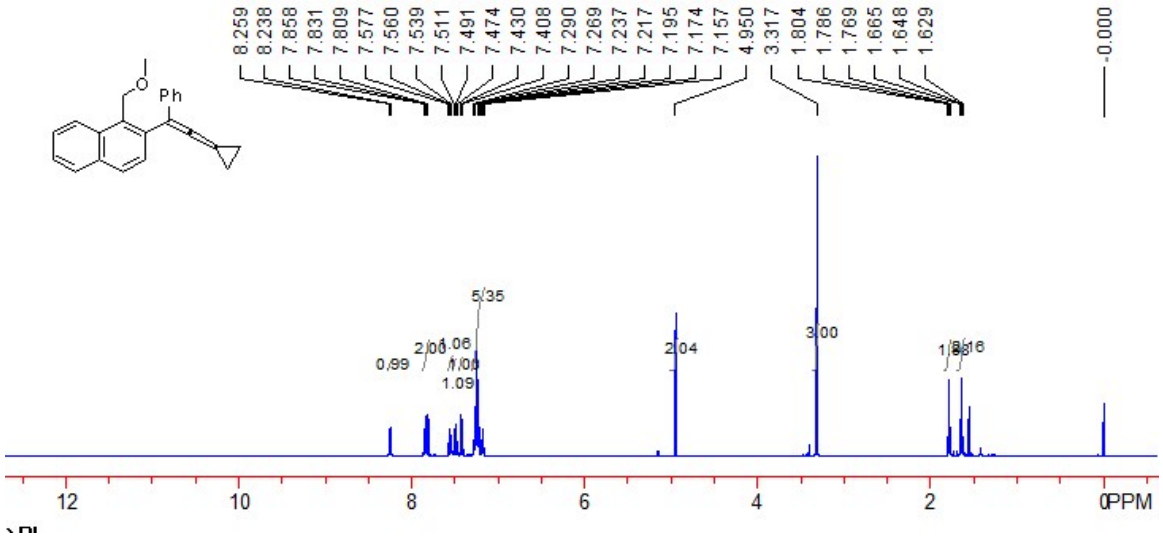

Compound **2l**. 51.0 mg, yield: 75%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.79-1.83 (m, 2H, $CH_2$), 2.02-2.13 (m, 4H, $2CH_2$), 2.78 (t, *J* = 7.6 Hz, 2H, $CH_2$), 3.59 (t, *J* = 6.4 Hz, 2H, $CH_2$), 4.53 (s, 3H, $CH_3$), 5.91 (s, 1H, =CH), 7.25-7.39 (m, 6H, Ar), 7.41-7.51 (m, 2H, Ar), 7.60 (d, *J* = 8.4 Hz, 1H, Ar), 7.76 (d, *J* = 8.4 Hz, 1H, Ar), 7.90 (d, *J* = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.0, 24.2, 28.5, 34.5, 69.8, 72.9, 118.9, 121.1, 123.7, 126.0, 126.3, 127.5, 127.7, 128.2, 128.3, 129.6, 131.9, 136.7, 138.6, 139.9, 140.8, 142.5. IR (neat) ν 3028, 2857, 1584, 1518, 1453, 1364, 1261, 1099, 833, 733 $cm^{-1}$. MS (%) m/e 340 ($M^+$, 22.91), 219 (20.56), 206 (100.00), 205 (37.58), 203 (33.76), 202 (25.20), 191 (28.65), 189 (20.16). HRMS (EI) calcd. for $C_{25}H_{24}O$: 340.1827, Found: 340.1821.

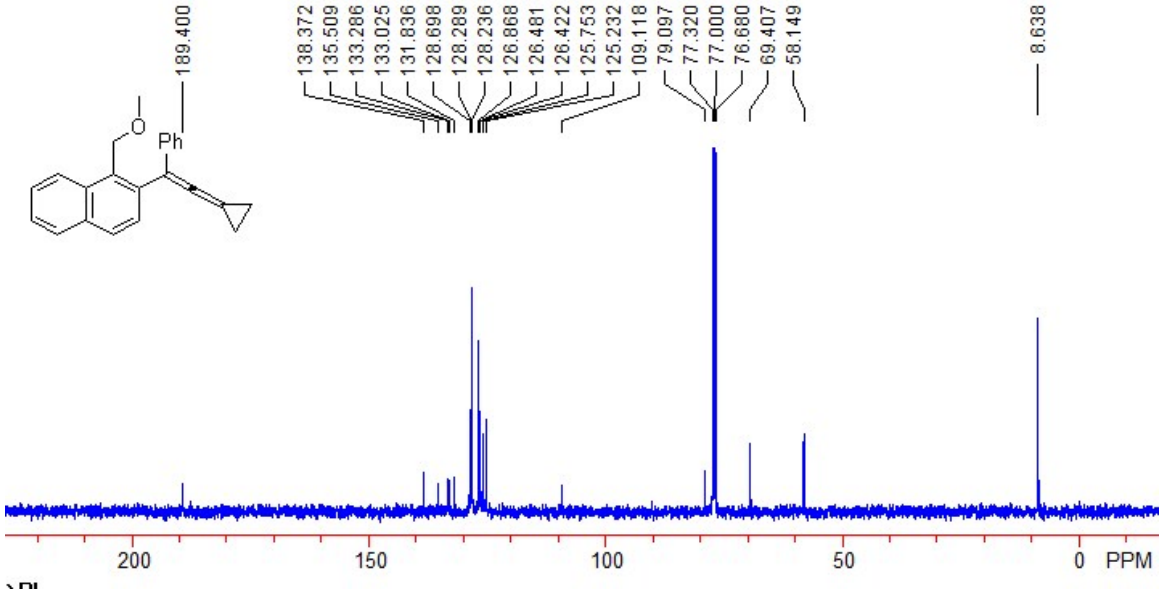


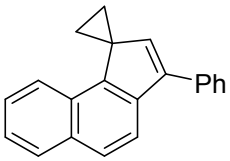


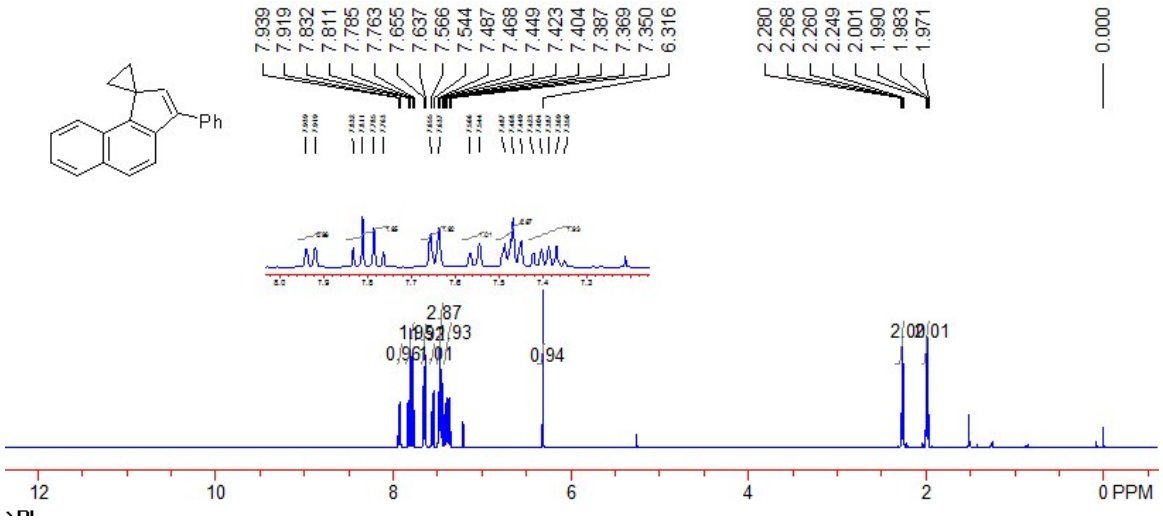

Compound **1m**. 83.0 mg, yield: 58%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.62-1.67 (m, 2H, $CH_2$), 1.76-1.81 (m, 2H, $CH_2$), 3.32 (s, 3H, $CH_3$), 4.95 (s, 2H, $CH_2$), 7.15-7.29 (m, 5H, Ar), 7.40-7.43 (m, 1H, Ar), 7.47-7.52 (m, 1H, Ar), 7.53-7.58 (m, 1H, Ar), 7.80-7.86 (m, 1H, Ar), 8.25 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 8.6, 58.1, 69.4, 79.1, 109.1, 125.2, 125.8, 126.4, 126.5, 126.9, 128.2, 128.3, 128.7, 131.8, 133.0, 133.3, 135.5, 138.4, 189.4. IR (neat) ν 3056, 2952, 2921, 2004, 1459, 1377, 1096, 831, 756, 742 cm$^{-1}$. MS (%) m/e 312 ($M^+$, 40.55), 284 (90.22), 281 (45.70), 279 (46.61), 269 (45.73), 266 (49.28), 265 (100.00), 253 (49.13), 252 (57.44). HRMS (EI) calcd. for $C_{23}H_{20}O$: 312.1514, Found: 312.1517.

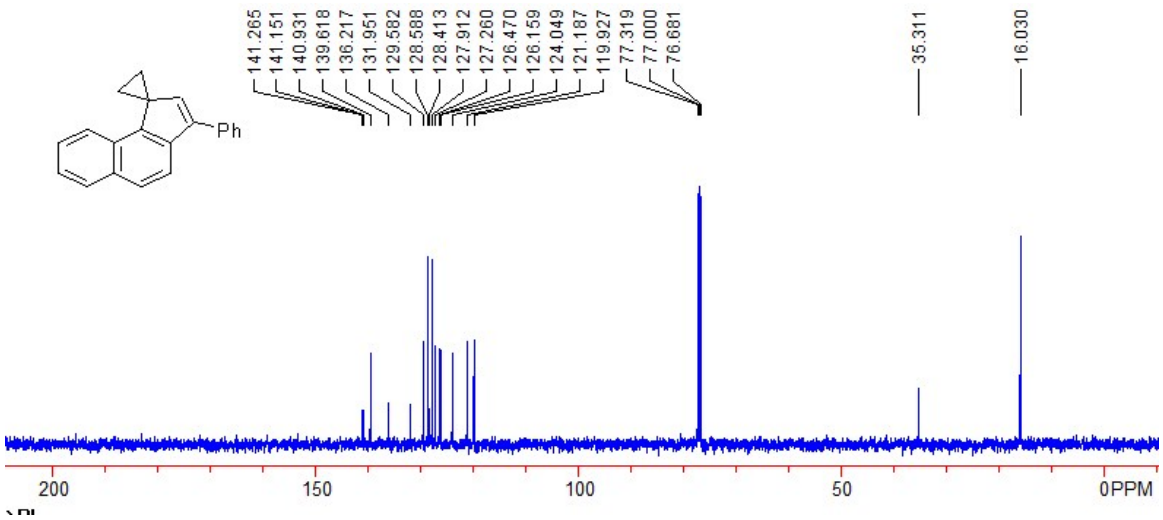


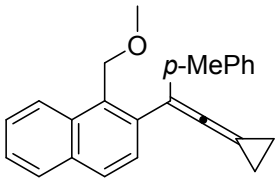


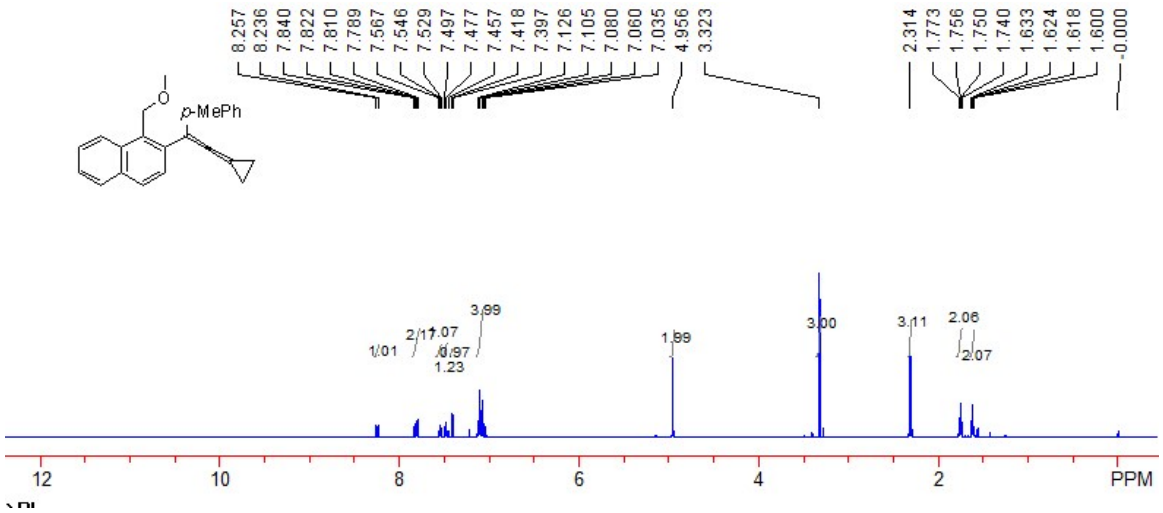

Compound **2m**. 34.1 mg, yield: 64%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.99 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 2.26 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 6.32 (s, 1H, =CH), 7.35-7.43 (m, 2H, Ar), 7.44-7.49 (m, 3H, Ar), 7.56 (d, $J$ = 8.8 Hz, 1H, Ar), 7.65 (d, $J$ = 7.2 Hz, 2H, Ar), 7.76-7.84 (m, 2H, Ar), 7.93 (d, $J$ = 8.0 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 16.0, 35.3, 119.9, 121.2, 124.0, 126.2, 126.5, 127.3, 127.9, 128.4, 128.6, 129.6, 132.0, 136.2, 139.6, 140.9, 141.2, 141.3. IR (neat) ν 3053, 2924, 1622, 1551, 1444, 1366, 1240, 1027, 945, 760 cm$^{-1}$. MS (%) m/e 268 ($M^+$, 100.00), 269 (23.81), 267 (57.69), 265 (29.11), 253 (28.26), 252 (37.79), 86 (51.81), 84 (80.23). HRMS (EI) calcd. for $C_{21}H_{16}$: 268.1252, Found: 268.1246.

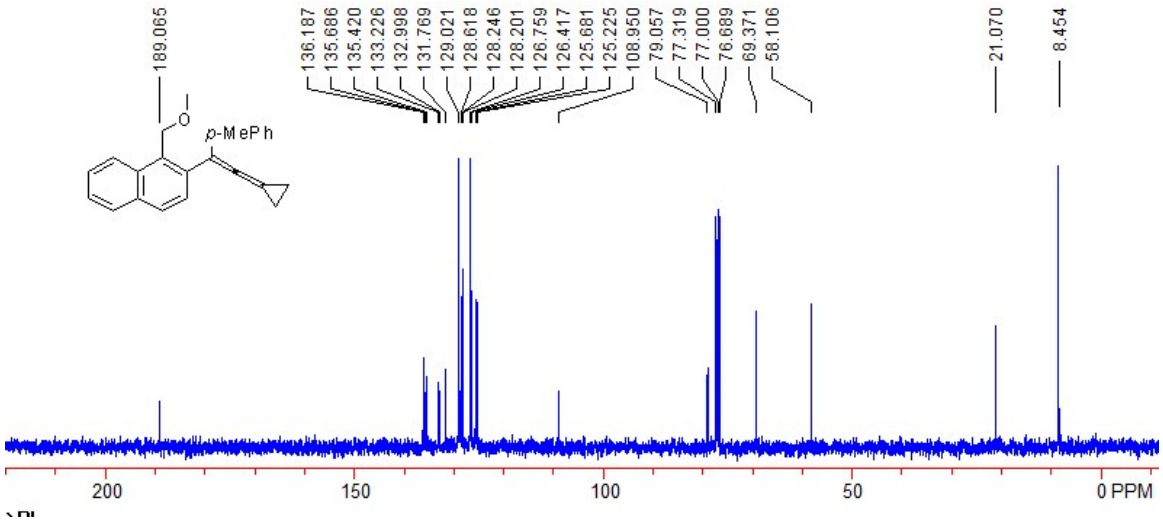


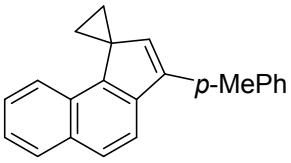


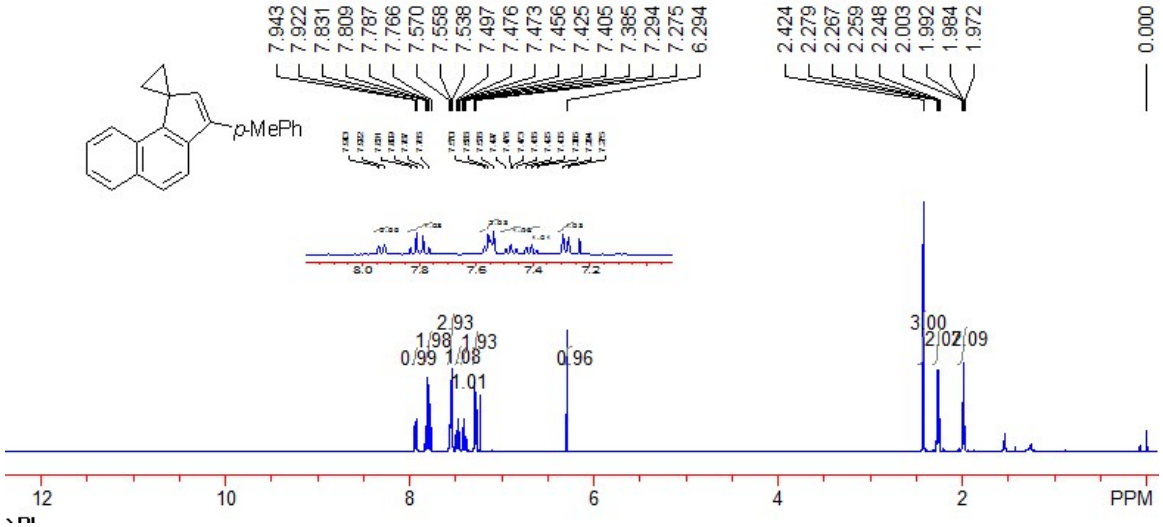

Compound **1n**. 159.1 mg, yield: 42%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.60-1.64 (m, 2H, $CH_2$), 1.74-1.78 (m, 2H, $CH_2$), 2.31 (s, 2H, $CH_2$), 3.32 (s, 3H, $CH_3$), 4.96 (s, 2H, $CH_2$), 7.03-7.13 (m, 4H, Ar), 7.41 (d, $J$ = 8.4 Hz, 1H, Ar), 7.45-7.50 (m, 1H, Ar), 7.52-7.57 (m, 1H, Ar), 7.78-7.84 (m, 2H, Ar), 8.25 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 8.5, 21.1, 58.1, 69.4, 79.1, 109.0, 125.2, 125.7, 126.4, 126.8, 128.20, 128.25, 128.6, 129.0, 131.8, 133.0, 133.2, 135.4, 135.7, 136.2, 189.1. IR (neat) ν 2985, 2921, 2003, 1508, 1458, 1394, 1094, 1044, 863, 728 cm$^{-1}$. MS (%) m/e 326 ($M^+$, 57.55), 298 (96.58), 283 (55.22), 281 (50.41), 280 (53.52), 279 (99.62), 266 (55.49), 265 (100.00). HRMS (EI) calcd. for $C_{24}H_{22}O$: 326.1671, Found: 326.1665.

