Silver-catalyzed formal [2π+2σ] cycloaddition of bicyclobutanes with naphthols as surrogates for arynes

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Supporting Information

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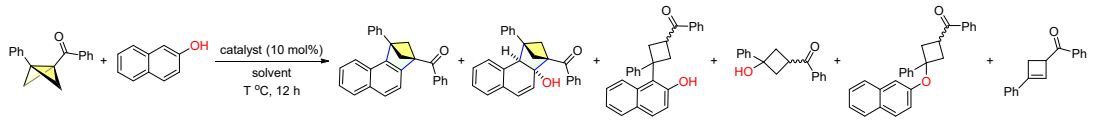
1 General Information

All reactions were performed in flame-dried glassware using conventional Schlenk techniques under a static pressure of nitrogen unless otherwise stated. Liquids and solutions were transferred with syringes. Bicyclo[1.1.0]butanes (BCBs) [1] and hydroxyarenes [2] were prepared according to reported procedures. $AgBF_4$ (98%, *Energy Chemical* and other commercially available reagents were purchased from *Sigma-Adrich*, *Leyan*, and *Bide* Chemical Company and used as received. All other solvents (1,2-dichloroethane, toluene, and CH_2Cl_2 *etc*.) were dried and purified following standard procedures. Technical grade solvents for extraction or chromatography (Petroleum ether, CH_2Cl_2, and ethyl acetate) were distilled prior to use. Analytical thin layer chromatography (TLC) was performed on silica gel 60 F254 glass plates by *Merck*. Flash column chromatography was performed on silica gel 60 (40–63 μm, 230–400 mesh, ASTM) by *Grace* using the indicated solvents. ^1H, ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker AV400 instruments. Chemical shifts are reported in parts per million (ppm) and are referenced to the residual solvent resonance as the internal standard ($CDCl_3$: δ = 7.26 ppm for ^1H NMR and $CDCl_3$: δ = 77.0 ppm for ^{13}C NMR). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplett, q = quartet, m = multiplet), coupling constants (Hz), and integration. The full-scan mass spectra were taken on a hybrid quadrupole-orbitrap mass spectrometer equipped with a heated electrospray ionization source (ThermoFischer Scientific, Bremen, Germany). X-ray data were taken on a Bruker SMART APEX II X-Ray diffractometer equipped with a large area CCD detector.

2 Optimization of the Reaction Conditions

Table S1. Optimization of dehydrative (3+2) annulation of BCBs [a]



1a **2a** **3aa** **4** **5** **6** **7** **8**

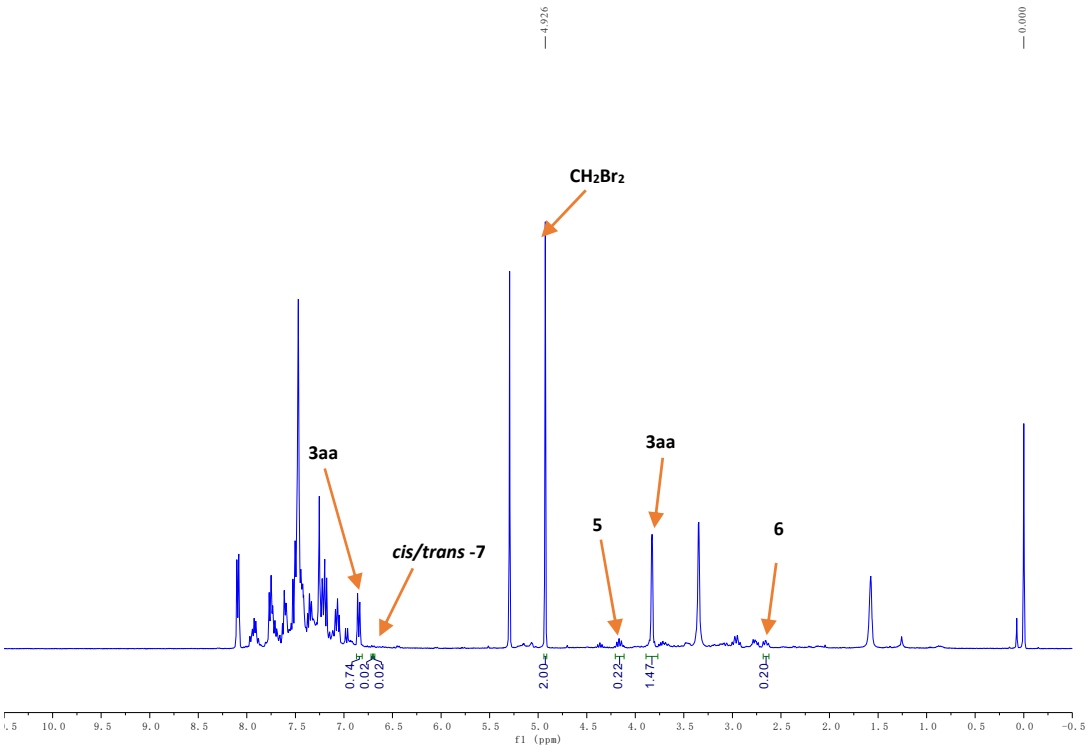
Entry	Catalyst	Solvent	T (°C)	Conversion of **1a** (%) [b]	**Yield** (%) [b]					
					3aa	**4**	**5**	**6**	**7**	**8**
1	$AgSbF_6$	CH_2Cl_2	25	100	53	0	45	0	0	3
2	$AgClO_4$	CH_2Cl_2	25	100	55	0	43	0	0	<3
3	AgOTf	CH_2Cl_2	25	100	39	0	58	0	0	5
4	**$AgBF_4$**	**CH_2Cl_2**	**25**	**100**	**74**	**0**	22	10	4	<3
5	$AgPF_6$	CH_2Cl_2	25	100	33	0	40	10	12	3
6	Ag_2CO_3	CH_2Cl_2	25	0	0	0	0	0	0	0
7	$Bi(OTf)_3$	CH_2Cl_2	25	100	36	0	53	0	0	8
8	$Ga(OTf)_3$	CH_2Cl_2	25	100	38	0	43	3	0	8
9	$Yb(OTf)_3$	CH_2Cl_2	25	65	15	25	0	0	13	9
10	$Eu(OTf)_3$	CH_2Cl_2	25	66	0	33	0	0	14	4
11	$Zn(OTf)_2$	CH_2Cl_2	25	67	0	30	19	0	15	4
12	$Co(OTf)_2$	CH_2Cl_2	25	100	44	0	54	0	0	8
13	$AlCl_3$	CH_2Cl_2	25	77	8	15	15	7	17	26
14	TMSOTf	CH_2Cl_2	25	100	32	0	65	0	0	3
15	$B(C_6F_5)_3$	CH_2Cl_2	25	100	23	0	38	13	2	23
16[c]	CF_3SO_3H	CH_2Cl_2	25	100	39	0	16	0	0	0
17	$HNTf_2$	CH_2Cl_2	25	100	20	0	35	0	0	0
18	$AgBF_4$	$CHCl_3$	25	100	0	25	36	0	8	<3
19	$AgBF_4$	DCE	25	100	73	0	26	8	0	0
20	**$AgBF_4$**	**toluene**	**25**	**100**	**0**	**56**	**14**	**0**	**20**	**3**
21	$AgBF_4$	THF	25	100	11	35	12	8	14	0
22	$AgBF_4$	EtOAc	25	100	40	4	41	15	15	3
23	$AgBF_4$	MeCN	25	100	0	47	10	0	15	8
24	$AgBF_4$	CH_2Cl_2	0	100	24	49	13	12	9	0
25[d]	**$AgBF_4$**	**CH_2Cl_2**	**0**	**100**	**5**	**66**	**12**	**18**	**12**	**3**
26	$AgBF_4$	CH_2Cl_2	15	100	60	14	19	10	7	<3
27	$AgBF_4$	CH_2Cl_2	40	100	72	0	27	0	0	4
28	$AgBF_4$	DCE	60	100	64	0	27	0	0	6
29[e]	$AgBF_4$	CH_2Cl_2	25	100	74	0	22	13	6	<3
30[f]	$AgBF_4$	CH_2Cl_2	25	100	74	0	19	7	5	<3

[a] Reaction conditions: **1a** (0.12 mmol, 1.2 equiv), **2a** (0.10 mmol, 1.0 equiv) and catalyst (10 mol%), solvent (2 mL), T °C, under N_2 for 12 h.
[b] Determined by ^1H NMR spectroscopy with CH_2Br_2 as an internal standard.
[c] CF_3SO_3H (20 mol%) was used.
[d] $NaBF_4$ (20 mol%) as an additive was introduced into the reaction system.
[e] **1a** (0.15 mmol, 1.5 equiv) and **2a** (0.10 mmol, 1.0 equiv) were used.
[f] **1a** (0.24 mmol, 1.2 equiv) and **2a** (0.20 mmol, 1.0 equiv) were used.

DCE = 1,2-dichloroethane

The representative NMR spectra under standard conditions (Table S1, Entry 4) and under dearomative (3+2) conditions (Table S1, Entry 25) are presented below.

Table S1. Entry 4:



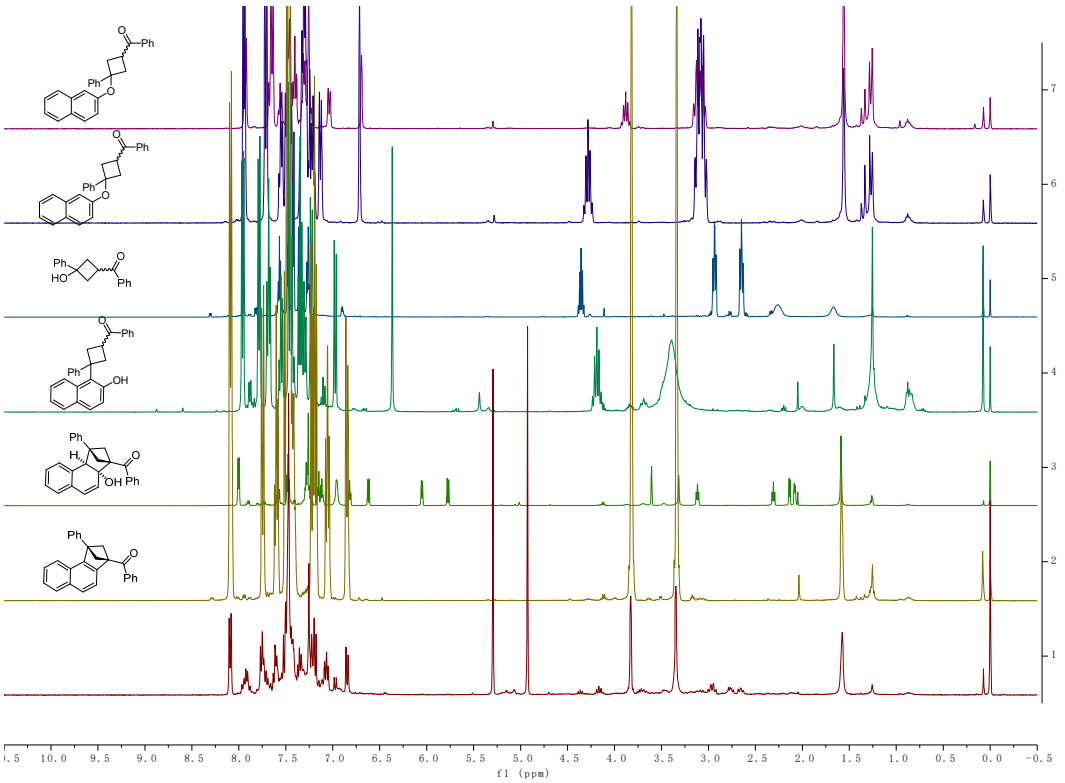
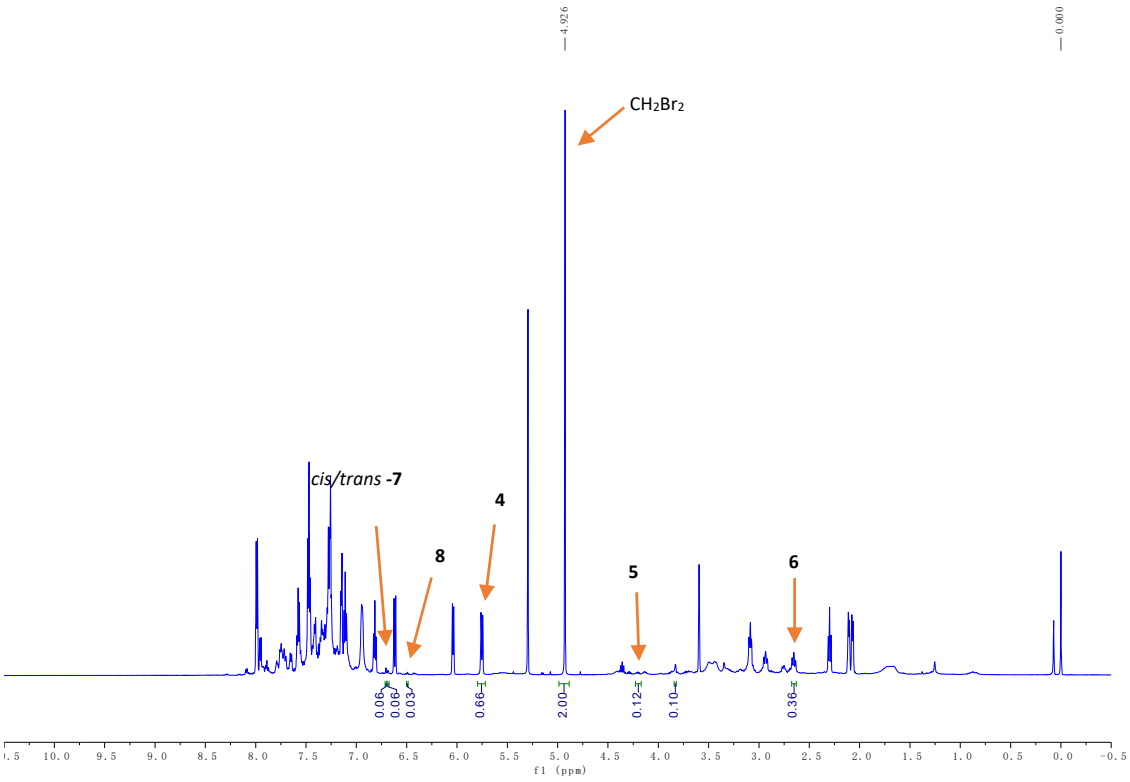
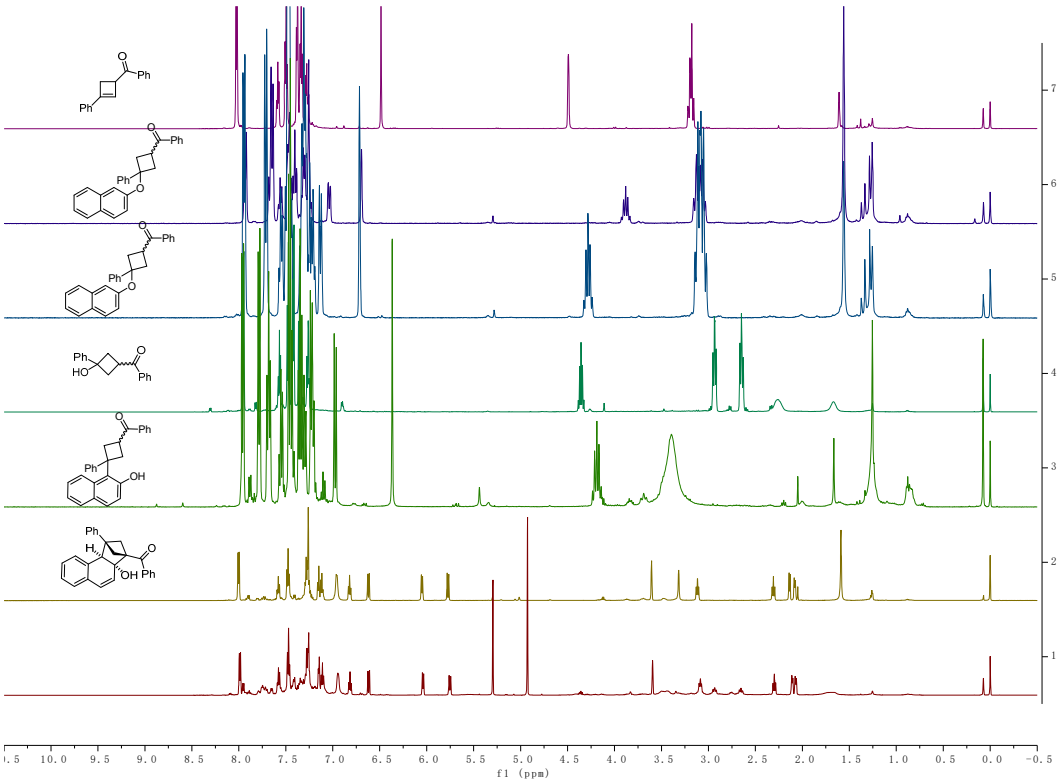
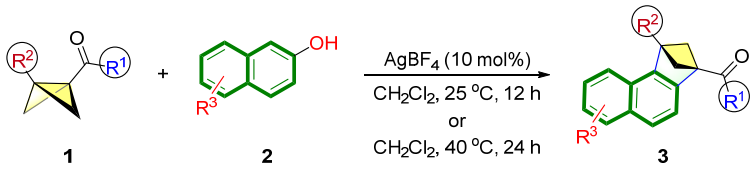


Table S1. Entry 25:



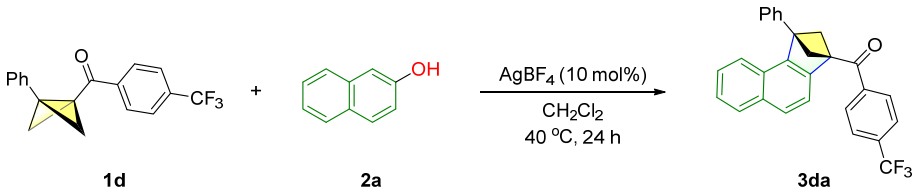


3 General Procedure for the Formal [2π+2σ] Cycloadditions of BCBs with Arynes (GP)



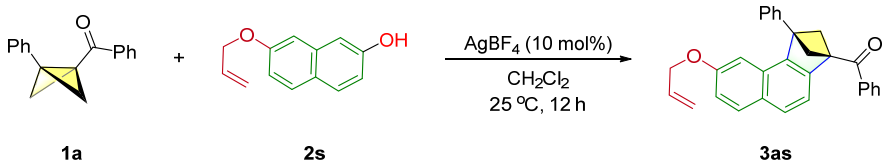
A 25 mL Schlenk tube, pre-dried in an oven and fitted with a Teflon-coated magnetic stir bar, was charged with BCB **1** (0.24 mmol, 1.2 equiv), hydroxyarene **2** (0.2 mmol, 1.0 equiv), and $AgBF_4$ (3.9 mg, 0.02 mmol, 10 mol%). The tube was evacuated and backfilled with nitrogen three times, followed by the addition of CH_2Cl_2 (2.0 mL). The reaction mixture was stirred at 25°C for 12 hours. After removal of the solvents under reduced pressure, the resulting crude product was purified through flash chromatography on a short silica gel column, yielding the target Benzobicyclo[2.1.1]hexenes **3**.

4 Scale-Up Experiments



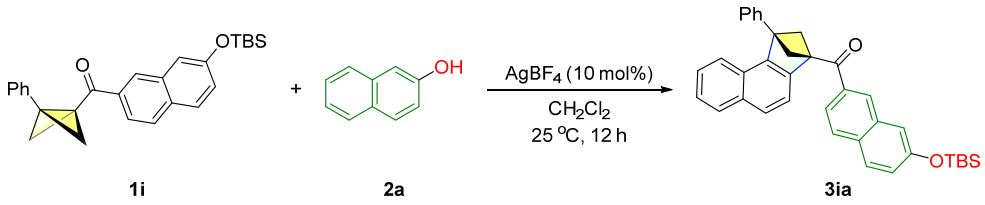
Into an oven-dried Schlenk tube equipped with a magnetic stir bar were sequentially added (3-phenylbicyclo[1.1.0]butan-1-yl)(4-(trifluoromethyl)phenyl)methanone **1d** (362.8 mg, 1.2 mmol, 1.2 equiv), naphthalen-2-ol **2a** (144.2 mg, 1.0 mmol, 1.0 equiv), and $AgBF_4$ (19.4 mg, 0.1 mmol, 10.0 mol%). The reaction vessel was subjected to three cycles of evacuation and backfilling with anhydrous N_2 to establish an inert atmosphere. Anhydrous CH_2Cl_2 (10 mL) was then introduced via syringe, and the resulting mixture was stirred at 40°C for 24 hours under a nitrogen atmosphere. After completion of the reaction, the solvent was carefully removed under reduced pressure using a rotary evaporator. The crude residue was purified by flash column chromatography on silica gel employing a gradient elution of petroleum ether/ethyl

acetate (100:1 to 50:1, v/v) to afford the desired product **3da** as a white solid (334.7 mg, 78% yield).



1a **2s** **3as**

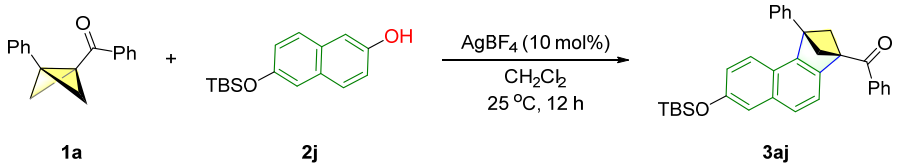
Into a flame-dried Schlenk flask equipped with a magnetic stir bar were sequentially charged phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone **1a** (281.2 mg, 1.2 mmol, 1.2 equiv), 6-(allyloxy)naphthalen-2-ol **2s** (200.2 mg, 1.0 mmol, 1.0 equiv), and $AgBF_4$ (19.4 mg, 0.1 mmol, 10.0 mol%). The reaction vessel was carefully evacuated and backfilled with anhydrous N_2 for three consecutive cycles to ensure an oxygen-free environment. Anhydrous CH_2Cl_2 (10 mL, freshly distilled over calcium hydride) was then introduced via cannula transfer, and the resulting mixture was allowed to stir at 25 °C for 12 hours under a positive pressure of nitrogen. Upon completion of the reaction as monitored by TLC analysis, the volatile components were removed under reduced pressure using a rotary evaporator. The crude product was purified by flash column chromatography on silica gel using a gradient elution of petroleum ether/ethyl acetate (100:1 to 50:1, v/v) as the mobile phase, yielding the desired product **3as** as a pale yellow crystalline solid (277.5 mg, 67% yield)



1i **2a** **3ia**

Into a flame-dried Schlenk flask equipped with a magnetic stir bar were sequentially added (7-((*tert*-butyldimethylsilyl)oxy)naphthalen-2-yl)(3-phenylbicyclo[1.1.0]butan-1-yl)methanone **1i** (199.0 mg, 0.48 mmol, 1.2 equiv), naphthalen-2-ol **2a** (57.7 mg, 0.4 mmol, 1.0 equiv), and $AgBF_4$ (7.8 mg, 0.04 mmol, 10.0 mol%). The reaction vessel was subjected to three cycles of evacuation and backfilling with anhydrous N_2 to establish an inert atmosphere. Anhydrous CH_2Cl_2 (4 mL, freshly distilled over calcium

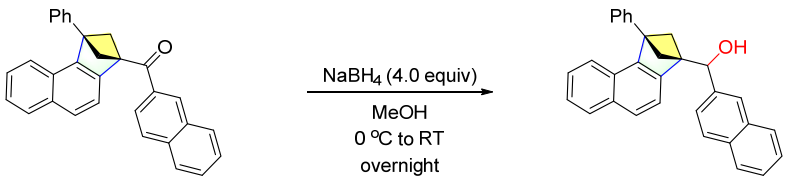
hydride) was then introduced via cannula transfer, and the resulting mixture was allowed to stir at 25°C for 12 hours under a positive pressure of nitrogen. Upon completion of the reaction as monitored by TLC analysis, the volatile components were removed under reduced pressure using a rotary evaporator. The crude product was purified by flash column chromatography on silica gel using a gradient elution of petroleum ether/ethyl acetate (100:1 to 50:1, v/v) as the mobile phase, yielding the desired product **3ia** as a pale yellow crystalline solid (241.8 mg, 56% yield).



1a **2j** **3aj**

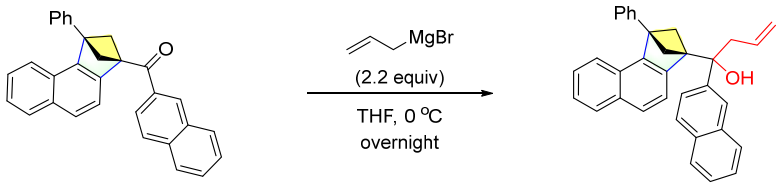
Into a flame-dried Schlenk flask equipped with a magnetic stir bar were sequentially charged phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone **1a** (281.2 mg, 1.2 mmol, 1.2 equiv), 6-((*tert*-butyldimethylsilyl)oxy)-naphthalen-2-ol **2j** (274.4 mg, 1.0 mmol, 1.0 equiv), and $AgBF_4$ (19.4 mg, 0.1 mmol, 10.0 mol%). The reaction vessel was carefully evacuated and backfilled with anhydrous N_2 for three consecutive cycles to ensure an oxygen-free environment. Anhydrous CH_2Cl_2 (10 mL, freshly distilled over calcium hydride) was then introduced via cannula transfer, and the resulting mixture was allowed to stir at 25°C for 12 hours under a positive pressure of nitrogen. Upon completion of the reaction as monitored by TLC analysis, the volatile components were removed under reduced pressure using a rotary evaporator. The crude product was purified by flash column chromatography on silica gel using a gradient elution of petroleum ether/ethyl acetate (100:1 to 50:1, v/v) as the mobile phase, yielding the desired product **3aj** as a pale yellow crystalline solid (273.5 mg, 56% yield).

5 Synthetic Transformations



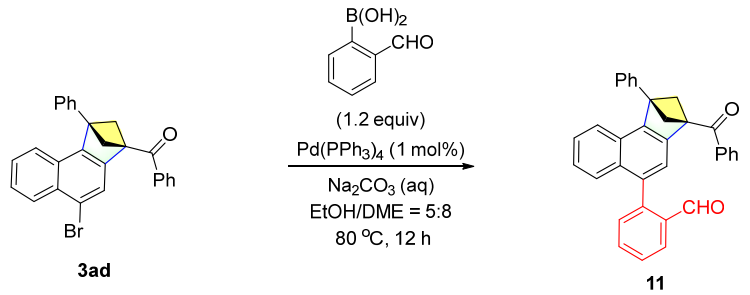
3ja **9**

Synthesis of (9): To a stirred solution of compound **3ja** (41.1 mg, 0.10 mmol, 1.0 equiv) in anhydrous methanol (2.0 mL) maintained at 0 °C under N_2 atmosphere, $NaBH_4$ (15.1 mg, 0.4 mmol, 4.0 equiv) was added. The resulting reaction mixture was allowed to warm to room temperature and stirred for 12 h. Upon completion of the reaction, as confirmed by thin-layer chromatography (TLC), the reaction was quenched by addition of saturated aqueous ammonium chloride solution (5 mL). The aqueous layer was extracted with ethyl acetate (3 × 5 mL), and the combined organic extracts were washed with brine (10 mL), dried over anhydrous $MgSO_4$, and filtered. The filtrate was concentrated in vacuo to afford the crude product, which was subsequently purified by flash column chromatography (silica gel, gradient elution: petroleum ether/EtOAc = 5:1, v/v) to yield compound **9** (39.1 mg, 95%) as a white solid.



3ja **10**

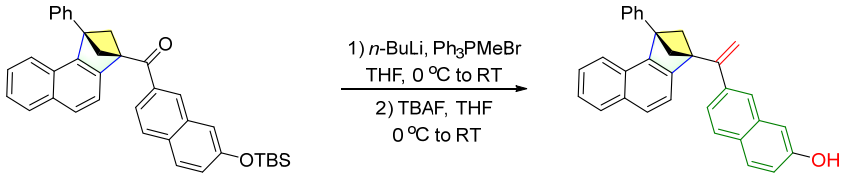
Synthesis of (10): In a flame-dried Schlenk flask under an inert atmosphere, compound **3ja** (41.1 mg, 0.10 mmol, 1.0 equiv) was dissolved in anhydrous THF (2.0 mL) and stirred. The solution was cooled to 0 °C, and then allylmagnesium bromide (0.22 mL, 0.22 mmol, 2.2 equiv) was added dropwise. The reaction mixture was subsequently stirred at room temperature for 12 hours. Upon completion, saturated aqueous ammonium chloride solution (2.0 mL) was added to quench the reaction. The mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic layers were filtered and concentrated under reduced pressure using a rotary evaporator. The crude product was purified by flash chromatography on silica gel using a petroleum ether/ethyl acetate (5:1, v/v) eluent to afford compound **10** (42.5 mg, 94%) as a colorless oil.



3ad **11**

Synthesis of (11): Under an argon atmosphere, compound **3ad** (43.9 mg, 0.10 mmol, 1.0 equiv) was dissolved in DME (0.5 mL) in a reaction vessel. To this solution was added $Pd(PPh_3)_4$ (1.2 mg, 0.001 mmol, 1 mol%). The mixture was stirred for 20 minutes. Subsequently, 3-formylphenylboronic acid (18.0 mg, 0.12 mmol, 1.2 equiv) and ethanol (EtOH, 0.8 mL) were added. After an additional 20 minutes, an aqueous solution of Na_2CO_3 (2 M, 0.2 mL) was introduced. The reaction mixture was then heated to reflux for 12 hours before being cooled to room temperature. The resulting precipitate was filtered off and washed with EtOAc (10 mL). The filtrate was concentrated to dryness. The residue was redissolved in EtOAc (5 mL), washed with water (3 × 5 mL), and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure. The crude product was purified by flash chromatography on silica gel using a petroleum ether/ethyl acetate (50:1, v/v) eluent to afford compound **11** as a colorless oil (37.9 mg, 85% yield).

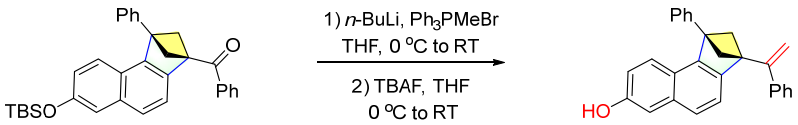
Note: *The deprotection of tert-butyldimethylsilyl ethers in compounds **3ia** and **3aj** via treatment with TBAF yielded corresponding naphthol products, which exhibited limited solubility in CH_2Cl_2. Consequently, the carbonyl groups in compounds **3ia** and **3aj** were converted into olefins to improve the solubility of naphthols **12** and **14**.*



3ia **12**

Synthesis of (12): In a flame-dried Schlenk flask under an inert atmosphere, methyltriphenylphosphonium bromide (314.4 mg, 0.88 mmol, 2.0 equiv) was dissolved

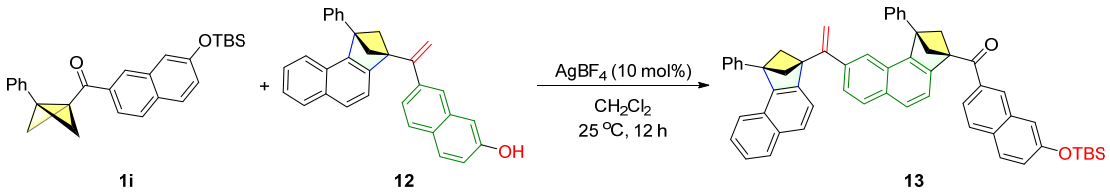
in THF (4.0 mL) and stirred. The solution was cooled to 0 °C, and then *n*-BuLi (2.5 M in hexane, 0.35 mL, 0.88 mmol, 2.0 equiv) was added dropwise. The reaction mixture was stirred at 0 °C for 30 minutes, after which a solution of compound **3ia** (240.0 mg, 0.44 mmol, 1.0 equiv) in anhydrous THF (4.0 mL) was added. The reaction mixture was stirred at room temperature overnight. The reaction was quenched with saturated aqueous NH_4Cl solution (3 mL). The mixture was extracted with ethyl acetate (3 × 5 mL). The combined organic layers were dried over anhydrous $MgSO_4$ and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using a petroleum ether/ethyl acetate (50:1, v/v) eluent to afford the intermediate. The intermediate was dissolved in anhydrous THF (3.0 mL). A solution of TBAF (1 M in THF, 0.88 mL, 0.88 mmol, 2.0 equiv) was added at 0 °C. The reaction mixture was stirred at 0 °C for 1 hour and then at room temperature until the intermediate was fully consumed, as monitored by thin-layer chromatography (TLC). The solvent was removed under reduced pressure, and the residue was diluted with water (4 mL). The aqueous layer was extracted with dichloromethane (3 × 5 mL). The combined organic layers were washed with brine (5 mL), dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using a hexane/ethyl acetate (5:1, v/v) eluent to afford compound **12** as a yellow solid (146.6 mg, 78% yield over two steps).



3aj **14**

Synthesis of (14): In a flame-dried Schlenk flask under an inert atmosphere, methyltriphenylphosphonium bromide (557.3 mg, 1.56 mmol, 2.0 equiv) was dissolved in anhydrous THF (7.0 mL) and stirred. The solution was cooled to 0 °C, and *n*-BuLi (2.5 M in hexane, 0.62 mL, 1.56 mmol, 2.0 equiv) was added dropwise. The reaction mixture was stirred at 0 °C for 30 minutes, after which a solution of compound **3aj** (382.5 mg, 0.78 mmol, 1.0 equiv) in anhydrous THF (5.0 mL) was added. The mixture was stirred at room temperature overnight. The reaction was quenched with saturated

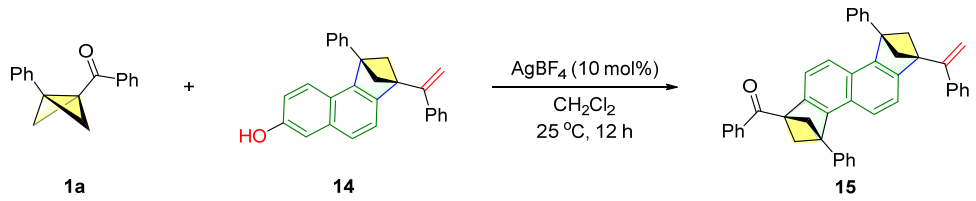
aqueous NH_4Cl solution (5 mL). The mixture was extracted with ethyl acetate (3 × 7 mL). The combined organic layers were dried over anhydrous Na_2SO_4. After evaporation, the residue was purified by flash chromatography on silica gel using a petroleum ether/ethyl acetate (50:1, v/v) solvent system to yield the intermediate. The intermediate was then dissolved in THF (5.0 mL). A solution of TBAF (1.56 mL, 1 M in THF, 1.56 mmol, 2.0 equiv) was added at 0 °C. The resulting mixture was stirred at 0 °C for 1 hour, and then allowed to stir at room temperature until the reaction was complete, as monitored by thin-layer chromatography (TLC). The solvent was removed under reduced pressure, and the residue was diluted with water (4 mL). The aqueous layer was extracted with dichloromethane (3 × 7 mL). The combined organic phases were washed with brine (5 mL), dried over anhydrous $MgSO_4$, filtered, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel using a hexane/ethyl acetate (5:1, v/v) eluent to afford compound **14** as a yellow solid (263.5 mg, 90% yield over two steps).