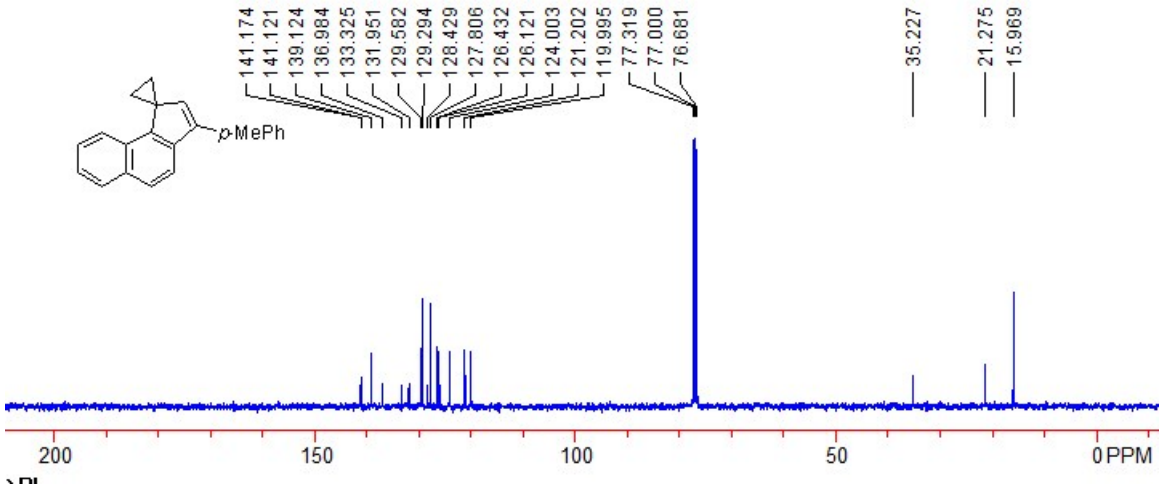


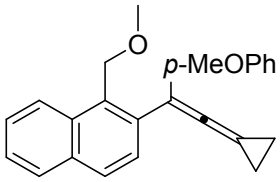


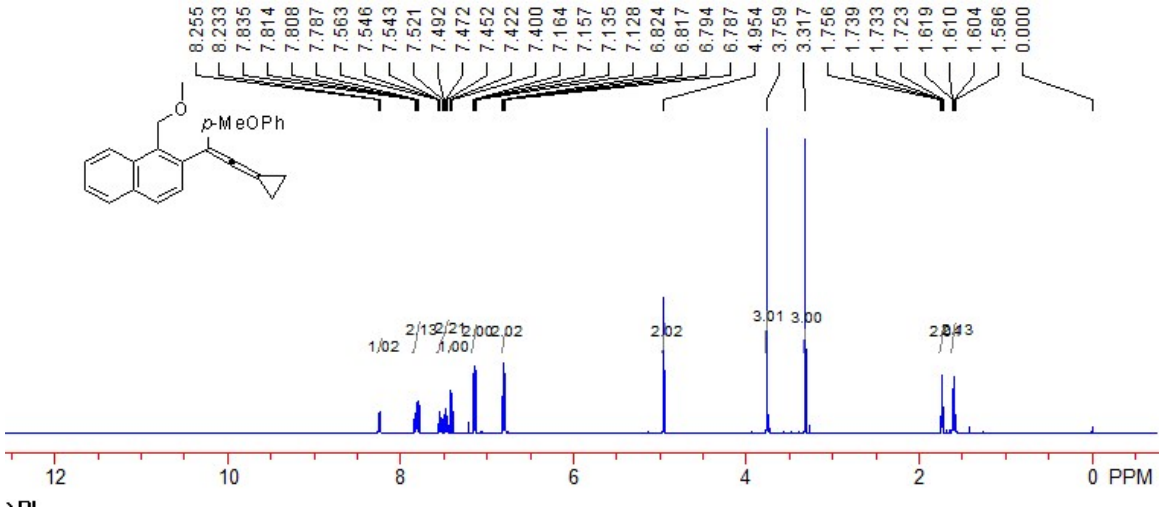

Compound **2n**. 34.1 mg, yield: 64%; yellow sold, Mp: 122-125 $^{o}$C. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.99 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.2 Hz, 2H, $CH_2$), 2.26 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.2 Hz, 2H, $CH_2$), 2.42 (s, 3H, $CH_3$), 6.29 (s, 1H, =$CH_2$) 7.27-7.30 (m, 2H, Ar), 7.38-7.43 (m, 1H, Ar), 7.45-7.50 (m, 1H, Ar), 7.53-7.57 (m, 3H, Ar), 7.76-7.84 (m, 2H, Ar), 7.93 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 16.0, 21.3, 35.2, 120.0, 121.2, 124.0, 126.1, 126.4, 127.8, 128.4, 129.3, 129.6, 132.0, 133.3, 137.0, 139.1, 141.1, 141.2. IR (neat) ν 2958, 2921, 2851, 1066, 1051, 1027, 824, 746 cm$^{-1}$. MS (%) m/e 282 ($M^+$, 100.00), 283 (26.42), 281 (28.76), 267 (46.15), 266 (31.99), 265 (35.73), 252 (25.21), 189 (15.69). HRMS (EI) calcd. for $C_{22}H_{18}$: 282.1409, Found: 282.1403.

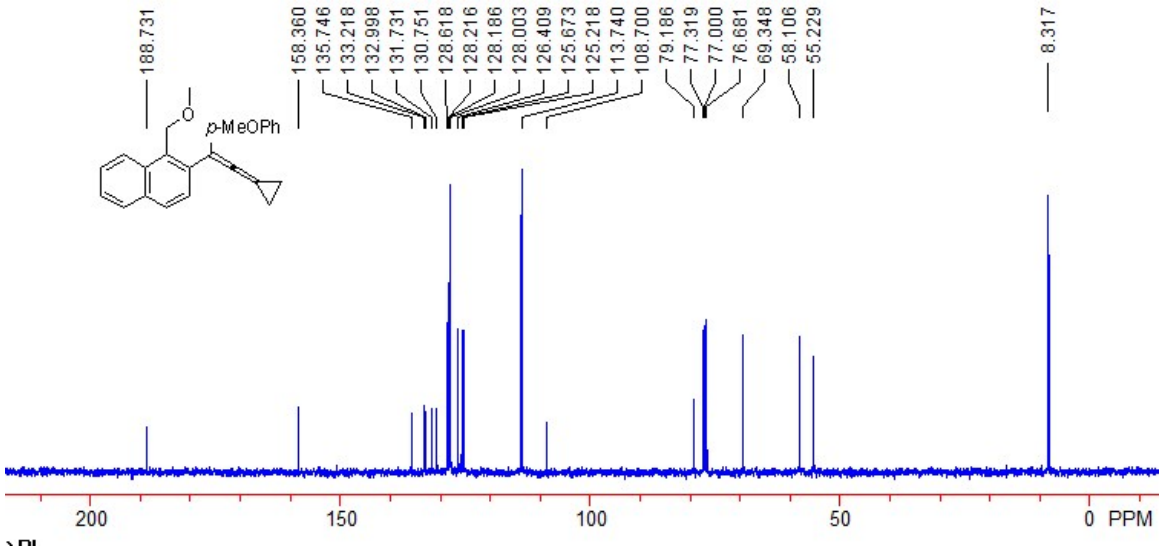


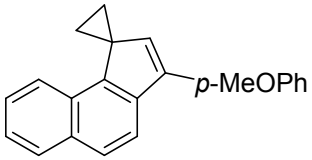


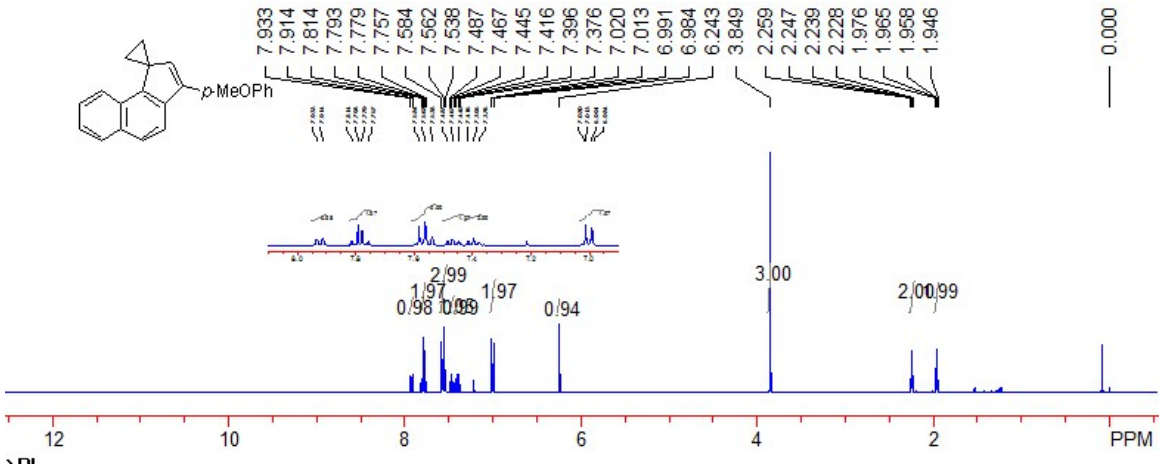

Compound **1o**. 100.3 mg, yield: 30%; white solid, Mp: 83-85 °C. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.58-1.62 (m, 2H, $CH_2$), 1.72-1.76 (m, 2H, $CH_2$), 3.32 (s, 3H, $CH_3$), 3.76 (s, 3H, $CH_3$), 4.95 (s, 2H, $CH_2$), 6.78-6.83 (m, 2H, Ar), 7.12-7.17 (m, 2H, Ar), 7.41 (d, $J$ = 8.8 Hz, 1H, Ar), 7.45-7.57 (m, 2H, Ar), 7.78-7.84 (m, 2H, Ar), 8.24 (d, $J$ = 8.8 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 8.3, 55.2, 58.1, 69.3, 79.2, 108.7, 113.7, 125.2, 125.7, 126.4, 128.0, 128.19, 128.22, 128.6, 130.8, 131.7, 133.0, 133.2, 135.7, 158.4, 188.7. IR (neat) ν 2983, 2004, 1736, 1508, 1372, 1172, 1095, 1043, 817, 760 cm$^{-1}$. MS (%) m/e 342 ($M^+$, 87.52), 314 (100.00), 311 (93.77), 299 (68.56), 265 (68.94), 253 (51.80), 252 (71.68), 239 (55.26). HRMS (EI) calcd. for $C_{24}H_{22}O_2$: 342.1620, Found: 342.1619.

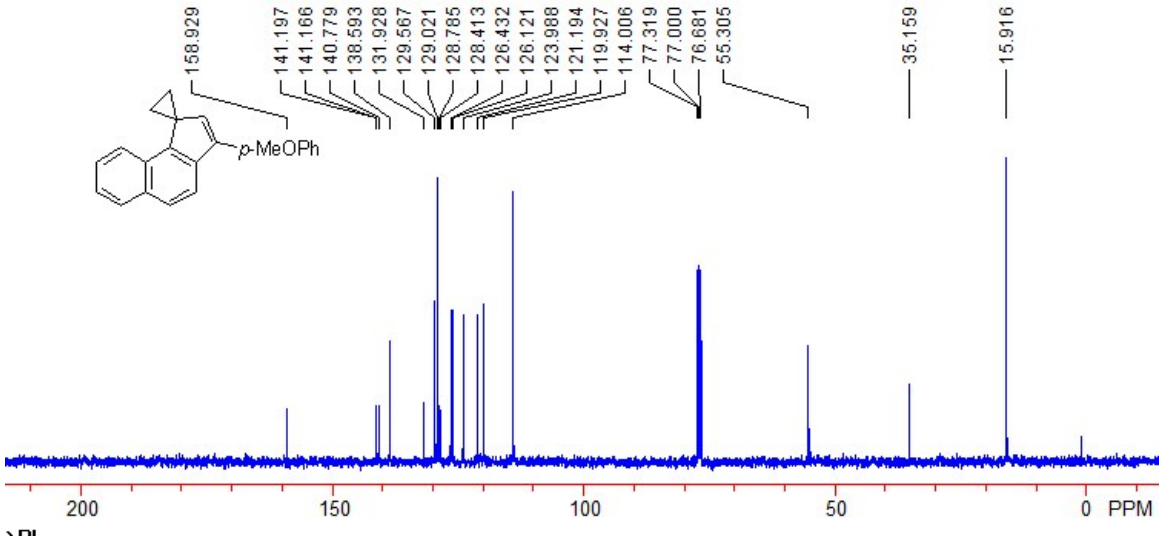


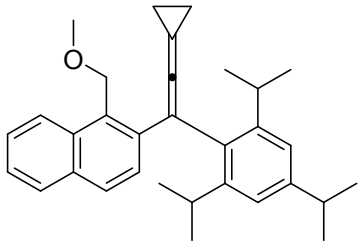


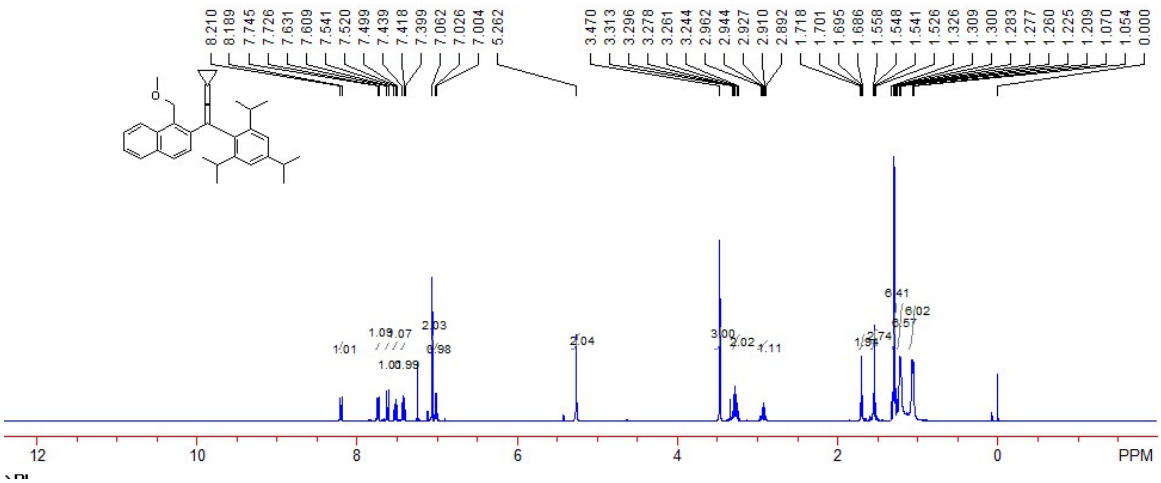

Compound **2o**. 30.6 mg, yield: 51%; white solid. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.96 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 2.24 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.6 Hz, 2H, $CH_2$), 3.85 (s, 3H, $CH_3$), 6.24 (s, 1H, =CH), 6.98-7.02 (m, 2H, Ar), 7.37-7.42 (m, 1H, Ar), 7.44-7.49 (m, 1H, Ar), 7.53-7.59 (m, 3H, Ar), 7.75-7.82 (m, 2H, Ar), 7.92 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.9, 35.2, 55.3, 114.0, 119.9, 121.2, 124.0, 126.1, 126.4, 128.4, 128.8, 129.0, 129.6, 131.9, 138.6, 140.8, 141.17, 141.20, 158.9. IR (neat) ν 2929, 1736, 1598, 1508, 1372, 1167, 1043, 940, 821, 766 cm$^{-1}$. MS (%) m/e 299 ($M^+$, 27.72), 298 (100.00), 297 (24.94), 283 (17.75), 267 (23.62), 265 (16.44), 252 (19.54), 239 (17.03). HRMS (EI) calcd. for $C_{22}H_{18}O$: 298.1358, Found: 298.1364.

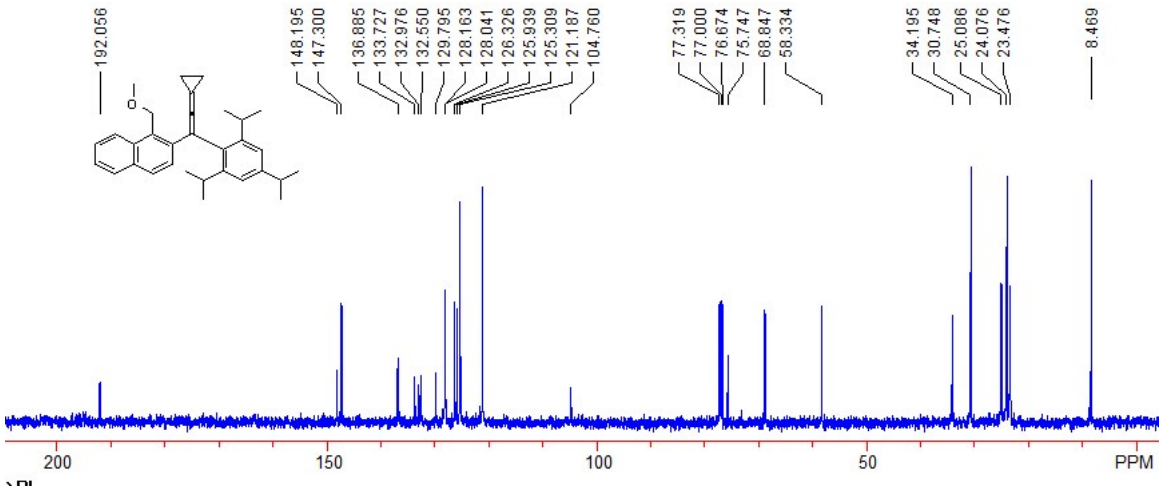


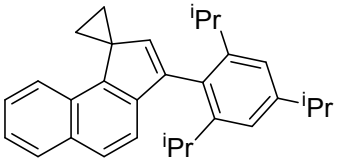


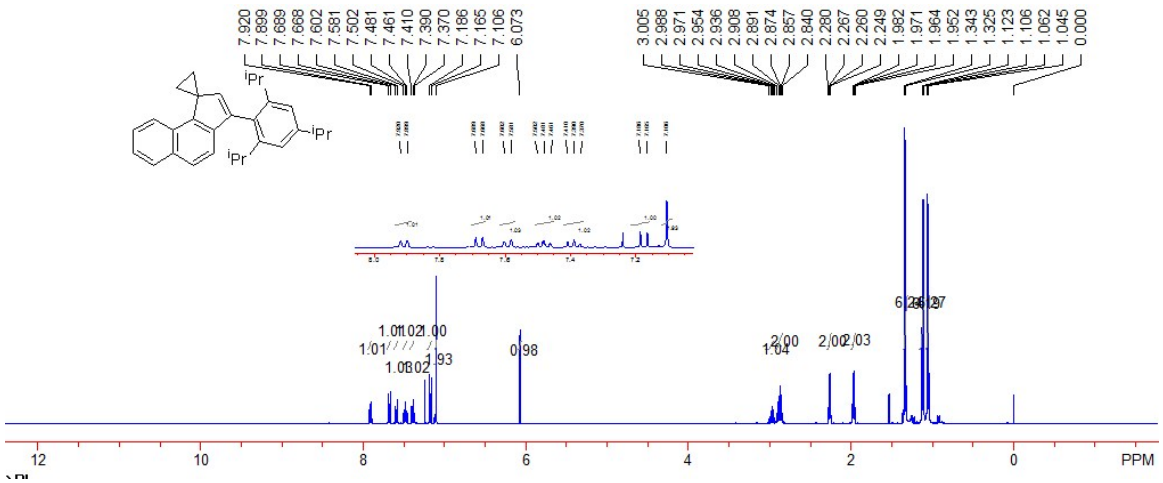
Compound **1p**. 430.4 mg, yield: 98%; pale yellow solid, Mp: 145-149 °C. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.06 (d, $J$ = 6.4 Hz, 6H, $2CH_3$), 1.21 (d, $J$ = 6.4 Hz, 6H, $2CH_3$), 1.26-1.33 (m, 6H, $2CH_3$), 1.52-1.56 (m, 2H, $CH_2$), 1.68-1.72 (m, 2H, $CH_2$), 2.89-2.97 (m, 1H, CH), 3.24-3.32 (m, 1H, CH), 3.47 (s, 3H, $CH_3$), 5.26 (s, 2H, $CH_2$), 7.02 (d, $J$ = 8.8 Hz, 1H, Ar), 7.06 (s, 2H, Ar), 7.39-7.44 (m, 1H, Ar), 7.49-7.55 (m, 1H, Ar), 7.62 (d, $J$ = 8.8 Hz, 1H, Ar), 7.74 (d, $J$ = 7.6 Hz, 1H, Ar), 8.20 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 8.5, 23.5, 24.1, 25.1, 30.7, 34.2, 58.3, 68.8, 75.7, 104.8, 121.2, 125.3, 125.9, 126.3, 128.0, 128.2, 129.8, 132.6, 133.0, 133.7, 136.9, 147.3, 148.2, 192.1. IR (neat) ν 2958, 2926, 2868, 1994, 1740, 1460, 1372, 1238, 1098, 823 cm$^{-1}$. MS (%) m/e 438 ($M^+$, 91.07), 410 (52.14), 407 (70.21), 396 (49.08), 395 (100.00), 321 (59.45), 291 (47.33), 279 (56.74). HRMS (EI) calcd. for $C_{32}H_{38}O$: 438.2923, Found: 438.2928.

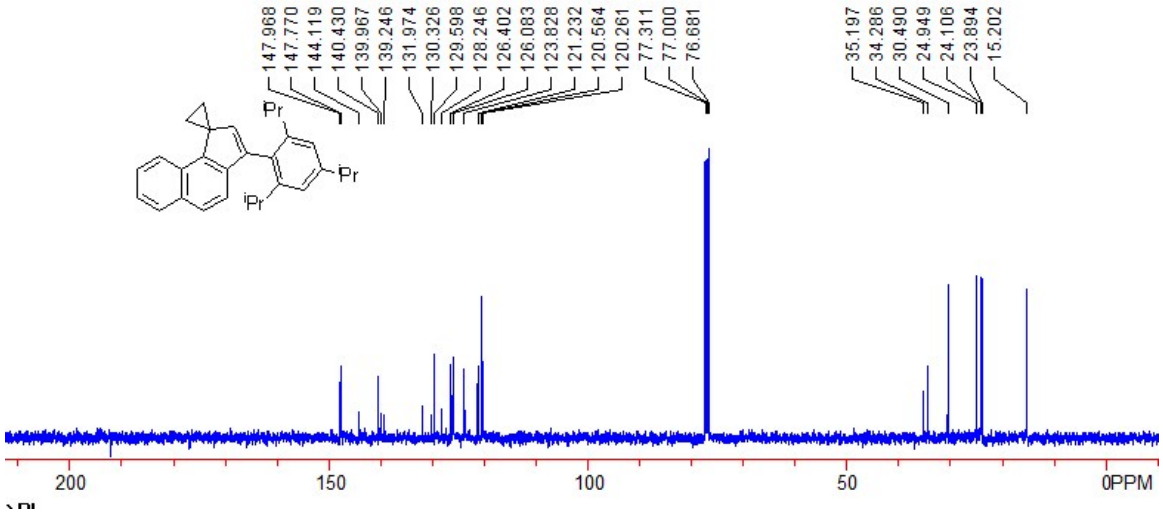


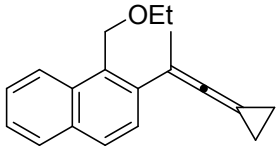


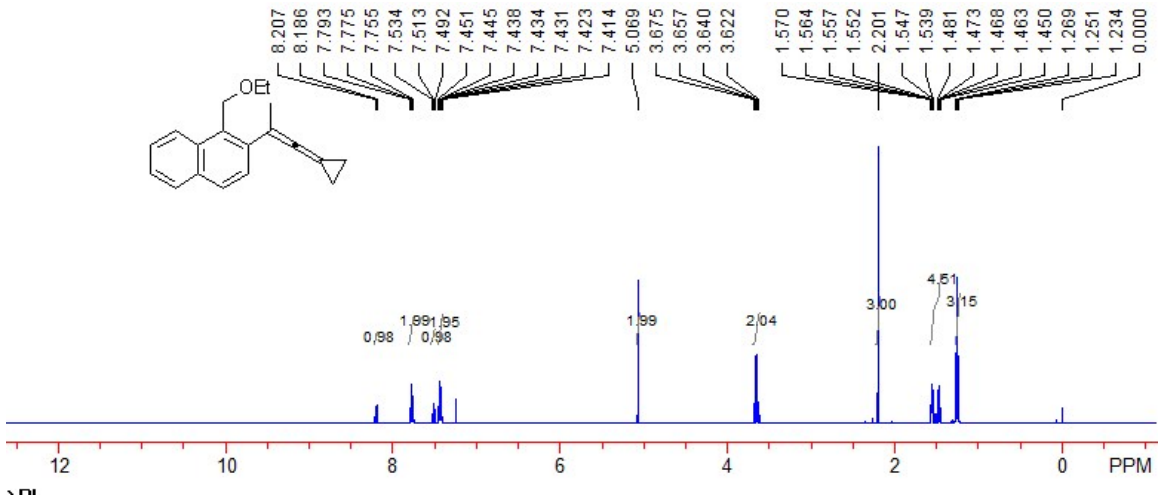

Compound **2p**. 30.2 mg, yield: 38%; white solid. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.05 (d, $J$ = 6.8 Hz, 6H, $2CH_3$), 1.12 (d, $J$ = 6.8 Hz, 6H, $2CH_3$), 1.33 (d, $J$ = 7.2 Hz, 6H, $2CH_3$), 1.97 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.2 Hz, 2H, $CH_2$), 2.26 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.2 Hz, 2H, $CH_2$), 2.84-2.91 (m, 2H, 2CH), 2.93-3.01 (m, 1H, CH), 6.07 (s, 1H, =CH), 7.11 (s, 2H, Ar), 7.18 (d, $J$ = 8.4 Hz, 1H, Ar), 7.37-7.41 (m, 2H, Ar), 7.46-7.51 (m, 1H, Ar), 7.59 (d, $J$ = 8.4 Hz, 1H, Ar), 7.68 (d, $J$ = 8.4 Hz, 1H, Ar), 7.91 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 15.2, 23.9, 24.1, 24.9, 30.5, 34.3, 35.2, 120.3, 120.6, 121.2, 123.8, 126.1, 126.4, 128.2, 129.6, 130.3, 132.0, 139.2, 140.0, 140.4, 144.1, 147.8, 148.0. IR (neat) ν 2959, 2927, 2867, 1739, 1372, 1237, 1046, 987, 945, 747 cm$^{-1}$. MS (%) m/e 394 ($M^+$, 22.26), 395 (8.24), 380 (34.88), 379 (100.00), 364 (5.74), 321 (5.73), 293 (5.94).291 (6.85). HRMS (EI) calcd. for $C_{30}H_{34}$: 394.2661, Found: 394.2657.

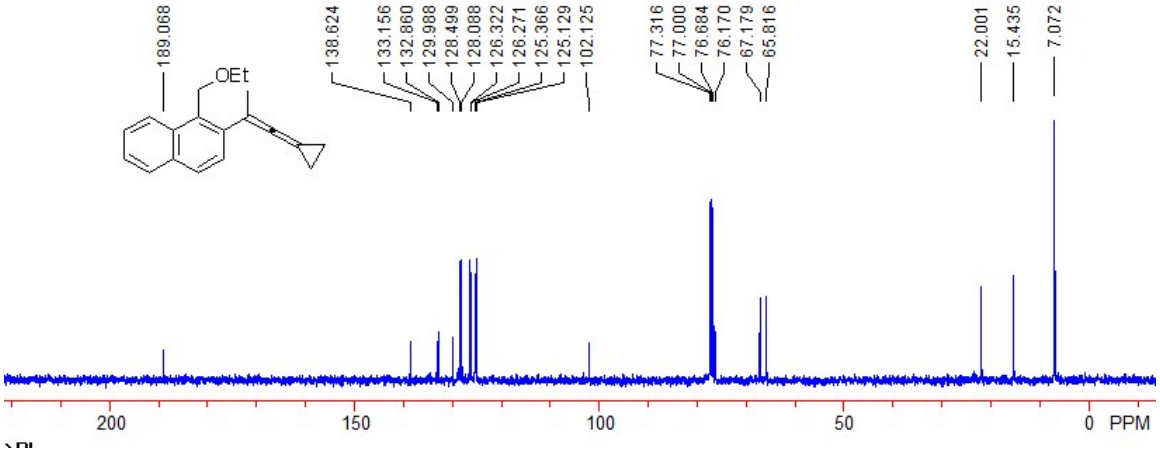


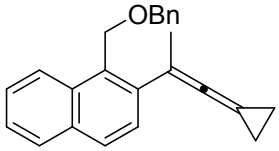


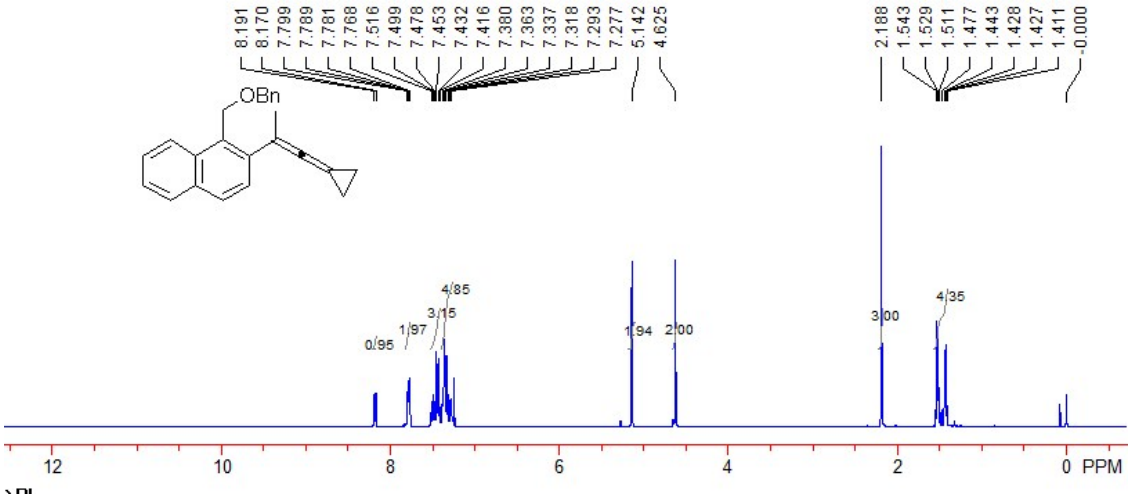

Compound **1q**. 245.5 mg, yield: 93%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.25 (t, $J$ = 7.2 Hz, 3H, $CH_3$), 1.45-1.57 (m, 4H, $2CH_2$), 2.20 (s, 3H, $CH_3$), 3.65 (q, $J$ = 7.2 Hz, 2H, $CH_2$), 5.07 (s, 2H, $CH_2$), 7.41-7.46 (m, 2H, Ar), 7.49-7.54 (m, 1H, Ar), 7.75-7.80 (m, 2H, Ar), 8.20 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 15.4, 22.0, 65.8, 67.2, 76.2, 102.1, 125.1, 125.4, 126.27, 126.32, 128.1, 128.5, 130.0, 132.9, 133.2, 138.6, 189.1. IR (neat) ν 3048, 2973, 2865, 2016, 1346, 1090, 905, 817, 746, 680 cm$^{-1}$. MS (%) m/e 264 ($M^+$, 11.73), 236 (100.00), 207 (76.66), 203 (79.61), 202 (98.58), 192 (75.98), 191 (81.14), 178 (96.10), 165 (78.51). HRMS (EI) calcd. for $C_{19}H_{20}O$: 264.1514, Found: 264.1506.

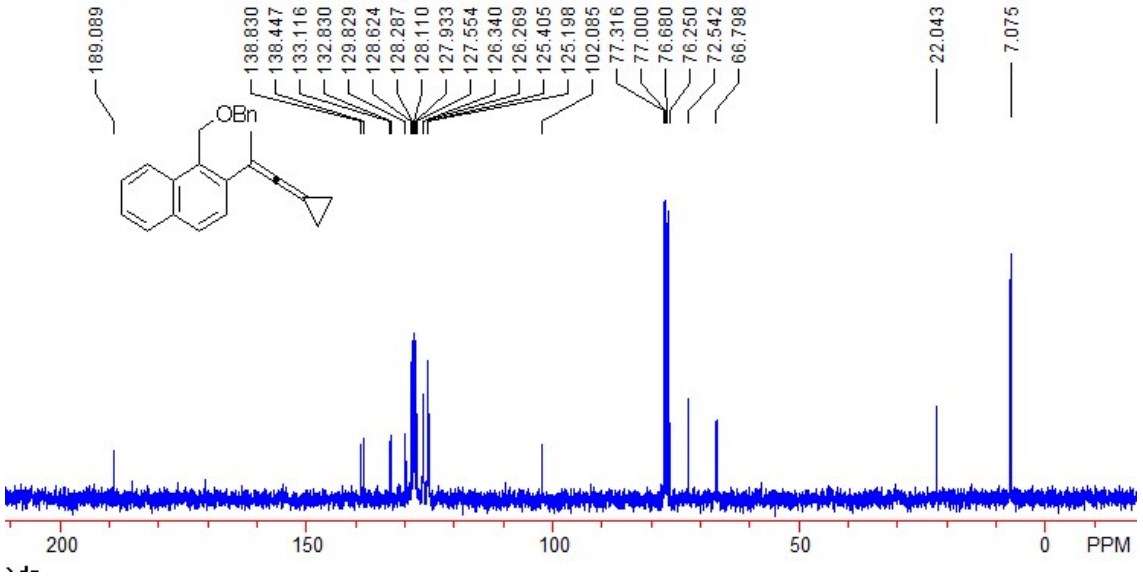


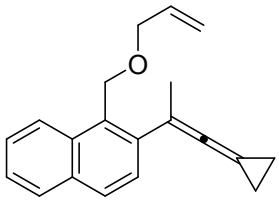


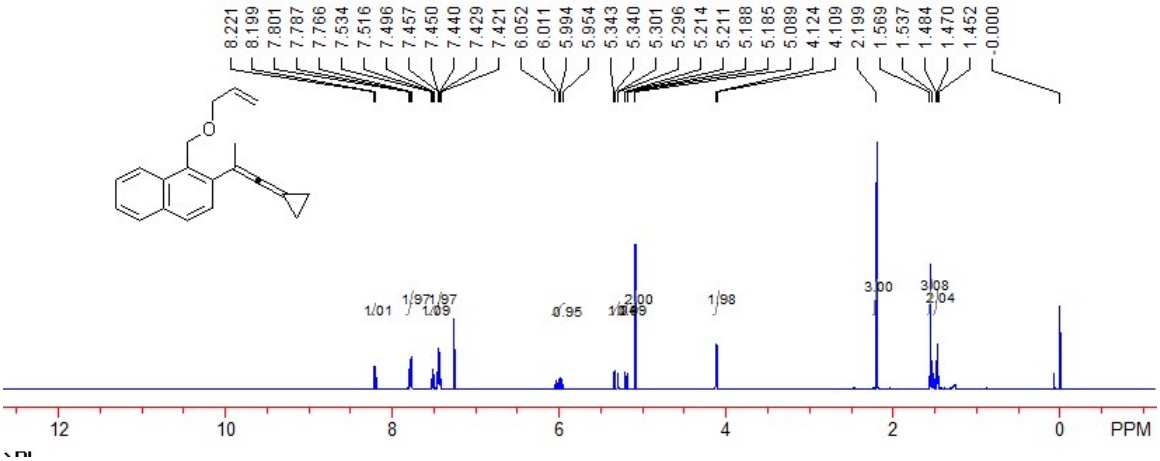

Compound **1r**. 300.8 mg, yield: 92%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.41-1.55 (m, 4H, $2CH_2$), 2.19 (s, 3H, $CH_3$), 4.63 (s, 2H, $CH_2$), 5.14 (s, 2H, $CH_2$), 7.27-7.38 (m, 5H, Ar), 7.41-7.52 (m, 3H, Ar), 7.76-7.80 (m, 2H, Ar), 8.18 (d, $J$ = 8.4 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 22.0, 66.8, 72.5, 76.3, 102.1, 125.2, 125.4, 126.27, 126.34, 127.6, 127.9, 128.1, 128.3, 128.6, 129.8, 132.8, 133.1, 138.4, 138.8, 189.1. IR (neat) ν 2981, 2907, 2016, 1507, 1071, 862, 848, 818, 731, 696 cm$^{-1}$. MS (%) m/e 326 ($M^+$, 3.57), 235 (71.23), 207 (44.45), 193 (100.00), 192 (59.86), 191 (45.20), 179 (43.78), 178 (53.01), 91 (97.66). HRMS (EI) calcd. for $C_{24}H_{22}O$: 326.1671, Found: 326.1672.