1i **12** **13**

Into a flame-dried Schlenk tube, (7-((*tert*-butyldimethylsilyl)oxy)naphthalen-2-yl)(3-phenylbicyclo[1.1.0]butan-1-yl)methanone **1i** (54.1 mg, 0.1 mmol, 2.0 equiv), 7-(1-(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)vinyl)naphthalen-2-ol **12** (21.2 mg, 0.05 mmol, 1.0 equiv), and $AgBF_4$ (1.0 mg, 0.005 mmol, 10 mol%) were sequentially added. The tube was subjected to three cycles of evacuation and backfilling with N_2. Subsequently, anhydrous CH_2Cl_2 (4.0 mL) was introduced via syringe. The reaction mixture was maintained at 25 °C with constant stirring for 12 hours. Upon completion, the solvent was evaporated under reduced pressure using a rotary evaporator. The crude product was purified by flash column chromatography on silica gel using a gradient elution of petroleum ether/ethyl acetate (100:1 to 50:1, v/v)

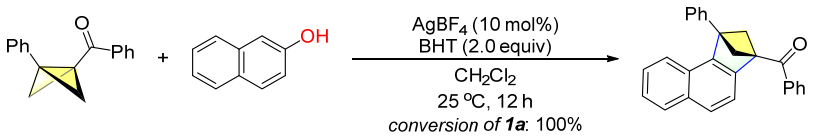
as the mobile phase, yielding the desired product **13** as a pale yellow solid (18.4 mg, 45% yield).



1a **14** **15**

Into a flame-dried Schlenk tube, phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone **1a** (23.4 mg, 0.1 mmol, 2.0 equiv), (7-hydroxy-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)methanone **14** (18.7 mg, 0.05 mmol, 1.0 equiv), and $AgBF_4$ (1.0 mg, 0.005 mmol, 10 mol%) were sequentially added. The tube was subjected to three cycles of evacuation and backfilling with N_2. Subsequently, anhydrous CH_2Cl_2 (4.0 mL) was introduced via syringe. The reaction mixture was maintained at 25 °C with constant stirring for 12 hours. Upon completion, the solvent was evaporated under reduced pressure using a rotary evaporator. The crude product was purified by flash column chromatography on silica gel using a gradient elution of petroleum ether/ethyl acetate (100:1 to 50:1, v/v) as the mobile phase, yielding the desired product **15** as a pale yellow crystalline solid (60% NMR yield of **15** was determined by ^1H NMR with CH_2Br_2 as an internal standard; 12.0 mg, 41% isolated yield due to the low solubility in petroleum ether/ethyl acetate and CH_2Cl_2).

6 Procedure for the Control Experiments



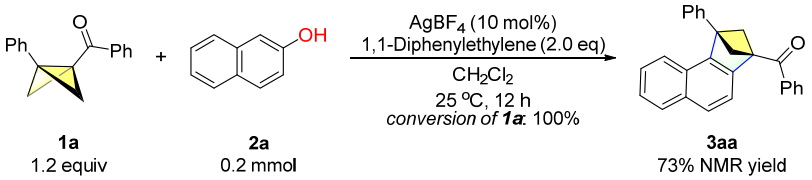
1a
1.2 equiv

2a
0.2 mmol

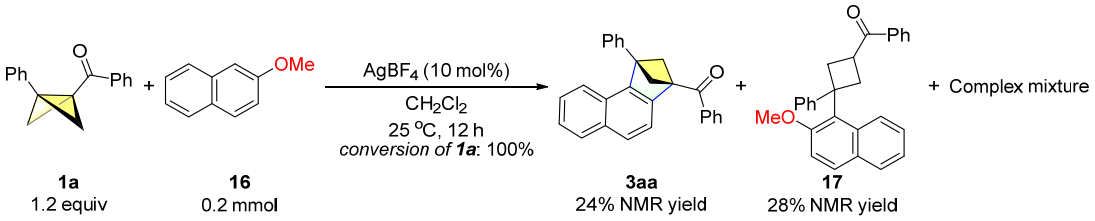
3aa
74% NMR yield

In a flame-dried Schlenk tube, BCB **1a** (56.2 mg, 0.24 mmol, 1.2 equiv), naphthalen-2-ol **2a** (28.8 mg, 0.2 mmol, 1.0 equiv), BHT (88.1 mg, 0.4 mmol, 2.0 equiv), and $AgBF_4$ (3.9 mg, 0.02 mmol, 10.0 mol%) were sequentially added. The tube was then evacuated and backfilled with N_2 (3 times). Subsequently, CH_2Cl_2 (2.0 mL) was introduced into the tube. The reaction mixture was stirred at 12 °C for 12 hours.

Afterward, the solvent was removed under reduced pressure, and the residue was dissolved in $CDCl_3$ (0.5 mL). The conversion of **1a** (100%) and the NMR yield of **3aa** (74%) were determined by ^1H NMR analysis using CH_2Br_2 as the internal standard. Additionally, no corresponding radical trapping products were detected by ^1H NMR and HRMS.



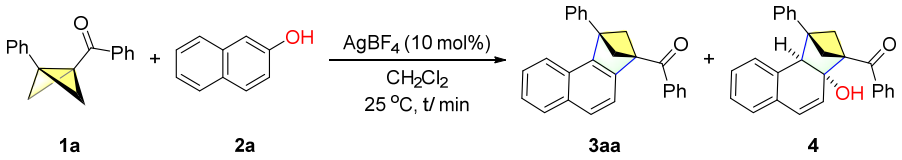
To a flame-dried Schlenk tube was added BCB **1a** (56.2 mg, 0.24 mmol, 1.2 equiv), naphthalen-2-ol **2a** (28.8 mg, 0.2 mmol, 1.0 equiv), and $AgBF_4$ (3.9 mg, 0.02 mmol, 10.0 mol%). The tube was then evacuated and backfilled with N_2 (3 times). Subsequently, 1,1-diphenylethylene (72.1 mg, 0.4 mmol, 2.0 equiv) and CH_2Cl_2 (2.0 mL) were added to the tube. The reaction mixture was stirred at 25 °C for 12 hours. Afterward, the solvent was removed under reduced pressure, and the residue was dissolved in $CDCl_3$ (0.5 mL). The conversion of **1a** (100%) and the NMR yield of **3aa** (73%) were determined by ^1H NMR analysis using CH_2Br_2 as the internal standard. Additionally, no corresponding radical trapping products were detected by ^1H NMR and HRMS.



In a flame-dried Schlenk tube, BCB **1a** (56.2 mg, 0.24 mmol, 1.2 equiv), 2-methoxynaphthalene **16** (31.6 mg, 0.2 mmol, 1.0 equiv), and $AgBF_4$ (3.9 mg, 0.02 mmol, 10.0 mol%) were sequentially added. The tube was then evacuated and backfilled with N_2 (3 times). Subsequently, CH_2Cl_2 (2.0 mL) was introduced into the tube. The reaction mixture was stirred at 12 °C for 12 hours. Afterward, the solvent was removed under reduced pressure, and the residue was dissolved in $CDCl_3$ (0.5

mL). The conversion of **1a** (100%), the NMR yield of **3aa** (24%), and the NMR yield of **17** (28%) were determined by ^{1}H NMR analysis using CH_2Br_2 as the internal standard.

Table S2 Monitoring the reaction process



1a **2a** **3aa** **4**

Entry	t/min	Conversion of **1a** (%)[b]	Yield of **3aa** (%)[b]	Yield of **4** (%)[b]
1	1	11	0	9
2	5	42	0	34
3	15	100	42	32
4	45	100	63	12
5	60	100	66	9
6	120	100	69	8
7	720	100	74	0

[a]Reaction conditions: **1a** (0.12 mmol, 1.2 equiv), **2a** (0.10 mmol, 1.0 equiv) and $AgBF_4$ (10 mol%), CH_2Cl_2 (2 mL), 25 °C, under N_2 for t min. [b]Determined by ^{1}H NMR spectroscopy with CH_2Br_2 as an internal standard.

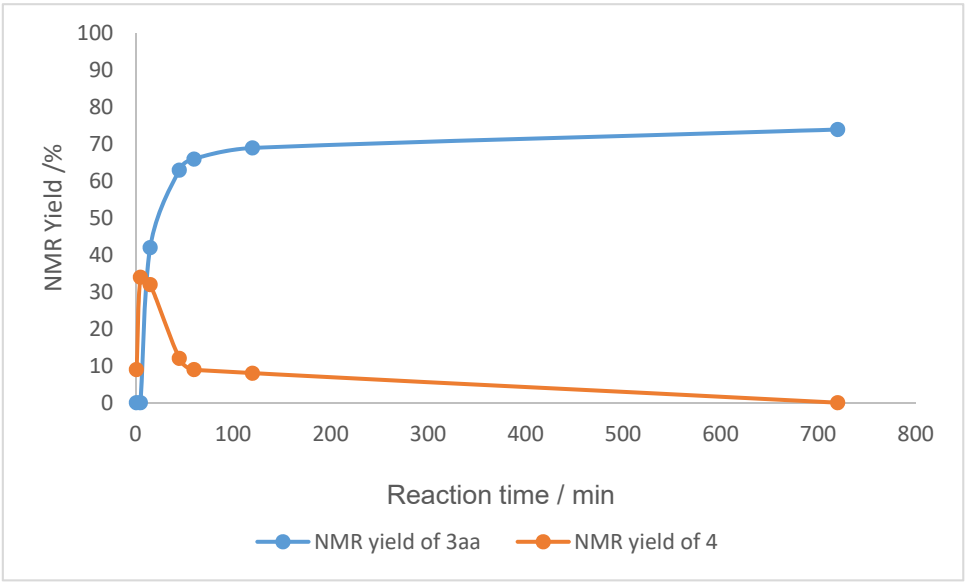
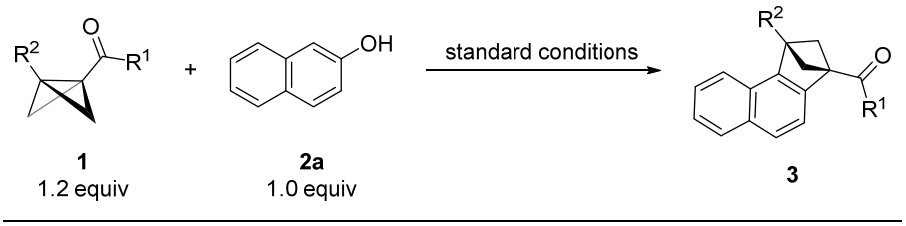


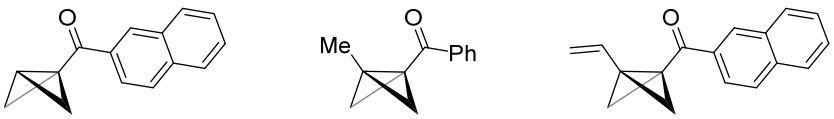
Figure S1 The kinetics of the cyclization behavior of BCB

7 Unsuccessful Substrates

Schemes S1 and S2 present the BCBs and hydroxyarene substrates that failed in the preliminary tests. The reactions were conducted in accordance with the General Procedure (GP) and examined using crude ^{1}H NMR, with CH_2Br_2 as the internal standard.

Scheme S1 Unsuccessful BCBs





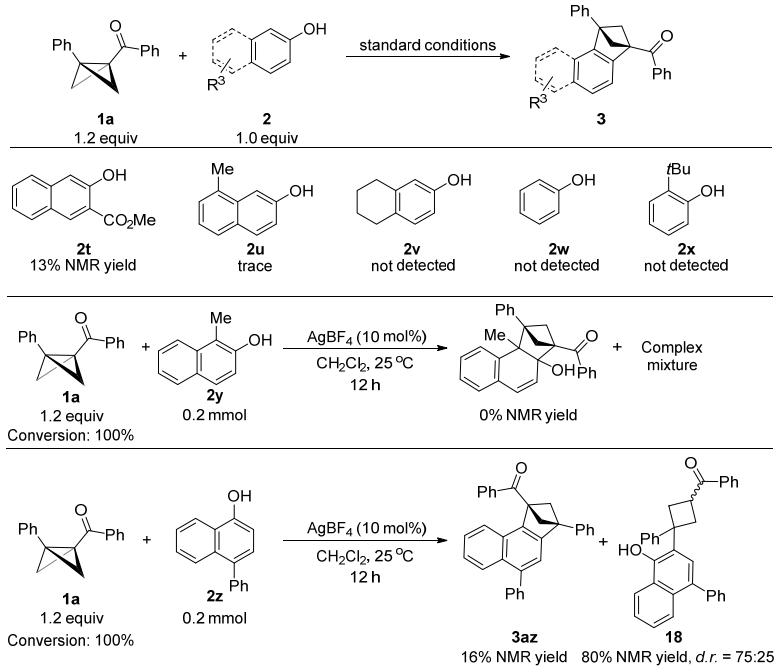
1s Conversion: 100%

1t Conversion: 100%

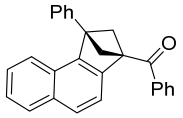
1u Conversion: 100%

The monosubstituted BCB ketone (**1s**), as well as the alkyl (**1t**) and vinyl (**1u**) BCB ketones, were investigated under standard conditions. However, these BCB substrates decomposed rapidly, yielding various unidentified byproducts.

Scheme S2 Unsuccessful hydroxyarenes



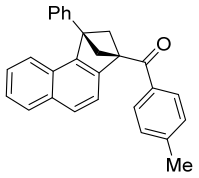
8 Characterization Data



3aa
$C_{27}H_{20}O$
M = 360.46 g/mol

phenyl-(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)methanone (**3aa**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3aa** as a white solid (50.4 mg, 70% yield).

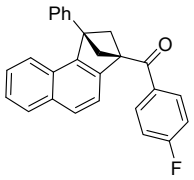
3aa: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.52-7.40 (m, 8H), 7.23-7.17 (m, 2H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 3.82 (s, 2H), 3.34 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.0, 150.0, 147.8, 141.2, 135.8, 133.4, 132.4, 129.5, 129.0, 128.8, 128.6, 127.6, 127.3, 126.7, 125.7, 125.1, 124.2, 122.5, 118.4, 72.5, 59.6, 55.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{21}O$: 361.1587; found: 361.1584.



3ba
$C_{28}H_{22}O$
M = 374.48 g/mol

(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(*p*-tolyl)-methanone (**3ba**): Prepared from (3-phenylbicyclo[1.1.0]butan-1-yl)(*p*-tolyl)methanone (**1b**, 59.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ba** as a yellow solid (38.4 mg, 51% yield).

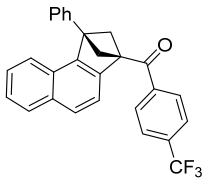
3ba: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.51-7.39 (m, 6H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.23-7.18 (m, 2H), 7.06 (d, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 8.8 Hz, 1H), 3.81 (s, 2H), 3.33 (s, 2H), 2.43 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.5, 150.2, 147.9, 144.4, 141.2, 133.3, 132.4, 129.7, 129.3, 129.0, 128.8, 127.6, 127.3, 126.7, 125.7, 125.0, 124.1, 122.6, 118.4, 72.5, 59.6, 55.4, 21.7 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1740.



3ca
$C_{27}H_{19}FO$
M = 378.45 g/mol

(4-fluorophenyl)(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)-methanone (**3ca**): Prepared from (4-fluorophenyl)(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1c**, 60.5 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ca** as a yellow solid (45.9 mg, 61% yield).

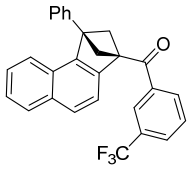
3ca: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.14-8.11 (m, 2H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.53-7.43 (m, 6H), 7.25-7.21 (m, 1H), 7.17-7.13 (m, 3H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 8.8 Hz, 1H), 3.80 (s, 2H), 3.34 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 197.3, 165.9 (d, *J* = 254.2 Hz), 149.7, 147.8, 141.0, 132.4, 132.2 (d, *J* = 9.3 Hz), 129.0, 128.8, 127.7, 127.3, 126.7, 125.8, 125.2, 124.3, 122.5, 118.2, 115.8 (d, *J* = 21.8 Hz), 72.4, 59.5, 55.5 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ –104.08 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{20}FO$: 379.1493; found: 379.1486.



3da
$C_{28}H_{19}F_3O$
M = 428.45 g/mol

(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(4-(trifluoromethyl)-phenyl)methanone (**3da**): Prepared from (3-phenylbicyclo[1.1.0]butan-1-yl)(4-(trifluoromethyl)phenyl)methanone (**1d**, 72.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3da** as a white solid (71.9 mg, 83% yield).

3da: $\mathbf{R_f}$ = 0.40(petroleum ether/EtOAc = 50/1).**^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.20 (d, *J* = 8.0 Hz, 2H), 7.77-7.73 (m, 3H), 7.53-7.43 (m, 6H), 7.24-7.21 (m, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 3.82 (s, 2H), 3.35 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.1, 149.4, 147.8, 140.8, 138.3, 134.6 (q, *J* = 32.4 Hz), 132.5, 129.8, 129.0, 128.9, 127.7, 127.4, 126.7, 125.9, 125.7 (q, *J* = 37.0 Hz), 125.3, 124.4, 123.5 (q, *J* = 271.2 Hz), 122.5, 118.0, 72.4, 59.6, 55.6 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -63.09 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{20}F_3O$: 429.1461; found: 429.1451.

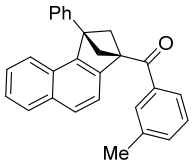


3ea
$C_{28}H_{19}F_3O$
M = 428.45 g/mol

(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(3-(trifluoromethyl)-phenyl)methanone (**3ea**): Prepared from (3-phenylbicyclo[1.1.0]butan-1-yl)(3-(trifluoromethyl)phenyl)methanone (**1e**, 36.3 mg, 0.12 mmol) and naphthalen-2-ol (**2a**, 14.4 mg, 0.1 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash

chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ea** as a white solid (34.3 mg, 80% yield).

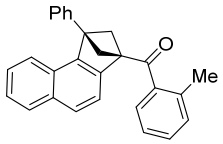
3ea: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.37 (s, 1H), 8.25 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 8.0 Hz, 1H), 7.54-7.42 (m, 6H), 7.25-7.22 (m, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.08 (t, *J* = 7.2 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 3.83 (s, 2H), 3.36 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 197.7, 149.4, 147.8, 140.9, 136.3, 132.7, 132.5, 131.5 (q, *J* = 32.6 Hz), 129.8 (q, *J* = 3.5 Hz), 129.3, 129.1, 128.9, 127.7, 127.4, 126.7, 126.1 (q, *J* = 3.8 Hz), 125.9, 125.5 (q, *J* = 273.0 Hz), 125.4, 124.4, 122.6, 118.0, 72.4, 59.5, 55.6 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ –62.85 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{20}F_3O$: 429.1461; found: 429.1461.



3fa
$C_{28}H_{22}O$
M = 374.48 g/mol

(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(*m*-tolyl)methanone (**3fa**): Prepared from (3-phenylbicyclo[1.1.0]butan-1-yl)(*m*-tolyl)methanone (**1f**, 59.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3fa** as a white solid (45.3 mg, 60% yield).

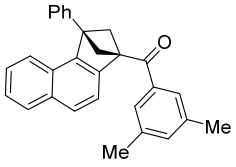
3fa: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.90 (s, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.51-7.45 (m, 5H), 7.41 (d, *J* = 6.8 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.23-7.18 (m, 2H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 8.4 Hz, 1H), 3.81 (s, 2H), 3.33 (s, 2H), 2.40 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.2, 150.2, 147.8, 141.2, 138.5, 135.9, 134.2, 132.4, 129.7, 129.0, 128.8, 128.4, 127.6, 127.3, 126.9, 126.7, 125.7, 125.1, 124.1, 122.6, 118.4, 72.5, 59.7, 55.4, 21.4 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1736.



3ga
$C_{28}H_{22}O$
M = 374.48 g/mol

(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(*o*-tolyl)methanone (**3ga**): Prepared from (3-phenylbicyclo[1.1.0]butan-1-yl)(*o*-tolyl)methanone (**1g**, 59.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ga** as a white solid (41.5 mg, 55% yield).

3ga: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.77-7.74 (m, 2H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.48-7.40 (m, 6H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.24-7.18 (m, 3H), 7.04 (dd, *J* = 8.4, 6.8 Hz, 1H), 6.83 (d, *J* = 8.8 Hz, 1H), 3.76 (s, 2H), 3.31 (s, 2H), 2.63 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 202.4, 149.8, 147.8, 141.2, 139.0, 136.2, 132.4, 132.3, 131.7, 130.0, 129.0, 128.8, 127.6, 127.3, 126.7, 125.6, 125.5, 125.1, 124.1, 122.5, 118.3, 72.3, 60.4, 55.2, 21.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1739.

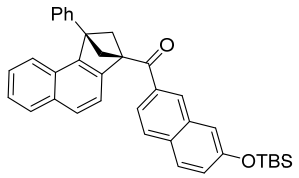


3ha
$C_{29}H_{24}O$
M = 388.51 g/mol

(3,5-dimethylphenyl)(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)-methanone (**3ha**): Prepared from (3,5-dimethylphenyl)(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1h**, 63.0 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ha** as a white solid (42.8 mg, 55% yield).

3ha: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 8.4 Hz, 1H), 7.68 (s, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.48-7.45 (m, 4H), 7.44-7.39 (m,

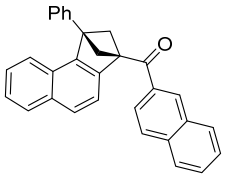
1H), 7.24-7.19 (m, 3H), 7.06 (t, *J* = 8.4 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 3.81 (s, 2H), 3.32 (s, 2H), 2.35 (s, 6H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.4, 150.3, 147.8, 141.3, 138.3, 136.0, 135.1, 132.4, 129.0, 128.8, 127.6, 127.25, 127.21, 126.7, 125.6, 125.1, 124.1, 122.6, 118.4, 72.6, 59.7, 55.4, 21.3 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{29}H_{25}O$: 389.1900; found: 389.1989.



3ia
$C_{37}H_{36}O_2Si$
M = 540.78 g/mol

(7-((*tert*-butyldimethylsilyl)oxy)naphthalen-2-yl)(1-phenyl-1,2-dihydro-3*H*-1,3-methano-cyclopenta[*a*]naphthalen-3-yl)methanone (**3ia**): Prepared from ((7-((*tert*-butyldimethylsilyl)oxy)naphthalen-2-yl)(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1i**, 99.5 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ia** as a white solid (59.7 mg, 55% yield).

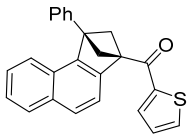
3ia: $\mathbf{R_f}$ = 0.25 (petroleum ether/EtOAc = 50/1) **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.43 (s, 1H), 8.01 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.78-7.75 (m, 2H), 7.51-7.46 (m, 5H), 7.44-7.40 (m, 1H), 7.24-7.19 (m, 4H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 1H), 3.90 (s, 2H), 3.39 (s, 2H), 1.01 (s, 9H), 0.24 (s, 6H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.0, 154.2, 150.3, 147.8, 141.2, 133.8, 133.4, 132.4, 131.5, 130.3, 129.2, 129.0, 128.8, 128.2, 127.7, 127.3, 126.8, 125.7, 125.2, 124.9, 124.1, 122.8, 122.6, 118.5, 116.6, 72.6, 59.8, 55.5, 25.6, 18.2, -4.4 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{37}H_{37}O_2Si$: 541.2557; found: 541.2550.



3ja
$C_{31}H_{22}O$
M = 410.52 g/mol

naphthalen-2-yl(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)-methanone (**3ja**): Prepared from naphthalen-2-yl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1j**, 68.2 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ja** as a white solid (53.1 mg, 65% yield).

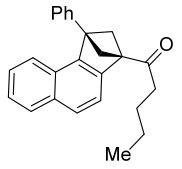
3ja: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1).**^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.17 (d, *J* = 8.8 Hz, 1H), 7.94-7.86 (m, 3H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.54-7.48 (m, 6H), 7.45-7.40 (m, 1H), 7.24-7.20 (m, 2H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 8.8 Hz, 1H), 3.91 (s, 2H), 3.40 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.9, 150.2, 147.9, 141.2, 135.7, 133.1, 132.45, 132.43, 131.7, 129.7, 129.0, 128.8, 128.7, 128.5, 127.8, 127.7, 127.3, 126.80, 126.75, 125.7, 125.2, 124.7, 124.2, 122.6, 118.4, 72.6, 59.7, 55.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{31}H_{23}O$ 411.1743; found: 411.1735.



3ka
$C_{25}H_{18}OS$
M = 366.48 g/mol

(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(thiophen-2-yl)methanone (**3ka**): Prepared from (3-phenylbicyclo[1.1.0]butan-1-yl)(thiophen-2-yl)methanone (**1k**, 57.7 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ka** as a white solid (41.0 mg, 56% yield).

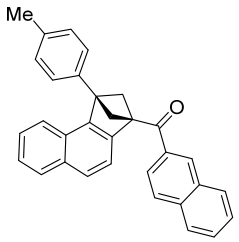
3ka: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.77-7.74 (m, 2H), 7.71-7.70 (m, 1H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.50-7.40 (m, 5H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.14-7.12 (m, 1H), 7.06 (t, *J* = 8.0 Hz, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 3.77 (s, 2H), 3.34 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 191.5, 149.9, 147.7, 142.8, 141.0, 134.2, 133.9, 132.4, 129.0, 128.8, 128.2, 127.6, 127.3, 126.7, 125.7, 125.1, 124.2, 122.5, 118.1, 72.2, 59.2, 55.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{25}H_{19}OS$: 367.1151; found: 367.1143.



3la
$C_{25}H_{24}O$
M = 340.47 g/mol

1-(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)pentan-1-one (**3la**): Prepared from 1-(3-phenylbicyclo[1.1.0]butan-1-yl)pentan-1-one (**1l**, 51.4 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3la** as a colorless oil (42.0 mg, 62% yield).

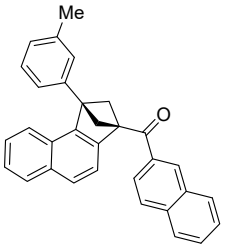
3la: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.51-7.44 (m, 3H), 7.42-7.38 (m, 3H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 7.6 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 3.55 (s, 2H), 3.18 (s, 2H), 2.72 (t, *J* = 7.6 Hz, 2H), 1.76-1.68 (m, 2H), 1.46-1.37 (m, 2H), 0.96 (t, *J* = 7.6 Hz, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 209.5, 148.8, 147.8, 141.2, 132.4, 129.0, 128.8, 127.6, 127.3, 126.6, 125.5, 125.1, 124.0, 122.4, 117.7, 70.7, 59.5, 55.4, 39.9, 25.4, 22.5, 13.9 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{25}H_{25}O$: 341.1900; found: 341.1892.



3ma
$C_{32}H_{24}O$
M = 424.54 g/mol

naphthalen-2-yl(1-(*p*-tolyl)-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)-methanone (**3ma**): Prepared from naphthalen-2-yl(3-(*p*-tolyl)bicyclo[1.1.0]butan-1-yl)methanone (**1m**, 71.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ma** as a yellow solid (54.5 mg, 64% yield).

3ma: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.93-7.85 (m, 3H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.53-7.47 (m, 2H), 7.37 (d, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.6 Hz, 2H), 7.22-7.19 (m, 2H), 7.10 (t, *J* = 8.0 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 1H), 3.88 (s, 2H), 3.37 (s, 2H), 2.46 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.9, 150.2, 147.9, 138.1, 136.9, 135.7, 133.2, 132.44, 132.42, 131.7, 129.7, 129.5, 129.0, 128.7, 128.5, 127.8, 127.7, 126.8, 126.6, 125.7, 125.1, 124.7, 124.1, 122.7, 118.4, 72.7, 59.8, 55.3, 21.3 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{32}H_{25}O$: 425.1900; found: 425.1893.

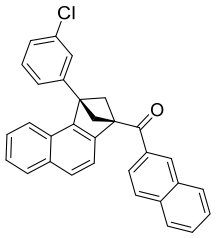


3na
$C_{32}H_{24}O$
M = 424.54 g/mol

naphthalen-2-yl(1-(*m*-tolyl)-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)-methanone (**3na**): Prepared from naphthalen-2-yl(3-(*m*-tolyl)bicyclo[1.1.0]butan-1-yl)methanone (**1n**, 71.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica

gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3na** as a white solid (55.7 mg, 66% yield).

3na: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.58 (s, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 7.93-7.85 (m, 3H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.54-7.48 (m, 2H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 9.6 Hz, 2H), 7.25-7.19 (m, 3H), 7.09 (t, *J* = 8.0 Hz, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 3.90 (s, 2H), 3.39 (s, 2H), 2.43 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.9, 150.2, 147.9, 141.1, 138.4, 135.7, 133.1, 132.43, 132.40, 131.7, 129.7, 129.0, 128.72, 128.71, 128.5, 128.0, 127.8, 127.7, 127.4, 126.8, 125.7, 125.1, 124.7, 124.1, 123.8, 122.7, 118.4, 72.7, 59.7, 55.5, 21.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{32}H_{25}O$: 425.1900; found: 425.1894.

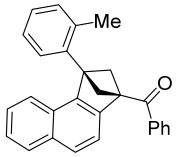


3oa
$C_{31}H_{21}ClO$
M = 444.96 g/mol

(1-(3-chlorophenyl)-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(naphthalen-2-yl)-methanone (**3oa**): Prepared from (3-(3-chlorophenyl)bicyclo[1.1.0]butan-1-yl)(naphthalen-2-yl)methanone (**1o**, 71.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3oa** as a white solid (64.9 mg, 73% yield).

3oa: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): 8.57 (s, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.53-7.48 (m, 3H), 7.43-7.39 (m, 2H), 7.38-7.34 (m, 1H), 7.26-7.23 (m, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 7.13 (t, *J* = 7.8 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 1H), 3.88 (s, 2H), 3.38 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.5, 150.0, 147.2, 143.3, 135.7, 134.8, 133.0, 132.4, 131.7, 130.1, 129.7, 129.1, 128.8, 128.6, 127.8, 127.55, 127.51, 127.0, 126.8, 126.0, 125.4,

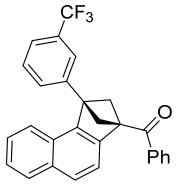
125.0, 124.6, 124.3, 122.3, 118.4, 72.6, 59.6, 55.0 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{31}H_{22}ClO$: 445.1354; found: 445.1351.



3pa
$C_{28}H_{22}O$
M = 374.48 g/mol

phenyl(1-(*o*-tolyl)-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)methanone (**3pa**): Prepared from phenyl(3-(*o*-tolyl)bicyclo[1.1.0]butan-1-yl)methanone (**1p**, 59.6 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3pa** as a white solid (56.7 mg, 76% yield).

3pa: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 8.0 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.52-7.45 (m, 3H), 7.35-7.27 (m, 4H), 7.23-7.18 (m, 2H), 7.07 (t, *J* = 8.0 Hz, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 4.02-3.98 (m, 1H), 3.88-3.84 (m, 1H), 3.39 (d, *J* = 5.2 Hz, 1H), 3.34 (d, *J* = 5.6 Hz, 1H), 2.34 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.1, 150.4, 146.9, 139.1, 137.3, 135.8, 133.4, 132.2, 130.9, 129.5, 128.9, 128.6, 128.1, 127.7, 127.4, 126.4, 126.1, 125.1, 124.2, 121.7, 118.5, 73.7, 72.6, 59.4, 56.1, 21.1 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1740.

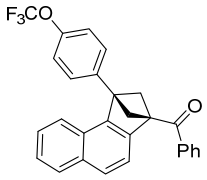


3qa
$C_{28}H_{19}F_3O$
M = 428.45 g/mol

phenyl(1-(3-(trifluoromethyl)phenyl)-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)-methanone (**3qa**): Prepared from phenyl-(3-(3-(trifluoromethyl)phenyl)-bicyclo[1.1.0]butan-1-yl)methanone (**1q**, 34.3 mg, 0.12 mmol) and naphthalen-2-ol (**2a**, 14.4 mg, 0.1 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash

chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3qa** as a white solid (26.2 mg, 61% yield).

3qa: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.08 (d, *J* = 7.8 Hz, 2H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.72-7.69 (m, 2H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.63-7.61 (m, 2H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.50-7.47 (m, 2H), 7.25-7.23 (m, 1H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.09 (t, *J* = 7.8 Hz, 1H), 6.76 (d, *J* = 9.0 Hz, 1H), 3.86 (s, 2H), 3.37 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.5, 149.9, 147.0, 142.3, 135.7, 133.6, 132.4, 131.3 (q, *J* = 32.0 Hz), 130.3, 129.5, 129.4, 129.2, 128.7, 127.5, 126.0, 125.5, 124.3, 124.2 (q, *J* = 3.8 Hz), 124.1 (q, *J* = 270.7 Hz),123.6 (q, *J* = 3.7 Hz), 122.1, 118.5, 72.4, 59.6, 55.1 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -62.58 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{20}F_3O$: 429.1461; found: 429.1454.

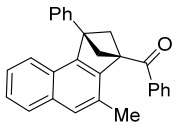


3ra
$C_{28}H_{19}F_3O_2$
M = 444.45 g/mol

phenyl-(1-(4-(trifluoromethoxy)phenyl)-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]-naphthalen-3-yl)methanone (**3ra**): Prepared from phenyl-(3-(4-(trifluoromethoxy)phenyl)-bicyclo[1.1.0]butan-1-yl)methanone (**1r**, 76.4 mg, 0.24 mmol) and naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ra** as a yellow solid (63.9 mg, 72% yield).

3ra: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.08 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.53-7.45 (m, 5H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 8.8 Hz, 1H), 3.80 (s, 2H), 3.33 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.6, 149.9, 148.4, 147.2, 140.0, 135.7, 133.5, 132.4, 129.5, 129.1, 128.6, 128.2, 127.5, 125.9, 125.3, 124.3, 122.2, 121.3, 120.5 (q, *J* = 255.8 Hz), 118.4,

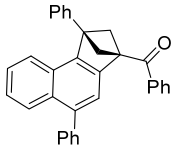
72.4, 59.5, 54.8 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ –57.70 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{20}F_3O_2$: 445.1410; found: 445.1402.



3ab
$C_{28}H_{22}O$
M = 374.48 g/mol

(4-methyl-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3ab**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 3-methylnaphthalen-2-ol (**2b**, 61.6 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ab** as a white solid (47.3 mg, 63% yield).

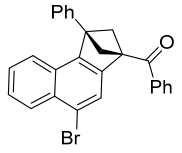
3ab: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 7.6 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.50-7.41 (m, 7H), 7.33 (s, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.77 (d, *J* = 8.8 Hz, 1H), 3.84 (s, 2H), 3.23 (s, 2H), 2.14 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 200.7, 149.3, 148.0, 141.3, 136.3, 133.3, 132.8, 129.2, 128.8, 128.6, 128.3, 128.2 127.2, 126.7, 126.4, 126.2, 124.8, 124.3, 122.4, 72.4, 59.3, 54.9, 19.7 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1737.



3ac
$C_{33}H_{24}O$
M = 436.55 g/mol

(1,5-diphenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)methanone (**3ac**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 4-phenylnaphthalen-2-ol (**2c**, 44.1 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ac** as a white solid (61.6 mg, 71% yield).

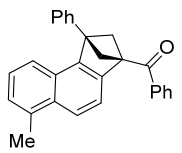
3ac: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.6 Hz, 2H), 7.82 (d, *J* = 8.8 Hz, 1H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.50-7.42 (m, 7H), 7.40-7.32 (m, 5H), 7.18-7.13 (m, 2H), 7.08-7.04 (m, 1H), 6.95 (d, *J* = 8.4 Hz, 1H), 3.89 (s, 2H), 3.37 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.9, 149.6, 147.2, 141.2, 141.1, 137.6, 135.7 133.5, 130.2, 129.5, 128.9, 128.6, 128.1, 127.9, 127.3, 127.1, 127.0, 126.7, 125.5, 124.3, 122.8, 119.6, 72.3, 59.6, 55.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{25}O$: 437.1900; found: 437.1895.



3ad
$C_{27}H_{19}BrO$
M = 439.35 g/mol

(5-bromo-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3ad**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 4-bromonaphthalen-2-ol (**2d**, 44.6 mg, 0.2 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ad** as a yellow solid (55.0 mg, 63% yield).

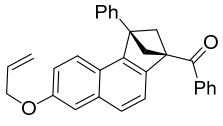
3ad: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.17 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 7.6 Hz, 2H), 7.63 (t, *J* = 7.2 Hz, 1H), 7.52-7.46 (m, 5H), 7.44-7.40 (m, 3H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.09 (t, *J* =8.0 Hz, 1H), 6.87 (d, *J* = 8.4 Hz, 1H), 3.81 (s, 2H), 3.33 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.1, 150.5, 147.9, 140.6, 135.5, 133.7, 130.3, 129.4, 129.0, 128.9, 128.8, 128.0, 127.5, 126.7, 126.4, 125.8, 123.1, 122.7, 118.7, 72.3, 59.5, 55.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{20}BrO$: 439.0692; found: 439.0684.



3ae
$C_{28}H_{22}O$
M = 374.48 g/mol

(6-methyl-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3ae**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 5-methylnaphthalen-2-ol (**2e**, 31.6 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ae** as a white solid (52.4 mg, 70% yield).

3ae: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.6 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.49-7.40 (m, 7H), 7.22 (d, *J* = 8.4 Hz, 1H), 7.07 (d, *J* = 6.8 Hz, 1H), 6.96 (t, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 8.4 Hz, 1H), 3.81 (s, 2H), 3.34 (s, 2H), 2.61 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.0, 149.7, 148.3, 141.3, 135.8, 135.0, 133.4, 131.6, 129.5, 128.8, 128.6, 127.7, 127.2, 126.7, 125.4, 125.0, 121.14, 121.06, 118.0, 72.3, 59.5, 55.6, 20.2 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1735.

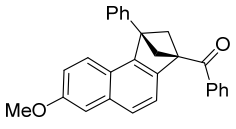


3af
$C_{30}H_{24}O_2$
M = 416.52 g/mol

(7-(allyloxy)-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3af**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 6-(allyloxy)naphthalen-2-ol (**2f**, 40.0 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3af** as a white solid (47.3 mg, 57% yield).

3af: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 8.0 Hz, 2H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.48-7.39 (m, 7H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 7.05 (s, 1H), 6.81-6.74 (m, 2H), 6.10-6.00 (m, 1H), 5.40 (d, *J* = 17.2 Hz, 1H), 5.26 (d, *J* = 10.4 Hz, 2H), 4.56 (d, *J* = 4.8 Hz, 2H), 3.78 (s, 2H), 3.31 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.1, 155.0, 148.1, 147.7, 141.2, 135.8, 133.5, 133.4, 133.2, 129.5, 128.8, 128.6, 127.3, 126.7, 124.1, 123.6, 123.4, 119.5,

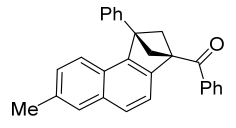
118.8, 117.6, 107.6, 72.1, 68.6, 59.5, 55.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{30}H_{25}O_2$: 417.1849; found: 417.1843.



3ag
$C_{28}H_{22}O_2$
M = 390.48 g/mol

(7-methoxy-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3ag**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 6-methoxynaphthalen-2-ol (**2g**, 34.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 30/1) afforded **3ag** as a white solid (43.6 mg, 56% yield).

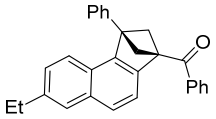
3ag: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 20/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 7.6 Hz, 2H), 7.60 (t, *J* = 7.2Hz, 1H), 7.49-7.41 (m, 7H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 7.04 (s, 1H), 6.75 (s, 2H), 3.83 (s, 3H), 3.78 (s, 2H), 3.32(s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.1, 156.1, 148.1, 147.6, 141.2, 135.8, 133.6, 133.4, 129.5, 128.8, 128.6, 127.3, 126.7, 124.1, 123.5, 123.3, 119.3, 118.8, 106.2, 72.1, 59.5, 55.5, 55.1 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O_2$: 391.1693; found: 391.1686.



3ah
$C_{28}H_{22}O$
M = 374.48 g/mol

(7-methyl-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3ah**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 6-methylnaphthalen-2-ol (**2h**, 31.6 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ah** as a white solid (48.2 mg, 64% yield).

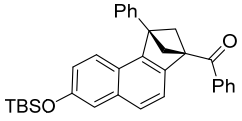
3ah: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.51 (s, 1H), 7.48-7.39 (m, 8H), 7.14 (d, *J* = 8.0 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 1H), 6.74 (d, *J* = 8.8 Hz, 1H), 3.79 (s, 2H), 3.32 (s, 2H), 2.36 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.0, 149.0, 147.7, 141.2, 135.8, 133.6, 133.4, 132.7, 129.5, 128.8, 128.6, 128.2, 127.6, 127.2, 126.7, 125.9, 124.2, 122.3, 118.4, 72.3, 59.6, 55.4, 21.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1736.



3ai
$C_{29}H_{24}O$
M = 388.51 g/mol

(7-ethyl-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3ai**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 6-ethylnaphthalen-2-ol (**2i**, 34.4 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ai** as a white solid (52.8 mg, 68% yield).

3ai: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.2 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.54 (s, 1H), 7.48-7.41 (m, 8H), 7.15 (d, *J* = 7.2 Hz, 1H), 6.96 (d, *J* = 9.0 Hz, 1H), 6.78 (d, *J* = 9.0 Hz, 1H), 3.80 (s, 2H), 3.33 (s, 2H), 2.67 (q, *J* = 7.2 Hz, 2H), 1.22 (t, *J* = 7.2 Hz, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.1, 149.1, 147.8, 141.3, 140.0, 135.8, 133.4, 132.7, 129.5, 128.8, 128.6, 127.23, 127.18, 126.7, 126.4, 126.1, 124.4, 122.4, 118.4, 72.3, 59.6, 55.4, 28.9, 15.4 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{29}H_{25}O$: 389.1900; found: 389.1892.

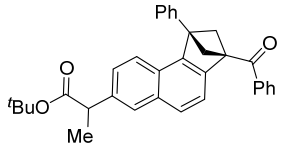


3aj
$C_{33}H_{34}O_2Si$
M = 490.72 g/mol

(7-((*tert*-butyldimethylsilyl)oxy)-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)methanone (**3aj**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-

yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 6-((*tert*-butyldimethylsilyl)oxy)naphthalen-2-ol (**2j**, 54.9 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3aj** as a pale yellow solid (54.2 mg, 55% yield).

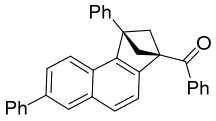
3aj: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.8 Hz, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.49-7.45 (m, 6H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.12-7.10 (m, 2H), 6.74-6.69 (m, 2H), 3.79 (s, 2H), 3.32 (s, 2H), 0.97 (s, 9H), 0.18 (s, 6H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 199.1, 151.9, 148.0, 147.7, 141.2, 135.8, 133.8, 133.4, 129.5, 128.8, 128.6, 127.2, 126.7, 124.0, 123.8, 123.3, 122.5, 118.7, 115.4, 72.1, 59.5, 55.5, 25.7, 18.2, -4.4 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{35}O_2Si$: 491.2401; found: 491.2396.



3ak
$C_{34}H_{32}O_3$
M = 488.63 g/mol

***tert*-butyl-2-(3-benzoyl-1-phenyl-2,3-dihydro-1*H*-1,3-methanocyclopenta[*a*]naphthalen-7-yl)-propanoate** (**3ak**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 28.1 mg, 0.12 mmol) and *tert*-butyl-2-(6-hydroxynaphthalen-2-yl)propanoate (**2k**, 27.2 mg, 0.1 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ak** as a yellow solid (19.5 mg, 40% yield).

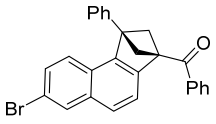
3ak: $\mathbf{R_f}$ = 0.25 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.08 (d, *J* = 7.2 Hz, 2H), 7.63-7.59 (m, 2H), 7.49-7.40 (m, 8H), 7.17 (d, *J* = 8.0 Hz, 1H), 7.05 (d, *J* = 9.2 Hz, 1H), 6.81 (d, *J* = 8.8 Hz, 1H), 3.80 (s, 2H), 3.63 (q, *J* = 7.2 Hz, 1H), 3.34 (s, 2H), 1.43 (d, *J* = 7.2 Hz, 3H), 1.37 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.0, 173.7, 149.8, 147.8, 141.1, 136.9, 135.8, 133.5, 132.5, 129.5, 128.8, 128.6, 127.3, 126.9, 126.72, 126.67, 125.9, 124.9, 122.8, 118.5, 80.5, 72.4, 59.6, 55.5, 46.4, 28.0, 18.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{34}H_{33}O_3$: 489.2424; found: 489.2416.



3al
$C_{33}H_{24}O$
M = 436.55 g/mol

(1,7-diphenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)methanone (**3al**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 6-phenylnaphthalen-2-ol (**2l**, 44.1 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3al** as a white solid (52.9 mg, 61% yield).

3al: R_f = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): 8.10 (d, *J* = 8.4 Hz, 2H), 7.96 (s, 1H), 7.62-7.56 (m, 4H), 7.52-7.39 (m, 9H), 7.37-7.30 (m, 2H), 7.23-7.20 (m, 1H), 6.92 (d, *J* = 8.8 Hz, 1H), 3.83 (s, 2H), 3.35 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.9, 150.1, 147.9, 141.1, 140.9, 136.7, 135.8, 133.5, 132.7, 129.5, 128.9, 128.7, 128.6, 127.4, 127.2, 127.1, 126.73, 126.71, 125.6, 125.5, 123.0, 118.8, 72.3, 59.7, 55.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{25}O$: 437.1900; found: 437.1895.

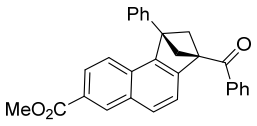


3am
$C_{27}H_{19}BrO$
M = 439.35 g/mol

(7-bromo-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3am**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 28.1 mg, 0.12 mmol) and 6-bromonaphthalen-2-ol (**2m**, 22.3 mg, 0.1 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3am** as a yellow solid (19.7 mg, 45% yield).

3am: **R_f** = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.07 (d, *J* = 8.0 Hz, 2H), 7.90 (s, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.50-7.46 (m, 4H), 7.44-7.39 (m, 4H), 7.19 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 9.2 Hz, 1H), 6.69 (d, *J* = 9.2 Hz, 1H), 3.81 (s,

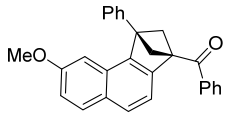
2H), 3.34 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.6, 150.5, 148.4, 140.7, 135.7, 133.54, 133.49, 130.8, 129.5, 129.1, 128.9, 128.7, 127.5, 126.6, 126.0, 124.3, 124.2, 119.3, 118.1, 72.4, 59.6, 55.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{20}BrO$: 439.0692; found: 439.0685.



3an
$C_{29}H_{22}O_3$
M = 418.49 g/mol

methyl-3-benzoyl-1-phenyl-2,3-dihydro-1*H*-1,3-methanocyclopenta[*a*]naphthalene-7-carboxylate (**3an**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and methyl-6-hydroxy-2-naphthoate (**2n**, 40.4 mg, 0.2 mmol) according to the **GP** at 40 °C for 24 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3an** as a white solid (33.3 mg, 40% yield).

3an: $\mathbf{R_f}$ = 0.20 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.52 (s, 1H), 8.07 (d, *J* = 8.0 Hz, 2H), 7.65-7.60 (m, 3H), 7.51-7.43 (m, 7H), 7.26 (s, 1H), 6.86 (d, *J* = 8.8 Hz, 1H), 3.91 (s, 3H), 3.84 (s, 2H), 3.37 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.5, 167.1, 152.8, 148.0, 140.6, 135.7, 133.6, 132.4, 131.4, 129.5, 129.3, 128.9, 128.7, 127.5, 127.2, 126.7, 125.6, 124.9, 122.7, 119.1, 72.4, 59.8, 55.5, 52.1 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{29}H_{23}O_3$: 419.1642; found: 419.1635.

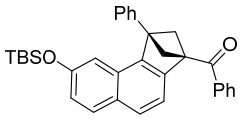


3ao
$C_{28}H_{22}O_2$
M = 390.48 g/mol

(8-methoxy-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (**3ao**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 7-methoxynaphthalen-2-ol (**2o**, 34.8 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica

gel using petroleum ether/EtOAc (100/1 to 30/1) afforded **3ao** as a white solid (54.8 mg, 70% yield).

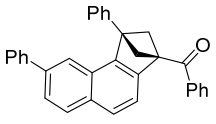
3ao: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 20/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.62-7.58 (m, 2H), 7.51-7.45 (m, 6H), 7.42-7.37 (m, 2H), 7.04 (d, *J* = 7.6 Hz, 1H), 6.87 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.09 (s, 1H), 3.80 (s, 2H), 3.34 (s, 2H), 3.27 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.0, 157.1, 150.3, 146.2, 141.4, 135.8, 133.4, 130.3, 129.5, 128.7, 128.6, 128.3, 128.2, 127.2, 127.0, 124.8, 118.1, 116.2, 99.7, 71.8, 59.6, 55.2, 54.4 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O_2$: 391.1693; found: 391.1685.



3ap
$C_{33}H_{34}O_2Si$
M = 490.72 g/mol

(8-((*tert*-butyldimethylsilyl)oxy)-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]-naphthalen-3-yl)(phenyl)methanone (**3ap**): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 7-methoxynaphthalen-2-ol (**2p**, 54.9 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ap** as a white solid (69.6 mg, 71% yield).

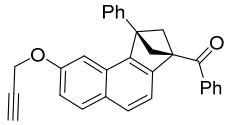
3ap: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.31 (d, *J* = 7.6 Hz, 2H), 7.86-7.79 (m, 2H), 7.70-7.58 (m, 8H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 8.8 Hz, 1H), 6.49 (s, 1H), 4.02 (s, 2H), 3.52 (s, 2H), 1.10 (s, 9H), 0.15 (s, 6H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.1, 153.1, 150.3, 146.1, 141.3, 135.8, 133.4, 130.4, 129.5, 128.9, 128.58, 128.55, 127.2, 126.7, 124.9, 121.4, 116.4, 109.3, 72.2, 59.5, 55.3, 25.6, 18.0, -4.7 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{35}O_2Si$: 491.2401; found: 491.2399.



3aq
$C_{33}H_{24}O$
M = 436.55 g/mol

(1,8-diphenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (3aq): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 7-phenylnaphthalen-2-ol (**2q**, 44.1 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ap** as a white solid (60.7 mg, 70% yield).

3aq: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.10 (d, *J* = 7.6 Hz, 2H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.61 (t, *J* = 7.2 Hz, 1H), 7.55-7.42 (m, 9H), 7.34-7.23 (m, 5H), 7.18 (d, *J* = 8.0 Hz, 1H), 7.10 (s, 1H), 3.85 (s, 2H), 3.38 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.9, 150.3, 148.4, 141.2, 140.4, 137.3, 135.8, 133.5, 131.6, 129.52, 129.45, 128.9, 128.65, 128.57, 127.8, 127.3, 127.2, 126.75, 126.71, 124.8, 123.5, 120.3, 118.4, 72.2, 59.7, 55.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{25}O$: 437.1900; found: 437.1894.

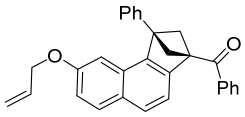


3ar
$C_{30}H_{22}O_2$
M = 414.50 g/mol

phenyl-(1-phenyl-8-(prop-2-yn-1-yloxy)-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)methanone (3ar): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 7-(prop-2-yn-1-yloxy)naphthalen-2-ol (**2r**, 39.6 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3ar** as a white solid (41.8 mg, 50% yield).

3ar: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 7.6 Hz, 2H), 7.65-7.58 (m, 2H), 7.51-7.41 (m, 8H), 7.06 (d, *J* = 8.0 Hz, 1H), 6.92

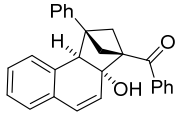
(dd, *J* = 9.2, 2.0 Hz, 1H), 6.16 (s, 1H), 4.12 (d, *J* = 1.6 Hz, 2H), 3.80 (s, 2H), 3.34 (s, 2H), 2.39 (s, 1H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.9, 155.0, 150.5, 146.4, 141.2, 135.8, 133.4, 130.5, 129.5, 128.9, 128.6, 128.5, 128.0, 127.3, 126.9, 124.9, 118.1, 116.6, 100.8, 78.3, 75.2, 71.9, 59.6, 55.2, 54.7 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{30}H_{23}O_2$: 415.1693; found: 415.1684.



3as
$C_{30}H_{24}O_2$
M = 416.52 g/mol

(8-(allyloxy)-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)-methanone (3as): Prepared from phenyl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1a**, 56.2 mg, 0.24 mmol) and 7-(allyloxy)naphthalen-2-ol (**2r**, 40.0 mg, 0.2 mmol) according to the **GP** at 25 °C for 12 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (100/1 to 50/1) afforded **3as** as a white solid (58.4 mg, 70% yield).

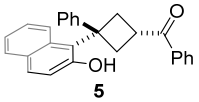
3as: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.09 (d, *J* = 8.4 Hz, 2H), 7.63-7.58 (m, 2H), 7.49-7.45 (m, 6H), 7.42-7.37 (m, 2H), 7.03 (d, *J* = 8.0 Hz, 1H), 6.91 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.10 (s, 1H), 5.88- 5.78 (m, 1H), 5.23-5.15 (m, 2H), 3.93 (d, *J* = 5.2 Hz, 2H), 3.79 (s, 2H), 3.33 (s, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 199.0, 155.9, 150.3, 146.2, 141.4, 135.8, 133.4, 132.9, 130.3, 129.5, 128.8, 128.6, 128.25, 128.21, 127.2, 126.9, 124.8, 118.4, 117.3, 116.3, 100.7, 71.8, 67.7, 59.6, 55.2 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{30}H_{25}O_2$: 417.1849; found: 417.1841.



4
$C_{27}H_{22}O_2$
M = 378.47 g/mol

(3a-hydroxy-1-phenyl-1,2,3a,9b-tetrahydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)(phenyl)methanone (**5**): $\mathbf{R_f}$ = 0.50 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (600 MHz,

$CDCl_3$): δ 8.00 (d, *J* = 7.2 Hz, 2H), 7.58 (t, *J* = 7.8 Hz, 1H), 7.49-7.46 (m, 2H), 7.30-7.25 (m, 3H), 7.15 (d, *J* = 7.2 Hz, 1H), 7.12 (t, *J* = 7.2 Hz, 1H), 6.96 (s, 2H), 6.82 (t, *J* = 7.2 Hz, 1H), 6.62 (d, *J* = 9.6 Hz, 1H), 6.05 (d, *J* = 7.2 Hz, 1H), 5.77 (d, *J* = 10.2 Hz, 1H), 3.61 (s, 1H), 3.32 (s, 1H), 3.12 (t, *J* = 7.8 Hz, 1H), 2.31 (t, *J* = 8.4 Hz, 1H), 2.14 (d, *J* = 6.6 Hz, 1H), 2.08 (d, *J* = 7.2 Hz, 1H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 202.9, 140.7, 137.5, 133.1, 132.6, 131.8, 129.7, 129.6, 129.2, 128.4, 128.1, 127.5, 126.9, 126.73, 126.71, 126.65, 126.5, 80.0, 62.8, 57.5, 55.4, 43.8, 42.1 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{23}O_2$: 379.1693; found: 379.1685.

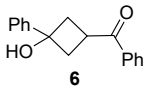


5

$C_{27}H_{22}O_2$

M = 378.47 g/mol

(*cis*)-(3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutyl)(phenyl)methanone (**5**): **R_f** = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H), 7.70-6.67 (m, 2H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.47-7.41 (m, 3H), 7.37-7.29 (m, 3H), 7.24-7.18 (m, 2H), 6.97 (d, *J* = 8.8 Hz, 1H), 6.37 (s, 1H), 4.24-4.17 (m, 1H), 3.53-3.23 (s, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 202.1, 150.7, 147.0, 135.5, 133.3, 132.2, 129.6, 128.71, 128.66, 128.63, 128.60, 128.5, 126.40, 126.37, 126.2, 125.7, 124.4, 122.6, 118.8, 45.9, 40.7, 38.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{23}O_2$: 379.1693; found: 379.1687.

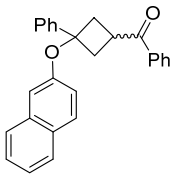


6

$C_{17}H_{16}O_2$

M = 252.31 g/mol

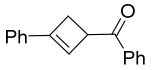
(3-hydroxy-3-phenylcyclobutyl)(phenyl)methanone. colorless oil. (**6**): **R_f** = 0.30 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.95 (d, *J* = 7.8 Hz, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.48-7.46 (m, 2H), 7.42 (d, *J* = 7.8 Hz, 2H), 7.36-7.34 (m, 2H), 7.28-7.25 (m, 1H), 4.39-4.33 (m, 1H), 2.93 (t, *J* = 10.8 Hz, 2H), 2.65 (t, *J* = 10.8 Hz, 2H), 2.26 (broad s, 1H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 200.6, 145.9, 135.5, 133.1, 128.7, 128.5, 128.4, 127.4, 124.7, 75.0, 39.3, 35.8 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{17}H_{17}O_2$: 253.1223; found: 253.1217.



***cis/trans*-7**
$C_{27}H_{22}O_2$
M = 378.47 g/mol

(*cis/trans*)-(3-(naphthalen-2-yloxy)-3-phenylcyclobutyl)(phenyl)methanone.

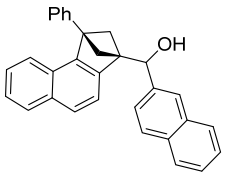
Major isomer: colorless oil. $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 8.8 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.51-7.44 (m, 5H), 7.35-7.28 (m, 4H), 7.25-7.19 (m, 1H), 7.13 (dd, *J* = 9.2, 2.4 Hz, 1H), 6.72 (s, 1H), 4.33-4.24 (m, 1H), 3.14-3.02 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 200.2, 153.1, 143.0, 135.3, 134.0, 133.3, 129.3, 128.7, 128.6, 128.4, 127.5, 127.2, 126.8, 126.1, 125.1, 123.7, 120.1, 112.0, 80.9, 37.3, 35.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{23}O_2$: 379.1693; found: 379.1694. **Minor isomer**: colorless oil. $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.68-7.64 (m, 4H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.49-7.44 (m, 3H), 7.42-7.39 (m, 2H), 7.33-7.30 (m, 2H), 7.26 (s, 1H), 7.04 (dd, *J* = 8.8, 2.0 Hz, 1H), 6.69 (s, 1H), 3.93-3.84 (m, 1H), 3.16-3.03 (m, 4H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 199.3, 152.8, 143.1, 135.3, 134.0, 133.3, 129.2, 128.9, 128.74, 128.69, 128.4, 127.6, 127.5, 126.7, 126.0, 125.0, 123.6, 120.0, 111.2, 77.9, 38.9, 33.7 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{27}H_{23}O_2$: 379.1693; found: 379.1692.



8
$C_{17}H_{14}O$
M = 234.30 g/mol

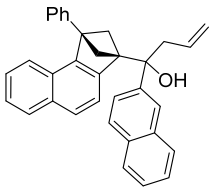
phenyl(3-phenylcyclobut-2-en-1-yl)methanone. colorless oil. (**8**) $\mathbf{R_f}$ = 0.45 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.02 (d, *J* = 7.8 Hz, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.51-7.48 (m, 2H), 7.38 (d, *J* = 7.8 Hz, 2H), 7.35-7.32 (m, 2H), 7.29-7.26 (m, 1H), 6.49 (s, 1H), 4.49 (s, 1H), 3.22-3.16 (m, 2H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 199.2, 147.5, 135.9, 133.7, 133.1, 128.6, 128.3, 128.23, 128.19, 125.6, 124.7,

45.8, 32.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{17}H_{15}O$: 235.1117; found: 235.1112.



9
$C_{31}H_{24}O$
M = 412.53 g/mol

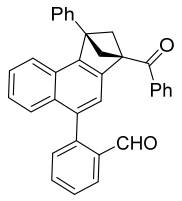
naphthalen-2-yl(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)methanol (**9**): $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.93 (s, 1H), 7.86-7.81 (m, 3H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.50-7.45 (m, 2H), 7.39-7.30 (m, 5H), 7.16 (t, *J* = 7.2 Hz, 1H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.77 (d, *J* = 8.8 Hz, 1H), 5.56 (s, 1H), 3.38-3.35 (m, 1H), 3.32-3.28 (m, 1H), 2.91 (d, *J* = 5.2 Hz, 1H), 2.66 (d, *J* = 4.8 Hz, 1H), 2.28 (broad s, 1H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 149.5, 149.4, 142.0, 139.7, 133.2, 133.0, 132.2, 129.0, 128.6, 128.1, 128.0, 127.7, 127.4, 126.9 126.7, 126.2, 126.0, 125.4, 125.2, 124.82, 124.79, 123.6, 122.5, 118.0, 73.2, 69.1, 67.3, 56.2, 55.9 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{31}H_{25}O$: 413.1900; found: 413.1896.



10
$C_{34}H_{28}O$
M = 452.60 g/mol

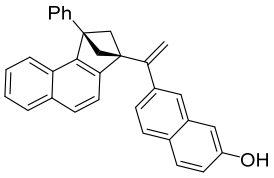
1-(naphthalen-2-yl)-1-(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]-naphthalen-3-yl)but-3-en-1-ol (**10**): $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.10 (s, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.83-7.80 (m, 2H), 7.67-7.63 (m, 3H), 7.50-7.33 (m, 8H), 7.12 (d, *J* = 7.6 Hz, 1H), 6.95 (dd, *J* = 8.0, 6.8 Hz, 1H), 6.73 (d, *J* = 8.4 Hz, 1H), 5.65-5.55 (m, 1H), 5.30 (d, *J* = 16.8 Hz, 1H), 5.16 (d, *J* = 10.4 Hz, 1H), 3.44-3.37 (m, 2H), 3.27 (dd, *J* = 14.0, 5.2 Hz, 1H), 3.05 (d, *J* = 4.0 Hz, 1H), 3.00 (dd, *J* = 14.0, 9.2 Hz, 1H), 2.82 (d, *J* = 4.0 Hz, 1H), 2.55 (s, 1H) ppm. **^{13}C NMR** (100 MHz,

$CDCl_3$): δ 149.6, 149.0, 142.1, 141.5, 133.0, 132.3, 131.8, 128.8, 128.6, 128.2, 127.7, 127.5, 127.2, 126.9, 126.7, 126.1, 125.9, 125.3, 125.0, 124.7, 124.4, 123.6, 122.4, 120.6, 120.1, 75.6, 69.0, 67.4, 59.4, 54.5, 42.9 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{34}H_{29}O$: 453.2213; found: 453.2210.



11
$C_{34}H_{24}O_2$
M = 464.56 g/mol

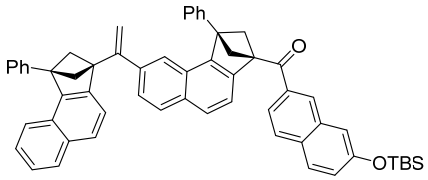
2-(3-benzoyl-1-phenyl-2,3-dihydro-1*H*-1,3-methanocyclopenta[*a*]naphthalen-5-yl)-benzaldehyde (**11**): $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 9.63 (s, 1H), 8.08 (d, *J* = 8.0 Hz, 2H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.64-7.57 (m, 2H), 7.52-7.44 (m, 8H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.18-7.13 (m, 2H), 7.08 (t, *J* = 7.2 Hz, 1H), 6.97 (d, *J* = 8.4 Hz, 1H), 3.98-3.95 (m, 1H), 3.90-3.86 (m, 1H), 3.42-3.39 (m, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 198.4, 191.8, 149.2 148.5, 144.7, 140.9, 135.5, 134.9, 133.7, 133.5, 132.3, 131.8, 131.4, 129.4, 128.9, 128.7, 128.0, 127.6, 127.5, 127.0, 126.8, 126.7, 125.9, 125.1, 123.0, 120.8, 72.9, 72.0, 59.6, 55.8 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{34}H_{25}O_2$: 465.1849; found: 465.1845.



12
$C_{32}H_{24}O$
M = 424.54 g/mol

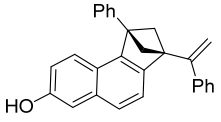
7-(1-(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)vinyl)-naphthalen-2-ol (**12**): $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.76 (s, 1H), 7.74-7.71 (m, 3H), 7.54 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.48-7.44 (m, 5H), 7.42-7.38 (m, 1H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.18 (t, *J* = 7.8 Hz, 1H), 7.06 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.05-7.02 (m, 2H), 6.84 (d, *J* = 8.4 Hz, 1H), 5.78 (s, 1H), 5.36 (s, 1H), 5.05 (s, 1H), 3.78 (s, 2H), 3.13 (s, 2H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 153.6, 152.4,

148.4, 147.0, 142.0, 137.6, 134.4, 132.1, 129.5, 129.0, 128.7, 128.2, 127.7, 127.5, 127.0, 126.8, 125.3, 124.9, 124.7, 123.6, 123.0, 122.5, 118.5, 117.8, 114.7, 109.9, 72.6, 55.9, 54.8 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{32}H_{25}O$: 425.1900; found: 425.1891.



13
$C_{59}H_{52}O_2Si$
M = 821.15 g/mol

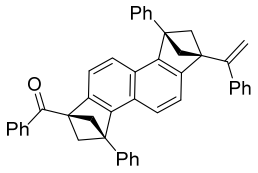
(7-((*tert*-butyldimethylsilyl)oxy)naphthalen-2-yl)(1-phenyl-8-(1-(1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)vinyl)-1,2-dihydro-3*H*-1,3-methano-cyclopenta[*a*]naphthalen-3-yl)methanone (**13**): $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.40 (s, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 7.84 (d, *J* = 9.0 Hz, 1H), 7.79-7.76 (m, 3H), 7.57 (d, *J* = 9.0 Hz, 1H), 7.52-7.49 (m, 3H), 7.46-7.41 (m, 4H), 7.26-7.25 (m, 3H), 7.23-7.19 (m, 4H), 7.08 (t, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 8.4 Hz, 1H), 6.90-6.87 (m, 2H), 6.85 (d, *J* = 8.4 Hz, 1H), 6.79 (t, *J* = 7.2 Hz, 1H), 5.56 (s, 1H), 5.19 (s, 1H), 3.85 (s, 2H), 3.28 (s, 2H), 3.25 (s, 2H), 2.89 (s, 2H), 1.01 (s, 9H), 0.24 (s, 6H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 199.1, 154.2, 151.9, 151.0, 148.3, 147.9, 146.6, 142.2, 140.9, 136.3, 133.8, 133.4, 132.2, 131.8, 131.5, 130.3, 129.2, 129.1, 129.0, 128.63, 128.56, 128.2, 127.9, 127.6, 126.92, 126.90, 126.88, 126.4, 125.2, 125.0, 124.5, 123.7, 123.5, 122.8, 122.5, 120.9, 118.5, 118.4, 116.6, 114.7, 72.9, 72.4, 59.7, 55.6, 55.4, 54.6, 25.7, 18.2, -4.3 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{59}H_{53}O_2Si$: 820.3737; found: 820.3728.



14
$C_{28}H_{22}O$
M = 374.48 g/mol

(7-hydroxy-1-phenyl-1,2-dihydro-3*H*-1,3-methanocyclopenta[*a*]naphthalen-3-yl)-(phenyl)methanone (**14**): $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (600 MHz,

$CDCl_3$): δ 7.53 (d, *J* = 7.2 Hz, 2H), 7.47-7.44 (m, 4H), 7.40-7.38 (m, 1H), 7.33-7.28 (m, 4H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.04 (s, 1H), 6.73 (d, *J* = 9.0 Hz, 1H), 6.67 (d, *J* = 8.4 Hz, 1H), 5.65 (s, 1H), 5.27 (s, 1H), 4.84 (s, 1H), 3.69 (s, 2H), 3.07 (s, 2H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 151.4, 149.9, 148.8, 147.2, 142.0, 139.7, 133.2, 128.7, 128.2, 127.5, 127.1, 127.0, 126.8, 124.5, 123.4, 122.7, 119.1, 117.9, 114.1, 109.8, 72.2, 55.7, 54.8 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{23}O$: 375.1743; found: 375.1734.

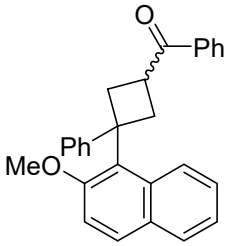


15

$C_{45}H_{34}O$

M = 590.77 g/mol

(3,8-diphenyl-6-(1-phenylvinyl)-3,6,7,8-tetrahydro-1,3:6,8-dimethanodicyclopenta-[*a*,*f*]-naphthalen-1(2*H*)-yl)(phenyl)methanone (15): R_f = 0.35 (petroleum ether/ EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.01 (d, *J* = 7.2 Hz, 2H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.46-7.36 (m, 14H), 7.33-7.27 (m, 3H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 6.60 (d, *J* = 8.4 Hz, 1H), 6.58 (d, *J* = 8.4 Hz, 1H), 5.59 (s, 1H), 5.20 (s, 1H), 3.74 (s, 2H), 3.67 (s, 2H), 3.27 (s, 2H), 3.04 (s, 2H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 199.0, 150.7, 149.0, 148.3, 147.8, 147.0, 142.0, 141.4, 139.5, 135.7, 133.3, 129.5, 128.8, 128.7, 128.6, 128.2, 127.5, 127.2, 127.0, 126.9, 126.8, 126.7, 126.6, 119.7, 119.5, 118.6, 118.2, 114.0, 72.25, 72.18, 59.4, 55.7, 55.6, 55.0 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{45}H_{35}O$: 591.2682 found: 591.2682.



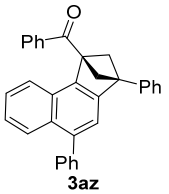
17

$C_{28}H_{24}O_2$

M = 392.50 g/mol

(*cis/trans*)-(3-(2-methoxynaphthalen-1-yl)-3-phenylcyclobutyl)(phenyl)methanone (17)

Major isomer: colorless oil. $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.92 (d, *J* = 7.8 Hz, 2H), 7.75-7.72 (m, 5H), 7.55-7.52 (m, 1H), 7.45-7.41 (m, 3H), 7.35-7.30 (m, 3H), 7.27-7.24 (m, 1H), 7.22-7.18 (m, 1H), 4.15-4.09 (m, 1H), 3.94 (s, 3H), 3.36 (broad s, 2H), 3.21 (t, *J* = 10.8 Hz, 2H) ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{25}O_2$: 393.1849; found: 393.1845. **Minor isomer**: colorless oil. $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 7.89-7.87 (m, 2H), 7.81 -7.79(m, 2H), 7.55-7.52 (m, 2H), 7.35-7.30 (m, 3H), 7.27-7.24 (m, 4H), 7.22-7.18 (m, 2H), 7.10-7.07 (m, 1H), 3.96 (s, 3H), 3.83-3.78 (m, 1H), 3.61-3.55 (m, 2H), 3.50 (broad s, 2H). ppm. (***cis/trans***)-**17: ^{13}C NMR** (150 MHz, $CDCl_3$): δ 201.1, 200.9, 154.9, 154.1, 148.1, 147.2, 135.8, 135.5, 133.0, 132.8, 132.3, 131.9, 129.91, 129.89, 129.6, 129.0, 128.9, 128.7, 128.64, 128.61, 128.57, 128.54, 128.47, 128.45, 128.4, 128.1, 126.6, 126.4, 126.1, 125.73, 125.72, 125.68, 125.5, 124.7, 123.0, 122.9, 114.4, 114.0, 56.13, 56.07, 47.1, 46.2, 40.3, 38.6, 37.3 29.7 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{28}H_{25}O_2$: 393.1849; found: 393.1847.