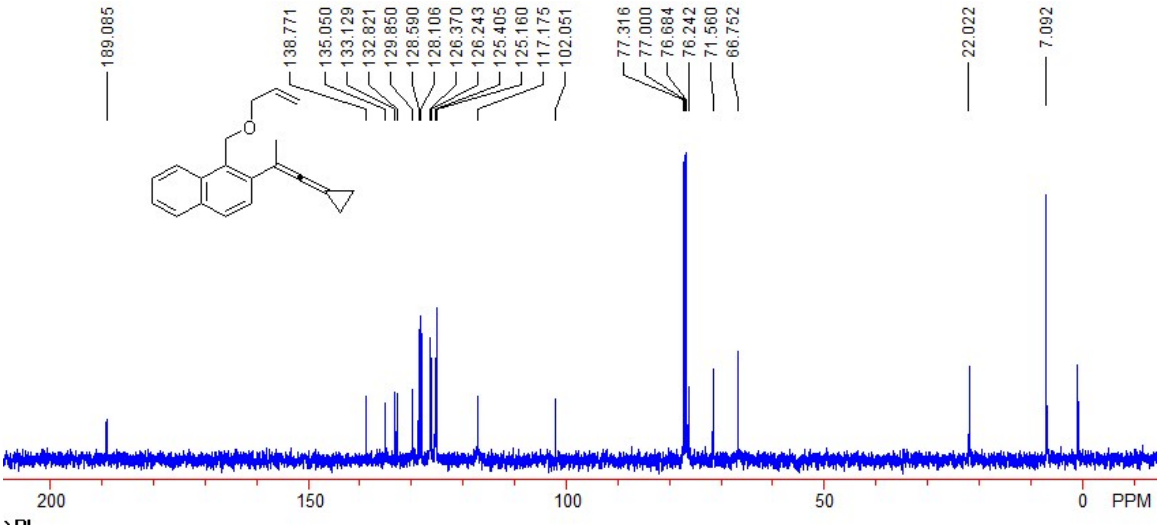


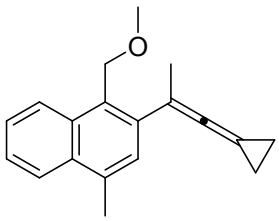


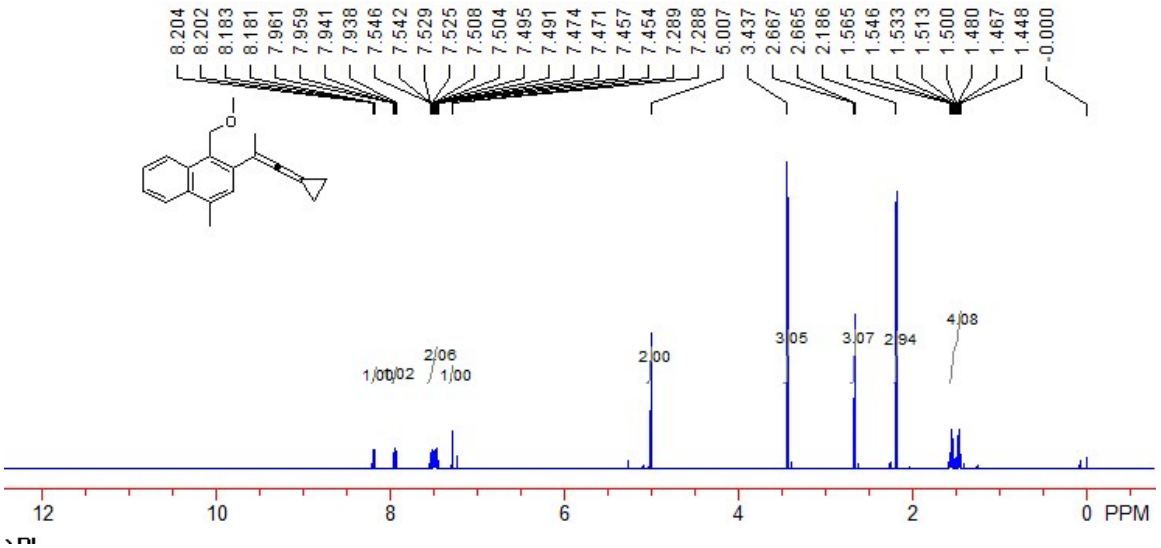

Compound **1q**. 100.2 mg, yield: 37%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.45-1.57 (m, 4H, $2CH_2$), 2.20 (s, 3H, $CH_3$), 4.12 (d, $J$ = 6.0 Hz, 2H, $CH_2$), 5.09 (s, 2H, $CH_2$), 5.20 (dd, 1H, $J_1$ = 1.2 Hz, $J_2$ = 10.8 Hz, 1H, =$CH_2$), 5.32 (dd, $J_1$ = 1.2 Hz, $J_2$ = 17.6 Hz, 1H, =$CH_2$), 5.95-6.06 (m, 1H, =CH), 7.42-7.46 (m, 2H, Ar), 7.49-7.54 (m, 1H, Ar), 7.76-7.81 (m, 2H, Ar), 8.21 (d, $J$ = 8.8 Hz, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 22.0, 66.8, 71.6, 76.2, 102.1, 117.2, 125.2, 125.4, 126.2, 126.4, 128.1, 128.6, 129.9, 132.8, 133.1, 135.1, 138.8, 189.1. IR (neat) ν 2979, 2908, 2016, 1259, 1072, 1009, 848, 817, 746, 682 cm$^{-1}$. MS (%) m/e 276 ($M^+$, 1.90), 207 (100.00), 202 (79.15), 193 (76.17), 192 (89.26), 191 (80.32), 179 (77.02), 178 (93.18), 165 (74.37). HRMS (EI) calcd. for $C_{20}H_{20}O$: 276.1514, Found: 276.1511.

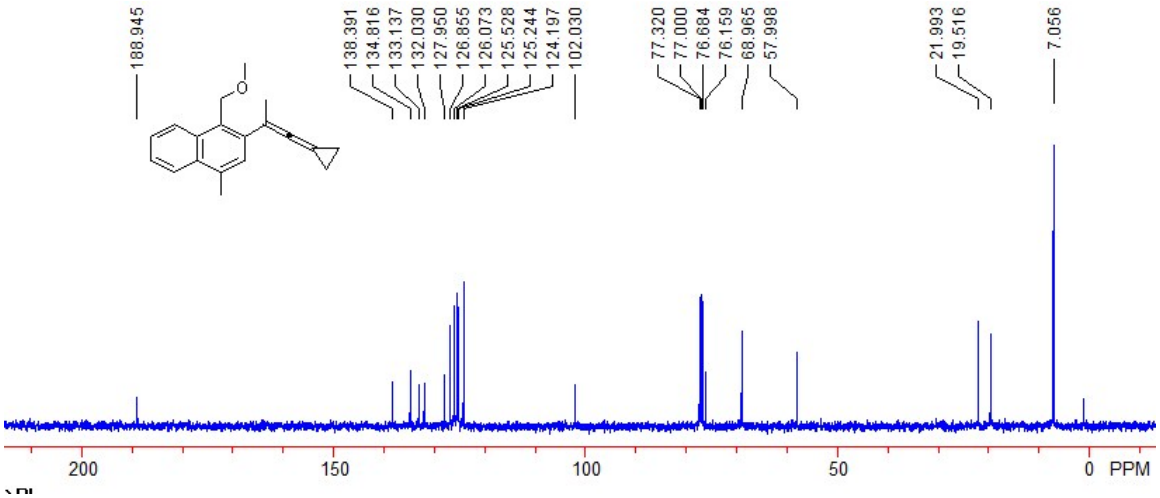


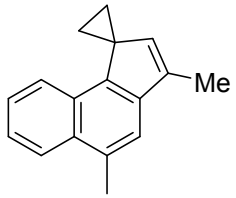


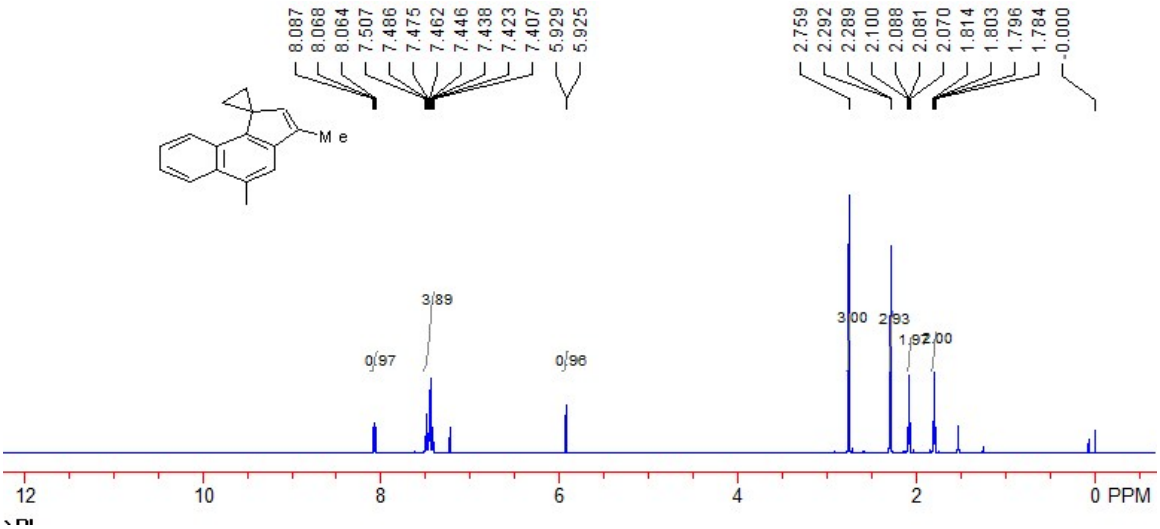
Compound **1t**. 150.3 mg, yield: 86%; white solid, Mp: 73-75 °C. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.44-1.57 (m, 4H, $2CH_2$), 2.19 (s, 3H, $CH_3$), 2.67 (d, $J$ = 0.8 Hz, 3H, $CH_3$), 3.44 (s, 3H, $CH_3$), 5.01 (s, 2H, $CH_2$), 7.29 (d, $J$ = 0.4 Hz, 1H, Ar), 7.45-7.55 (m, 2H, Ar), 7.93-7.97 (m, 2H, Ar), 8.18-8.21 (m, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 7.1, 19.5, 22.0, 58.0, 69.0, 76.2, 102.0, 124.2, 125.2, 125.5, 126.1, 126.9, 128.0, 132.0, 133.1, 134.8, 138.4, 188.9. IR (neat) ν 2966, 2905, 2870, 2013, 1600, 1376, 1193, 1093, 953, 748 cm$^{-1}$. MS (%) m/e 264 ($M^+$, 24.20), 249 (47.88), 236 (100.00), 221 (45.48), 219 (51.15), 203 (70.83), 202 (80.22), 189 (47.15), 178 (49.88). HRMS (EI) calcd. for $C_{19}H_{20}O$: 264.1514, Found: 264.1517.

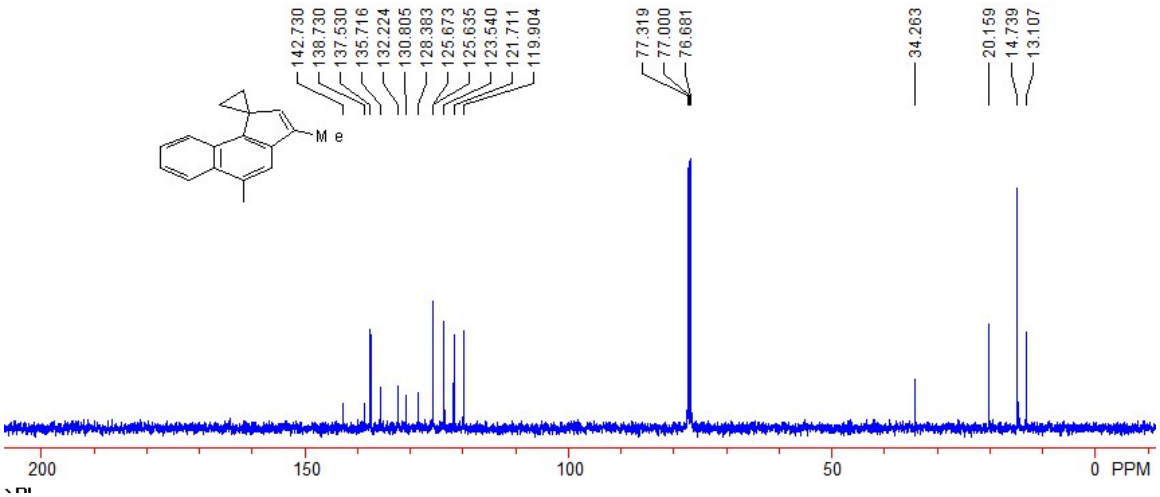




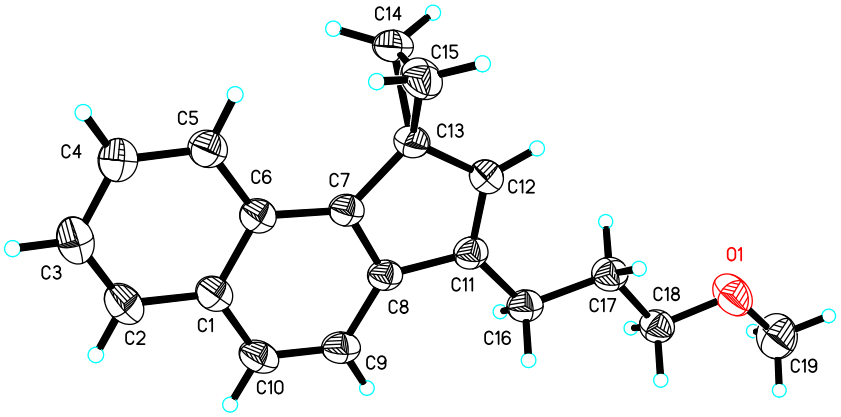




Compound **2p**. 26.4 mg, yield: 65%; pale yellow oil. $^{1}$H NMR ($CDCl_3$, 400 MHz, TMS) δ 1.80 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.2 Hz, 2H, $CH_2$), 2.08 (dd, $J_1$ = 4.8 Hz, $J_2$ = 7.2 Hz, 2H, $CH_2$), 2.29 (d, $J$ = 1.2 Hz, 3H, $CH_3$), 2.76 (s, 3H, $CH_3$), 5.93 (d, $J$ = 1.2 Hz, 1H, =CH), 7.40-7.51 (m, 4H, Ar), 8.06-8.09 (m, 1H, Ar). $^{13}$C NMR ($CDCl_3$, 100 MHz, TMS) δ 13.1, 14.7, 20.2, 34.3, 119.9, 121.7, 123.5, 125.6, 125.7, 128.4, 130.8, 132.2, 135.7, 137.5, 138.7, 142.7. IR (neat) ν 2957, 2923, 2854, 1514, 1407, 1047, 997, 887, 779, 752 cm$^{-1}$. MS (%) m/e 220 ($M^+$, 91.96), 219 (22.98), 205 (100.00), 203 (31.26), 202 (33.78), 190 (41.20), 189 (44.59), 101 (25.70). HRMS (EI) calcd. for $C_{17}H_{16}$: 220.1252, Found: 220.1243.




142.730
138.730
137.530
135.716
132.224
130.805
128.383
125.673
125.635
123.540
121.711
119.904
77.319
77.000
76.681
34.263
20.159
14.739
13.107
Me
200
150
100
50
0 PPM

## 6. X-ray Crystal Data of 2h




The crystal data of **2h** have been deposited in CCDC with number 1522831. Empirical formula: $C_{19}H_{20}O$, Formula weight: 264.35, Crystal system: Monoclinic, Space group: P 21/c, Unit cell dimensions: a = 8.8590(15) Å, α = 90°; b = 21.377(4) Å, β = 106.440(4)°; c = 8.0979(14) Å, γ = 90°. Volume: 870.8(3) $Å^3$, Z = 4, Density (calculated): 1.194 $Mg/m^3$, F(000) = 568, Crystal size: 0.200 x 0.160 x 0.120 $mm^3$, Final R indices [I>2sigma(I)]: R1 = 0.0449, wR2 = 0.1150.

## 7. UV/FL spectra and quantum yields of 2n and 2o

**Sample preparation**: To a 100 mL Volumetric flask was added **2n** or **2o** (0.01 mmol) and diluted with $CH_2Cl_2$ to 100 mL. The solution was shook several times and then was moved 1.0 mL to another 100 mL of volumetric flask and diluted with $CH_2Cl_2$ to 100 mL. The solution was shook several times and then was moved 1.0 mL to another 10 mL of volumetric flask and diluted with $CH_2Cl_2$ to 10 mL, the solution was shook several times for using.

**Quantum yield determination**: All the quantum yields of samples were determined based on 1.0 x $10^{-6}$ mol/L tryptophan in $H_2O$ ($\Phi$ = 0.14).