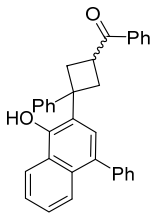


3az

$C_{33}H_{24}O$

M = 436.55 g/mol

(3,5-diphenyl-2,3-dihydro-1*H*-1,3-methanocyclopenta[*a*]naphthalen-1-yl)-(phenyl) methanone (**3az**): $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.13 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.47-7.41 (m, 8H), 7.40-7.36 (m, 4H), 7.33 (t, *J* = 7.2 Hz, 1H), 7.19-7.17 (m, 1H), 7.15-7.12 (m, 2H), 3.78 (s, 2H), 3.35 (s, 2H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 200.6, 151.6, 146.8, 141.2, 138.7, 138.1, 136.0, 133.4, 130.2, 129.9, 129.5, 128.70, 128.68, 128.2, 127.3, 127.1, 127.0, 126.9, 126.6, 126.0, 124.2, 123.9, 119.3, 72.5, 59.8, 54.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{25}O$: 437.1900; found: 437.1893.

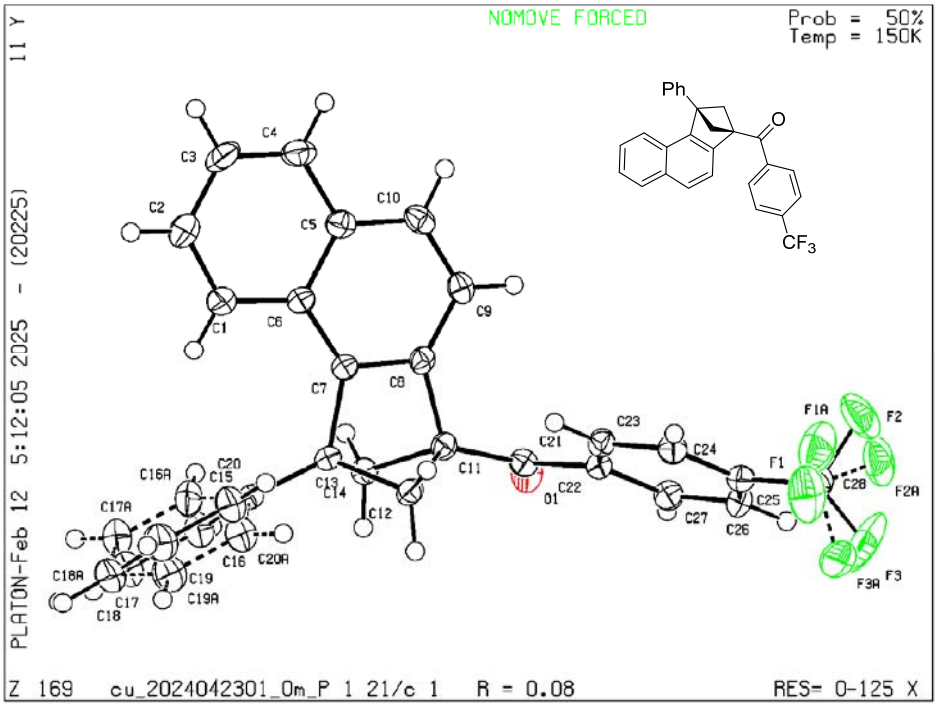


18
$C_{33}H_{26}O_2$
M = 454.57 g/mol

(*cis/trans*)-(3-(1-hydroxy-4-phenylnaphthalen-2-yl)-3-phenylcyclobutyl)(phenyl)-methanone (**18**): **Major isomer:** white solid. $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 7.2 Hz, 2H), 7.55-7.46 (m, 5H), 7.44-7.34 (m, 8H), 7.26 (t, *J* = 7.2 Hz, 1H), 5.06 (s, 1H), 4.13-4.07 (m, 1H), 3.26-3.17 (m, 4H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 200.3, 147.1, 145.7, 140.8, 135.4, 133.2, 133.1, 131.3, 130.3, 129.0, 128.6, 128.5, 128.3, 128.2, 127.0, 126.7, 126.3, 126.0, 125.9, 125.8, 125.3, 125.2, 120.8, 45.0, 37.5 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{27}O_2$: 455.2006; found: 455.2001. **Minor isomer**: white solid. $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.4 Hz, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 2H), 7.77 (s, 1H), 7.60 (d, *J* = 7.8 Hz, 2H), 7.56-7.53 (m, 3H), 7.49-7.42 (m, 5H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.33-7.30 (m, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 5.00 (s, 1H), 4.01-3.95 (m, 1H), 3.20 (d, *J* = 9.6 Hz, 4H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$): δ 200.4, 148.9, 146.0, 140.9, 135.4, 133.2, 132.9, 131.8, 130.4, 129.1, 128.7, 128.39, 128.37, 127.1, 127.0, 126.3, 126.0, 125.8, 125.42, 125.36, 125.3, 121.7, 44.9, 37.0, 36.7 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{33}H_{27}O_2$: 455.2006; found: 455.2002.

9 Crystal Structure of 3da

Note: The thermal ellipsoids are 50% probability level. The crystals are grown by slow solvent (CH_2Cl_2/*n*-Hexane) evaporation at room temperature. CCDC number of **3da** is 2423216.



Datablock: cu_2024042301_0m_a_pl

Bond precision: C-C = 0.0050 A Wavelength=1.54178

Cell: a=14.9924(5) b=12.7608(4) c=10.9520(4)
alpha=90 beta=91.202(1) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	2094.82(12)	2094.82(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H19 F3 O	C28 H19 F3 O
Sum formula	C28 H19 F3 O	C28 H19 F3 O
Mr	428.43	428.43
Dx,g cm-3	1.359	1.358
Z	4	4
Mu (mm-1)	0.826	0.826
F000	888.0	888.0
F000'	890.99	
h,k,lmax	18,15,13	18,15,13
Nref	3862	3836
Tmin,Tmax	0.796,0.862	0.648,0.752
Tmin'	0.768	

Correction method= # Reported T Limits: Tmin=0.648 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.993 Theta(max)= 68.466

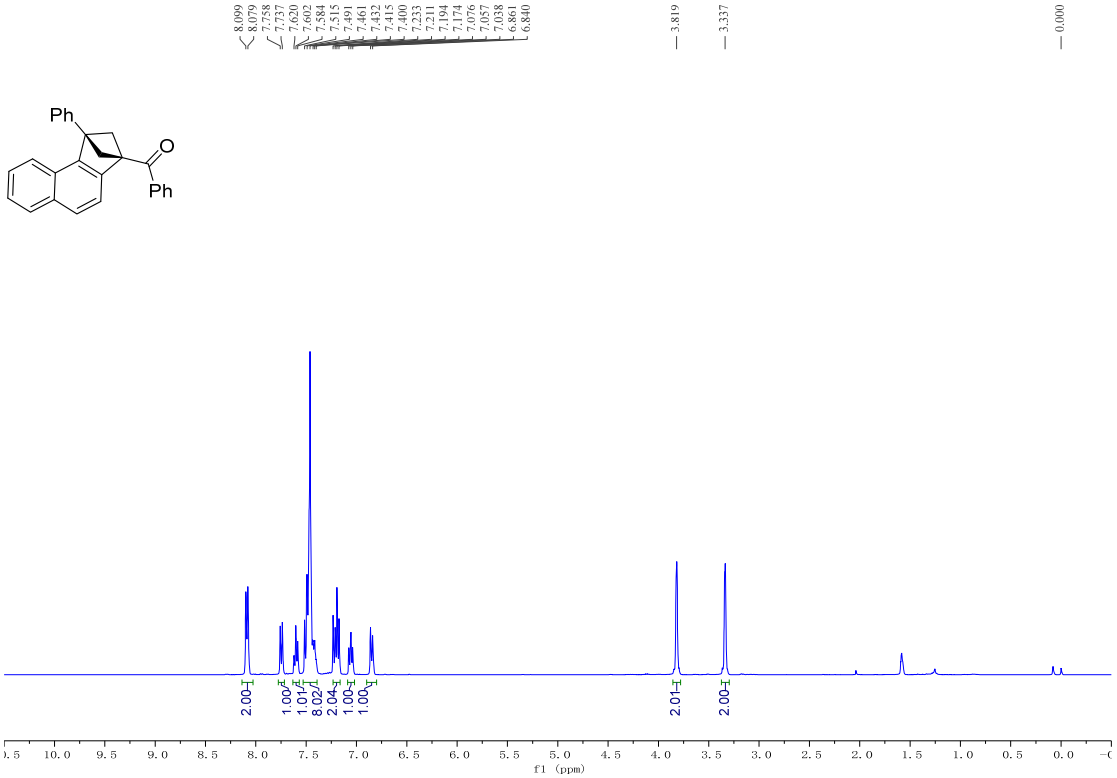
R(reflections)= 0.0809(3652) wR2(reflections)= 0.1891(3836)

S = 1.258 Npar= 351

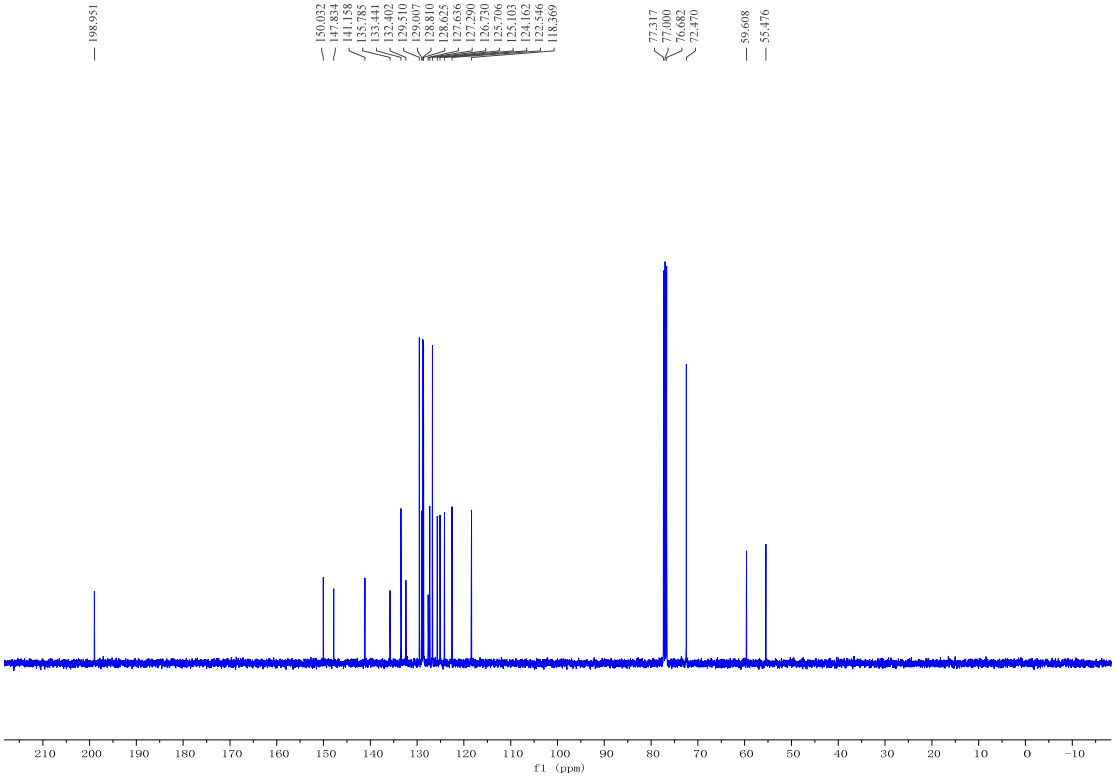
10 NMR Spectra

^{1}H and ^{13}C NMR Spectra for Compound 3aa:

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

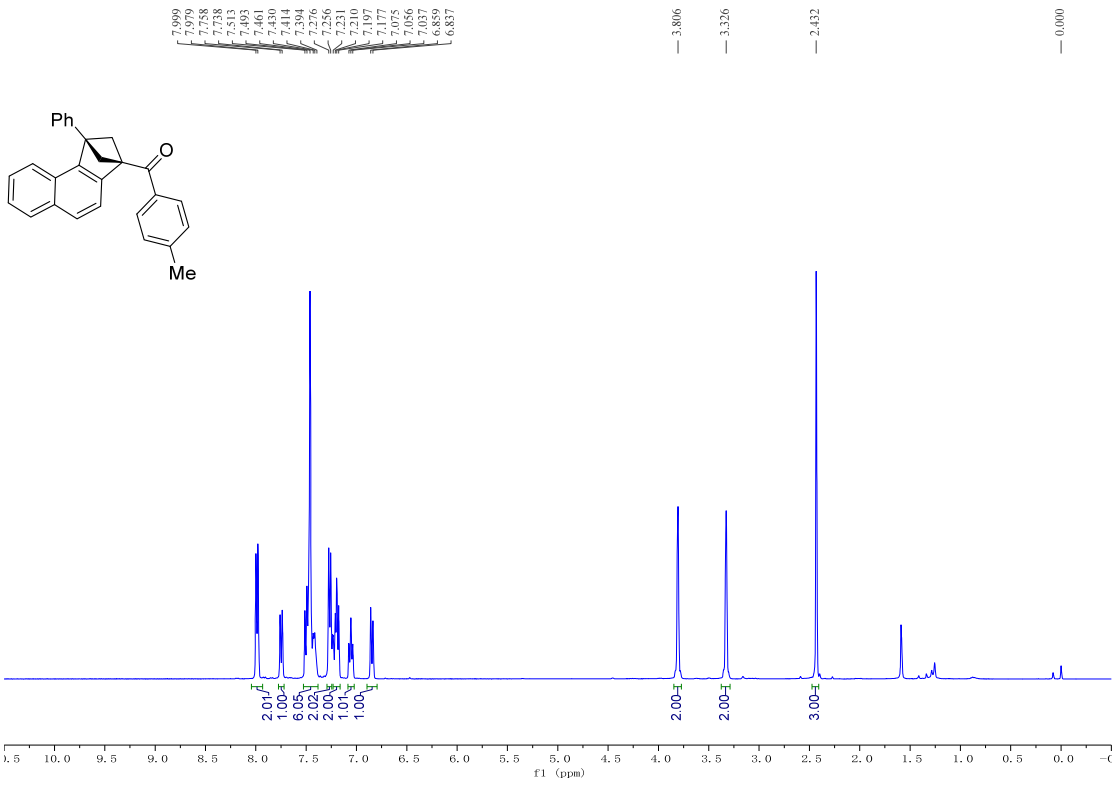


^{13}C NMR (100 MHz, $CDCl_3$)

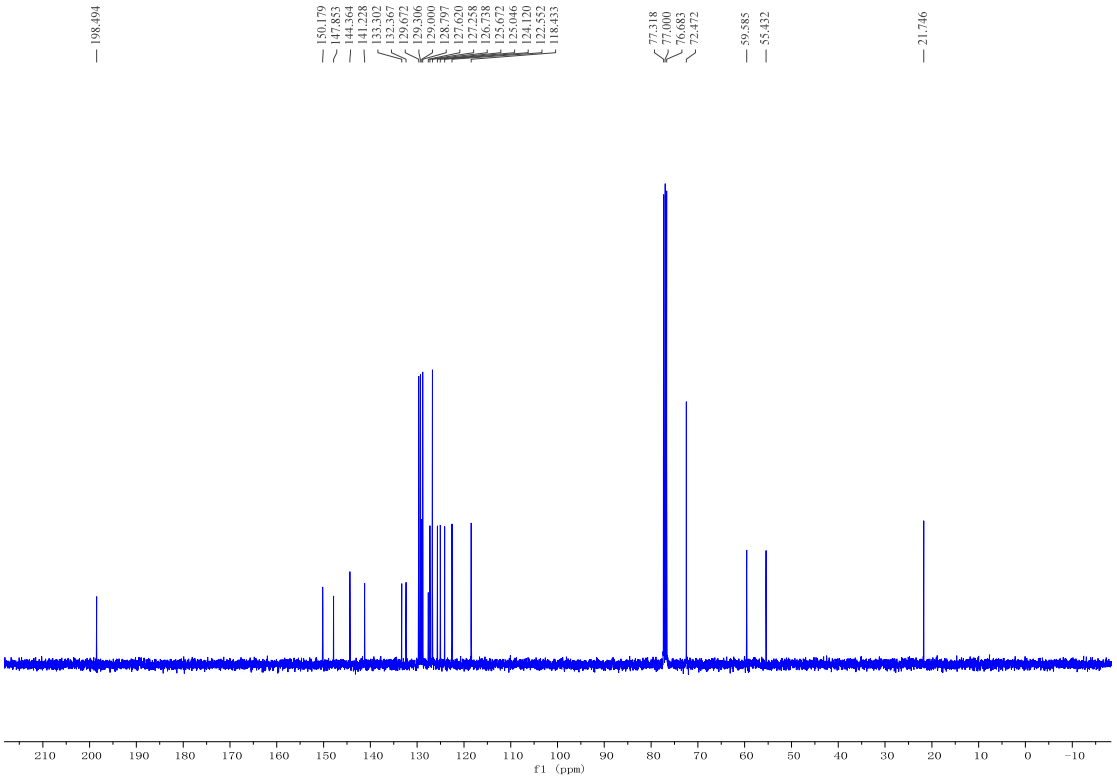


^{1}H and ^{13}C NMR Spectra for Compound 3ba:

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

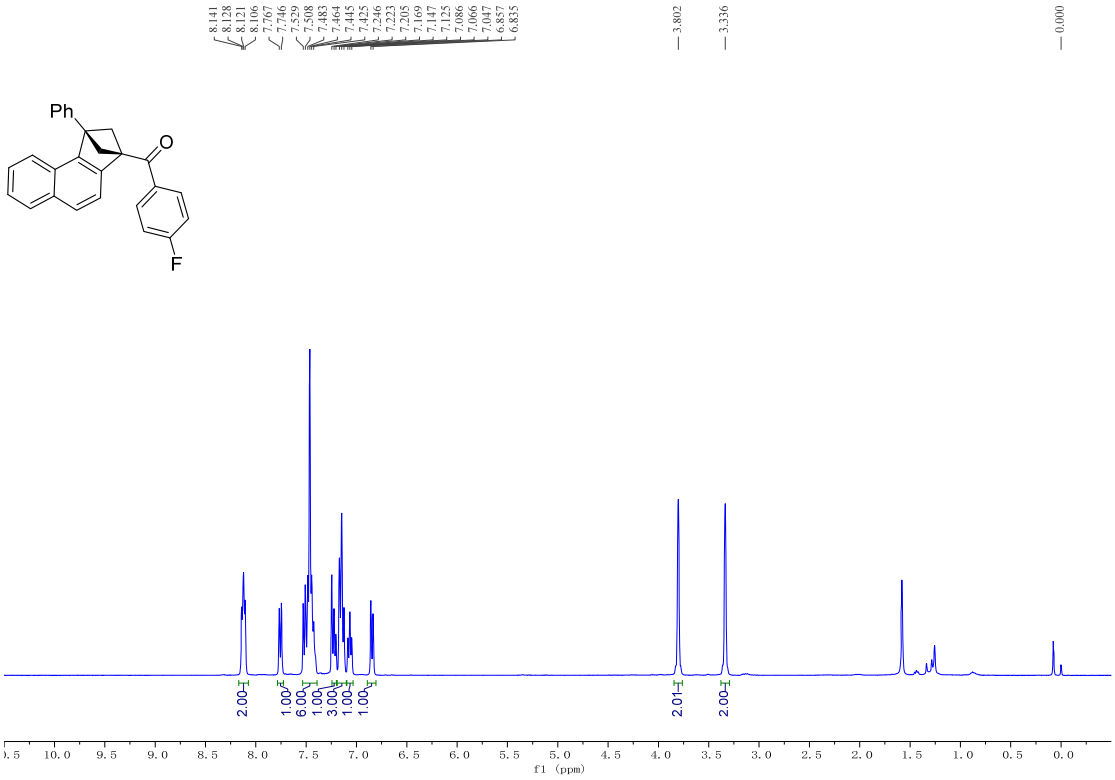


^{13}C NMR (100 MHz, $CDCl_3$)

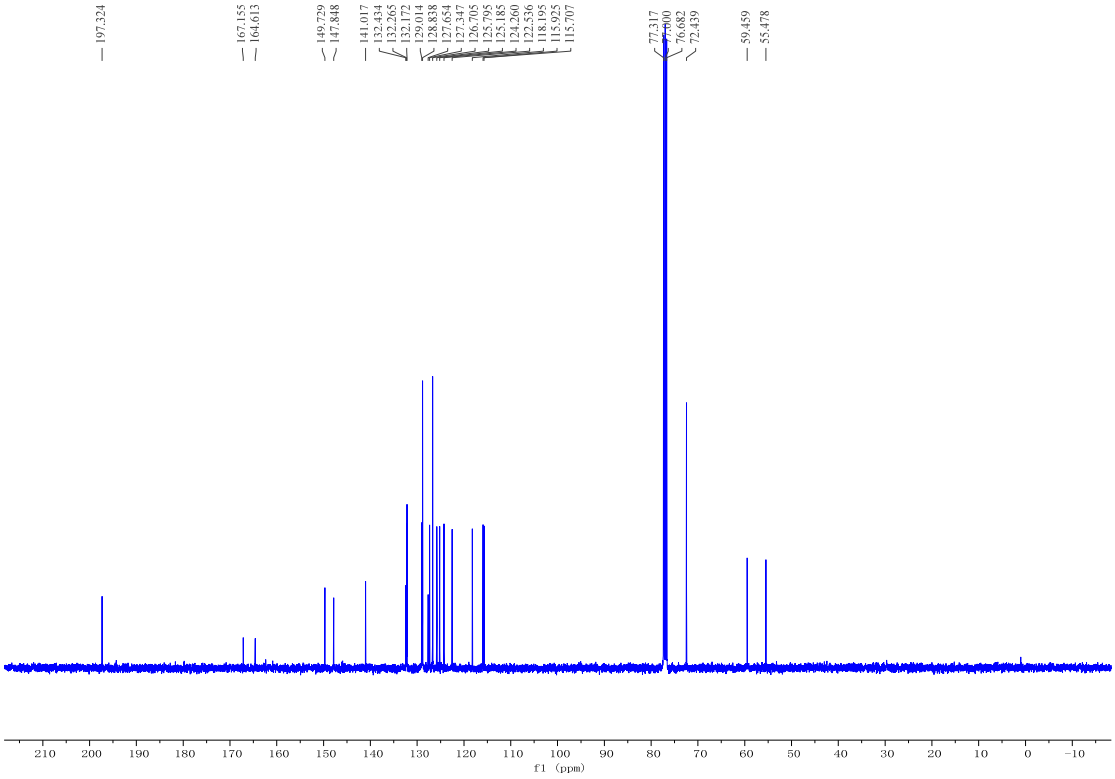


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound 3ca:

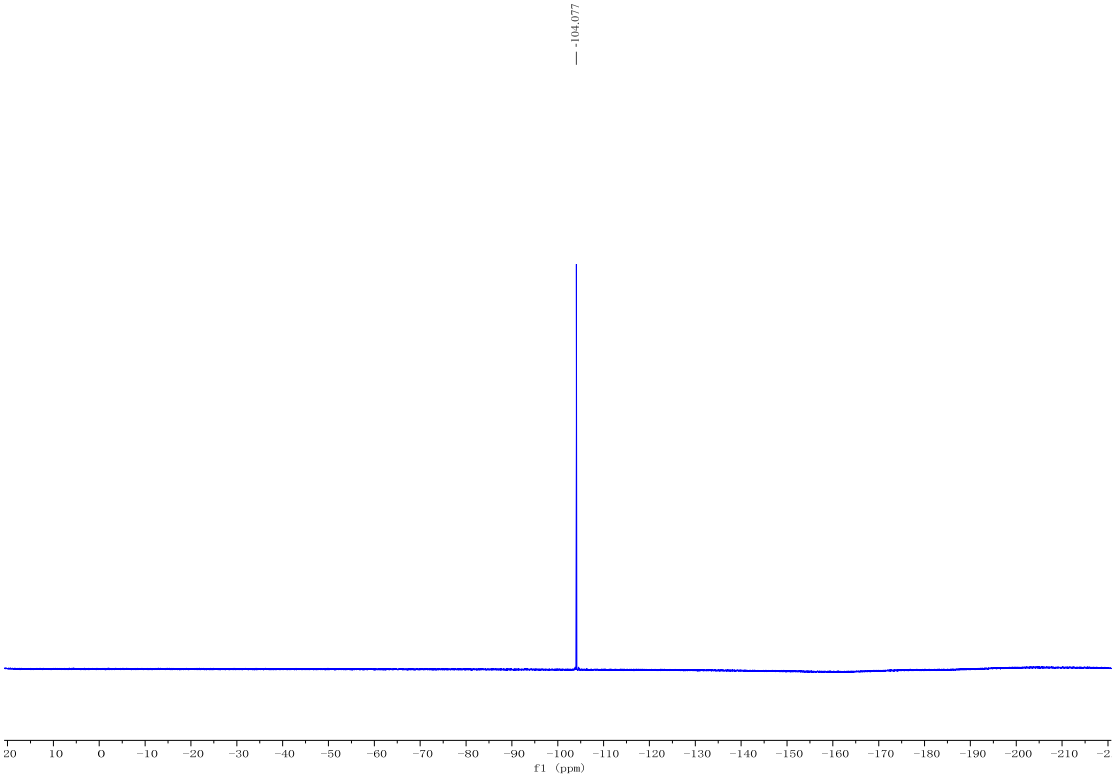
^{1}H NMR (400 MHz, $CDCl_3$)



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

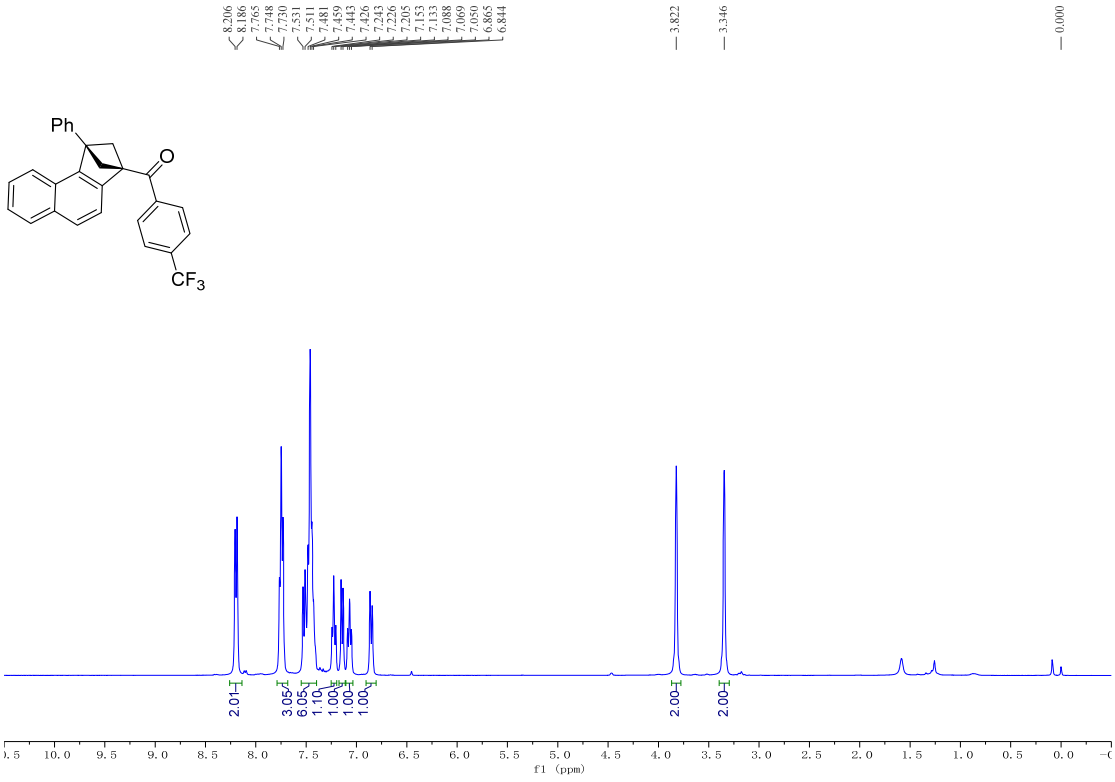


^{19}F NMR (376 MHz, $CDCl_3$)

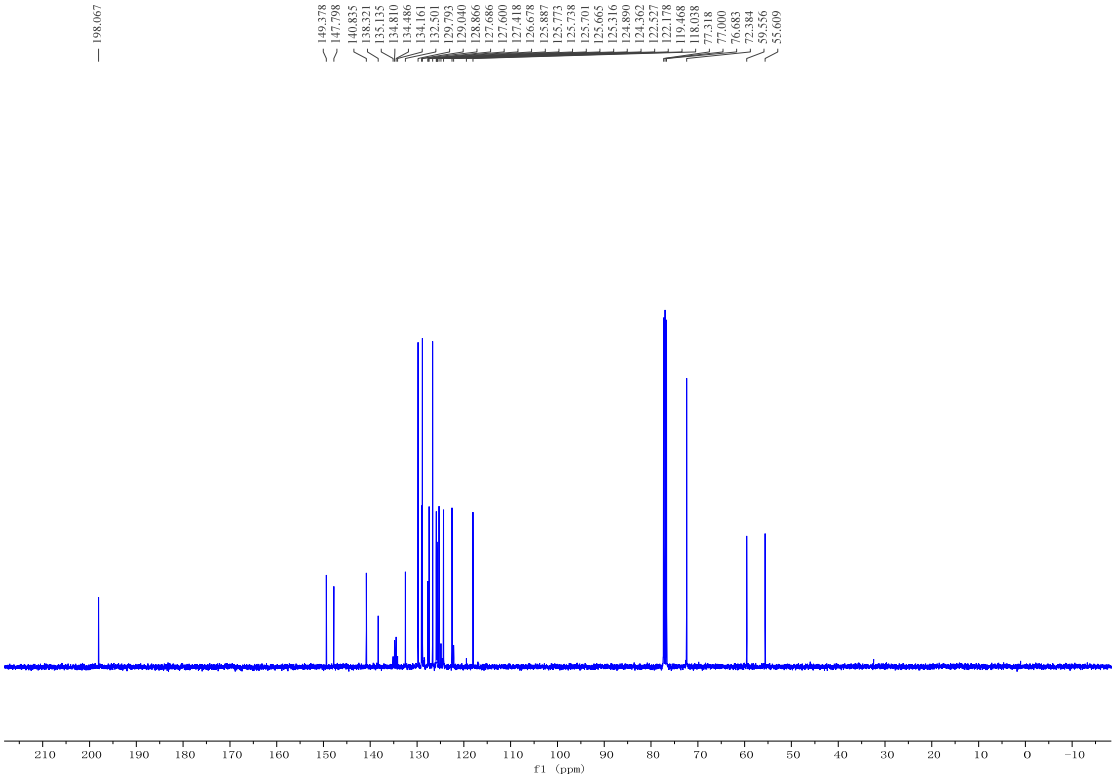


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound 3da:

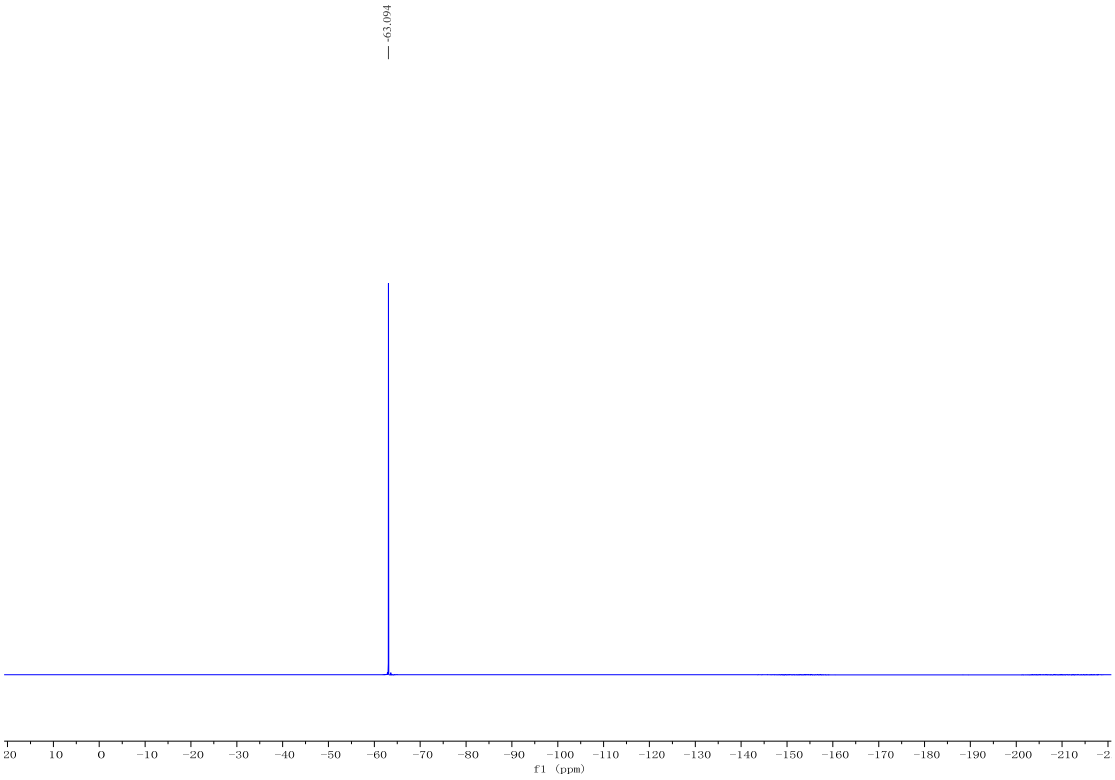
^{1}H NMR (400 MHz, $CDCl_3$)



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

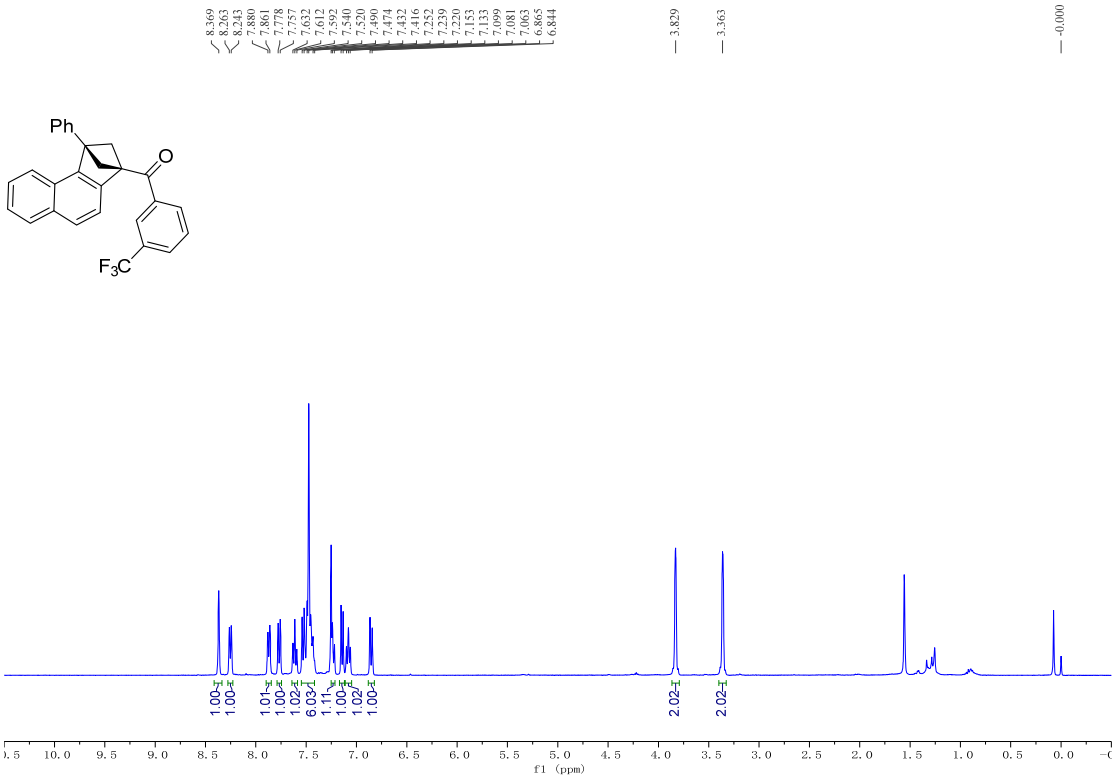


^{19}F NMR (376 MHz, $CDCl_3$)

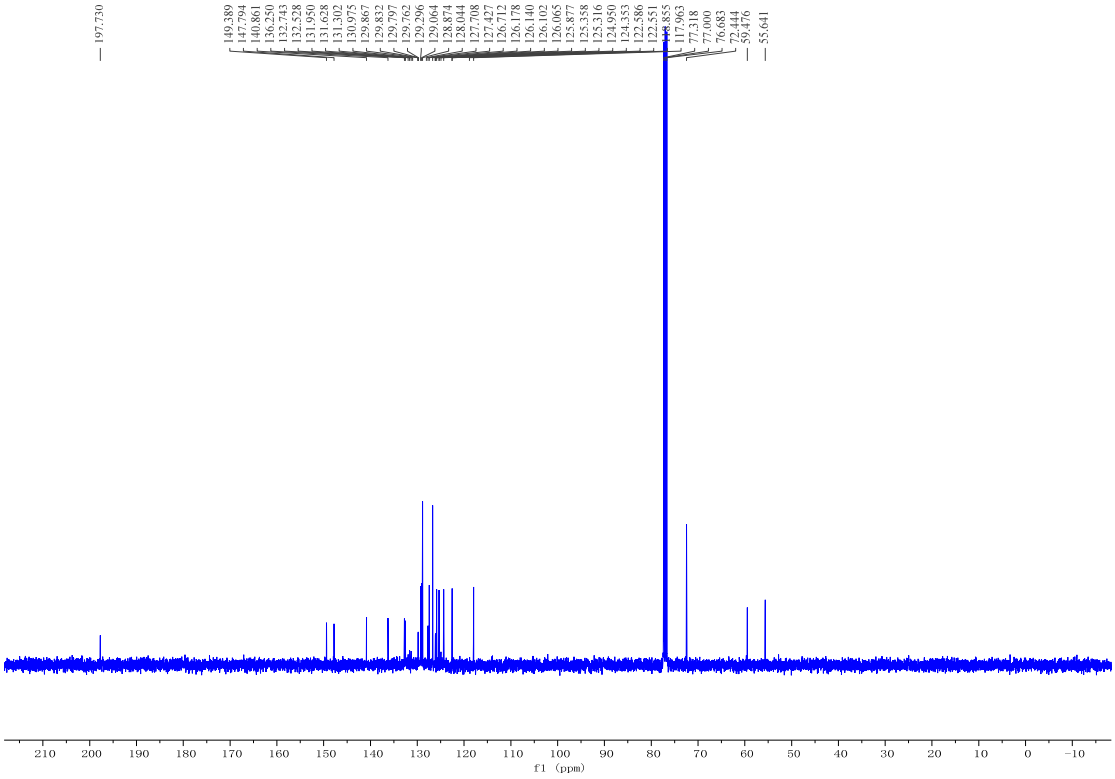


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound 3ea:

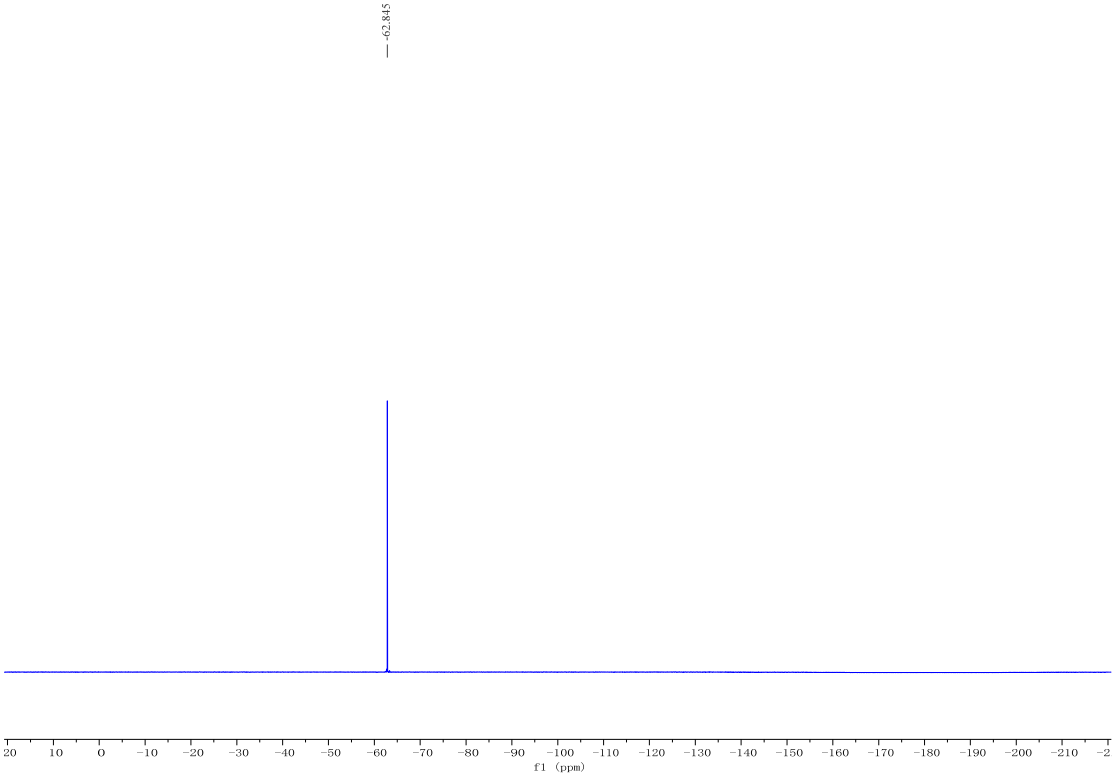
^{1}H NMR (400 MHz, $CDCl_3$)



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

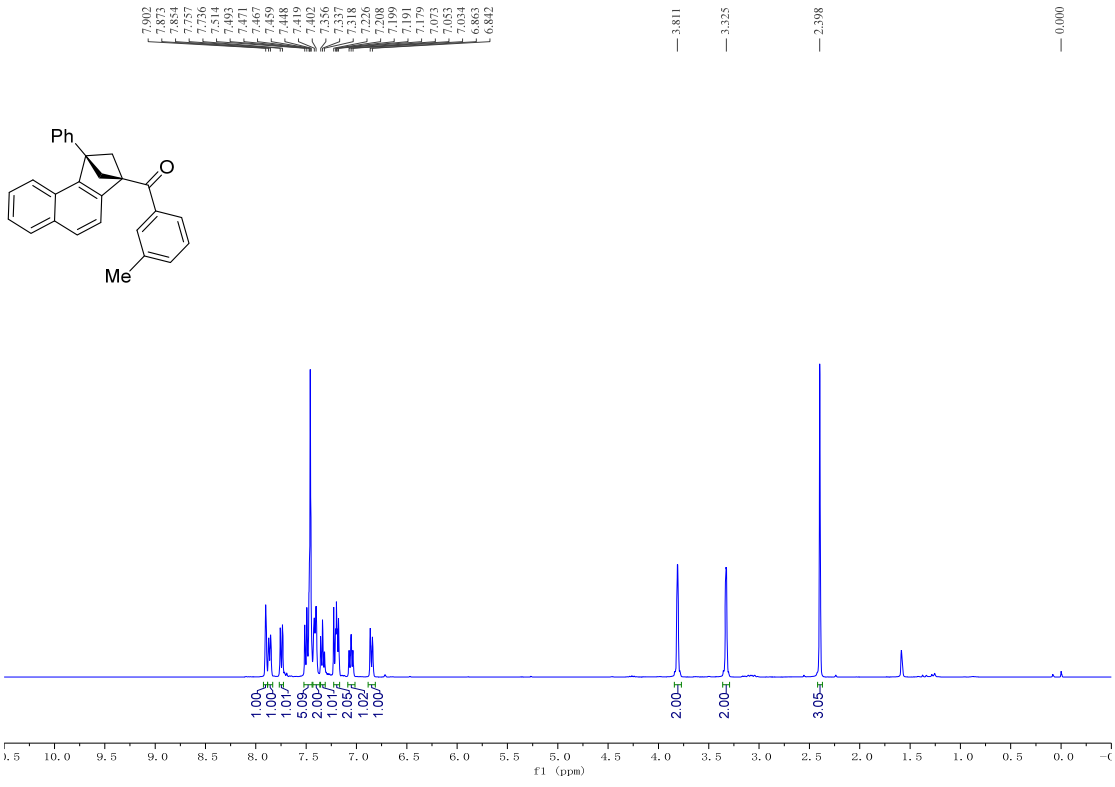


^{19}F NMR (376 MHz, $CDCl_3$)

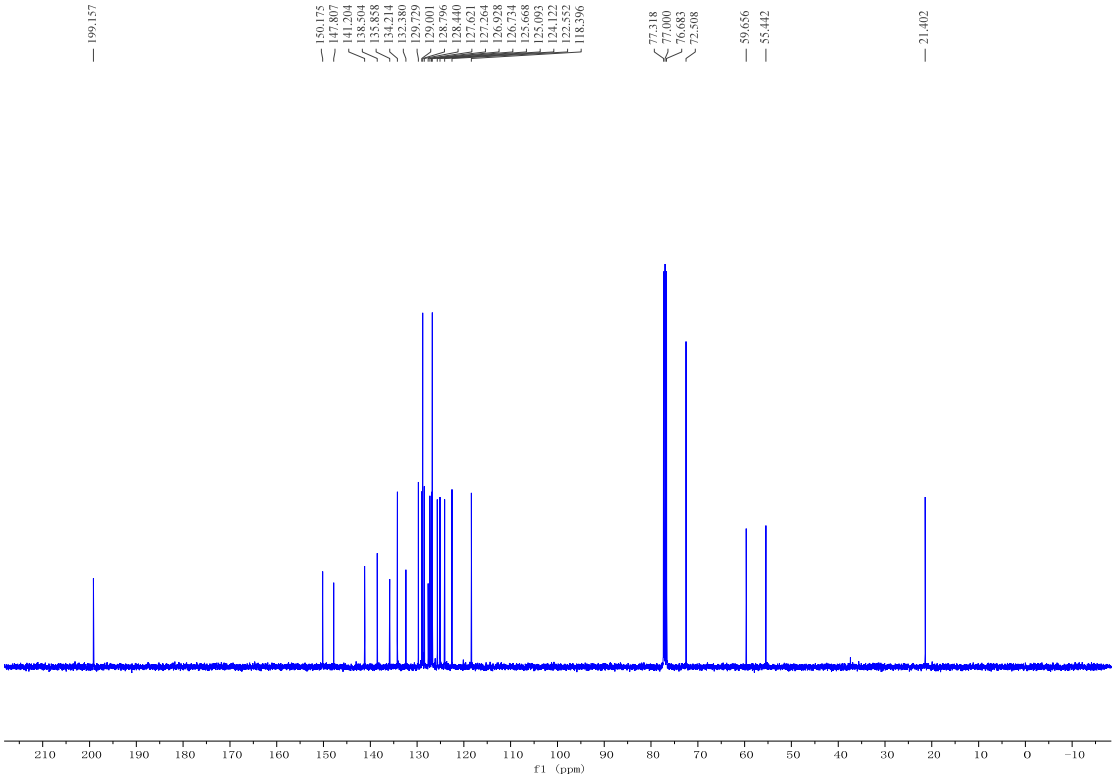


^{1}H and ^{13}C NMR Spectra for Compound 3fa:

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

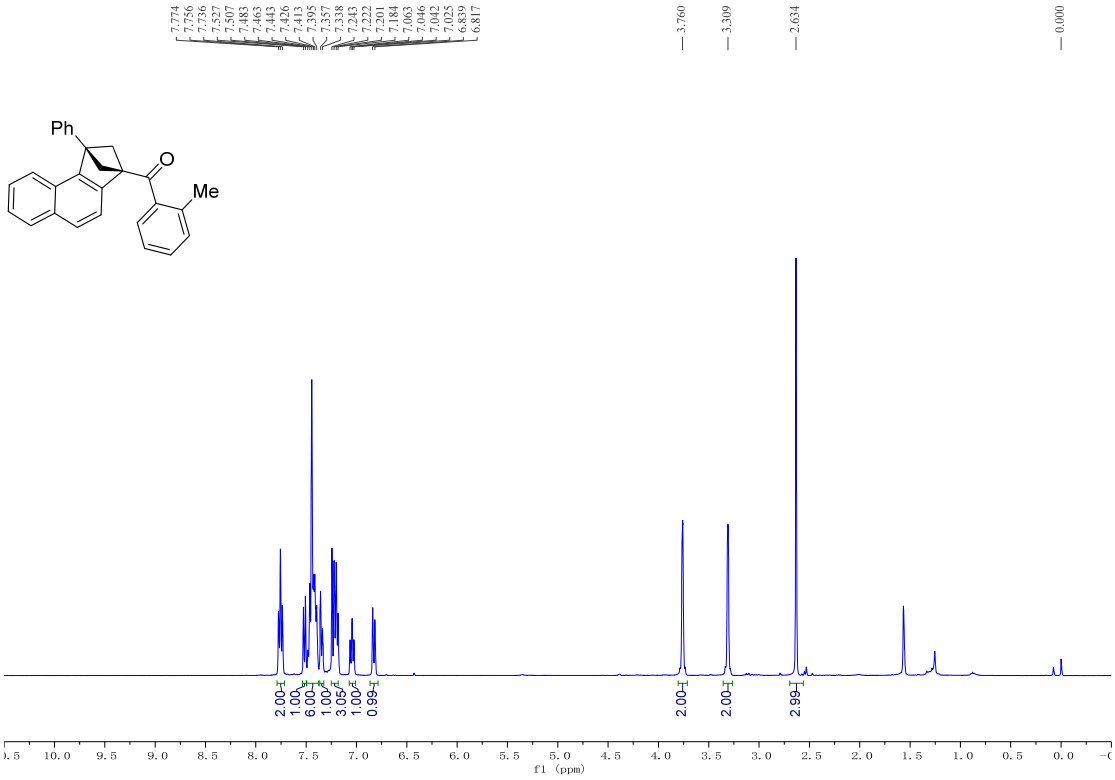


^{13}C NMR (100 MHz, $CDCl_3$)

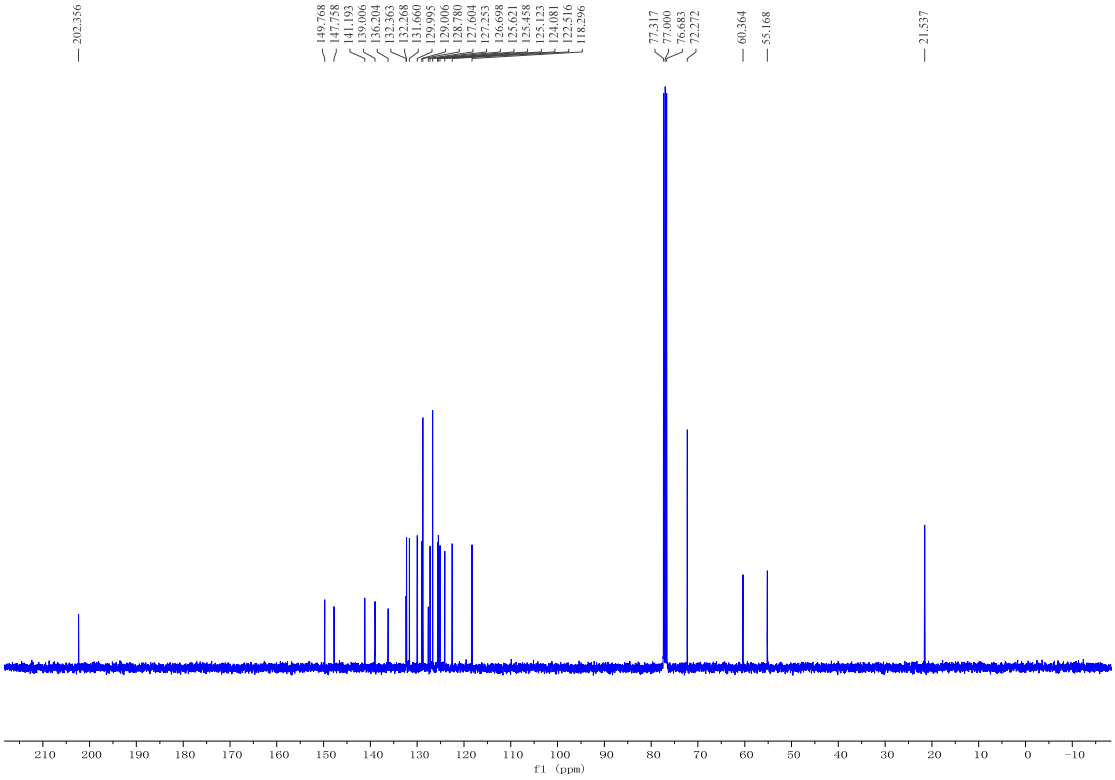


^{1}H and ^{13}C NMR Spectra for Compound 3ga:

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

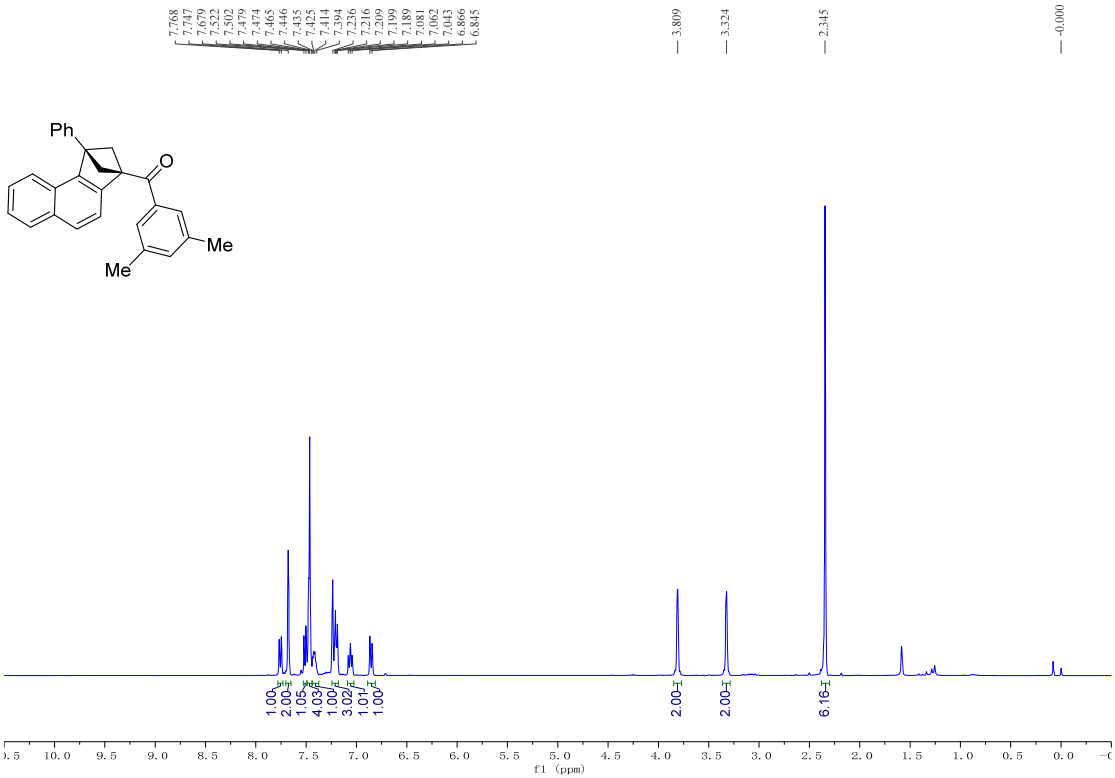


^{13}C NMR (100 MHz, $CDCl_3$)

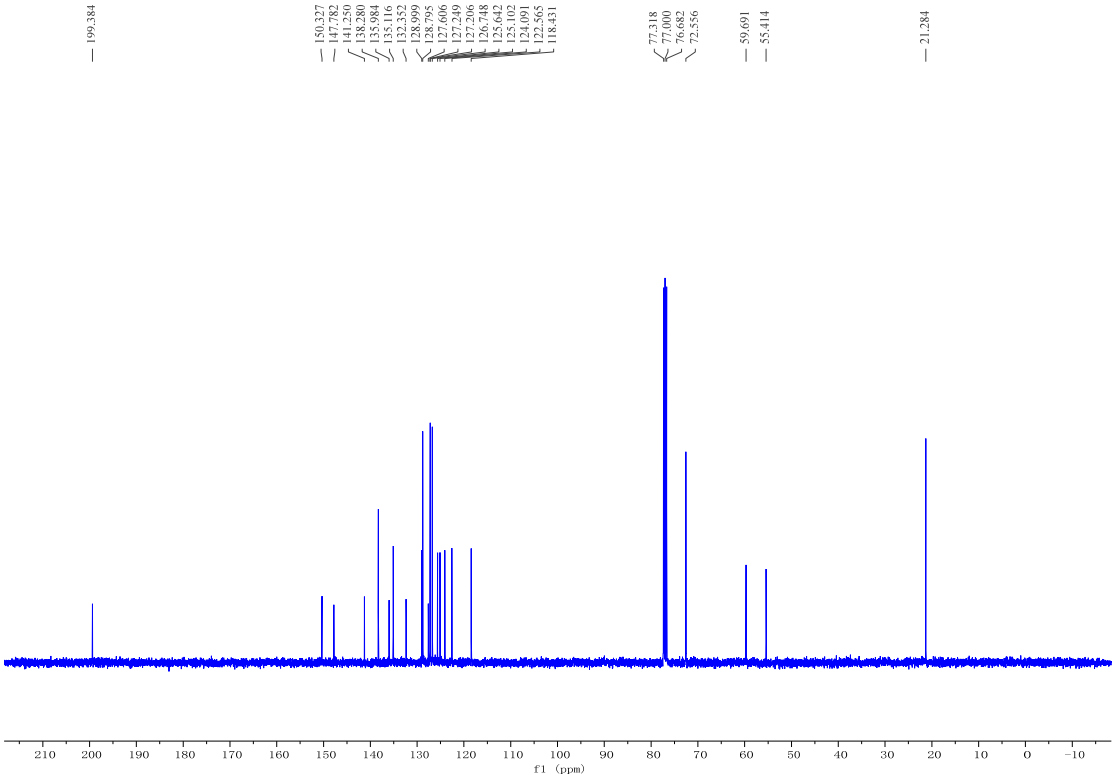


^{1}H and ^{13}C NMR Spectra for Compound 3ha:

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

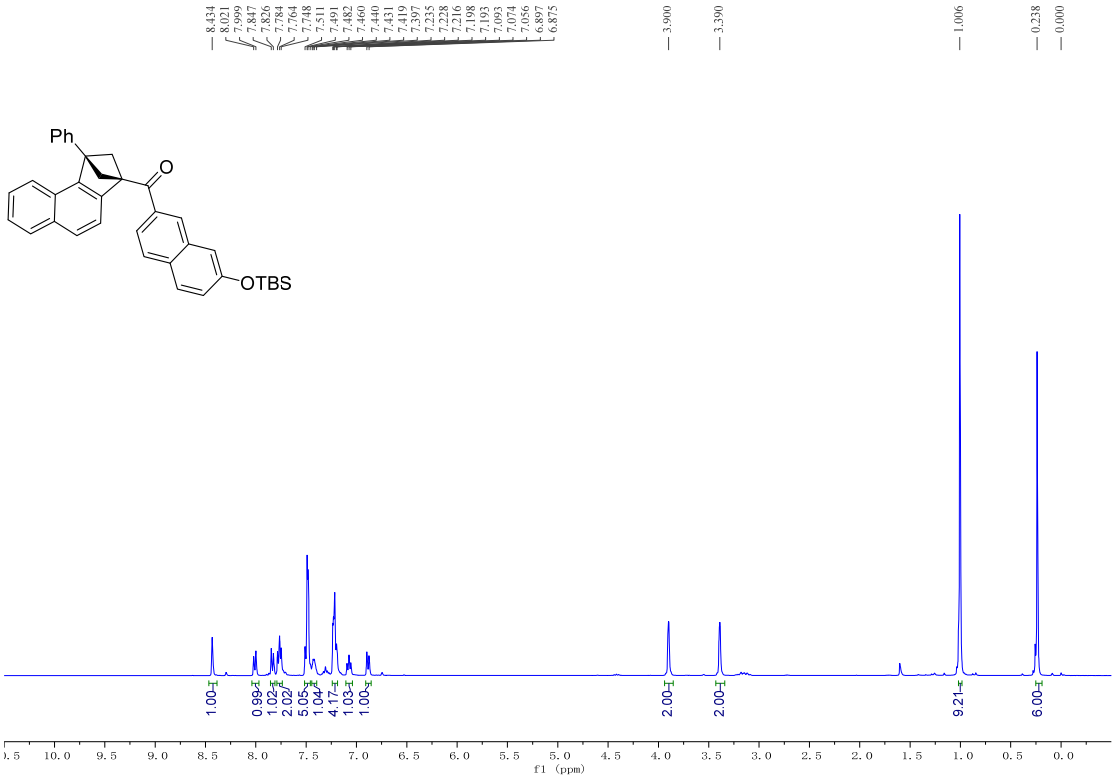


^{13}C NMR (100 MHz, $CDCl_3$)

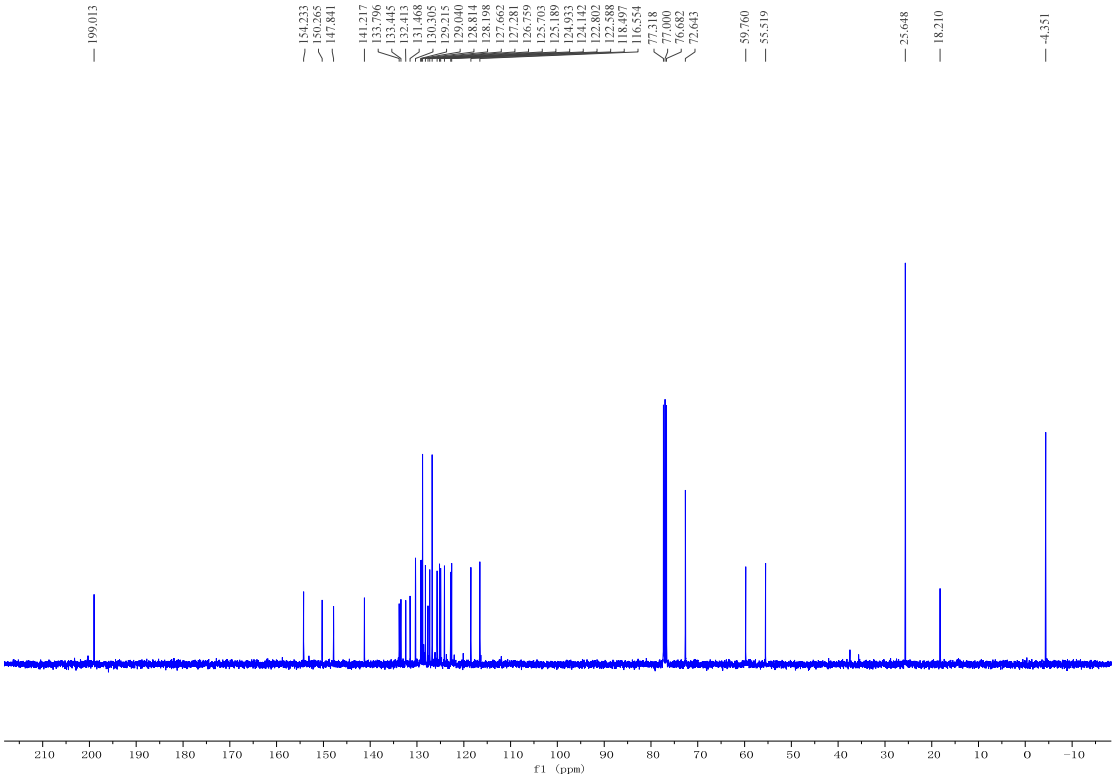


^{1}H and ^{13}C NMR Spectra for Compound 3ia:

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

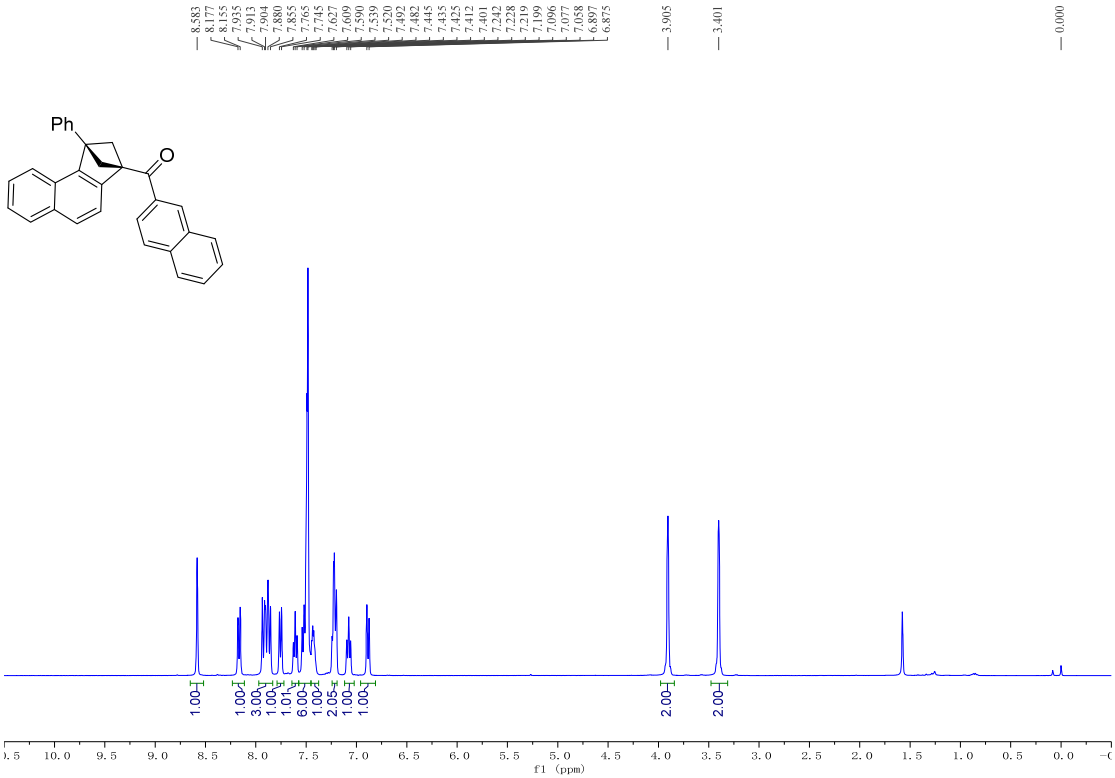


^{13}C NMR (100 MHz, $CDCl_3$)

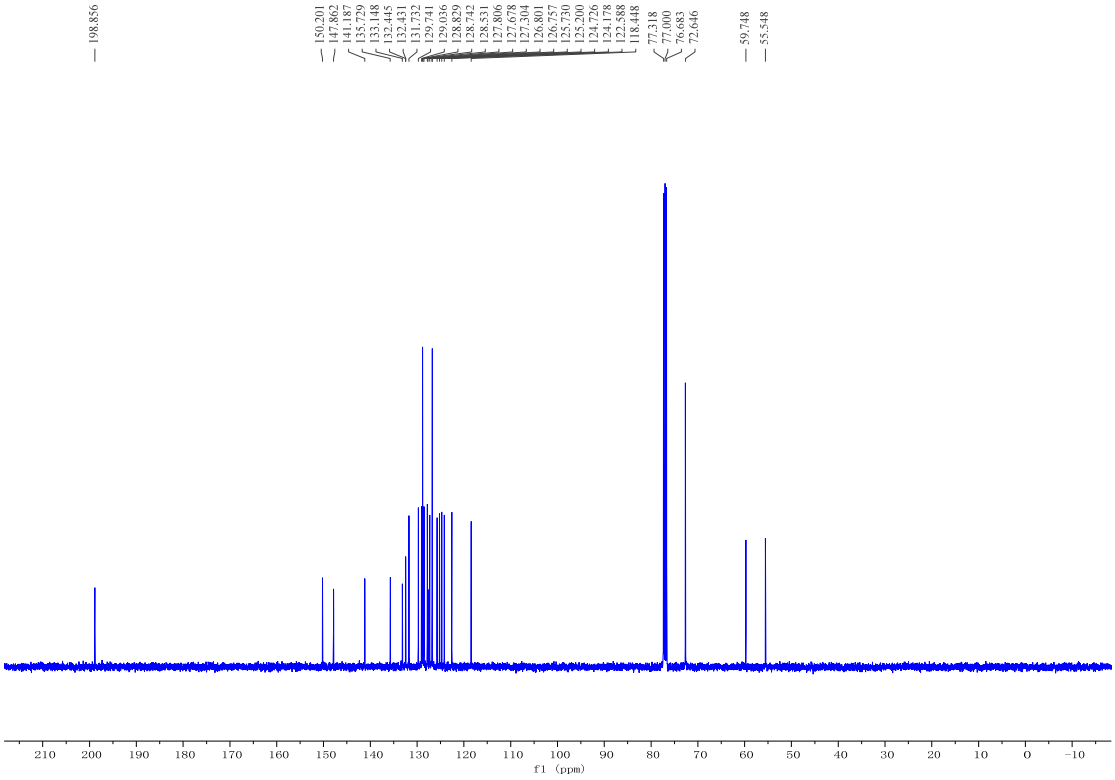


^{1}H and ^{13}C NMR Spectra for Compound 3ja

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

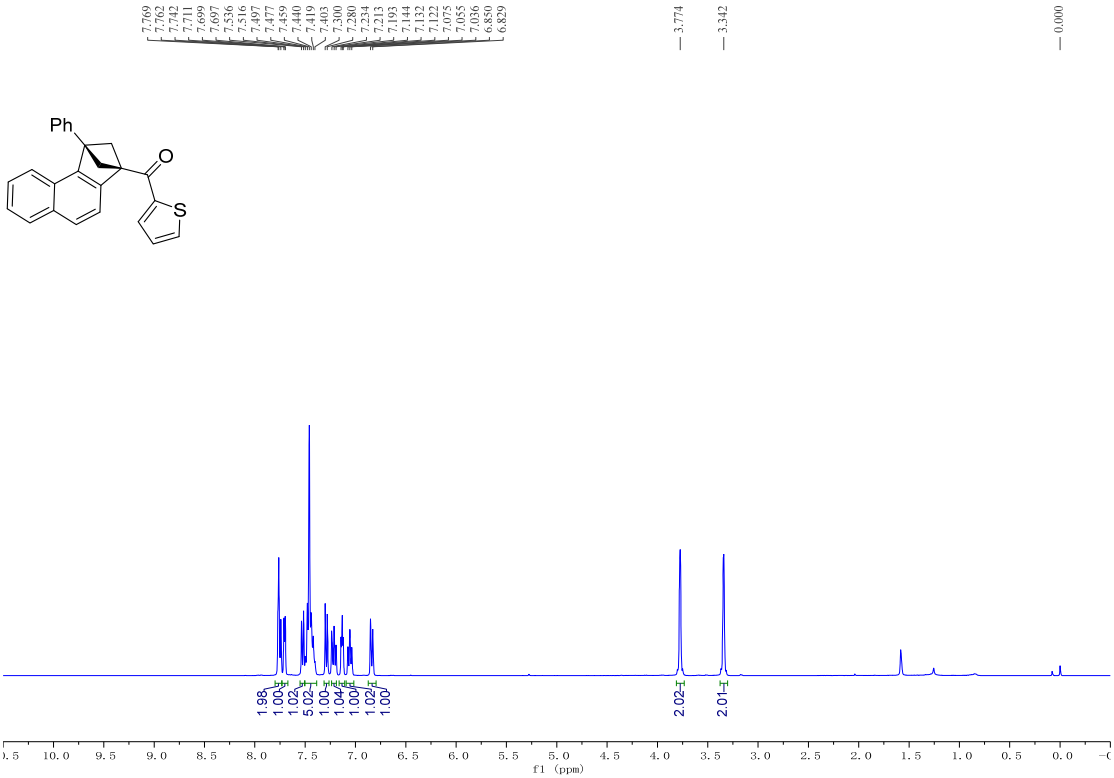


^{13}C NMR (100 MHz, $CDCl_3$)