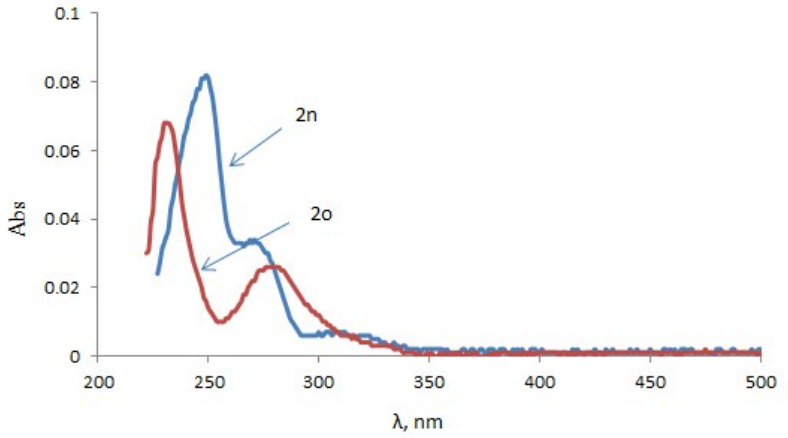



**Figure S1**. UV spectra: sample preparation: 1.0 x $10^{-6}$ mol/L in $CH_2Cl_2$, with 4.0 nm slit.

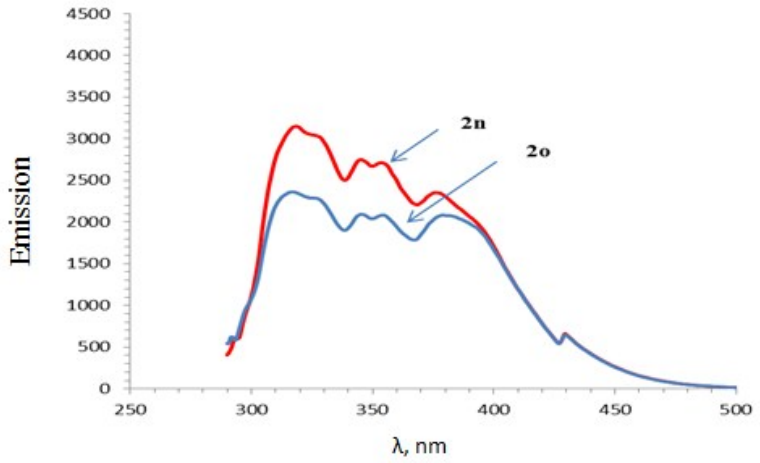
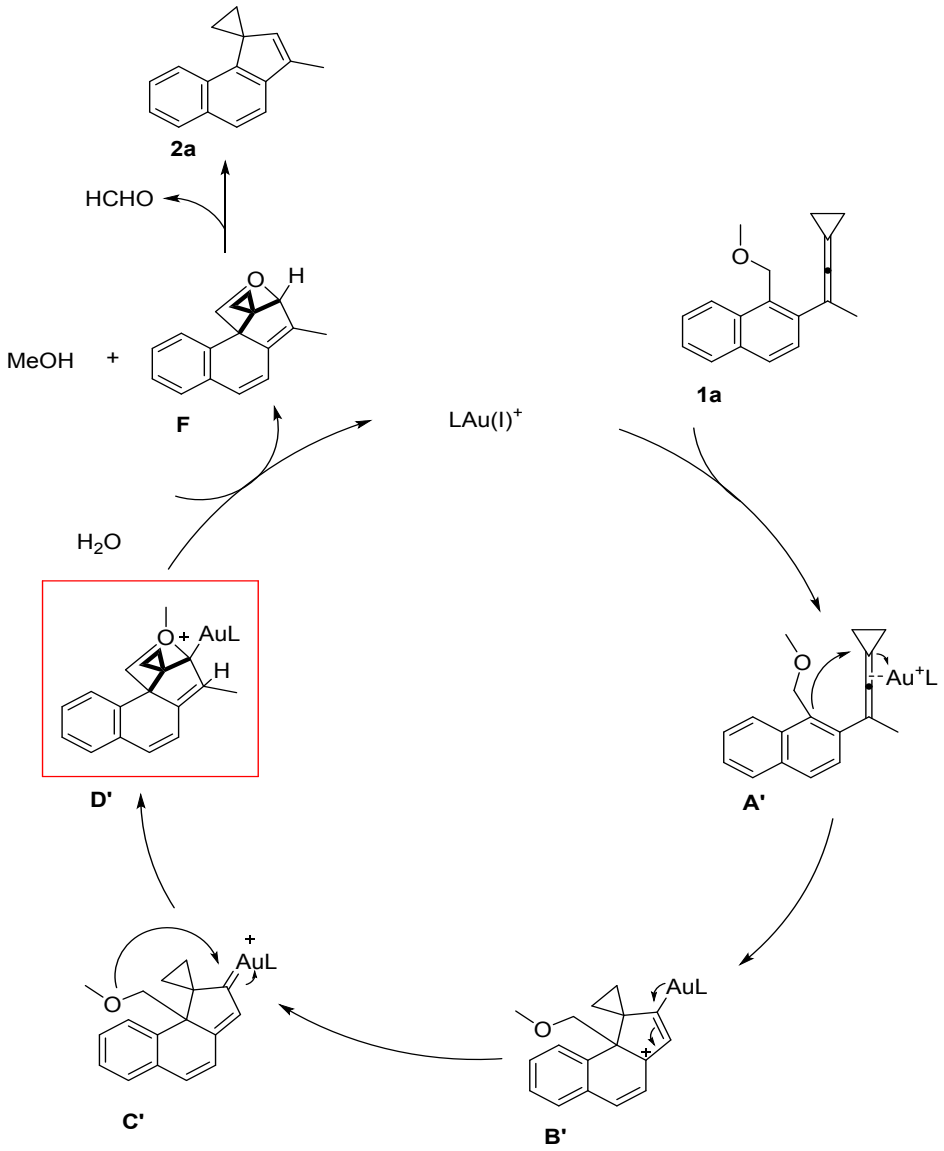


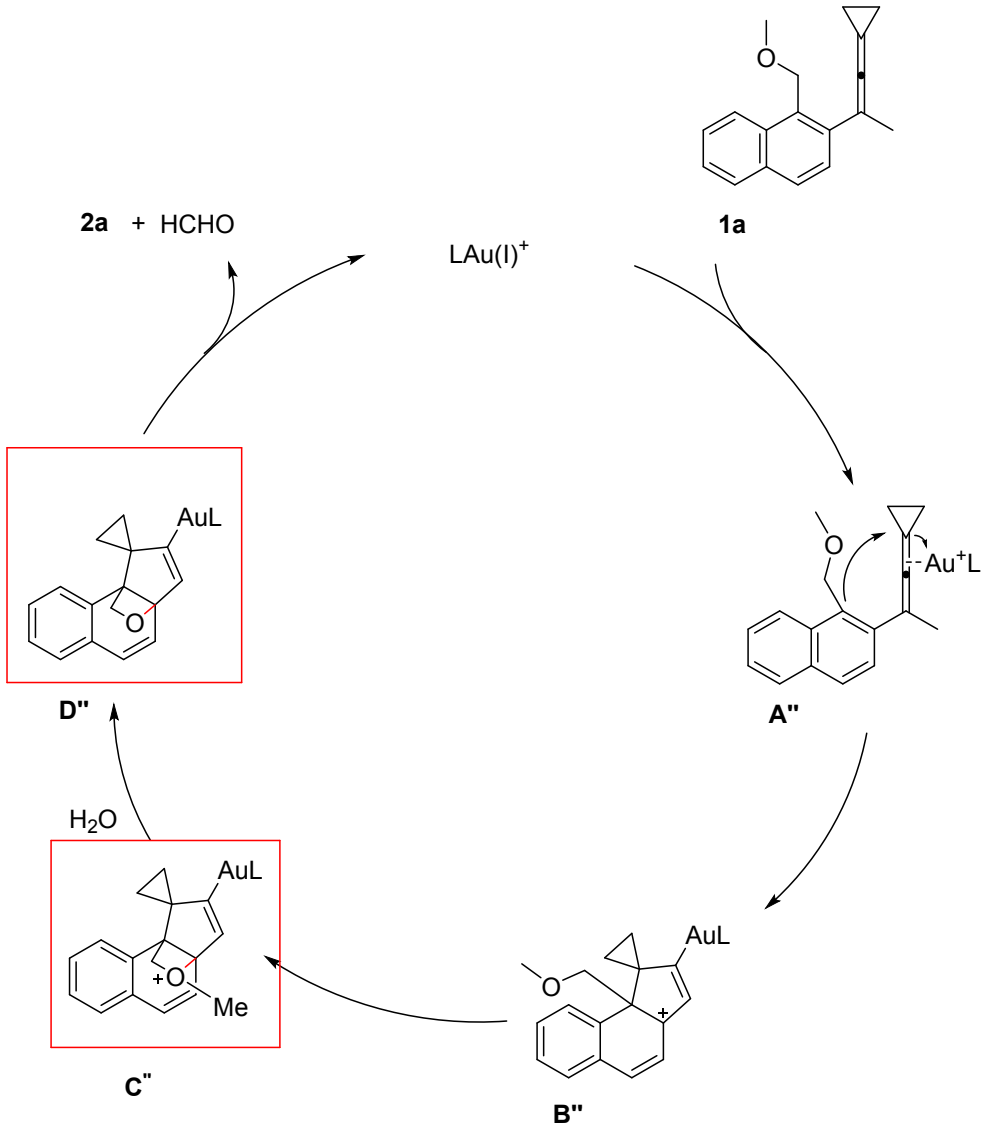

**Figure S2**. Fluorescence emission of **2n** and **2o**: samples were measured in $CH_2Cl_2$, $c$ = 1.0 $\mu$M. excitation at 271 nm with 5.0 nm EX slit and 5.0 nm EM slit, quantum yield of **2n** ($\Phi$ = 0.017), quantum yield of **2o** ($\Phi$ = 0.020).

## 8. Other plausible reaction mechanisms



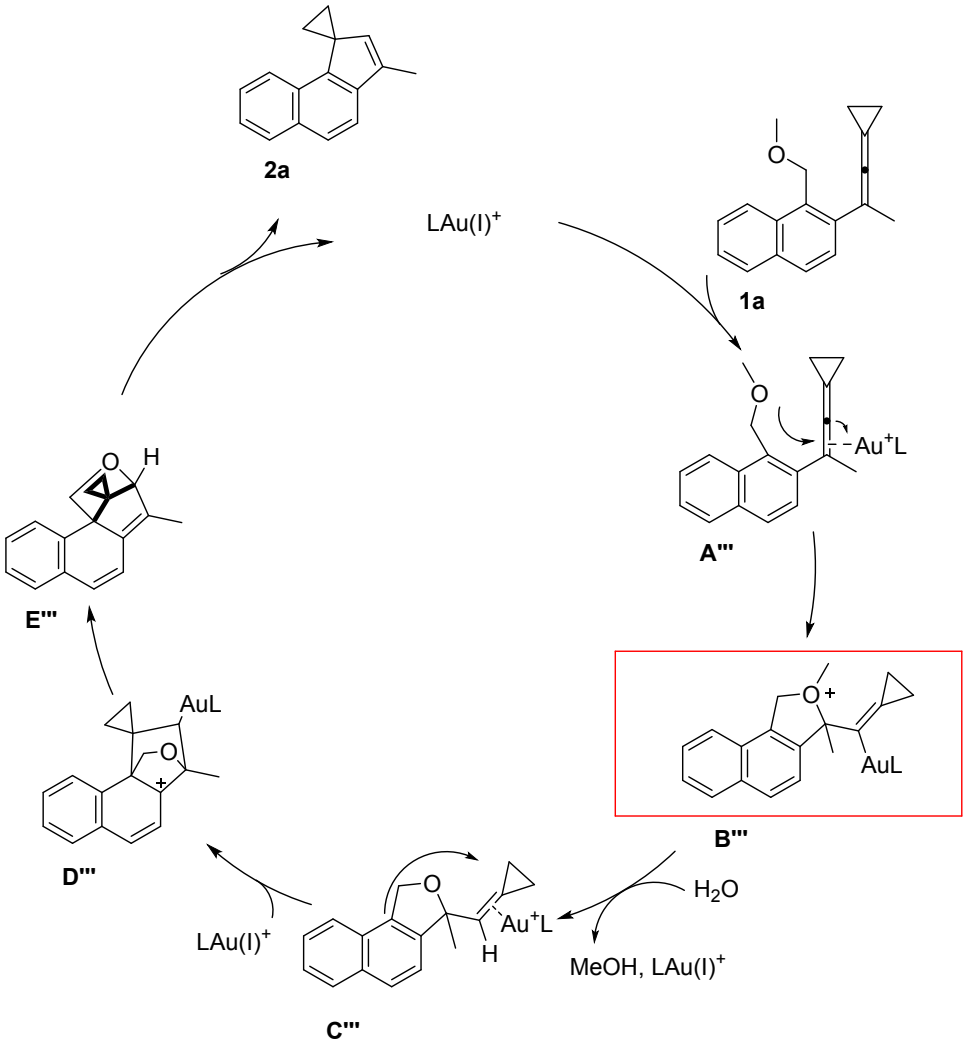

**Scheme S3. The reaction mechanism via gold carbene pathway**

The proposed intermediate in red basket can neither be located by DFT calculation in gas phase nor in THF at pbe1pbe/6-31G(d)/SDD level probably because of the existence of the positive charge on O atom.




**Scheme S4. The second possible reaction mechanism.**

The proposed intermediate in red basket can not be located by DFT calculation in gas phase at pbe1pbe/6-31G(d)/SDD level.




**Scheme S5. The third possible reaction mechanism**

The proposed intermediate in red basket can not be located by DFT calculation in gas phase at pbe1pbe/6-31G(d)/SDD level/.

## 9. Calculation Details

The geometries of compounds not involving **Au** atom have been optimized at pbe1pbe/6-31G(d) level; and the geometries of compounds involving **Au** atom have been optimized at pbe1pbe/6-31G(d)/SDD level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. The conformational space of flexible systems has first been searched manually. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single-point energies calculated at the pbe1pbe/6-311+G(d,p)/SDD)// pbe1pbe/6-311+G(d)/SDD level to yield free energy $G_{298}$ at 298.15 K. All quantum mechanical calculations have been performed with Gaussian 09.

**Table S2. The total energies, enthalpies and free energies of all species in gas phase shown in Scheme 4**

| | $E_{tot}$ | $H_{298}$ | $G_{298}$ |
|---|---|---|---|
| **1a** | -770.961439 | -770.631632 | -770.697144 |
| **1a-A** | -2065.229111 | -2064.286390 | -2064.431966 |
| **1a-TS1** | -2065.201262 | -2064.258623 | -2064.398661 |
| **1a-B** | -2065.221732 | -2064.276951 | -2064.415126 |
| **1a-C** | -731.755908 | -731.454370 | -731.512342 |
| **1a-D** | -2026.048650 | -2025.132750 | -2025.270488 |
| **1a-TS2** | -2025.981785 | -2025.068974 | -2025.204252 |
| **1a-E** | -2025.998710 | -2025.084724 | -2025.218814 |
| **1a-TS3** | -2025.934290 | -2025.023571 | -2025.158254 |
| **1a-F** | -731.751107 | -731.449698 | -731.504243 |
| **1a-TS4** | -731.714106 | -731.415974 | -731.471898 |
| **1a-P** | -617.384959 | -617.119497 | -617.170783 |

**Table S3. The total energies, enthalpies and free energies of all species in THF shown in Scheme 4, ε=7.4257**

| | $E_{sol}$ | $H_{sol}$ | $G_{sol}$(kcal/mol) |
|---|---|---|---|
| **1a** | -771.163769 | -770.833962 | -770.899474 |
| **1a-A** | -2065.771855 | -2064.829134 | -2064.974710 |
| **1a-TS1** | -2065.743799 | -2064.801160 | -2064.941198 |
| **1a-B** | -2065.765517 | -2064.820736 | -2064.958911 |
| **1a-C** | -731.945265 | -731.643727 | -731.701699 |
| **1a-D** | -2026.580008 | -2025.664109 | -2025.801847 |
| **1a-TS2** | -2026.509825 | -2025.597014 | -2025.732292 |
| **1a-E** | -2026.527687 | -2025.613701 | -2025.747791 |
| **1a-TS3** | -2026.471572 | -2025.560853 | -2025.695536 |
| **1a-F** | -731.938413 | -731.637004 | -731.691549 |
| **1a-TS4** | -731.906164 | -731.608031 | -731.663955 |
| **1a-P** | -617.539244 | -617.273782 | -617.325068 |

## 10. Archive Entries

### 1a


1\1\GINC-A730\FOpt\RPBE1PBE\6-31G(d)\C18H18O1\SIOC001\25-Feb-2017\0\\#
p opt pbe1pbe/6-31g(d)\\Title Card Required\\0,1\C,4.550386773,-0.2126
867605,-3.3731779607\C,5.9194692658,-0.1131698997,-3.3989346807\C,6.55
25163121,1.1216059833,-3.6791222667\C,5.7594732243,2.2770583323,-3.945
0338424\C,4.3476175316,2.141645097,-3.8942786255\C,3.7603111783,0.9299
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7155516,-4.2518163229\H,3.7280344922,3.0205608223,-4.0354926252\H,2.67
69226242,0.8527214004,-3.578662204\C,7.7803026656,3.6112339388,-4.2295
038874\C,8.553291943,2.4481709057,-3.9629452001\H,9.6365347713,2.53180
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73956,4.3535754819,-5.4323826415\H,6.1598939775,5.4695686893,-5.118295
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456,-4.6736632204\H,3.4898249269,6.6170084242,-3.029313681\H,4.5815102
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7\C,9.5653529392,4.8984181552,-5.5636210122\H,10.0581693202,5.87225689
38,-5.6192611907\H,10.3350214385,4.1350471182,-5.3958561587\H,9.108186
501,4.6806790909,-6.5370266636\C,8.5228327878,4.8817688242,-4.47158837
98\C,8.2899753157,5.94004251,-3.7228892006\C,8.0676364215,6.9653507527
,-2.9746679542\C,7.2825694543,8.182563736,-2.6979177667\H,6.2406917643
,8.0546053183,-2.4103824433\H,7.4858788817,9.0757245947,-3.2863183146\
C,8.3530187516,7.7061289109,-1.7324012554\H,9.2784233876,8.2766755725,
-1.6748979371\H,8.0367460461,7.2623692947,-0.7903988276\\Version=ES64L
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pole=0.0304902,0.4537564,-0.2550277\Quadrupole=1.879712,4.7474136,-6.6
271256,-1.0626002,0.4853688,-0.8717924\PG=C01 [X(C18H18O1)]\\@