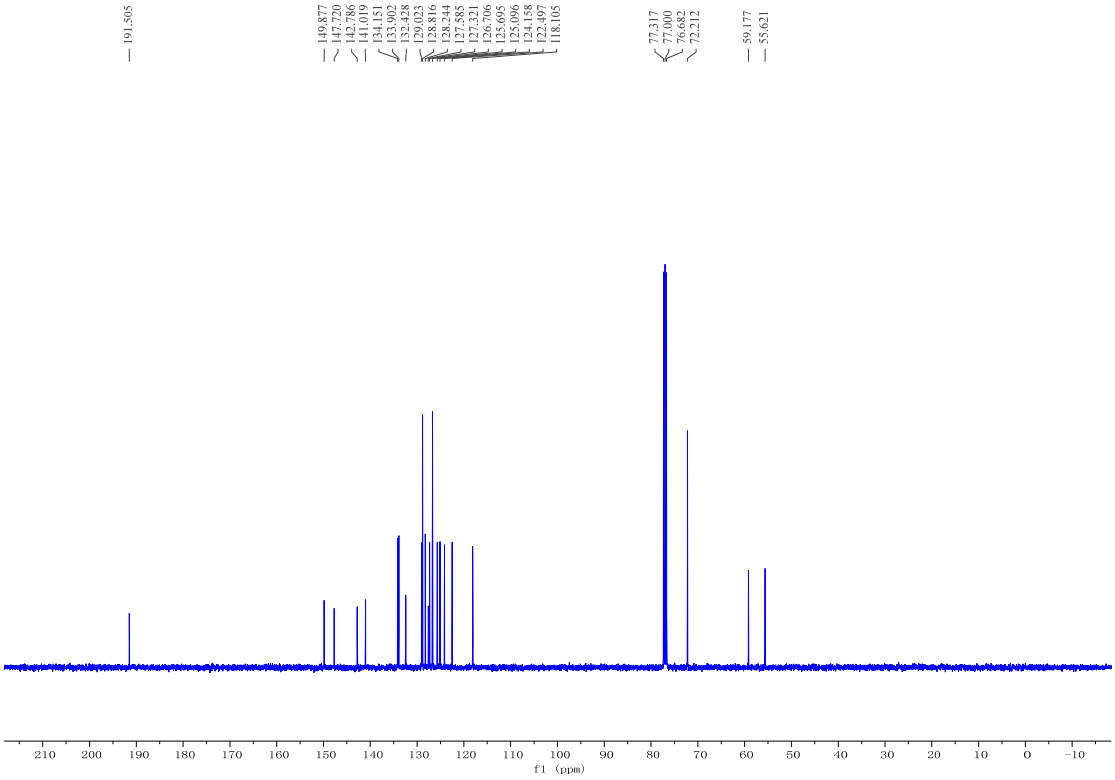


^{1}H and ^{13}C NMR Spectra for Compound 3ka

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

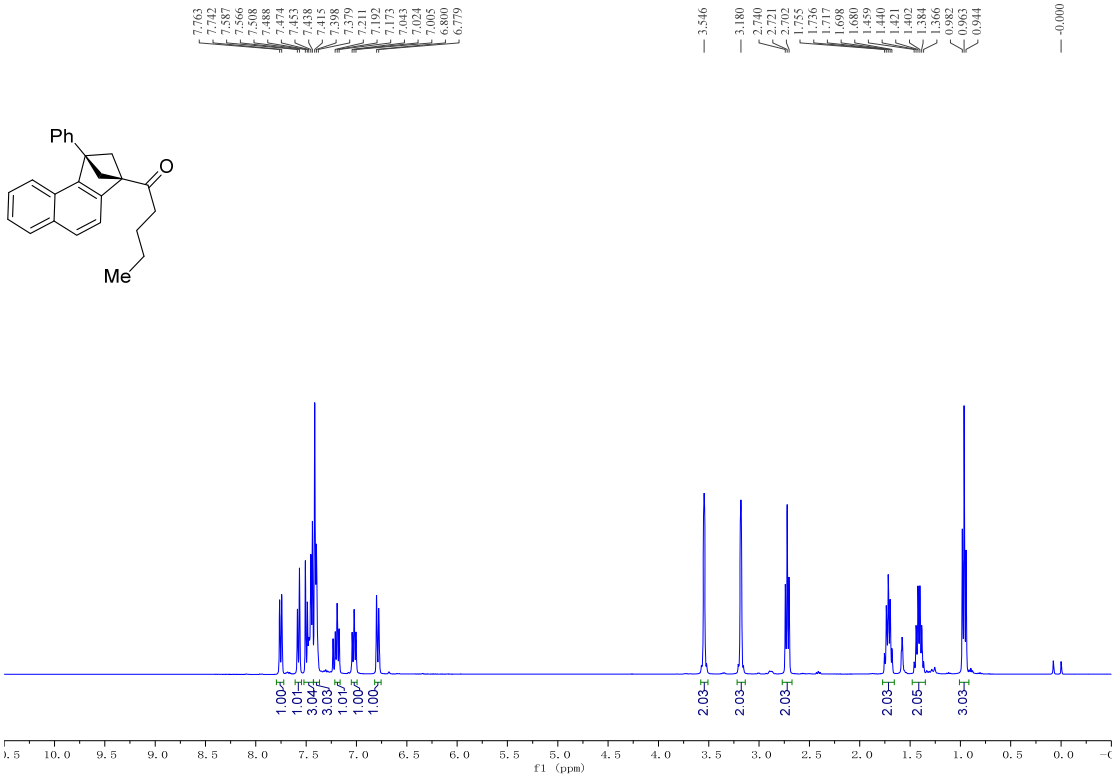


^{13}C NMR (100 MHz, $CDCl_3$)

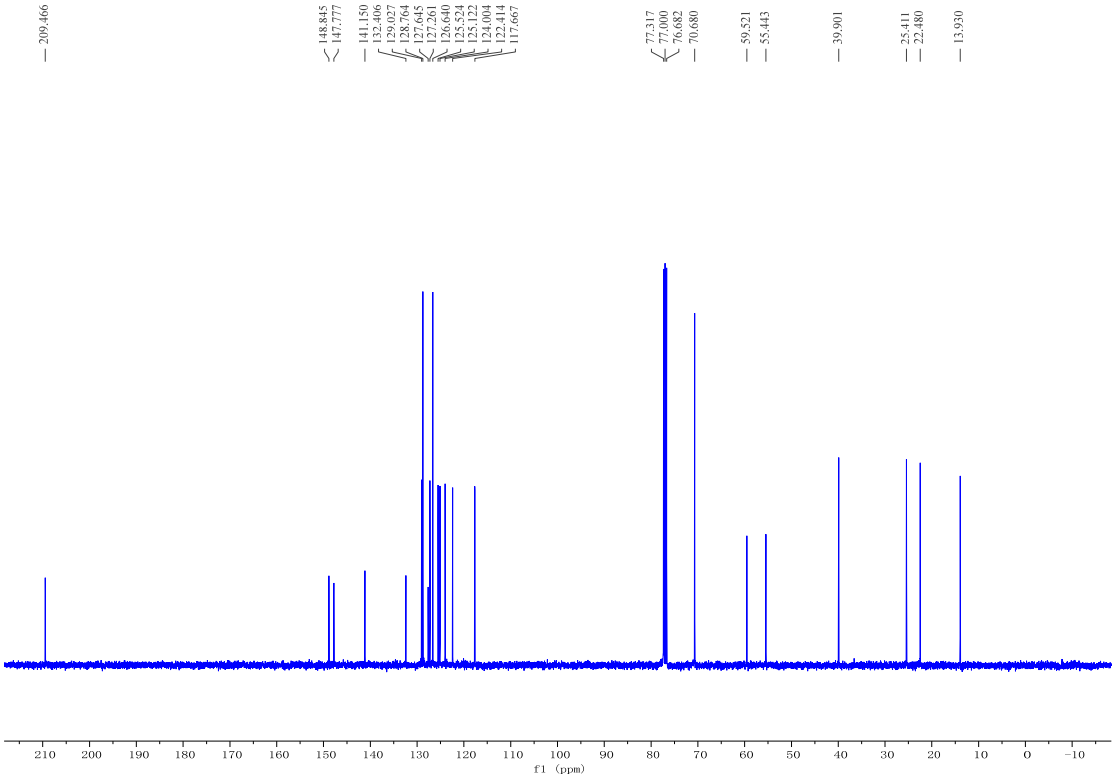


^{1}H and ^{13}C NMR Spectra for Compound 3la

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

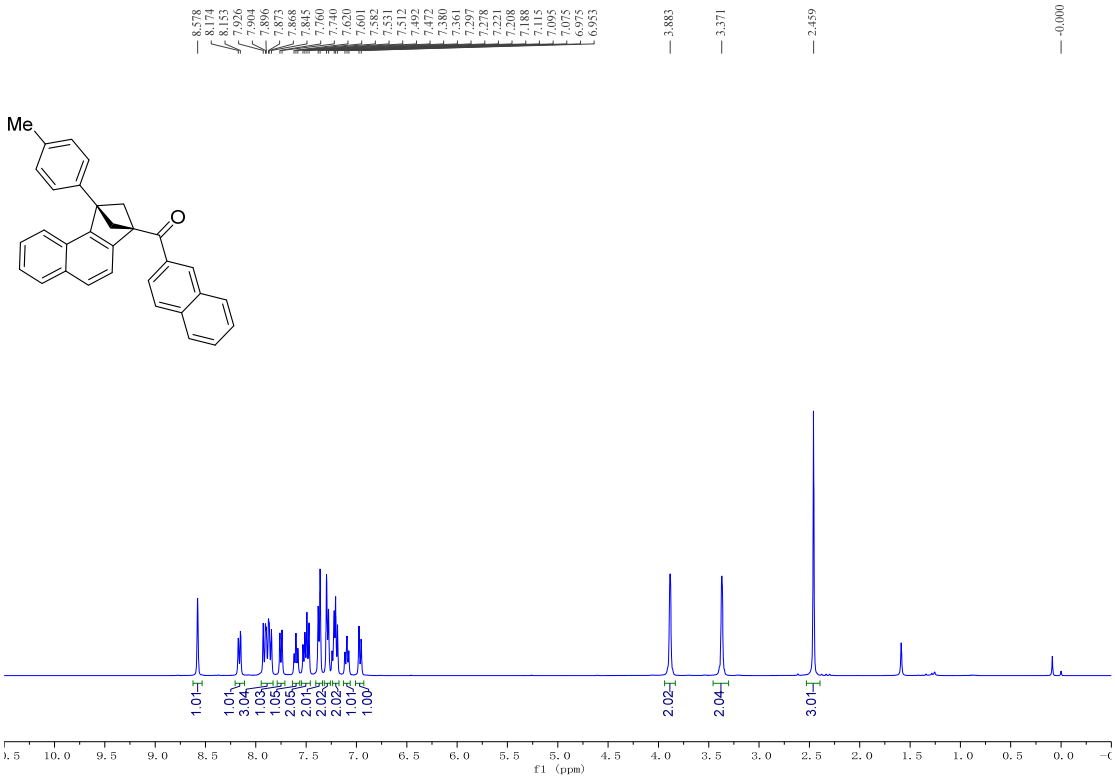


^{13}C NMR (100 MHz, $CDCl_3$)

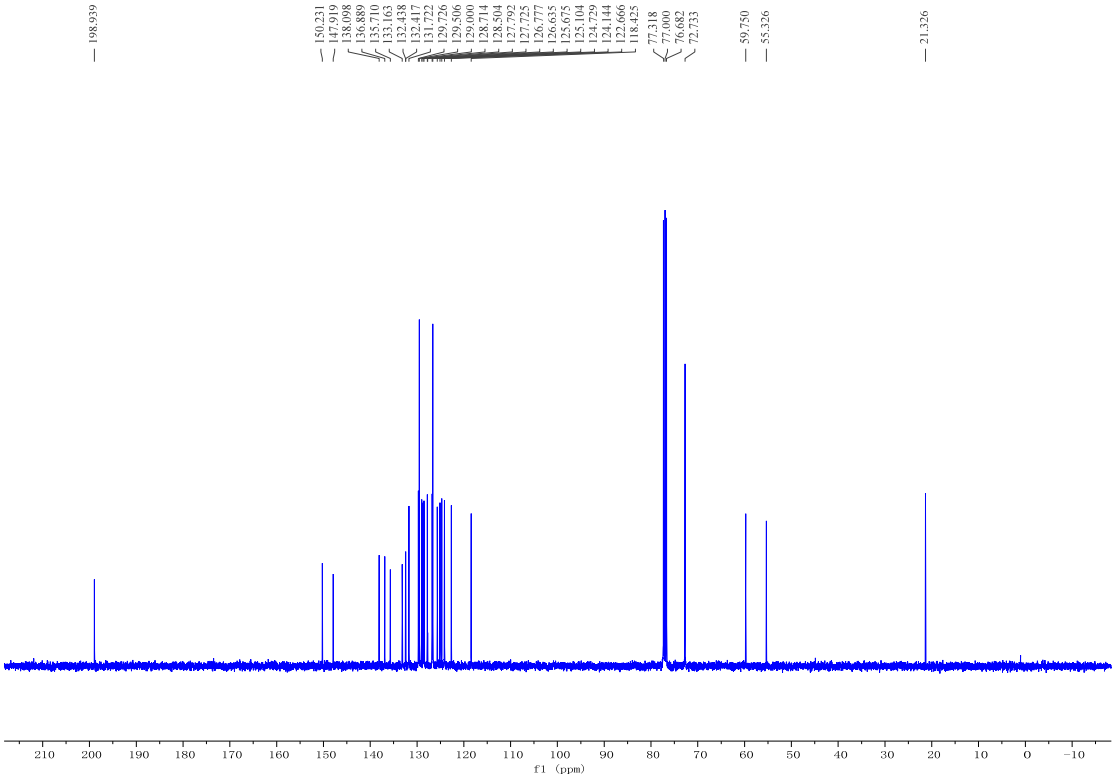


^{1}H and ^{13}C NMR Spectra for Compound 3ma

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

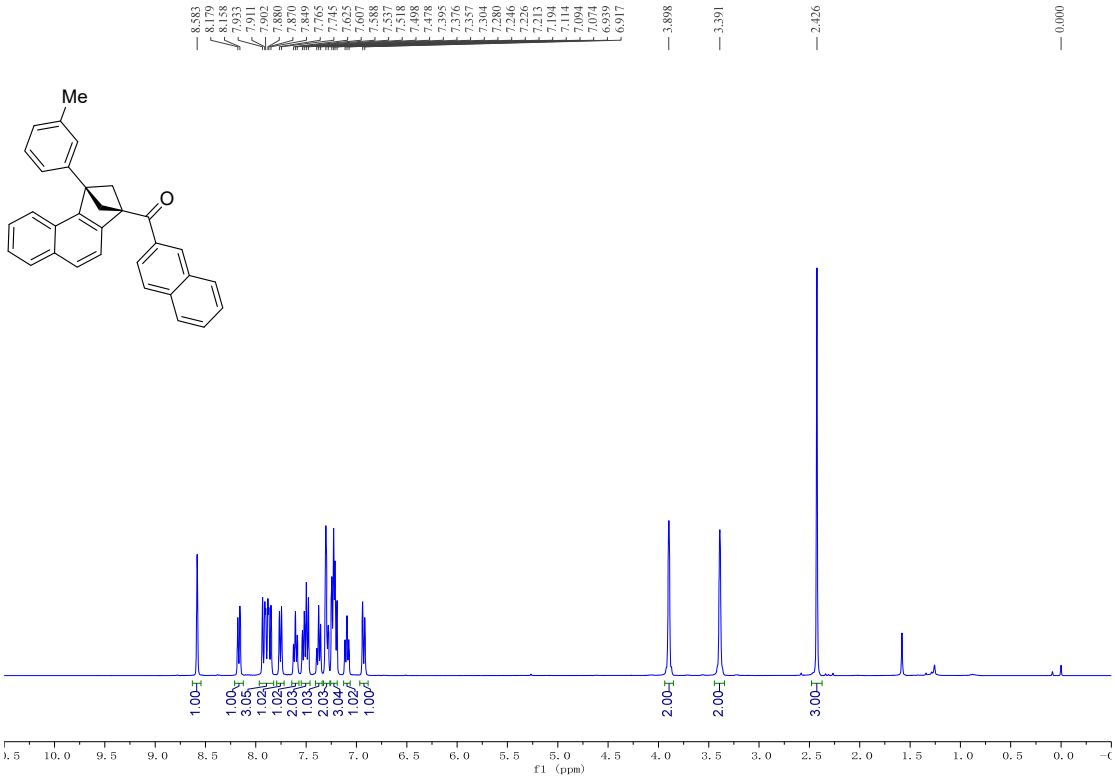


^{13}C NMR (100 MHz, $CDCl_3$)

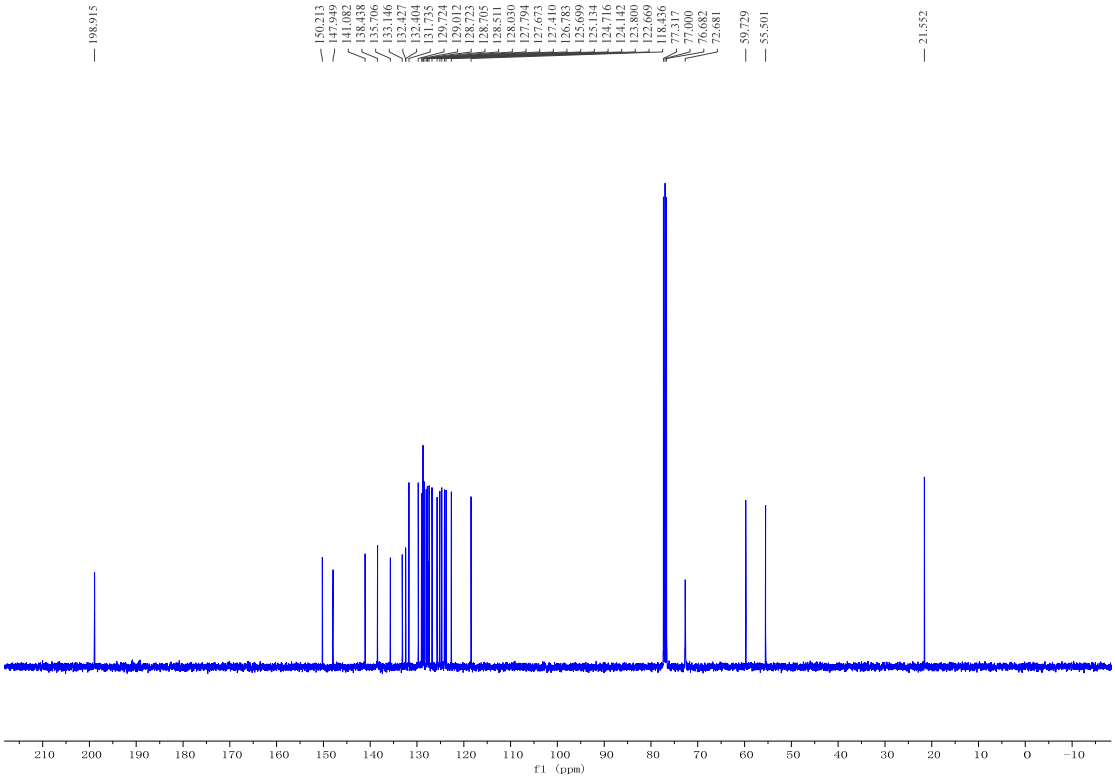


^{1}H and ^{13}C NMR Spectra for Compound 3na

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

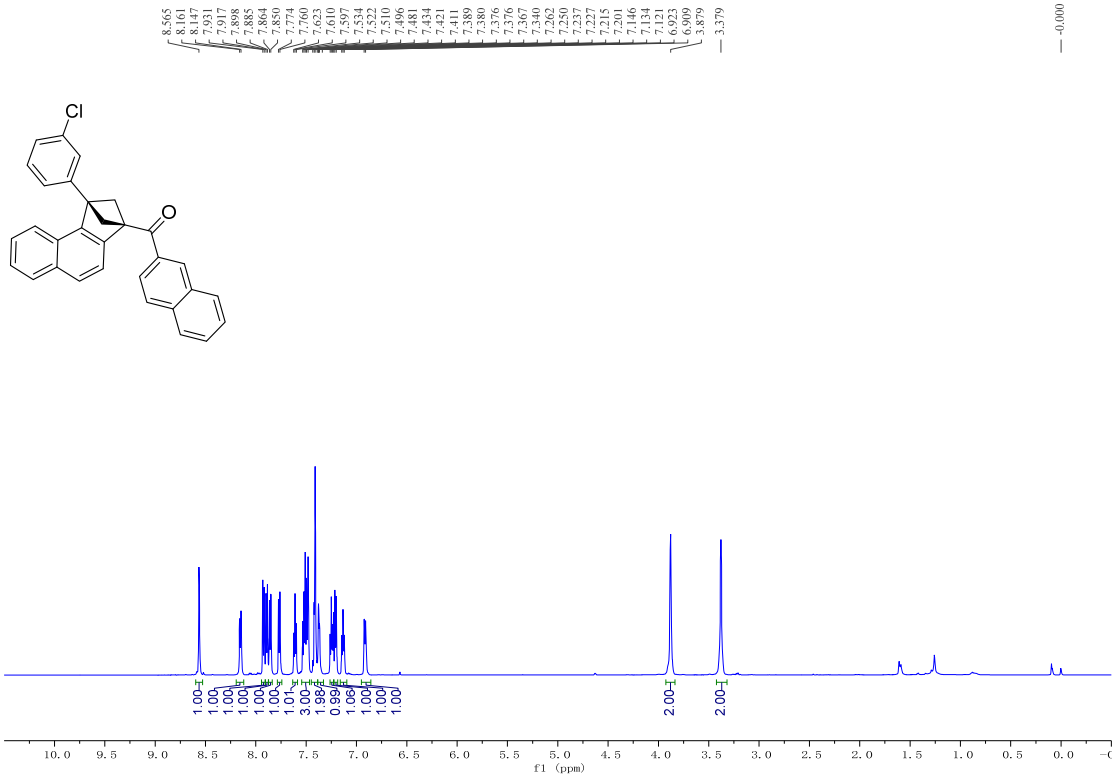


^{13}C NMR (100 MHz, $CDCl_3$)

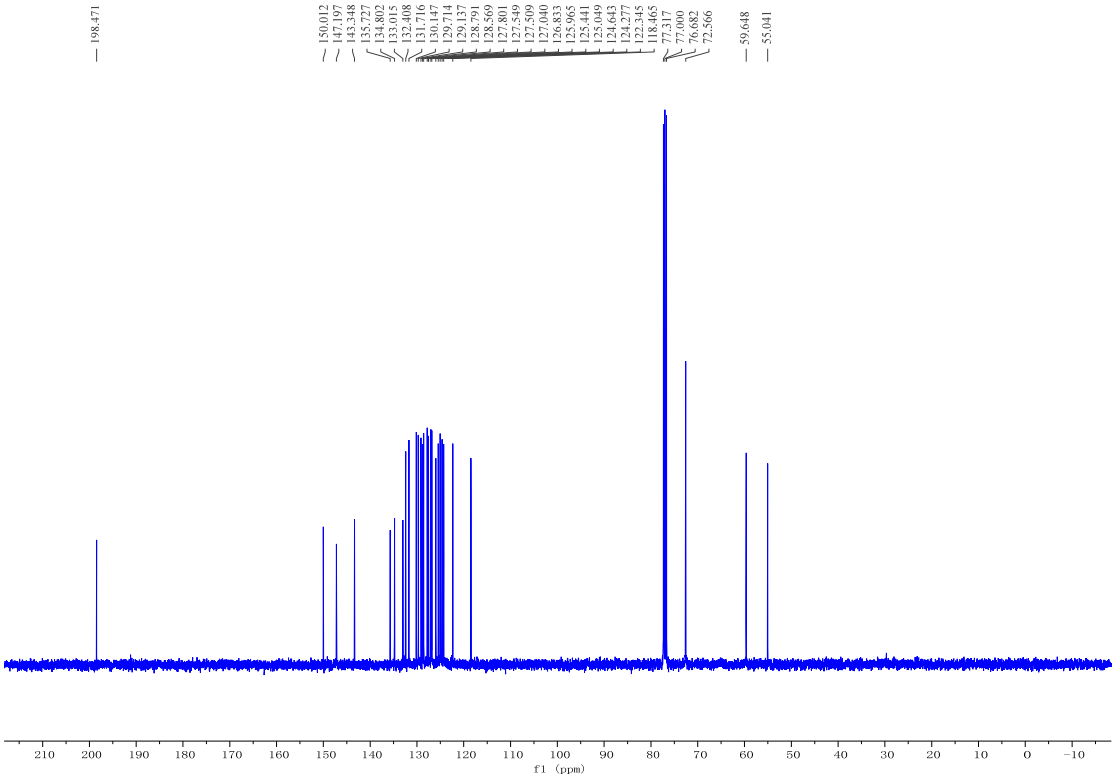


^{1}H and ^{13}C NMR Spectra for Compound 3oa

^{1}H NMR (600 MHz, $CDCl_3$)

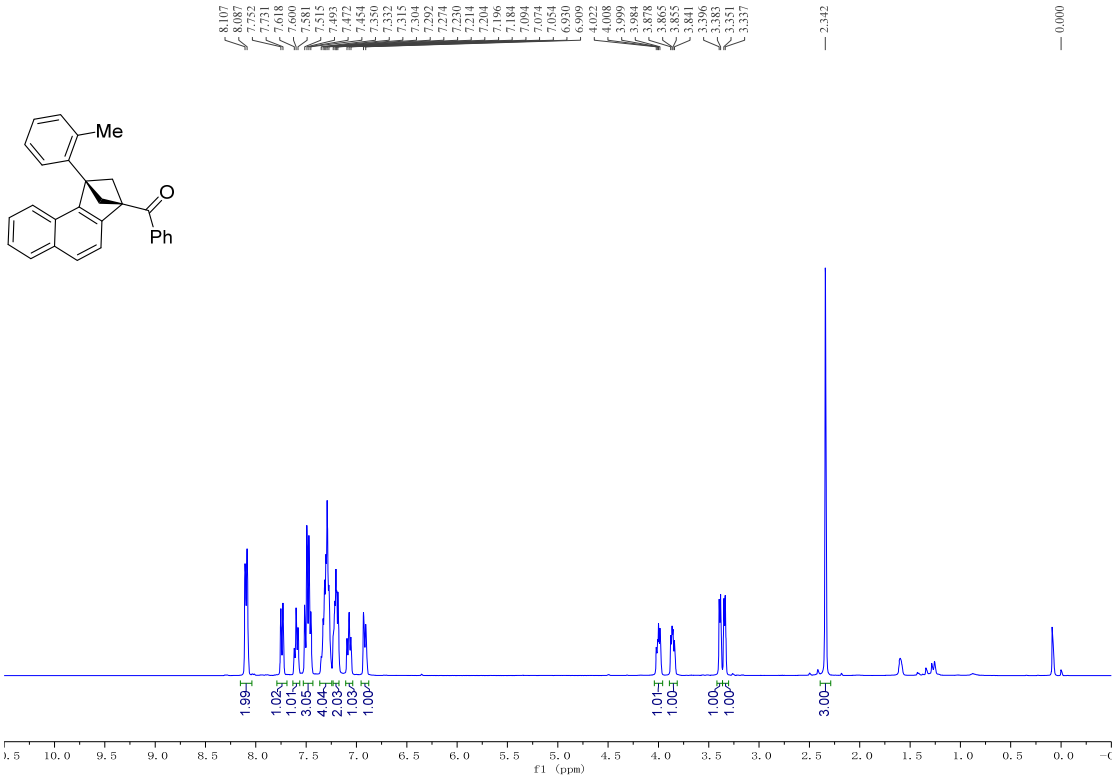


^{13}C NMR (100 MHz, $CDCl_3$)

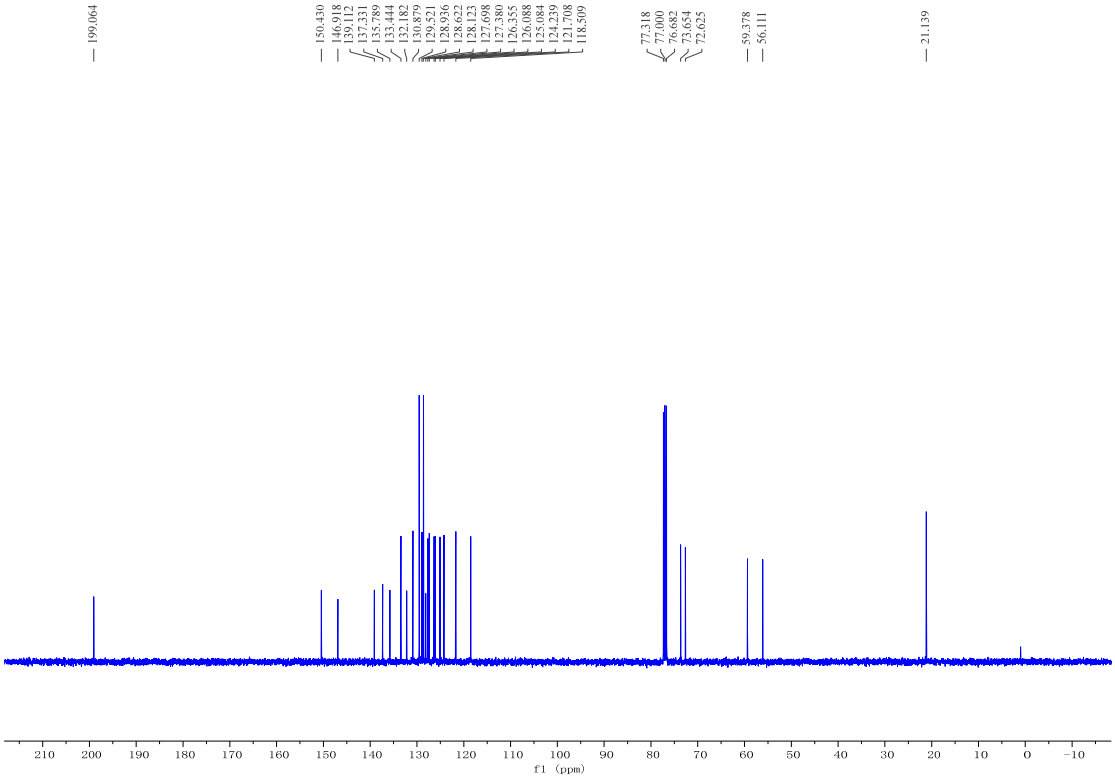


^{1}H and ^{13}C NMR Spectra for Compound 3pa

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

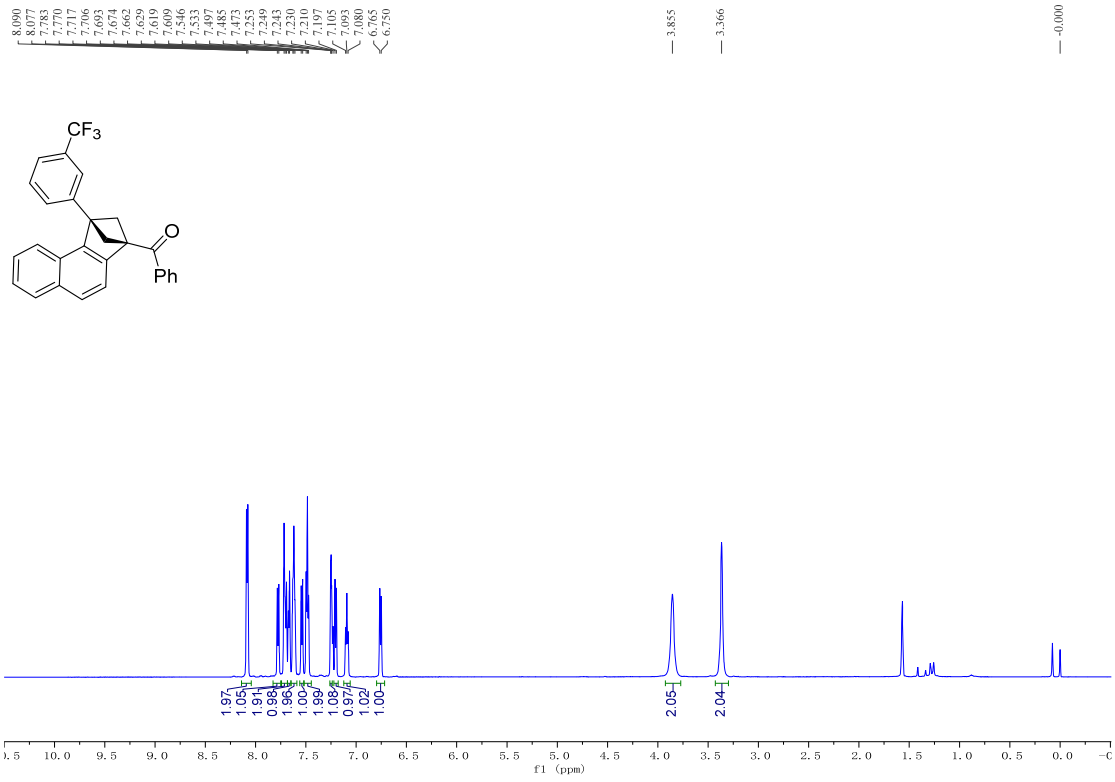


^{13}C NMR (100 MHz, $CDCl_3$)