### 1a-A


1\1\GINC-A756\FOpt\RPBE1PBE\GenECP\C45H54Au1N2O1(1+)\SIOC001\25-Feb-20
17\0\\#p opt genecp pbe1pbe\\Title Card Required\\1,1\Au,0.507842697,0
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414765599,1.4261232584,0.7447348384\H,5.2825070659,-0.5331422512,1.373
8831396\H,5.1804778736,2.2037261083,0.8606032716\C,2.4286285216,0.5611
050331,0.2118587447\N,3.1730687072,1.6912937841,0.2682922567\N,3.25136
33768,-0.4159970195,0.6623676812\C,2.7049818756,2.9979391727,-0.106767
0929\C,2.8088427686,3.3869942094,-1.4517638034\C,2.1804290975,3.830817
8095,0.8947200502\C,2.3423649674,4.6604067945,-1.7854340197\C,1.733237
4095,5.0949612322,0.5044035129\C,1.8080417436,5.5052702489,-0.82081372
34\H,2.4055025175,4.9971369904,-2.8165972523\H,1.32459125,5.7693685875
,1.2520340065\H,1.4560444549,6.4938888736,-1.1021270266\C,2.8933354302
,-1.8024122663,0.7922895888\C,2.3710229497,-2.2442958167,2.0185036633\
C,3.1071300577,-2.6553845234,-0.302330106\C,2.0513550807,-3.5999143829
,2.1253627635\C,2.7661597822,-4.00004873,-0.1405376852\C,2.2459092252,

-4.469552156,1.0590622002\H,1.6524535998,-3.9802279355,3.061947133\H,2
.9203632508,-4.6908338267,-0.9648746875\H,1.999277655,-5.5223489453,1.
1670137659\C,2.1016845007,3.4164257811,2.3527139353\C,0.6585365477,3.4
280125035,2.8645071672\C,3.0024836611,4.297363973,3.2248315666\H,2.465
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88,2.8392359736\H,4.0447519203,4.2638819137,2.8894363327\H,2.6799077,5
.3442787534,3.2005422817\H,2.9699059999,3.9631691472,4.2677301653\C,3.
4080365363,2.4950804873,-2.523244477\C,4.6590867262,3.1311961792,-3.13
78344543\C,2.3768635968,2.1497895401,-3.6019173389\H,3.7153372371,1.55
37699847,-2.0533804838\H,5.4128988926,3.3523959777,-2.3746699682\H,5.1
079917459,2.4550079604,-3.8738031161\H,4.4208348521,4.0691759369,-3.65
16204523\H,1.4982871519,1.6635766767,-3.1618120867\H,2.0378879867,3.04
6199126,-4.1336623137\H,2.815018534,1.4700047661,-4.3418281951\C,3.674
0711346,-2.1712486638,-1.6238388529\C,2.6206959434,-2.2632766325,-2.73
30309865\C,4.9477479235,-2.9309900813,-2.0061088339\H,3.9433932934,-1.
1143651352,-1.5153749012\H,1.7273118368,-1.6818467905,-2.4757279433\H,
3.0244924473,-1.8773635188,-3.6761749241\H,2.3137790162,-3.3023848139,
-2.9007858771\H,5.7109132691,-2.8546049774,-1.2243866726\H,4.747921252
9,-3.9950047809,-2.1744523311\H,5.3677780513,-2.5243219726,-2.93253447
53\C,2.1451245644,-1.3178630754,3.198787239\C,2.9419067217,-1.76787193
29,4.4273319943\C,0.6526864359,-1.1939978811,3.5219057333\H,2.50172738
46,-0.3185216669,2.9247405472\H,4.0133721897,-1.8327878657,4.209767660
1\H,2.8039317741,-1.0579422221,5.250179672\H,2.6139425675,-2.751457167
2,4.7815277171\H,0.0917211709,-0.834903875,2.6513186504\H,0.2271067438
,-2.1575980728,3.8247246968\H,0.4985498943,-0.488771244,4.3465444661\C
,-2.5489113426,0.4467198311,-0.3724287445\C,-1.4210695915,0.1416901205
,-1.1660114093\C,-1.6129095942,-0.2434469015,-2.4559750294\C,-2.478093 7842,-
0.2626189684,-3.6400028296\H,-3.2150257781,-1.0573402723,-3.7431
903466\H,-2.793201003,0.6897300254,-4.0636819817\C,-0.9971329547,-0.63
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7331098554,-1.6787813891,-3.8634273984\C,-2.4502757703,1.5351883687,0.
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.3236794985,0.3169357916\H,-3.4191110858,1.9541466713,0.9203702872\C,-
3.7752347257,-0.3049333604,-0.5134510868\C,-3.7987359866,-1.6923490892
,-0.7643901471\C,-5.0028067634,0.4312350651,-0.485634473\C,-5.03635076
28,-2.3180568456,-1.0903111458\C,-6.1838585391,-0.1616652042,-0.816867
7373\H,-4.9809914705,1.496754886,-0.28537645\C,-5.1240485405,-3.703261
8493,-1.4051721174\C,-6.2362224673,-1.5399555805,-1.1457456797\H,-7.10
03468481,0.4215722525,-0.8459585987\C,-6.3191984819,-4.2687107617,-1.7
749429276\H,-4.2382050627,-4.3217275051,-1.336662073\C,-7.4532866252,-
2.1537573451,-1.5145885532\C,-7.4957027383,-3.4914891568,-1.8279290959
\H,-6.3628089919,-5.3255640453,-2.020717701\H,-8.3556940406,-1.5491386
863,-1.5476520065\H,-8.4357171963,-3.9548765294,-2.1131533924\C,-2.593
0920148,-2.5807260624,-0.5430562684\H,-2.319226886,-3.0981469278,-1.48
14267068\H,-1.7161909418,-1.9994274658,-0.2379190374\O,-2.9185698038,-
3.5172417267,0.4551185889\C,-1.8311217633,-4.3600094703,0.7492590858\H

,-1.5191028493,-4.9414908956,-0.1332420879\H,-0.9620881636,-3.7906470624,1.1126668665\H,-2.1632171787,-5.0478484077,1.529766975\\Version=ES64L-G09RevD.01\State=1-A\HF=-2065.2291111\RMSD=4.920e-09\RMSF=2.305e-06\Dipole=-0.738385,-0.1015998,-0.4568099\Quadrupole=25.4376139,-1.5730842,-23.8645298,11.9439807,14.4252113,4.7209198\PG=C01 [X(C45H54Au1N2O1)]\\@

**1a-TS1**

1\1\GINC-A743\FTS\RPBE1PBE\GenECP\C45H54Au1N2O1(1+)\SIOC001\20-Mar-2017\0\\#p opt=(calcfc,ts,noeigen) genecp pbe1pbe\\Title Card Required\\1,1\Au,-0.1799918799,-0.0246025508,-0.5407364125\C,-3.7359684463,-0.3779899383,1.7099284448\C,-3.2635683376,0.7639893131,2.2669072403\H,-4.6332816024,-0.946945383,1.8980146423\H,-3.6618969497,1.4002828919,3.0419660076\C,-1.7742481223,0.1028534901,0.7095613385\N,-2.0626366685,1.0409414263,1.6427446186\N,-2.812001726,-0.766475,0.7609760245\C,-1.2299617454,2.1661676932,1.966435796\C,-0.2702866117,2.0136444513,2.9805903237\C,-1.4319010096,3.3703284099,1.27250979\C,0.5271668525,3.1228916395,3.2745463303\C,-0.6121456505,4.4487931814,1.6144582051\C,0.3594612166,4.3269835348,2.6008339312\H,1.2810822077,3.0440398688,4.0531359446\H,-0.7415999537,5.3994342263,1.1042961687\H,0.982603785,5.1802491981,2.8544788272\C,-2.9242255413,-1.951510636,-0.0465522116\C,-3.5516070567,-1.8532650391,-1.2986150957\C,-2.4060029764,-3.1535717334,0.4626806748\C,-3.6269219509,-3.0176296204,-2.0663459175\C,-2.5124673484,-4.2864520046,-0.3470363402\C,-3.1098943356,-4.2199775674,-1.5998478189\H,-4.1041664311,-2.9824358488,-3.0417793716\H,-2.128251501,-5.2366348503,0.013846833\H,-3.1838195121,-5.1144750319,-2.212073583\C,-2.4877153012,3.5303609882,0.1941016484\C,-1.8480927954,3.809515203,-1.1700703759\C,-3.5010320688,4.6188263227,0.5616412517\H,-3.0361357498,2.5853777032,0.1088231329\H,-1.1626442337,3.0035398407,-1.4580388822\H,-2.6219632246,3.891864318,-1.9417988699\H,-1.2856072353,4.7505711485,-1.161533357\H,-3.9788832986,4.4139367694,1.5254842443\H,-3.0268457703,5.6043310268,0.6277520011\H,-4.2851852423,4.6797399863,-0.2007983899\C,-0.0879516503,0.7204319694,3.7548152513\C,-0.2921388603,0.9387146046,5.2576218065\C,1.2758637097,0.0842113439,3.469985953\H,-0.8540817795,0.0109230323,3.4221680591\H,-1.2722440786,1.378517927,5.4708998108\H,-0.2238900099,-0.0160234778,5.7902656899\H,0.4704989444,1.6044423889,5.6766412479\H,1.3917162804,-0.151988855,2.4061660603\H,2.0967061547,0.7482490593,3.7650387603\H,1.3848800654,-0.8482929944,4.0349166736\C,-1.7825547049,-3.2612830853,1.8419235451\C,-0.339508211,-3.7692310849,1.779592079\C,-2.6376928492,-4.1444414679,2.7575426448\H,-1.7537747463,-2.2589512586,2.284659613\H,0.2881202093,-3.1153897892,1.1644478058\H,0.0917231679,-3.8039969601,2.7864387632\H,-0.2859499648,-4.7822744815,1.364407443\H,-3.6642181892,-3.7699630576,2.8351715409\H,-2.6873545964,-5.1734752565,2.3842653342\H,-2.2094577069,-4.176291178,3.7654572608\C,-4.1423574687,-0.5578871723,-1.8240186978\C,-5.6428318343,-0.7004484493,-2.0990398061\C,-3.3961870774,-0.0716815419,-3.0699276812\H,-4.0232293886,0.2110846763,-1.051898936\H,-6.1852156865,-1.0293451282,-1.2062690322\H,-6.06299743

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83354\C,3.7547787831,-0.1694446831,-0.8420879221\C,2.5683994688,-2.279
0016925,-0.7298797049\C,4.8482217107,-0.7589370831,-0.12949089\C,3.589
5441707,-2.8554717172,-0.0270110682\H,1.6855997569,-2.8667358789,-0.95
76641528\C,6.0492288751,-0.0623933744,0.1761759654\C,4.7589540636,-2.1
242317323,0.2839747443\H,3.5164527542,-3.8920114063,0.293023811\C,7.07
77243786,-0.6729209597,0.8542064664\H,6.1871710705,0.9659277733,-0.140
9203606\C,5.8312629067,-2.7236889584,0.9867592833\C,6.9720570351,-2.01
57828639,1.2707307446\H,7.9844037622,-0.1139406159,1.0678133611\H,5.73
48238409,-3.7628837129,1.2916740455\H,7.7919213573,-2.4838054281,1.807
3326072\C,3.8517242868,1.2787842159,-1.2587147468\H,4.229715459,1.3858
053367,-2.280609715\H,4.5151180562,1.844029052,-0.5979902348\O,2.59251
02604,1.9556467207,-1.2480163314\C,1.6090331188,0.8373000542,-2.591728
0997\C,2.1160683804,2.2317445578,0.0647835611\H,1.1270533225,2.6779294
313,-0.037078795\H,2.0577147851,1.3221796344,0.6706188291\H,2.79657986
02,2.9500735905,0.5369686207\C,1.501465288,1.6304463495,-3.5975015478\
C,1.414265038,2.9630401054,-4.2173485564\H,0.4751363421,3.5022886657,-
4.1045346468\H,2.307343726,3.5839069279,-4.1819260931\C,1.4310709041,1
.735465788,-5.0829692535\H,2.33741892,1.5036722761,-5.6385399019\H,0.5
052146592,1.4190531086,-5.5588005057\C,0.7888523113,-1.3805076239,-2.9
322732659\H,0.3623255845,-2.2526531071,-2.433495052\H,-0.0216431163,-0
.889810149,-3.4777942619\H,1.5337161455,-1.7301705673,-3.6587479137\\V
ersion=ES64L-G09RevD.01\State=1-A\HF=-2065.2012622\RMSD=5.692e-09\RMSF
=1.454e-06\Dipole=-0.1970659,1.0117625,-0.3424954\Quadrupole=7.935865,
-2.8224624,-5.1134026,6.5447536,-1.5405264,-4.0182438\PG=C01 [X(C45H54
Au1N2O1)]\\@

**1a-B**

1\1\GINC-A744\FOpt\RPBE1PBE\GenECP\C45H54Au1N2O1(1+)\SIOC001\15-Mar-20
17\0\\#p opt genecp pbe1pbe\\Title Card Required\\1,1\Au,-1.0072937432
,-0.9502504332,1.094693915\C,-4.9911867282,-0.1197972943,-0.1166810499
\C,-4.9841432325,-1.4621051962,-0.3061550979\H,-5.765711014,0.61761242
33,-0.2603430032\H,-5.750144218,-2.1393459078,-0.6510384488\C,-2.93635
67119,-0.8678187245,0.4351611782\N,-3.7188740348,-1.9004964736,0.03689
17521\N,-3.7320404049,0.2230689037,0.3356928613\C,-3.2849537297,-3.267
7408532,-0.0243084741\C,-2.7106445173,-3.7337755268,-1.2183229709\C,-3
.4592573387,-4.078701802,1.1099017442\C,-2.2837777714,-5.0647250443,-1
.2458148731\C,-3.0236770614,-5.4037534073,1.0231552346\C,-2.4395807164
,-5.8926427289,-0.1399279762\H,-1.8388457509,-5.4621621468,-2.15414593
81\H,-3.1547375492,-6.064542875,1.8759778193\H,-2.118039212,-6.9296411
699,-0.1899624554\C,-3.3147591062,1.562053519,0.6534161591\C,-3.451452
3212,2.0087274528,1.9775442592\C,-2.795606333,2.3611983418,-0.37766863
13\C,-3.0174768715,3.305414264,2.2609421079\C,-2.3802289725,3.65042441
53,-0.0370787443\C,-2.4843944837,4.1171924674,1.2673510315\H,-3.103493

1291,3.6869442171,3.274780859\H,-1.9730336424,4.2998795747,-0.80728095
99\H,-2.1561237704,5.1240971531,1.509758423\C,-4.1000911608,-3.5743485
168,2.3894082108\C,-3.1379479904,-3.6778708573,3.5772120833\C,-5.41300
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1987\H,-2.2150850995,-3.1168410867,3.3873908509\H,-3.6058244069,-3.268
0201498,4.4793805815\H,-2.8721429037,-4.7203688493,3.7892175302\H,-6.1
183214695,-4.2120793065,1.8448411644\H,-5.2446054537,-5.3800131195,2.8
454834943\H,-5.8888690101,-3.9032185445,3.5756884922\C,-2.5432875348,-
2.8579894065,-2.4466427778\C,-3.238338981,-3.466841518,-3.6685141489\C
,-1.0634667008,-2.5815062339,-2.7324894541\H,-3.0214761608,-1.89281069
51,-2.2460940788\H,-4.2981120176,-3.6616217239,-3.4728395553\H,-3.1701
366349,-2.7824723223,-4.5209705398\H,-2.7748828751,-4.4130424313,-3.96
92770829\H,-0.5847177658,-2.0672250975,-1.8906075184\H,-0.5154271195,-
3.510949635,-2.9289322005\H,-0.9587592964,-1.9433716787,-3.6170624107\
C,-2.6869917219,1.8854997883,-1.8149782446\C,-1.2304325477,1.850409937
7,-2.2866634842\C,-3.5488368584,2.7442101844,-2.746683916\H,-3.0695028
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9\H,-1.175958383,1.4937626603,-3.3216349167\H,-0.7765476233,2.84766706
04,-2.2556914917\H,-4.5971994118,2.754266156,-2.4293494362\H,-3.199601
1886,3.7824270166,-2.771825544\H,-3.5062322865,2.3555303976,-3.7701157
446\C,-4.0457094556,1.14906336,3.077796699\C,-5.2846391217,1.806994715
1,3.6933931127\C,-3.0029247954,0.8201379231,4.150717198\H,-4.366770526
2,0.199286354,2.6345740973\H,-6.0407902538,2.0296304724,2.9330357333\H
,-5.7363578064,1.1431410709,4.4388012837\H,-5.0331125617,2.7463520576,
4.1979957237\H,-2.1420264044,0.3007640596,3.713552879\H,-2.6372100435,
1.7282309546,4.6436544066\H,-3.4411617852,0.1758142127,4.9219815492\C,
0.9949831894,-1.0006385715,1.8426558867\C,1.9275525254,-0.9122751362,0 .
6598615352\C,2.7928797092,-1.9320523305,0.2895114723\C,1.9029339716,0
.2646086491,-0.1402110803\C,3.6523368598,-1.8219730854,-0.8482536205\C
,2.7100195267,0.4033355666,-1.2343948626\H,1.2158877884,1.0622589625,0
.1264337149\C,4.5723121899,-2.828921918,-1.2376485478\C,3.6051529562,-
0.6252447501,-1.623567659\H,2.6724194523,1.3143915057,-1.8269336815\C,
5.3805580009,-2.6649141441,-2.3396672947\H,4.6701505794,-3.7434046463,
-0.6592079311\C,4.4456335447,-0.4869780919,-2.7518308845\C,5.318384335
9,-1.4866069698,-3.1091132532\H,6.0784190894,-3.4505838619,-2.61496222
26\H,4.3924550196,0.4322134347,-3.3301411718\H,5.9630864912,-1.3701732
737,-3.9750203124\C,2.8522911165,-3.1669944226,1.1284660761\H,3.539396
0875,-3.1108342908,1.9773644002\H,3.0575196375,-4.0781500489,0.5630927
552\O,1.5459100222,-3.4183644737,1.7685774388\C,1.1505778472,-2.254150
2719,2.6063147025\C,0.5336676299,-3.9743217104,0.870791525\H,-0.395040
2964,-4.0028721564,1.4363311011\H,0.4430892445,-3.3429930321,-0.013457
1715\H,0.8793610851,-4.9792726225,0.6253604192\C,1.0391783927,-2.59080
03152,3.8764096361\C,1.0274722327,-3.6412324119,4.89793172\H,0.2120461
365,-4.36337596,4.8945704189\H,1.9793821946,-4.0439620983,5.2402419773
\C,0.7022323681,-2.1968739238,5.2449259491\H,1.4344923293,-1.630983016
6,5.8177896044\H,-0.3339833754,-1.9440205363,5.465668911\C,1.168621331
2,0.1894174133,2.8041167116\H,0.9968257084,1.1404482902,2.2949843149\H