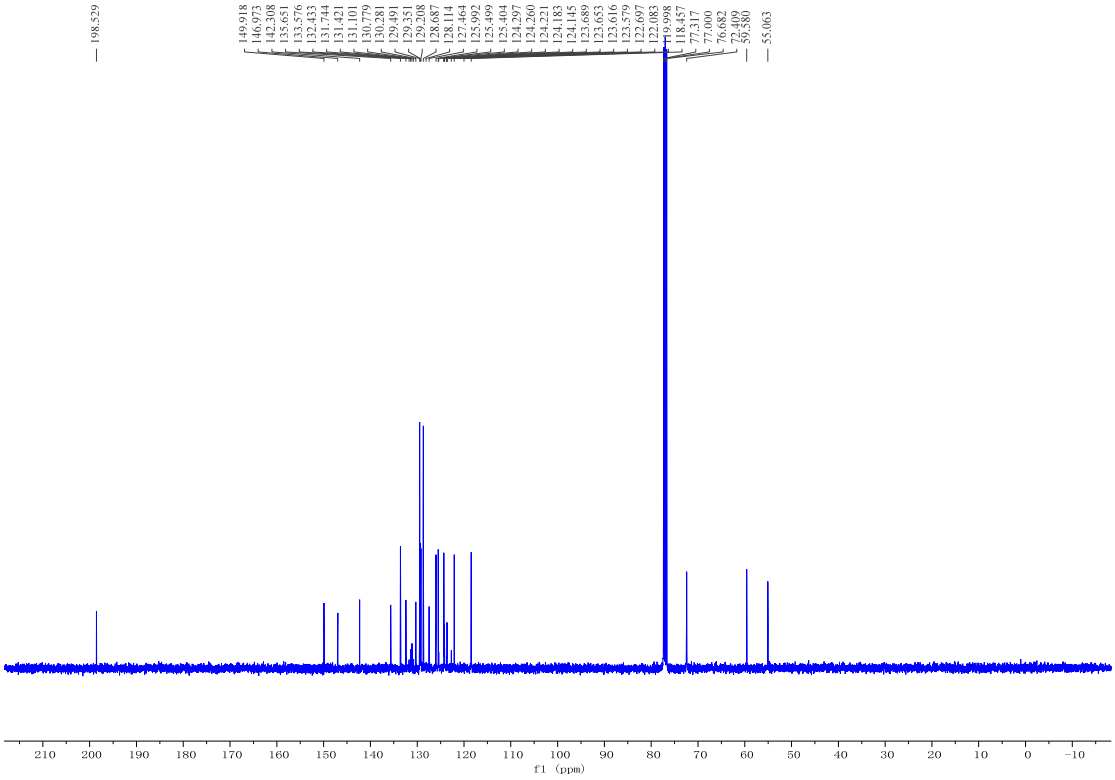


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound 3qa

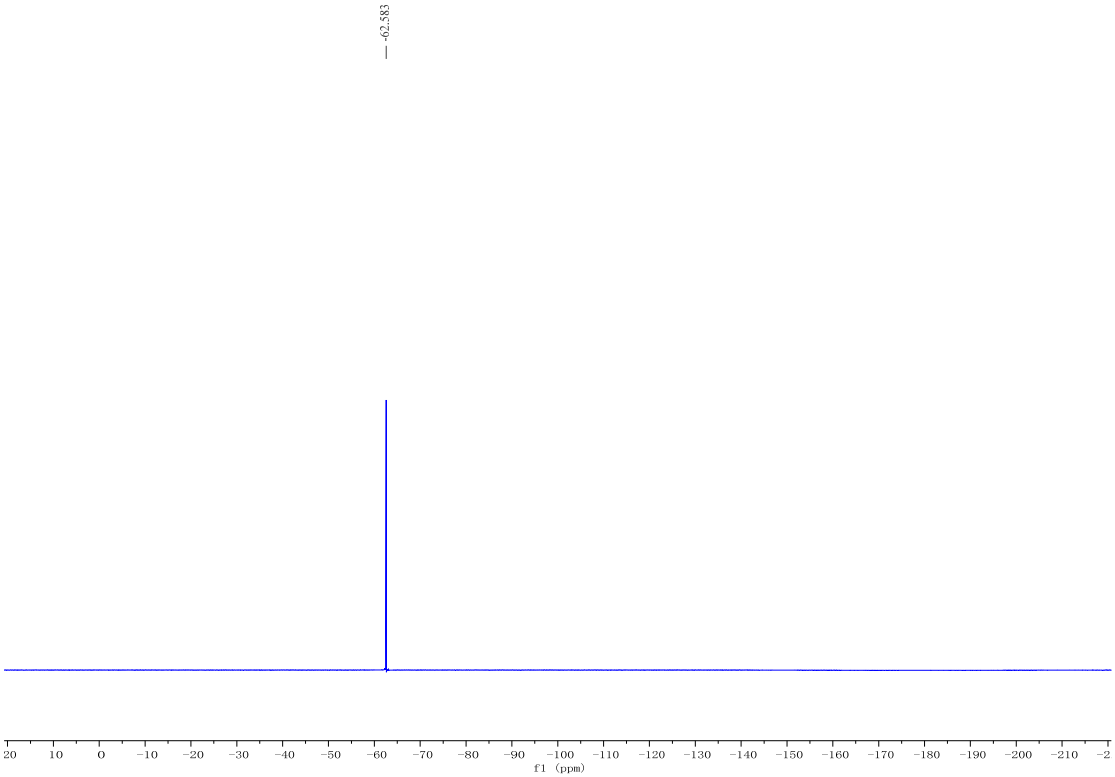
^{1}H NMR (600 MHz, $CDCl_3$)



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

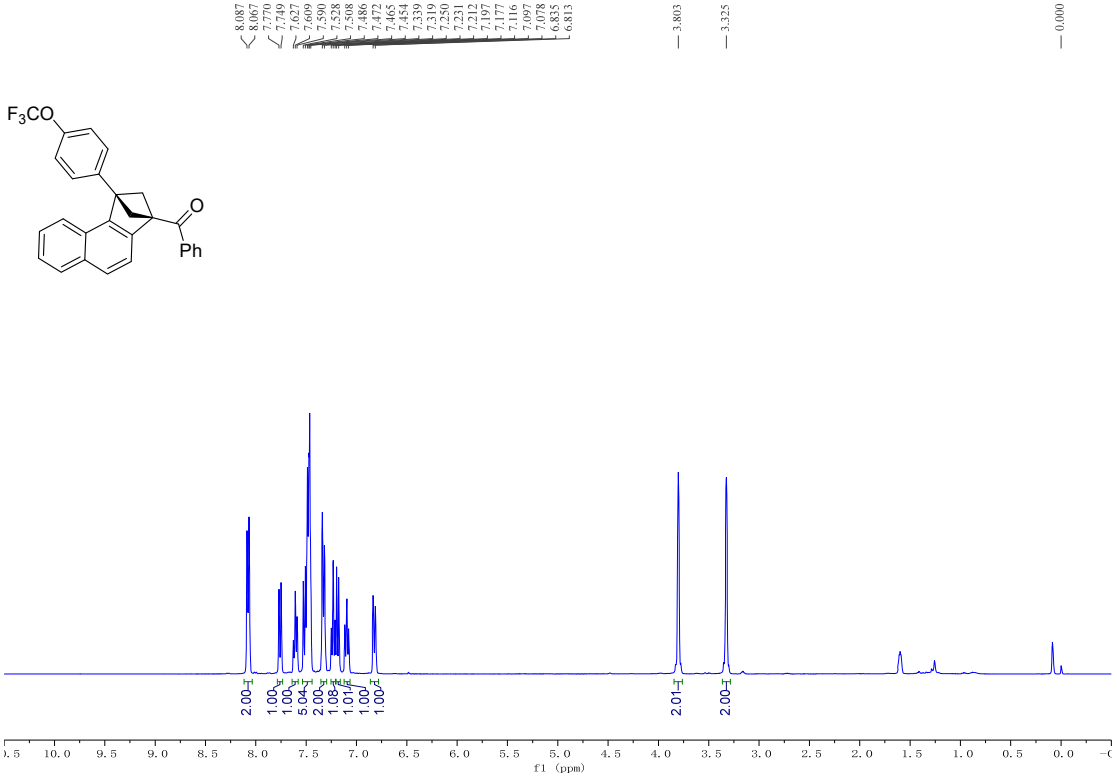


^{19}F NMR (376 MHz, $CDCl_3$)

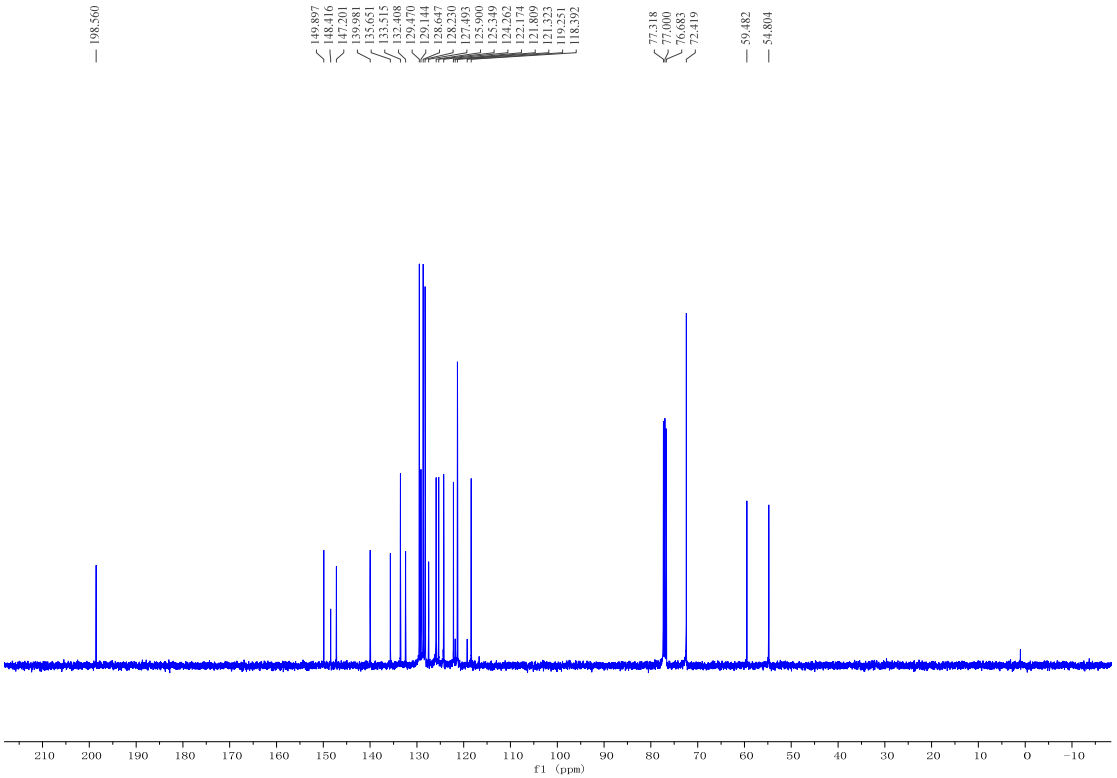


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound 3ra

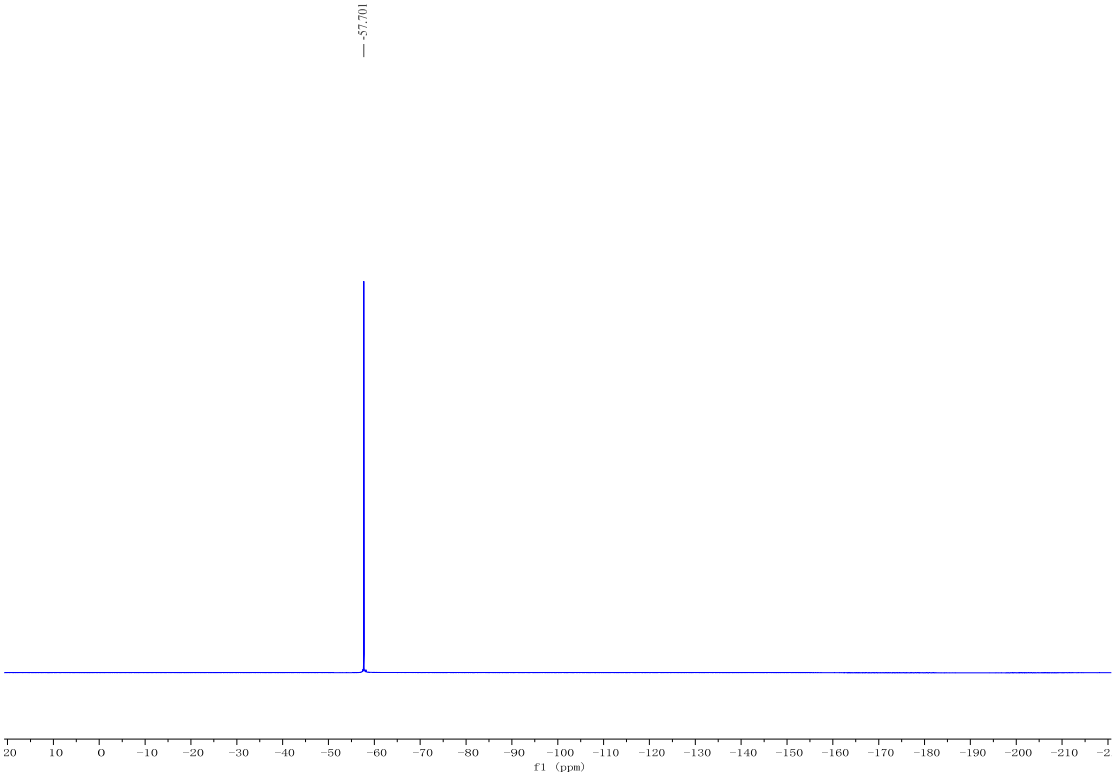
^{1}H NMR (400 MHz, $CDCl_3$)



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

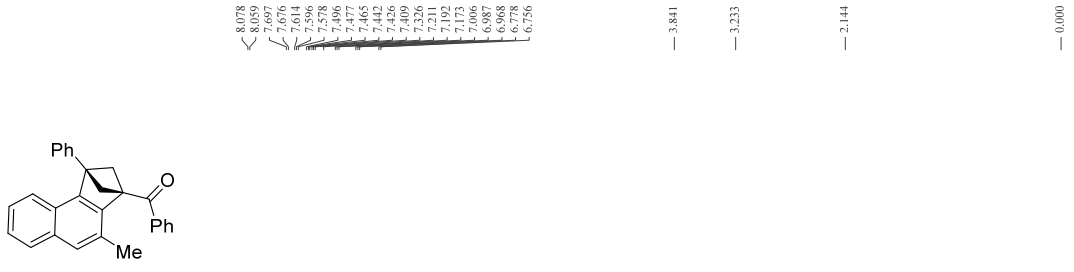


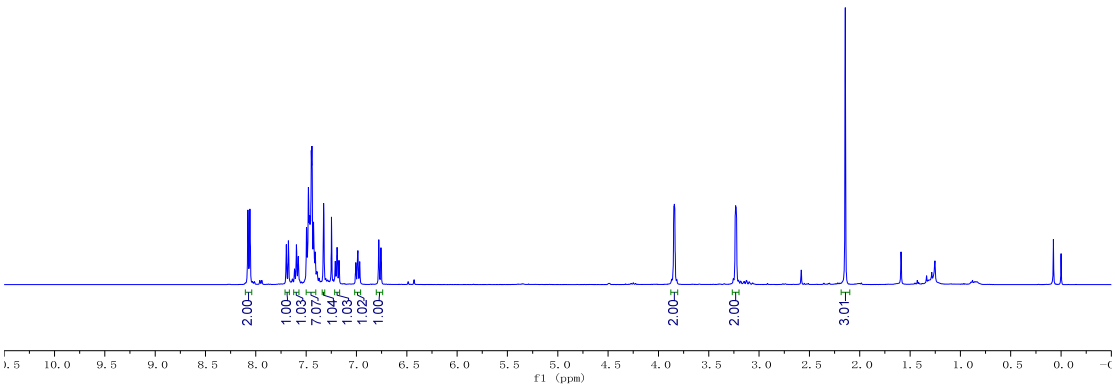
^{19}F NMR (376 MHz, $CDCl_3$)



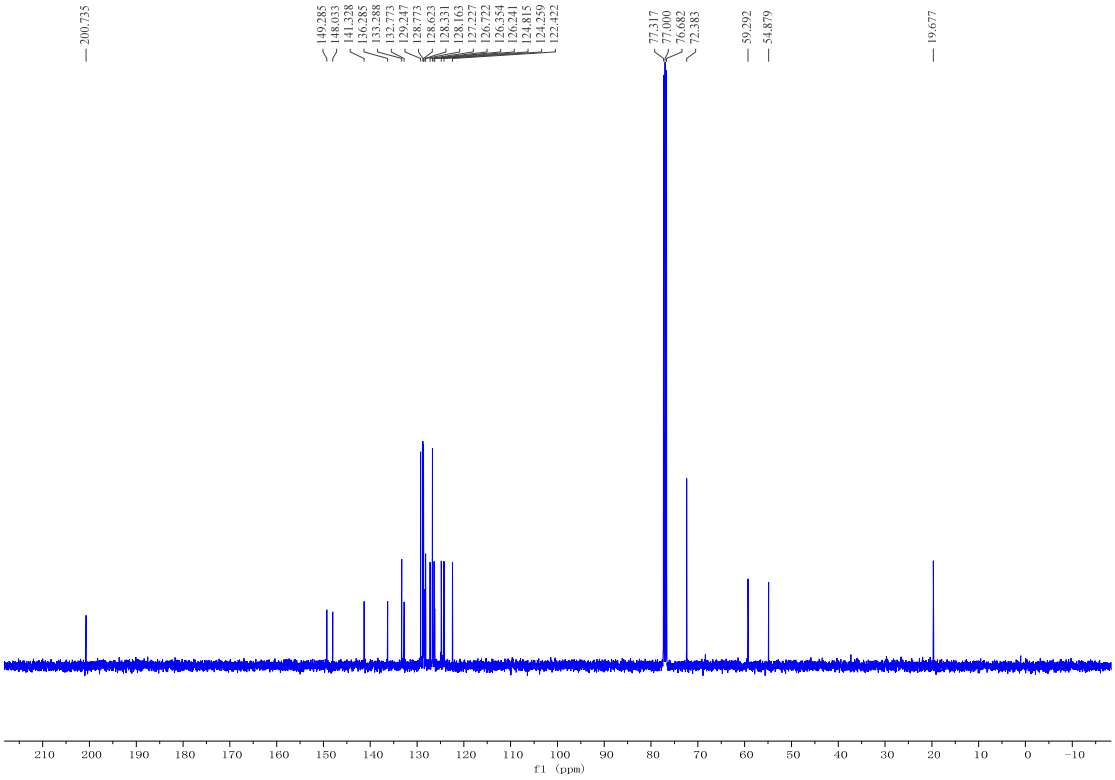
^{1}H and ^{13}C NMR Spectra for Compound 3ab

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



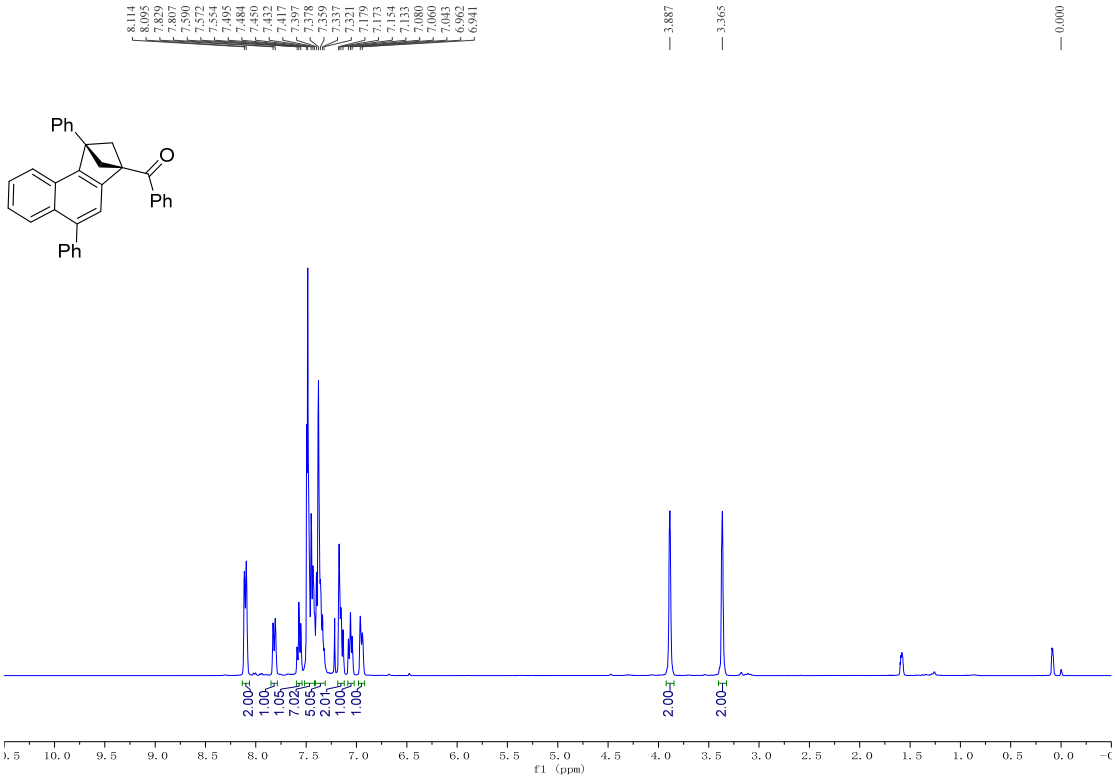


^{13}C NMR (100 MHz, $CDCl_3$)

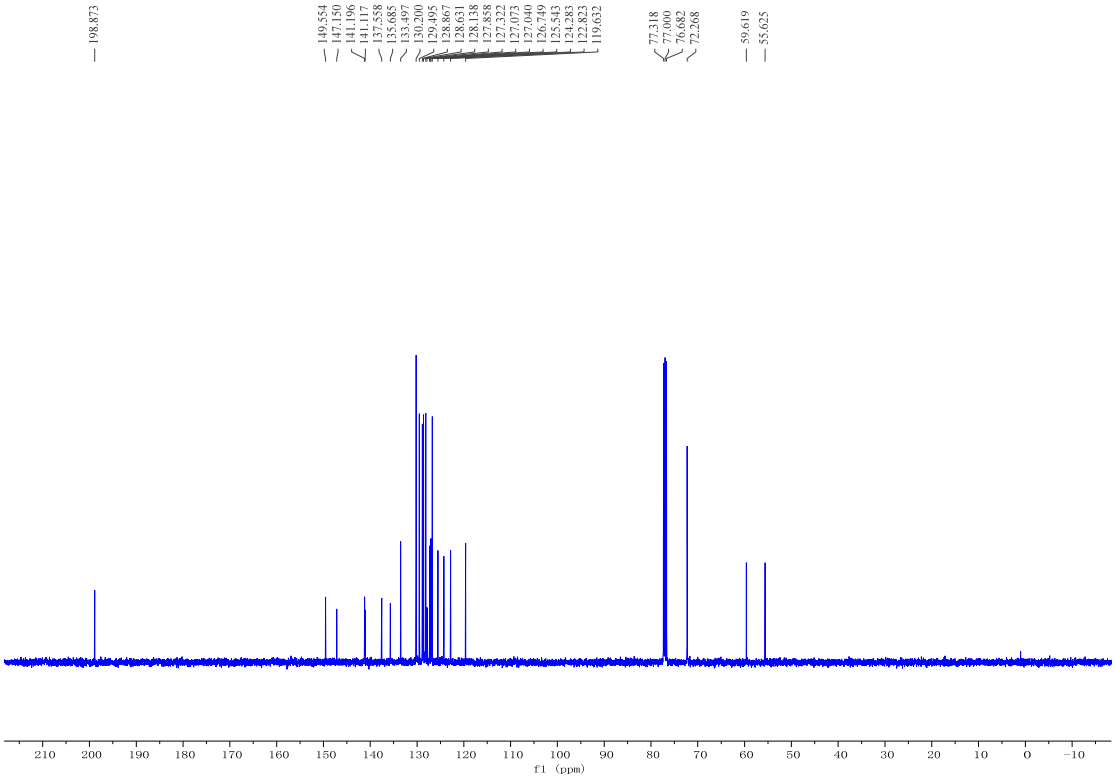


^{1}H and ^{13}C NMR Spectra for Compound 3ac

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

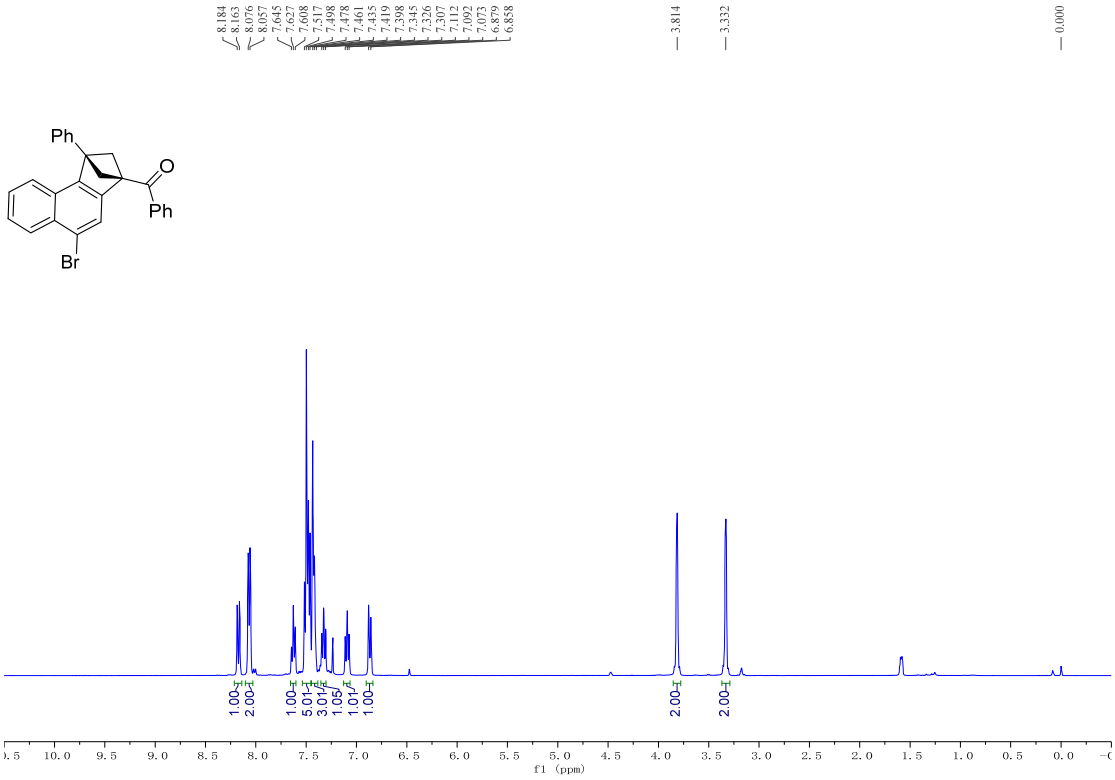


^{13}C NMR (100 MHz, $CDCl_3$)

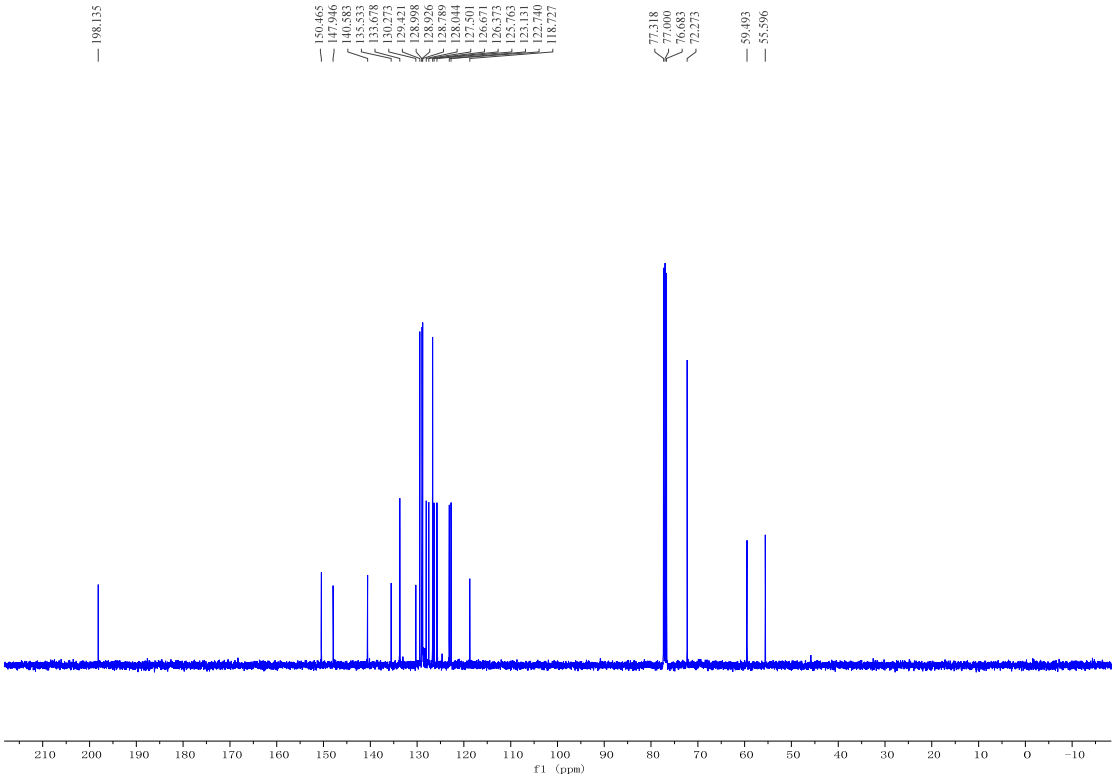


^{1}H and ^{13}C NMR Spectra for Compound 3ad

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

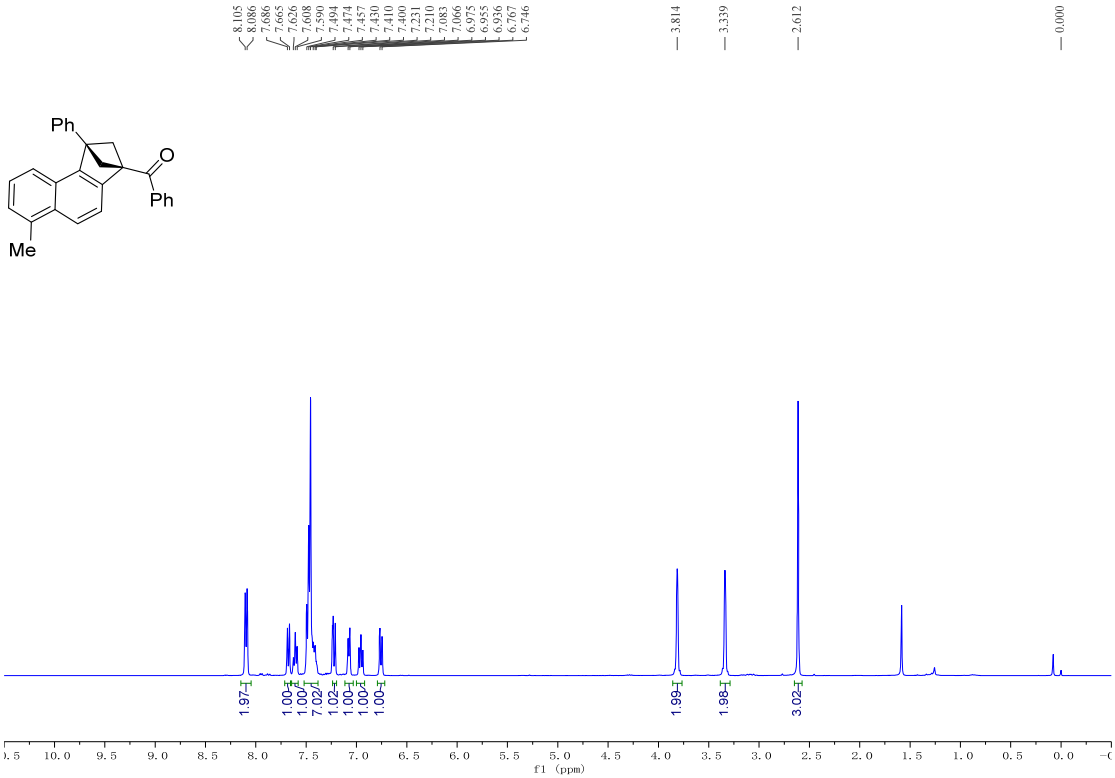


^{13}C NMR (100 MHz, $CDCl_3$)

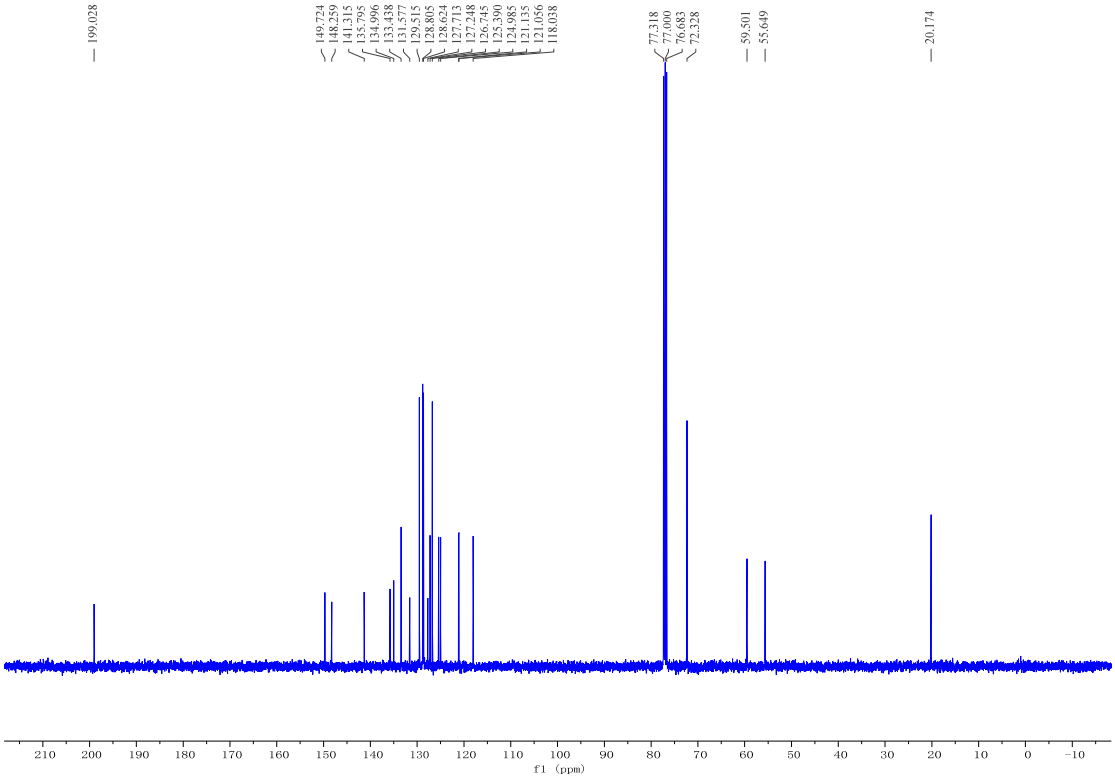


^{1}H and ^{13}C NMR Spectra for Compound 3ae

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

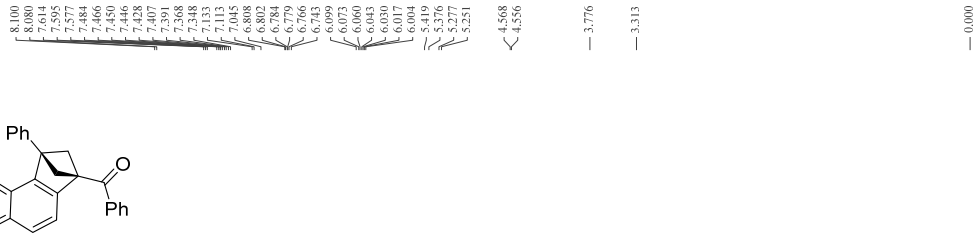


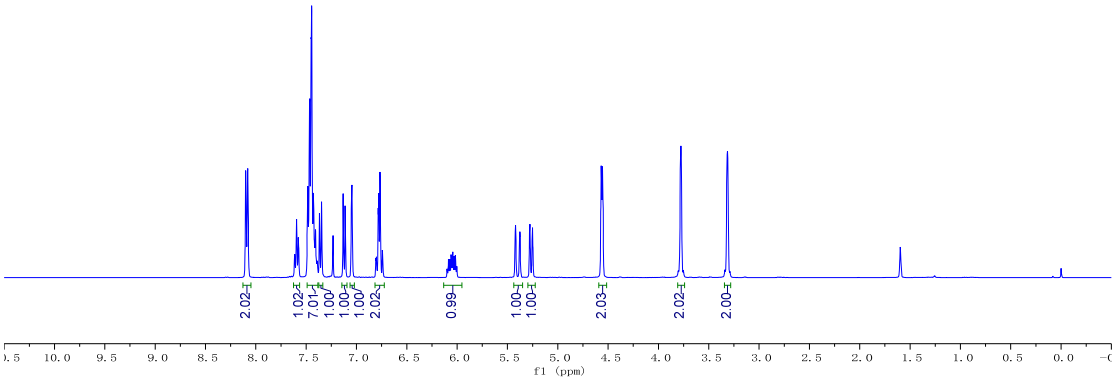
^{13}C NMR (100 MHz, $CDCl_3$)