,0.4572318752,0.1355719299,3.6325959957\H,2.1834504535,0.2084597107,3.
2271155275\\Version=ES64L-G09RevD.01\State=1-A\HF=-2065.2217319\RMSD=4
.965e-09\RMSF=3.011e-06\Dipole=0.0743185,-1.6749682,0.2282793\Quadrupo
le=6.0695484,2.9597764,-9.0293247,-13.8596875,-3.315809,-4.7974001\PG=
C01 [X(C45H54Au1N2O1)]\\@

**1a-C**

1\1\GINC-A740\FOpt\RPBE1PBE\6-31G(d)\C17H16O1\SIOC001\14-Mar-2017\0\\#
p opt pbe1pbe/6-31g(d)\\Title Card Required\\0,1\C,0.7525116232,-1.351
45097,0.7066136727\C,2.0530516323,-0.7030761899,0.304060109\C,3.126623
3862,-0.8051057686,1.1634204014\C,2.1714090284,0.0217458297,-0.9031069
61\C,4.3604913996,-0.1578057037,0.8624539141\C,3.3467144515,0.64788676
05,-1.2256097268\H,1.3166822789,0.0765208395,-1.573755059\C,5.49397742
69,-0.1987645077,1.7154427681\C,4.4640506824,0.5813700011,-0.357439329
6\H,3.4388477027,1.2054550231,-2.1547923047\C,6.6604668573,0.445121374
4,1.379748426\H,5.4446392261,-0.7408898674,2.6547390609\C,5.6818632681
,1.2311420789,-0.6751380538\C,6.759731748,1.1676321183,0.1720348973\H,
7.5143895148,0.3979566626,2.0501570261\H,5.7454469445,1.7861104388,-1.
6084817454\H,7.6880219639,1.6714551661,-0.0825862672\C,2.9099066097,-1
.6152788217,2.4118594434\H,2.4493782614,-0.99728374,3.1998932657\H,3.8
492673191,-2.0012693264,2.8126359621\O,2.1194915393,-2.7735952957,2.19
57912415\C,1.012487245,-2.6659678469,1.4032620425\C,0.2176965147,-3.71
71804272,1.2649220556\C,-0.0929501872,-5.104991505,1.5889741843\H,0.52
48636135,-5.8976387393,1.1676869811\H,-0.5024937964,-5.3409989762,2.57
1029113\C,-0.9653388032,-4.2949066748,0.6278052886\H,-1.958029484,-4.0
019618323,0.9706628435\H,-0.9276364365,-4.5556439076,-0.430411679\C,-0
.0917436334,-0.4004390556,1.5757540318\H,-0.3047436026,0.5258235681,1.
0310774653\H,-1.0397182304,-0.8774751846,1.8438097487\H,0.4268844813,-
0.1311342752,2.5018791801\H,0.1691901849,-1.5799293154,-0.1925058065\\
Version=ES64L-G09RevD.01\State=1-A\HF=-731.7559082\RMSD=3.713e-09\RMSF
=3.039e-05\Dipole=0.0683154,0.6593876,-0.1592735\Quadrupole=3.9104141,
-5.1013345,1.1909204,1.7258861,2.2778388,-1.6817273\PG=C01 [X(C17H16O1
)]\\@

**1a-D**

1\1\GINC-A738\FOpt\RPBE1PBE\GenECP\C44H52Au1N2O1(1+)\SIOC001\15-Mar-20
17\0\\#p opt genecp pbe1pbe\\Title Card Required\\1,1\C,-0.6631491308,
-7.4382313572,5.0291294779\C,-1.9486553301,-7.0082740959,4.9832401384\
H,-0.1865399978,-8.2067585139,5.6177726294\H,-2.8276723154,-7.32384316
76,5.5236513339\C,-0.7714857038,-5.7863606147,3.5047189918\N,-1.993849
0759,-5.9974327759,4.0444244215\N,0.041817756,-6.6778052466,4.11629330
02\C,-3.1773495987,-5.2665618305,3.6759175371\C,-3.4748566369,-4.08149
85727,4.3681153706\C,-3.9757706426,-5.7721600915,2.6370977482\C,-4.617
2523993,-3.3824842637,3.971669358\C,-5.105773207,-5.031451535,2.283787
3752\C,-5.4227457574,-3.8485174319,2.9400155578\H,-4.8807917933,-2.460
3221113,4.4822596356\H,-5.7485854578,-5.3895982024,1.4843271587\H,-6.3
08339186,-3.2897617785,2.6503944314\C,1.4460110821,-6.8257862429,3.847

0023145\C,1.8409787584,-7.7402132516,2.856734709\C,2.3561339023,-6.062
0561564,4.5951987321\C,3.2107039166,-7.8629216832,2.6122816497\C,3.713
4909601,-6.2284878458,4.3104162739\C,4.137860042,-7.1164751149,3.32942
98384\H,3.5556680689,-8.5593110663,1.8530758231\H,4.4489666719,-5.6590
592165,4.8722757544\H,5.1991361006,-7.2344674354,3.1286627365\C,-3.653
0025134,-7.0597256036,1.9013336072\C,-3.294231711,-6.782092746,0.43794
12918\C,-4.7992069878,-8.0702761236,2.0079381879\H,-2.7729152736,-7.51
38742341,2.3713204598\H,-2.4378311601,-6.1012820887,0.365160521\H,-3.0
34052016,-7.714678319,-0.0755701137\H,-4.1347209998,-6.3284918481,-0.0
997649099\H,-5.0492325194,-8.2851296864,3.0523246191\H,-5.7072209203,-
7.7033698419,1.516920933\H,-4.5204872665,-9.0123565089,1.5233905931\C,
-2.612815593,-3.5459372177,5.4964470969\C,-3.4135701505,-3.3974510843,
6.7938795015\C,-1.9504083887,-2.2224732047,5.1001179714\H,-1.810935231
4,-4.2679290649,5.6893446127\H,-3.8747077393,-4.3448116701,7.092722078
3\H,-2.7585774079,-3.0656669316,7.60688907\H,-4.2128793422,-2.65527022
37,6.6914222204\H,-1.3379811799,-2.340910953,4.1983462585\H,-2.6990736
011,-1.4473771411,4.9003559839\H,-1.3051825726,-1.8620017982,5.9094651
079\C,1.9211884911,-5.0883731482,5.6751717586\C,2.2510004186,-3.644452
2626,5.2823948857\C,2.5334839168,-5.4445279195,7.0334059925\H,0.832367
0331,-5.1548464582,5.7806290816\H,1.7547170426,-3.3684971324,4.3442520
142\H,1.9147930276,-2.9509603713,6.061461306\H,3.3316627903,-3.5053469
452,5.1565098239\H,2.285362779,-6.4694805664,7.3286081381\H,3.62554144
37,-5.3567198453,7.0203908537\H,2.1574287583,-4.7669563141,7.807702129
\C,0.8490359441,-8.5670749751,2.0589854491\C,1.1419617428,-10.06647616
65,2.1689409475\C,0.8139354744,-8.1162283289,0.5950093745\H,-0.1506821
037,-8.4003876503,2.476441803\H,1.1519141442,-10.3986833789,3.21242859
78\H,0.3760104123,-10.6402655238,1.6361296322\H,2.1109435395,-10.32386
98662,1.7275916722\H,0.5409931914,-7.0574255985,0.5134709956\H,1.78904
78214,-8.2547531162,0.1136223329\H,0.0781112826,-8.7020918593,0.032673
0143\C,2.3616760893,-3.1709384644,0.1057955876\C,3.3573314662,-2.10633
76384,-0.2981415145\C,3.6305905258,-1.0955857829,0.5976090327\C,4.0199
614096,-2.1640851849,-1.5434482762\C,4.6103044287,-0.1031810696,0.3048
49888\C,4.9631806201,-1.2203075649,-1.8582037756\H,3.7799114345,-2.960
4287538,-2.2435379796\C,4.9576688819,0.945275638,1.1941521926\C,5.2860
298018,-0.1785952344,-0.9532258577\H,5.4788512051,-1.2592241664,-2.814
2821449\C,5.9138699595,1.8716922332,0.8525886123\H,4.4764727543,1.0223
757188,2.1646980268\C,6.2642285123,0.7939911083,-1.2742639984\C,6.5739
844985,1.7992025848,-0.3923170083\H,6.1655207418,2.667210231,1.5479981
013\H,6.7683550214,0.7278995919,-2.2350993789\H,7.326479781,2.53920702
29,-0.647818449\C,2.8394289672,-1.0971781914,1.8695822238\H,2.72847641
72,-0.1037268187,2.3025258117\H,3.2594065481,-1.7606655684,2.635898643
8\O,1.4720219263,-1.5173757626,1.6431243804\C,1.2187904383,-2.50628239
22,0.8245146056\C,-0.124403682,-2.8679627045,0.6395775503\C,-0.8682724
512,-2.9661508723,-0.6556944403\H,-0.3900362296,-2.5784469307,-1.55361
44058\H,-1.515047515,-3.8216080089,-0.828095753\C,-1.2848811286,-1.960
3830415,0.3985803621\H,-2.2121875428,-2.1442427799,0.9344530386\H,-1.0
754854963,-0.9100487276,0.2075248028\Au,-0.3238898808,-4.3857052653,2.

1054228471\H,1.9347448662,-3.6454545636,-0.7841223648\C,3.0473335284,-
4.271391231,0.9412839059\H,3.4659643295,-3.8816162062,1.8734274067\H,2
.3435190281,-5.0712326098,1.1907391708\H,3.8695819032,-4.6943338158,0.
3561613556\\Version=ES64L-G09RevD.01\State=1-A\HF=-2026.0486495\RMSD=6
.750e-09\RMSF=1.597e-06\Dipole=0.616905,-0.0723559,0.144926\Quadrupole
=10.5799916,0.6768956,-11.2568872,21.6966764,-14.7660875,-10.530863\PG
=C01 [X(C44H52Au1N2O1)]\\@

**1a-TS2**

1\1\GINC-A749\FTS\RPBE1PBE\GenECP\C44H52Au1N2O1(1+)\SIOC001\26-Mar-201
7\0\\#p opt=(calcfc,ts,noeigen) genecp pbe1pbe\\Title Card Required\\1
,1\Au,0.2320611178,-0.167300115,-0.1060295596\C,4.4576508158,0.0648499
932,0.1975370794\C,4.1638279438,1.3883910688,0.1569218929\H,5.40081480
13,-0.4561623698,0.2540698255\H,4.7969543822,2.2620096203,0.1713735372
\C,2.2162152924,0.2574247065,0.0856870778\N,2.7878709453,1.4849225613,
0.0897107792\N,3.2531699945,-0.6092999988,0.1527647131\C,2.0499308374,
2.7178756825,0.0386033777\C,1.6859030265,3.2310118201,-1.2164916057\C,
1.7219243893,3.3469116162,1.2507709799\C,0.949538225,4.4182521684,-1.2
296040253\C,0.9804974678,4.5281101664,1.1775486369\C,0.5963693124,5.05
84965431,-0.0484306862\H,0.6531100807,4.8491500532,-2.1819645694\H,0.7
053938008,5.0426628363,2.0940619193\H,0.0265978553,5.9831134413,-0.083
3673361\C,3.1176109457,-2.0410421685,0.1686905577\C,3.0110553369,-2.68
77335418,1.4104055358\C,3.1029903294,-2.7250604818,-1.0572966858\C,2.8
723137082,-4.0772176237,1.3965122178\C,2.9612317029,-4.1139650451,-1.0
109410215\C,2.8461363053,-4.7839962897,0.2005385636\H,2.7864648259,-4.
6133585766,2.3376919093\H,2.9460157366,-4.6780006268,-1.9395860964\H,2
.7415987861,-5.8654073399,0.2131600976\C,2.1190385803,2.7806035626,2.6
017768418\C,0.8939858993,2.2323624121,3.3411005708\C,2.8670435598,3.80
74897842,3.4566459931\H,2.8010893302,1.9389991557,2.4348336703\H,0.398
7567211,1.454544177,2.7479766512\H,1.1891848694,1.7956328396,4.3020549
358\H,0.1647698116,3.0258604347,3.5427919824\H,3.7496036422,4.19534470
02,2.937143106\H,2.2310231254,4.6607680262,3.7165859048\H,3.1982785579
,3.3483100571,4.394437246\C,2.0714843395,2.564809421,-2.5237255666\C,3
.019546605,3.455693756,-3.333762759\C,0.8376266476,2.1791860505,-3.345
5958813\H,2.6090993454,1.638450159,-2.2915135124\H,3.9181332609,3.7121
712915,-2.7622270503\H,3.3330578061,2.9427325631,-4.249637153\H,2.5333
37614,4.392700191,-3.6280266574\H,0.1705985811,1.5168142488,-2.7822133
51\H,0.2644307528,3.0638697482,-3.6467796739\H,1.1428162454,1.65859790
33,-4.2604179522\C,3.2313851453,-2.0213180095,-2.3952907792\C,1.956062
9664,-2.181888934,-3.2287460731\C,4.4618950561,-2.5082379623,-3.167312
3484\H,3.3662018057,-0.9497170488,-2.208513596\H,1.0815743108,-1.78887
69808,-2.6974811151\H,2.0507765771,-1.6409761711,-4.1772149352\H,1.764
5743128,-3.2351160163,-3.4645789797\H,5.3799718338,-2.3792072731,-2.58
40901933\H,4.3793124161,-3.5692193695,-3.4282871501\H,4.5695857545,-1.
9460677218,-4.1013647818\C,3.024573092,-1.9394829012,2.7304905215\C,4.
1410771701,-2.4370952434,3.6531296525\C,1.6578854908,-2.025694449,3.41
76352992\H,3.2198383437,-0.880949175,2.5236411439\H,5.1216490279,-2.36

7081557,3.1704241566\H,4.1696488822,-1.8387807962,4.5704648675\H,3.987
8781157,-3.4815310857,3.9465162453\H,0.8682050197,-1.6291548468,2.7688
073913\H,1.4040453791,-3.0628781672,3.6654983749\H,1.6610191199,-1.450
0182173,4.3503653076\C,-2.3138849902,-2.008262034,-0.1197667453\C,-1.7
912041345,-0.5935051101,-0.4342737861\C,-1.8884216915,-3.1106647745,-1
.0842411633\H,-2.1289956447,-2.8416076368,-2.1162836626\H,-0.807852977
9,-3.2706212827,-1.0158589709\H,-2.3890458474,-4.0547661238,-0.8444941
162\C,-3.8127328673,-1.755200744,-0.0542812189\C,-4.678237742,-2.52864
31204,0.7280677448\C,-5.5799859601,-0.0575862066,-0.3618207772\C,-5.94
73325015,-2.0696522584,1.0015936674\H,-4.3155813597,-3.4489153441,1.17
82584485\C,-6.0951992344,1.1490883275,-0.8822839665\C,-6.4200263373,-0
.8310937192,0.4961644351\H,-6.6023565642,-2.644823774,1.6521761589\C,-
7.3644689221,1.5792976183,-0.5481370408\H,-5.4966254514,1.7565600526,-
1.5527123725\C,-7.7183838538,-0.3708088265,0.814085903\C,-8.1852778487
,0.8181113824,0.3031897615\H,-7.7344589206,2.5171075861,-0.9524792428\
H,-8.343035835,-0.974828399,1.4671352372\H,-9.182814781,1.1678662502,0
.5503217623\C,-4.2496661094,-0.5411207047,-0.6471018783\C,-2.610866488
,0.2499670715,0.4140658038\C,-2.8281169065,1.6620420196,0.7576420323\C
,-2.7757448982,0.5868755957,1.8333175817\C,-3.5228406353,-0.0705673392
,-1.8985644198\H,-3.7073401113,0.9946240943,-2.0785426252\H,-3.8915043
437,-0.6295718335,-2.7674246896\O,-2.128866386,-0.3030223411,-1.784786
7047\H,-3.8010267415,2.109784407,0.564528269\H,-1.9792041687,2.3283545
091,0.6121302241\H,-3.7223548597,0.3383140455,2.3094964877\H,-1.905879
0727,0.5009778286,2.4800627543\H,-1.9930348937,-2.2782498711,0.8950316
408\\Version=ES64L-G09RevD.01\State=1-A\HF=-2025.9817851\RMSD=5.644e-0
9\RMSF=1.455e-06\Dipole=-2.1661451,0.1469128,0.8772002\Quadrupole=43.0
062911,-11.8625355,-31.1437555,-1.0511081,-4.781568,-3.89959\PG=C01 [X
(C44H52Au1N2O1)]\\@

**1a-E**

1\1\GINC-A762\FOpt\RPBE1PBE\GenECP\C44H52Au1N2O1(1+)\SIOC001\14-Mar-20
17\0\\#p opt genecp pbe1pbe\\Title Card Required\\1,1\Au,0.1976367403,
-0.1244751877,-0.0550514128\C,4.4439981743,0.0025933361,0.0350334715\C
,4.1884697078,1.3336773796,0.0010053874\H,5.3722847035,-0.5472458341,0
.0486012258\H,4.8476587111,2.1876144544,-0.0216708282\C,2.2021229038,0
.2629304138,0.0322475723\N,2.8140293163,1.4715857179,0.0012902981\N,3.
218002465,-0.6334131406,0.0532802816\C,2.1244765097,2.732698175,-0.020
5371806\C,1.7349226088,3.2652272475,-1.2597375626\C,1.8800016393,3.378
1649775,1.2024555454\C,1.0686476486,4.4930128087,-1.2453670934\C,1.208
1790961,4.6014725589,1.157127262\C,0.8063703738,5.1545870575,-0.052534
8463\H,0.7543791915,4.9382019537,-2.1854611374\H,0.999452015,5.1292499
779,2.0836584702\H,0.2910388868,6.1111667193,-0.0657755728\C,3.0402469
992,-2.0590490858,0.0932157666\C,2.9758072057,-2.6884619087,1.34660234
93\C,2.9405179623,-2.7564262583,-1.1213620593\C,2.7901870947,-4.072458
3902,1.3581566286\C,2.7536929606,-4.1390396758,-1.0502023313\C,2.67787
71991,-4.7911868324,0.1742627244\H,2.7358206548,-4.5949561442,2.309355
4583\H,2.6710443999,-4.712657013,-1.9693050177\H,2.5382313679,-5.86833

08387,0.206205081\C,2.2931627141,2.7894532064,2.5385655242\C,1.0620680
093,2.3733267052,3.3501229942\C,3.1834163189,3.748724302,3.3338050735\
H,2.8789233774,1.8829321329,2.3487474439\H,0.4534104857,1.6523657843,2
.7926006283\H,1.3652574321,1.9107457065,4.2964965375\H,0.4315806581,3.
238364651,3.5866947723\H,4.0695224567,4.0426235727,2.7610952784\H,2.64
73219545,4.6632876412,3.6109572517\H,3.5198939675,3.2718598749,4.26098
18249\C,2.0119719236,2.5712760005,-2.5799535491\C,2.9355613057,3.41400
30264,-3.4656072616\C,0.7102954861,2.2241482156,-3.3092239368\H,2.5288
147513,1.6282608237,-2.3695038786\H,3.8804184938,3.6418712425,-2.96036
03253\H,3.1660152008,2.8777198644,-4.3928368345\H,2.4672278553,4.36573
99339,-3.7410274741\H,0.0614209187,1.5950337336,-2.6894643202\H,0.1520
86157,3.1282177645,-3.5792054075\H,0.9290344704,1.6816422494,-4.236114
2845\C,3.0168170397,-2.0691272035,-2.4718421637\C,1.6717608782,-2.1458
805611,-3.2013556925\C,4.1481812709,-2.6396636339,-3.3324319584\H,3.23
71947703,-1.0086044531,-2.3043293064\H,0.8723347038,-1.6907101204,-2.6
051302498\H,1.7271793836,-1.6175557282,-4.1601010453\H,1.3929463945,-3
.185730947,-3.4091652915\H,5.1149470598,-2.5737469135,-2.8218829682\H,
3.9739850606,-3.6922570811,-3.5822148161\H,4.2220309869,-2.0859849153,
-4.2748517558\C,3.0808154816,-1.9253616158,2.653766896\C,4.2176563536,
-2.4554066332,3.5322447832\C,1.7448189126,-1.945192873,3.404023424\H,3
.3082191576,-0.8786544759,2.4221008706\H,5.1775515777,-2.4298892928,3.
0055396441\H,4.3103504307,-1.8470199132,4.4386332762\H,4.0375067972,-3
.4891931463,3.8475356925\H,0.9436195444,-1.523738968,2.7857934012\H,1.
4606388109,-2.9673864318,3.6805879617\H,1.8150667575,-1.3567109945,4.3
261193459\C,-2.3130231835,-1.9530747433,0.1243238696\C,-1.827619223,-0
.5167285078,-0.2403356649\C,-1.7331039774,-3.1239168184,-0.6562948896\
H,-1.8969681062,-2.9831256957,-1.7285380225\H,-0.6546694553,-3.1800641
295,-0.4822827155\H,-2.1760238844,-4.079060217,-0.3535718796\C,-3.7959
151283,-1.7978515935,0.0774318491\C,-4.7789094876,-2.769947478,0.19290
83571\C,-5.5234237458,0.0231915158,0.0586706012\C,-6.0922529754,-2.354
8811928,0.3406397067\H,-4.5225568859,-3.8228269705,0.2583983174\C,-5.9
643655031,1.3425741943,-0.0703858995\C,-6.4927028861,-0.9924092421,0.2
957272402\H,-6.8655061245,-3.1008550419,0.5162348754\C,-7.3084056033,1
.6570654134,0.086799537\H,-5.2573199424,2.1325388171,-0.2978179144\C,-
7.8553332962,-0.6518490405,0.4515355224\C,-8.259163653,0.662601554,0.3
562649256\H,-7.6265402756,2.6918243383,-0.0031910383\H,-8.5794253764,-
1.4409465326,0.6366672493\H,-9.3050523269,0.9268514143,0.4751497668\C,
-4.1119489925,-0.3788261525,-0.1224417921\C,-2.857941183,0.297121223,0
.5155679099\C,-2.7153262054,1.7323011742,0.8999519828\C,-2.7300828725,
0.6587542702,1.9589250799\C,-3.6346032566,-0.1523107751,-1.6428347137\
H,-3.9063691052,0.8849368999,-1.8811177317\H,-4.1304315409,-0.83282645
05,-2.3464164526\O,-2.2576068027,-0.3473672163,-1.6269485527\H,-3.5747
137833,2.3944795294,0.8664751626\H,-1.7688062715,2.2057662255,0.651399
5684\H,-3.615549445,0.5987905912,2.5871985824\H,-1.7975460579,0.409648
6129,2.4587619573\H,-2.0731944082,-2.0696767743,1.1960829913\\Version=
ES64L-G09RevD.01\State=1-A\HF=-2025.9987096\RMSD=4.452e-09\RMSF=3.142e
-06\Dipole=-3.8239405,-0.5846469,0.5300418\Quadrupole=58.0467483,-14.9

035405,-43.1432078,6.8270167,-2.5068288,-1.5375929\PG=C01 [X(C44H52Au1
N2O1)]\\@

**1a-TS3**

1\1\GINC-A729\FTS\RPBE1PBE\GenECP\C44H52Au1N2O1(1+)\SIOC001\10-May-201
7\0\\#p genecp opt=(calcfc,ts,noeigen) pbe1pbe\\Title Card Required\\1
,1\C,-4.4542516478,-0.2766661881,-0.0615589495\C,-4.2182503733,1.05975
45195,-0.0786925595\H,-5.37456987,-0.8395100849,-0.0392967601\H,-4.889
7002053,1.9043791789,-0.0732545918\C,-2.2280250061,0.0177615745,-0.110
5340403\N,-2.8479166242,1.2187823424,-0.1086420293\N,-3.2219647998,-0.
897436581,-0.0811051995\C,-2.161204959,2.482831669,-0.1347399551\C,-1.
8034423019,3.0740046733,1.0878365166\C,-1.8772941478,3.0601671555,-1.3
831655266\C,-1.1129337416,4.2870178685,1.0290653288\C,-1.1845991031,4.
272755009,-1.3802177259\C,-0.8034613224,4.8789657736,-0.1893703925\H,-
0.818703547,4.7771051081,1.9530991964\H,-0.9430787429,4.7503290263,-2.
3255948501\H,-0.2685842093,5.8243833294,-0.2111319125\C,-3.0184884197,
-2.3222395384,-0.0772685268\C,-2.9840244933,-2.9918259769,-1.311166614
7\C,-2.8673343168,-2.9726541219,1.1577480306\C,-2.7799244672,-4.372885
8346,-1.2802377057\C,-2.6669334176,-4.3546569052,1.1271316753\C,-2.622
6086277,-5.0479490101,-0.0758630625\H,-2.7488188765,-4.9276872678,-2.2
13945965\H,-2.5477523336,-4.8953741144,2.0619484563\H,-2.4706293106,-6
.1237397406,-0.0746884546\C,-2.2825577213,2.4199421959,-2.6979884074\C
,-1.0526706966,1.9595030515,-3.4872978863\C,-3.1561589429,3.3580297113
,-3.5366025883\H,-2.8816345035,1.5287144138,-2.4771954338\H,-0.4604611
456,1.2400032031,-2.9097342044\H,-1.3571320047,1.4780717663,-4.4235028
17\H,-0.4035943336,2.8053271026,-3.7414669652\H,-4.0397595439,3.688978
971,-2.9807151686\H,-2.6050848866,4.2515650729,-3.8502013775\H,-3.4963
451766,2.8471395491,-4.4439085386\C,-2.1363014066,2.4544673896,2.43259
8654\C,-3.0074327336,3.3904245083,3.2767865808\C,-0.8665263227,2.05091
64184,3.1887069229\H,-2.7152185415,1.5404103203,2.2567179571\H,-3.9256
366133,3.670535088,2.7496405612\H,-3.2889065948,2.9013312588,4.2156562
1\H,-2.4748897374,4.3131196071,3.5322245838\H,-0.2663315146,1.33861334
11,2.610528022\H,-0.2390836281,2.9224446409,3.4085113903\H,-1.12624705
81,1.5796687172,4.1432816762\C,-2.9155477716,-2.2435172601,2.487408710
3\C,-1.5794395202,-2.3527900021,3.2294150273\C,-4.0733384286,-2.747435
409,3.3553058489\H,-3.0930660221,-1.179734081,2.2910283143\H,-0.752466
2912,-1.9570844274,2.628347489\H,-1.6203552155,-1.7877494514,4.1674357
526\H,-1.3457823389,-3.393823189,3.4799251243\H,-5.035679334,-2.644045
5044,2.8425000241\H,-3.9473665525,-3.803837139,3.6171854283\H,-4.12227
28943,-2.1784831333,4.2901246891\C,-3.1412400878,-2.276740264,-2.64039
67021\C,-4.3026347271,-2.8481952738,-3.4592816234\C,-1.8328550786,-2.3
139745982,-3.4371948406\H,-3.371284893,-1.2236622382,-2.4406079275\H,-
5.2437530701,-2.8132424801,-2.9004037806\H,-4.4329899668,-2.2735286821
,-4.3826750526\H,-4.1222882275,-3.8907252333,-3.7434603386\H,-1.013680
5377,-1.8555522656,-2.8703680614\H,-1.5447672878,-3.343708784,-3.67851
05124\H,-1.943072667,-1.7679684928,-4.3809678038\C,2.8907175871,-1.893
6756239,-0.658189477\C,2.4029579117,-3.2122692614,-1.1460096723\H,1.83

37211141,-3.7380662687,-0.3673584585\H,1.7598247748,-3.1287596601,-2.0
316557796\H,3.2554142357,-3.8451591911,-1.4128565189\C,4.1175640005,-1
.4196106613,-0.3809327716\C,5.3775705735,-2.0305650308,-0.7234549972\C
,5.3870315262,0.6028220499,0.5250798015\C,6.522004874,-1.3383625661,-0
.5450332982\H,5.3911750475,-3.0148401015,-1.1818654619\C,5.4837192754,
1.8364709338,1.168071619\C,6.564635566,-0.0092518008,0.0431120733\H,7.
469383967,-1.777224765,-0.8488194454\C,6.7083981049,2.4904079104,1.288
4745334\H,4.5993266897,2.2920131977,1.6032120927\C,7.7890587144,0.6584
261779,0.1719470033\C,7.8638292137,1.9047352729,0.7794285117\H,6.75788
70832,3.4529101306,1.7891445706\H,8.6906712473,0.1819172087,-0.2049960
754\H,8.820896405,2.4094027574,0.8710290142\C,4.0804641512,-0.12904488
96,0.4141140594\C,2.8192304875,0.5163467783,-0.1893234047\C,2.41954207
65,1.9625660223,-0.1932754026\C,2.7584984399,1.2577258599,-1.478835985
\C,3.4940955162,-0.5444163764,1.792902467\H,3.4856099693,0.3017136443,
2.4867337632\H,4.0210421251,-1.390965798,2.2417757288\O,2.1319733837,-
0.9239712406,1.5188834034\H,3.1335005159,2.6959553779,0.1668528738\H,1
.3788565225,2.2047366357,0.0086388812\H,3.7070356135,1.5007100415,-1.9
506990166\H,1.9528748342,1.0241247645,-2.1701071953\H,1.5149985078,-1.
3893474063,-0.5643823412\C,1.8868360948,-0.5904632683,0.1913277834\Au,
-0.236397267,-0.3269161356,-0.0675501969\\Version=ES64L-G09RevD.01\Sta
te=1-A\HF=-2025.93429\RMSD=8.338e-09\RMSF=1.734e-06\Dipole=0.1464761,-
0.0405895,-0.3330173\Quadrupole=29.6706575,-3.0249944,-26.6456631,2.74
95541,1.7936977,6.0165614\PG=C01 [X(C44H52Au1N2O1)]\\@

**1a-F**

1\1\GINC-A748\FOpt\RPBE1PBE\6-31G(d)\C17H16O1\SIOC001\03-Mar-2017\0\\#
p opt pbe1pbe/6-31g(d)\\Title Card Required\\0,1\C,4.835483949,-0.631
6678971,-4.094298337\C,6.1770802198,-0.4781264743,-3.7720730012\C,6.86
60083973,0.7048503701,-4.0709528495\C,6.1744497387,1.7634722799,-4.704
0293871\C,4.8343535597,1.5817914568,-5.0459199571\C,4.1619729302,0.400
8579212,-4.7405422992\H,8.7608828326,-0.0452568988,-3.3012832958\H,4.3
19814955,-1.557005639,-3.8523604408\H,6.713846139,-1.2869683071,-3.280
9128046\C,8.2800843445,0.8238985669,-3.7447030462\C,6.9141022637,3.019
7255095,-5.0522934247\H,4.3078438005,2.369313864,-5.576897965\H,3.1167
541407,0.2873443339,-5.0148526191\C,8.3338482728,3.1124120978,-4.50347
04051\C,8.9844752363,1.9560927814,-3.9568817137\H,10.0330907221,2.0138
980703,-3.6747191286\C,10.0997573523,4.9872196957,-4.4267573826\H,10.0
367761096,5.8570789059,-3.7592300926\H,10.7984570326,4.2725108406,-3.9
812026862\H,10.5381599829,5.3440917023,-5.3685856139\C,8.7610839036,4.
3875707316,-4.6655059001\C,6.4133013428,4.4237825518,-4.6550061603\C,7
.5978593105,5.108214675,-5.3079151727\H,7.6228912537,6.1997461085,-5.3
253140962\C,5.809805685,4.8110013228,-3.352813303\H,6.1813172601,5.700
1042331,-2.8488757033\H,5.5029829991,4.0105163692,-2.6838787644\C,5.02
91915656,4.9791027134,-4.6373667983\H,4.8864358063,5.9837359892,-5.028
8373296\H,4.1813965612,4.3188681235,-4.794285204\C,7.0595349657,3.2902
846631,-6.5847138137\H,6.0900351407,3.1896971622,-7.0895885105\H,7.782
1118315,2.6100154069,-7.0513770491\O,7.5081079047,4.6354014995,-6.6760

010945\\Version=ES64L-G09RevD.01\State=1-A\HF=-731.7511074\RMSD=4.899e
-09\RMSF=1.134e-05\Dipole=-0.0296573,-0.1595095,0.5129325\Quadrupole=3
.5273611,3.2131099,-6.740471,1.5389929,3.1080142,0.7597042\PG=C01 [X(C
17H16O1)]\\@

**1a-TS4**

1\1\GINC-A756\FTS\RPBE1PBE\6-31G(d)\C17H16O1\SIOC001\18-Mar-2017\0\\#p
opt=(calcfc,ts,noeigen) 6-31g(d) pbe1pbe geom=check\\Title Card Requi
red\\0,1\C,0.0115142297,0.0312150955,-0.0050615928\C,0.0119683467,0.03
91919274,1.3763662386\C,1.2157298447,0.0052813584,2.1038950677\C,2.454
5248805,-0.0520609068,1.4078489117\C,2.4250361108,-0.0663894663,0.0041
766362\C,1.2285921022,-0.0177700257,-0.6929477647\H,0.2216079091,0.079
1163411,4.0310257098\H,-0.9261358417,0.0615911223,-0.5528637353\H,-0.9
272557176,0.0793990708,1.9237457868\C,1.1930751455,0.0557125542,3.5420
026671\C,3.6799779594,-0.1807781564,2.1953474278\H,3.3529635194,-0.121
8936389,-0.5534886435\H,1.2389724716,-0.0248350968,-1.7795678528\C,3.5
943398424,0.088528848,3.6192510426\C,2.332958613,0.1117979111,4.279754
6808\H,2.288447242,0.1956800094,5.3623351771\C,5.2335386726,0.10457858
67,5.6192844652\H,6.2241853514,0.5336104702,5.7999060778\H,4.513692085
6,0.6626041114,6.2270126457\H,5.2499049698,-0.9293251953,5.9875578985\
C,4.8794932331,0.1417505934,4.1691152892\C,5.0824334149,0.2611791942,1
.8319292612\C,5.7684187731,-0.0326802929,3.1033970594\H,6.8495138493,-
0.0560433864,3.1964040384\C,5.3900277714,1.5141776544,1.0402932409\H,6
.148065686,2.1927075344,1.4208432989\H,4.5424728967,2.0019124601,0.565
6371236\C,5.8074476226,0.1686322064,0.5274865372\H,6.8586629239,-0.100
802222,0.5873817617\H,5.3028879426,-0.2478491701,-0.3379187614\C,4.224
5339678,-1.9904162024,2.2441767732\H,4.1960417492,-2.1548351242,1.1528
87478\H,3.377540493,-2.4658939887,2.7650681717\O,5.3737247826,-1.98761
79904,2.8299484605\\Version=ES64L-G09RevD.01\State=1-A\HF=-731.7141063
\RMSD=7.486e-09\RMSF=1.431e-06\Dipole=-0.4335442,0.8502539,-0.1639527\
Quadrupole=3.883439,-9.0008331,5.1173941,4.6598802,-0.2913677,1.559405
9\PG=C01 [X(C17H16O1)]\\@

**1a-P**

1\1\GINC-A735\FOpt\RPBE1PBE\6-31G(d)\C16H14\SIOC001\03-Mar-2017\0\\# p
opt pbe1pbe/6-31g(d)\\Title Card Required\\0,1\C,-6.7496693329,-2.421
4528011,0.1117187586\C,-5.3779292034,-2.3934466933,0.0614696658\C,-4.6
675626501,-1.1697470043,0.0063317975\C,-5.3996367704,0.0654214543,0.00
30394074\C,-6.8180024836,-0.0042282106,0.0559799081\C,-7.4733464286,-1
.2109032343,0.1087282417\H,-2.7253307209,-2.1114957011,-0.0411602447\H
,-7.2784234583,-3.3696912368,0.1536359502\H,-4.8090795131,-3.320806051
3,0.0632427574\C,-3.2491519182,-1.1583587617,-0.0451777336\C,-4.650567
4053,1.2683072957,-0.0531123963\H,-7.4032534845,0.90869794,0.055146268
\H,-8.5592768739,-1.2323731039,0.1485077078\C,-3.25681482,1.2380144245
,-0.1027750438\C,-2.5480890176,0.0190006851,-0.0988990931\H,-1.4615860
244,0.0154624756,-0.1379869758\C,-5.0554166483,2.6995115198,-0.0734113
462\C,-2.7346602997,2.6048495274,-0.1548268591\C,-3.7853400874,3.45091

4934,-0.1377009543\H,-3.7395667446,4.5355323301,-0.1658627118\C,-6.240
2436489,3.2669297619,0.6978187252\H,-6.0838932838,4.2244092493,1.18643
09849\H,-6.8335344325,2.5625128732,1.2725465583\C,-6.2933874656,3.2304
530324,-0.7849778454\H,-6.1741105168,4.1626646544,-1.3297015658\H,-6.9
254515725,2.4999265292,-1.280277059\C,-1.2835310979,2.9450218068,-0.21
57440715\H,-0.744810351,2.553881258,0.6569349679\H,-0.8083048306,2.509
9926678,-1.1043757432\H,-1.1307659552,4.0277609489,-0.248219115\\Versi
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e-05\Dipole=-0.0754853,0.3677383,-0.0063978\Quadrupole=3.0729868,4.331
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