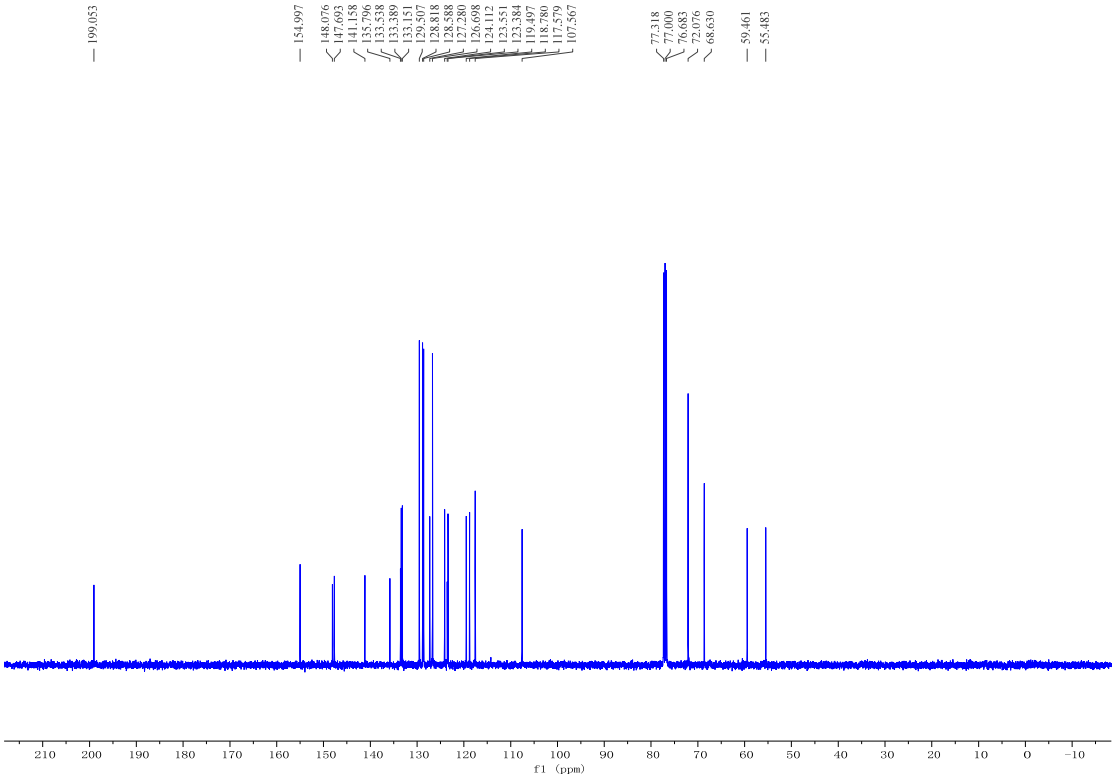
^{1}H and ^{13}C NMR Spectra for Compound 3af

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



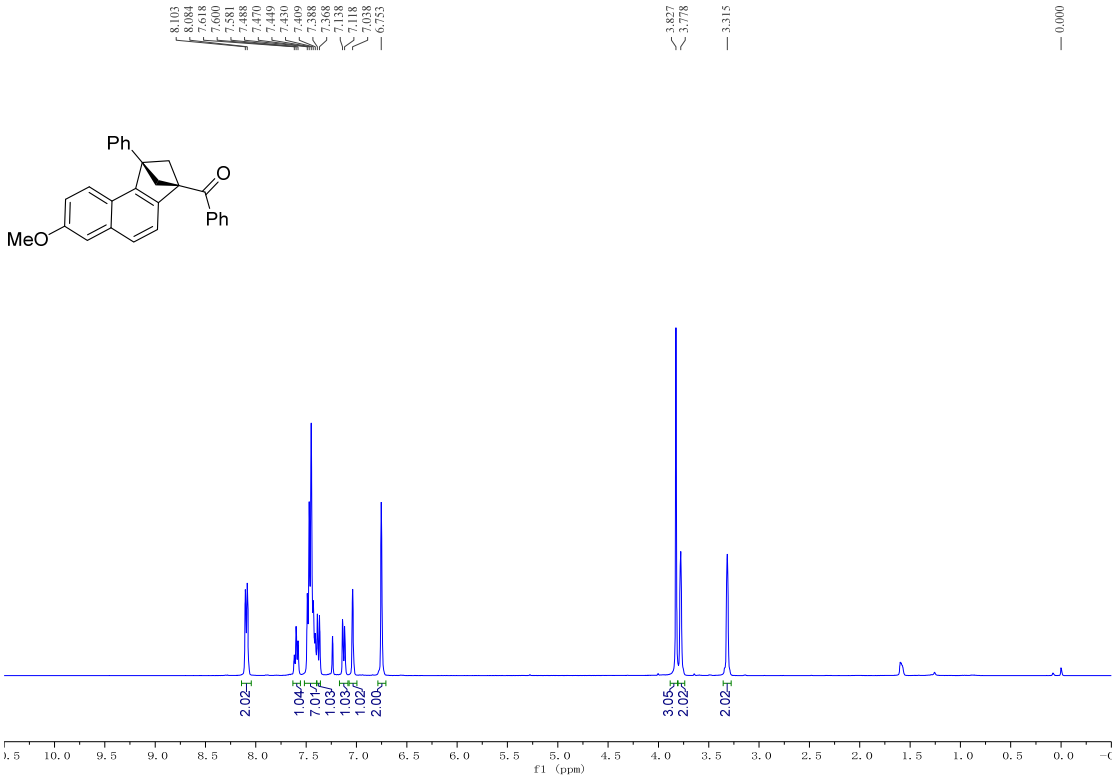


^{13}C NMR (100 MHz, $CDCl_3$)

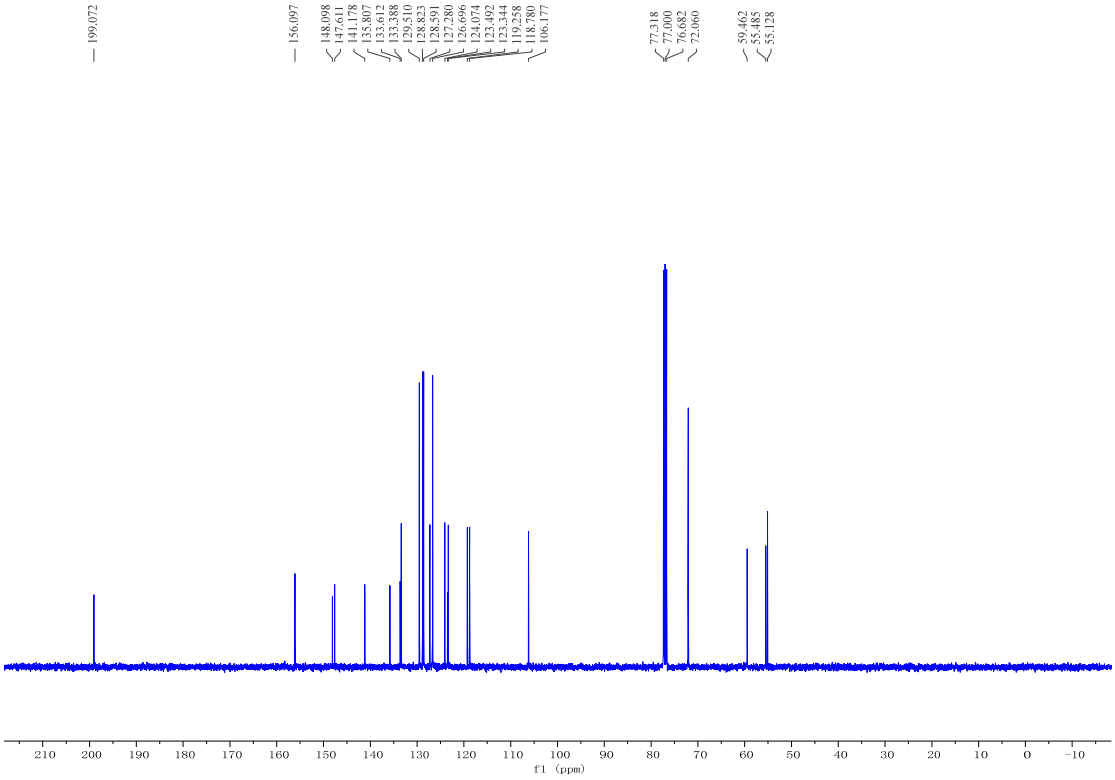


^{1}H and ^{13}C NMR Spectra for Compound 3ag

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

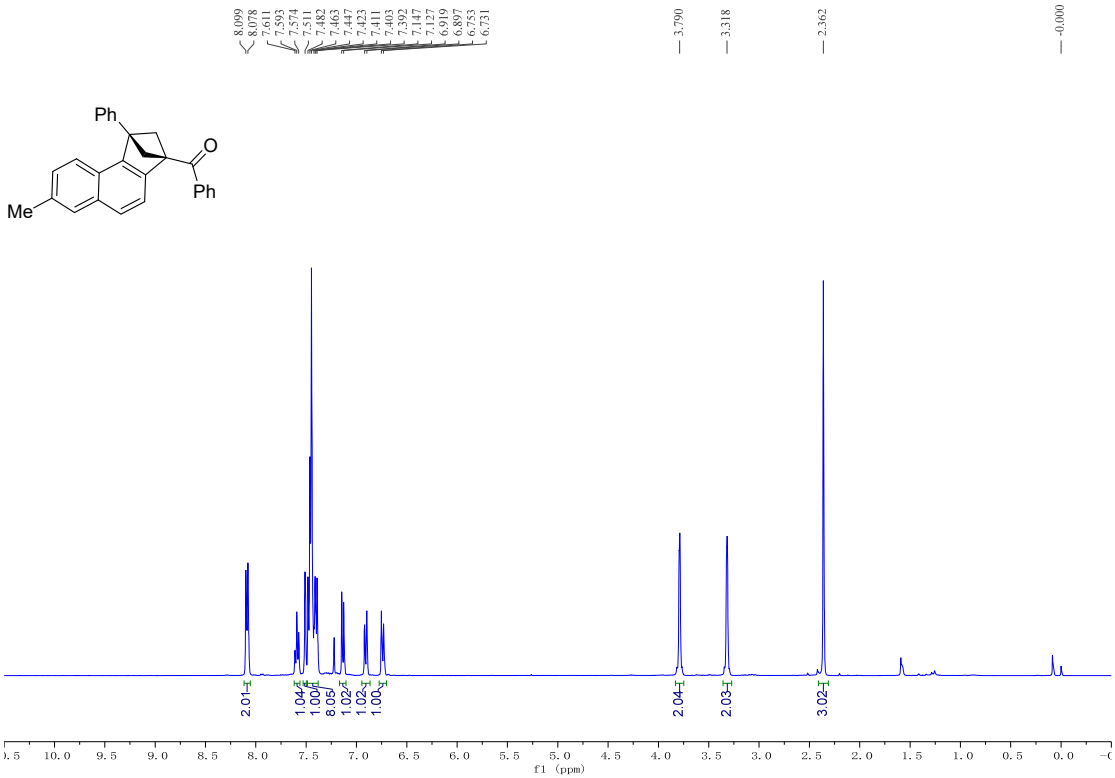


^{13}C NMR (100 MHz, $CDCl_3$)

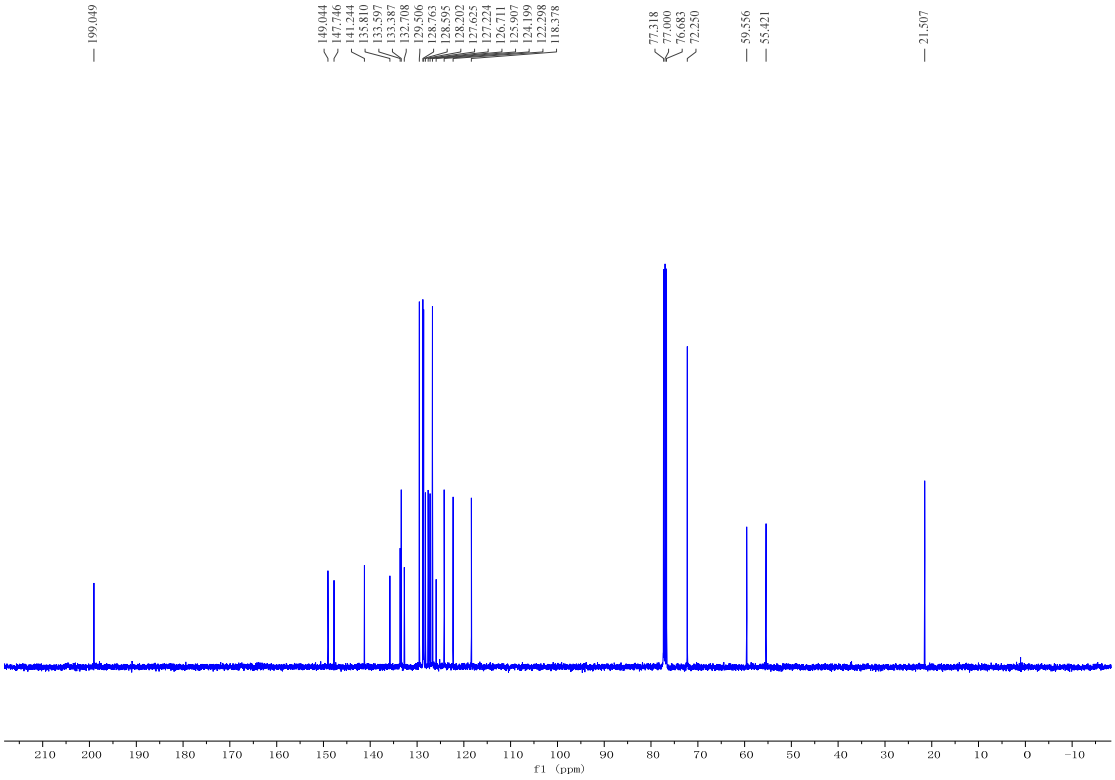


^{1}H and ^{13}C NMR Spectra for Compound 3ah

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

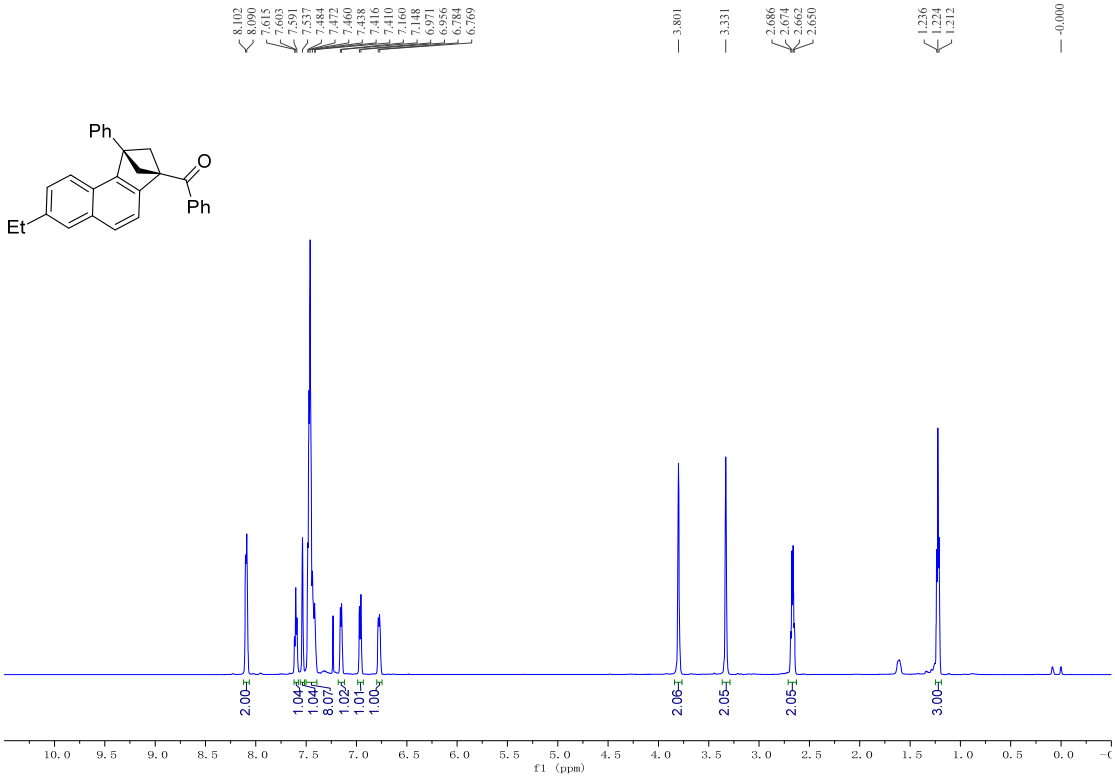


^{13}C NMR (100 MHz, $CDCl_3$)

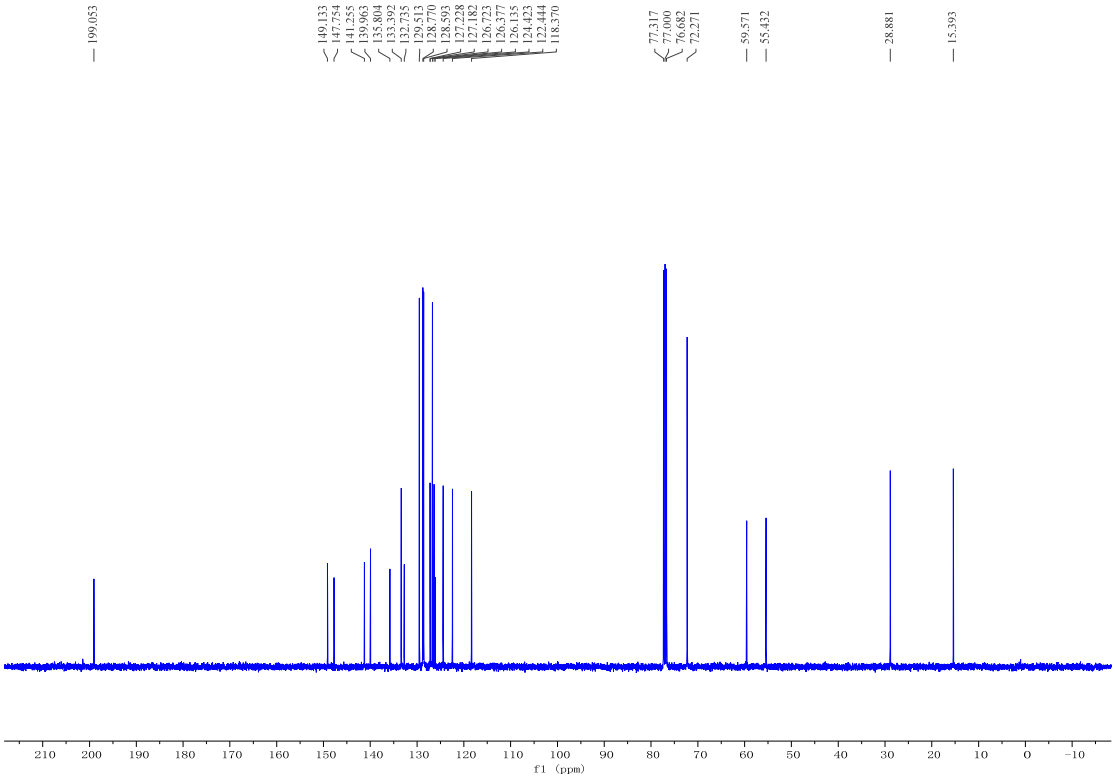


^{1}H and ^{13}C NMR Spectra for Compound 3ai

^{1}H NMR (600 MHz, $CDCl_3$)

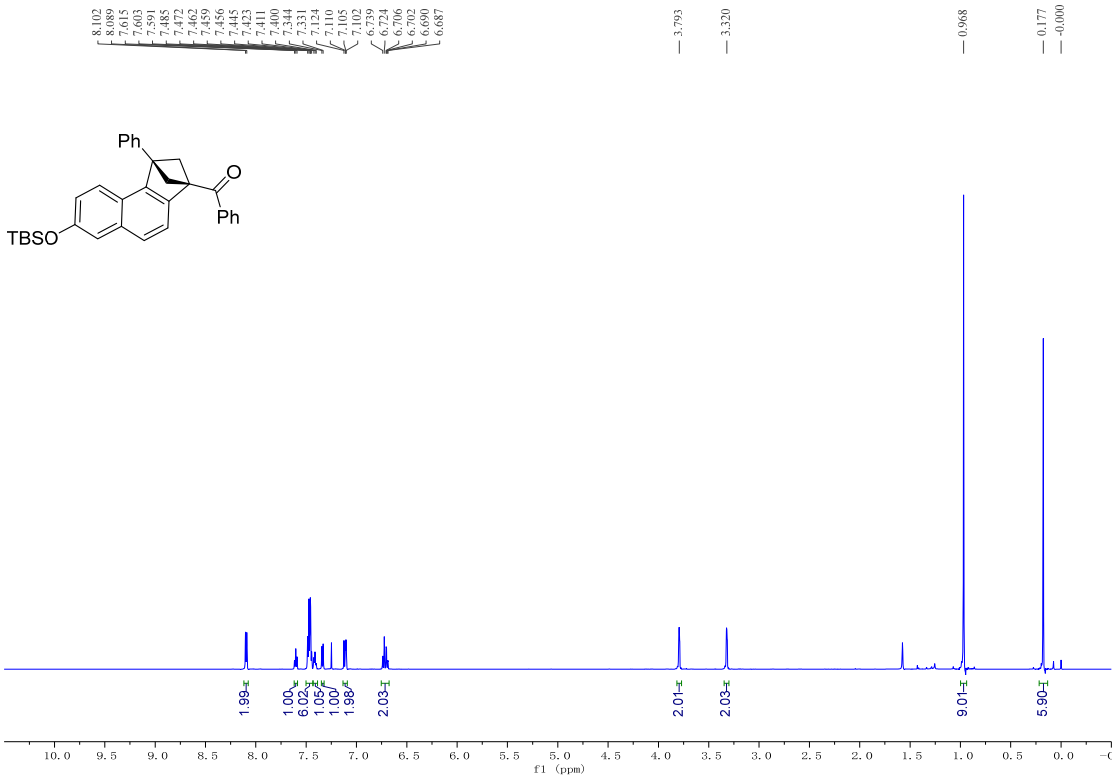


^{13}C NMR (100 MHz, $CDCl_3$)

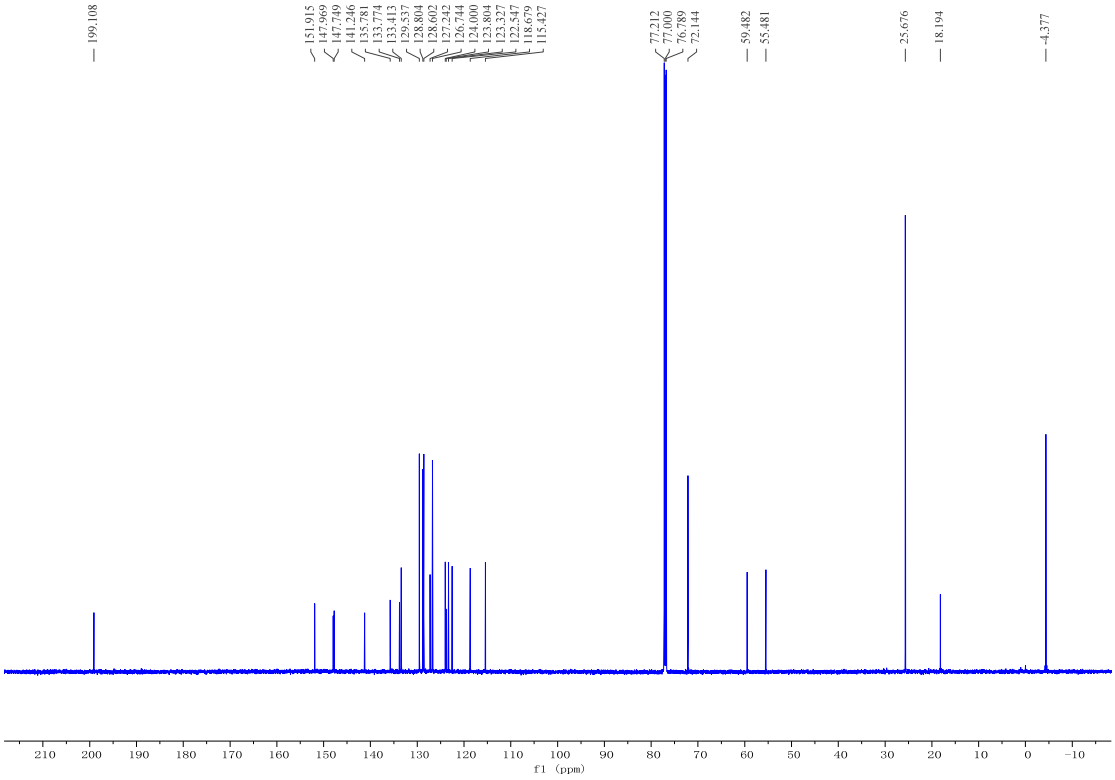


^{1}H and ^{13}C NMR Spectra for Compound 3aj

^{1}H NMR (600 MHz, $CDCl_3$)

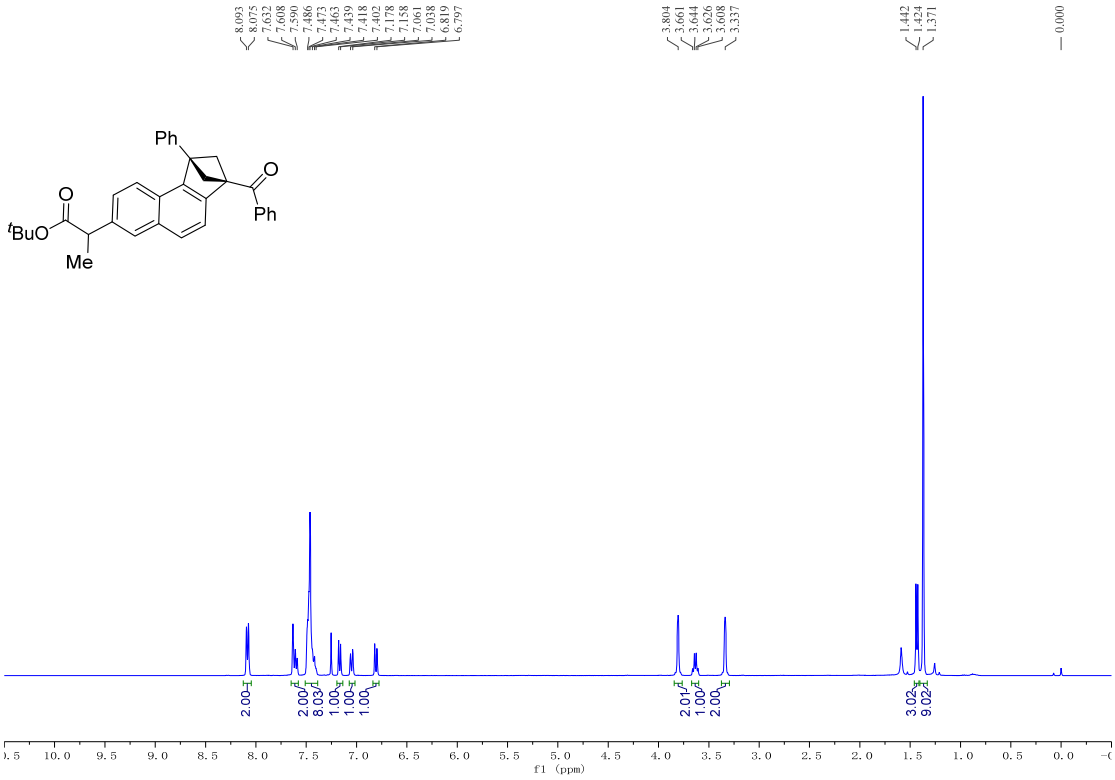


^{13}C NMR (150 MHz, $CDCl_3$)

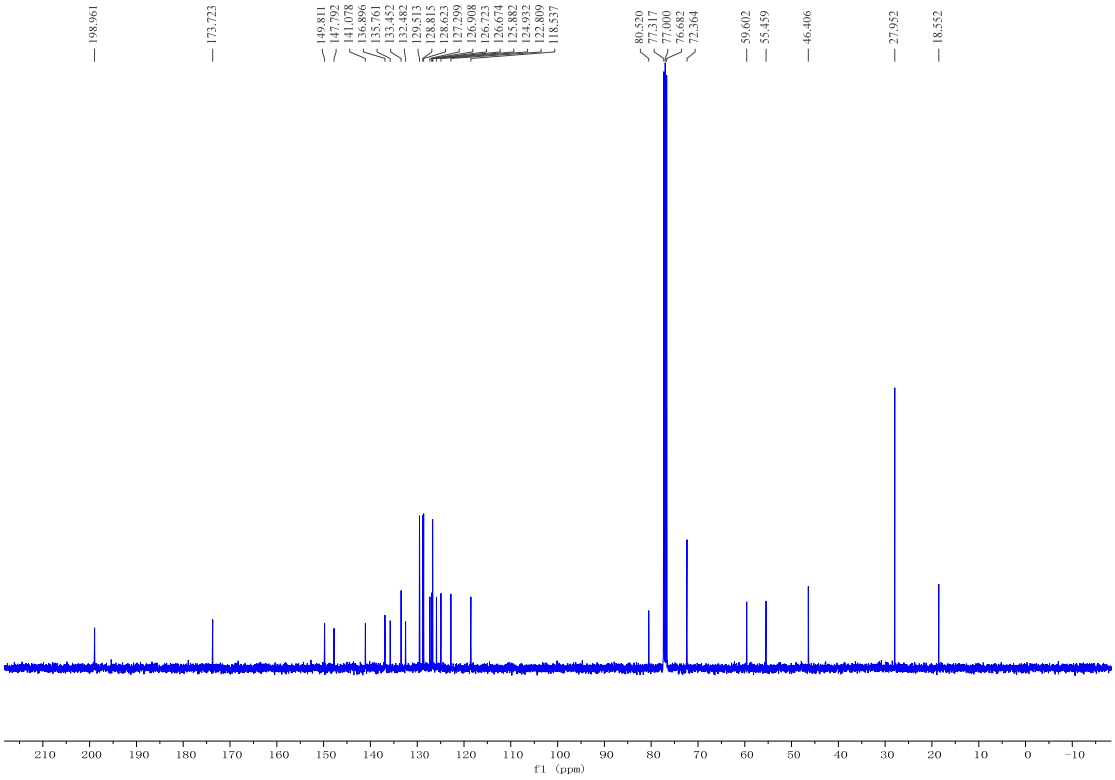


^{1}H and ^{13}C NMR Spectra for Compound 3ak

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

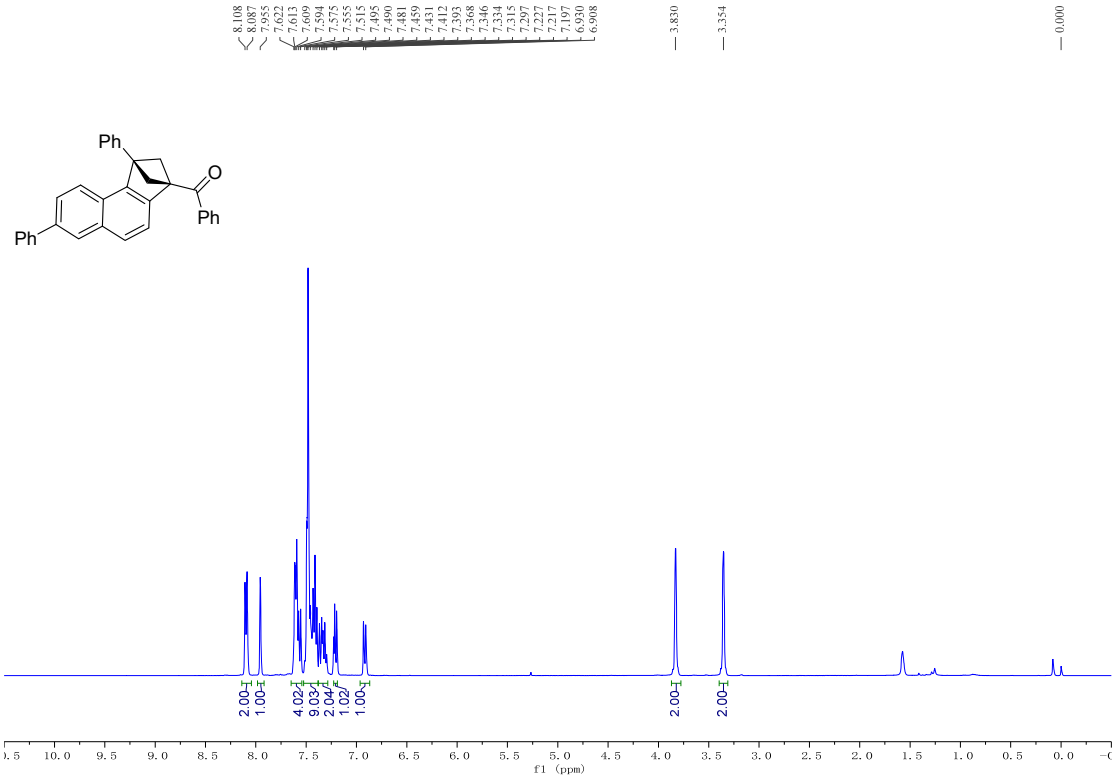


^{13}C NMR (100 MHz, $CDCl_3$)

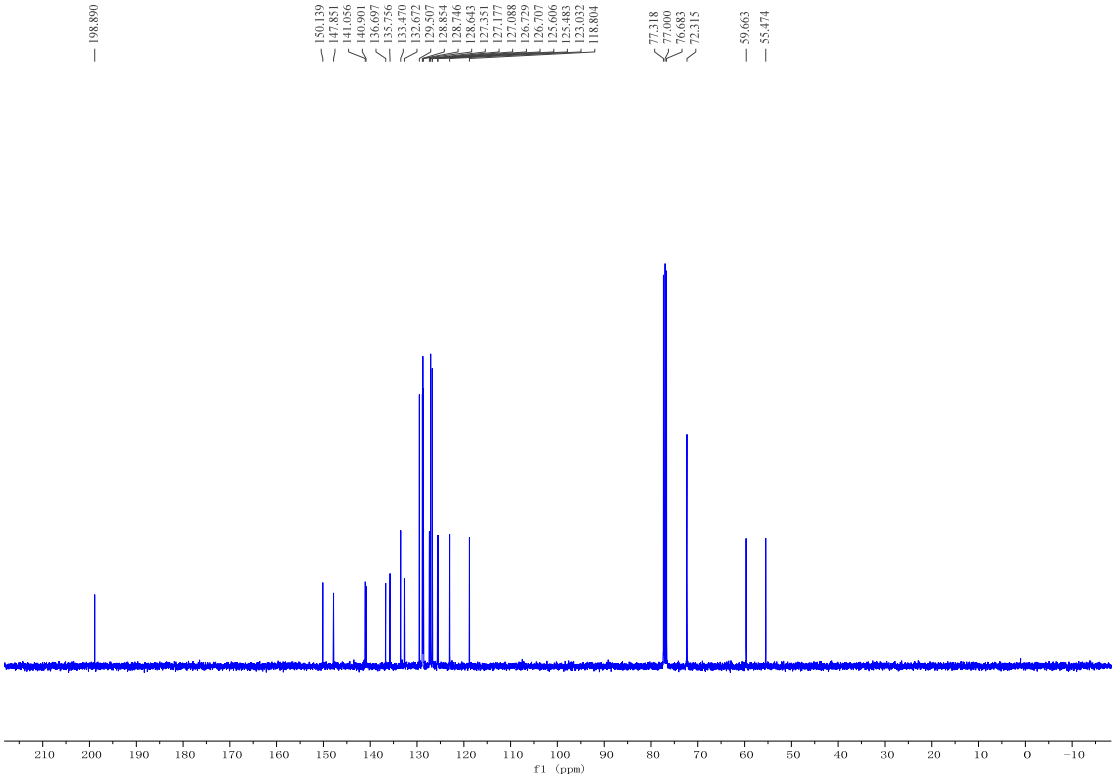


^{1}H and ^{13}C NMR Spectra for Compound 3al

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

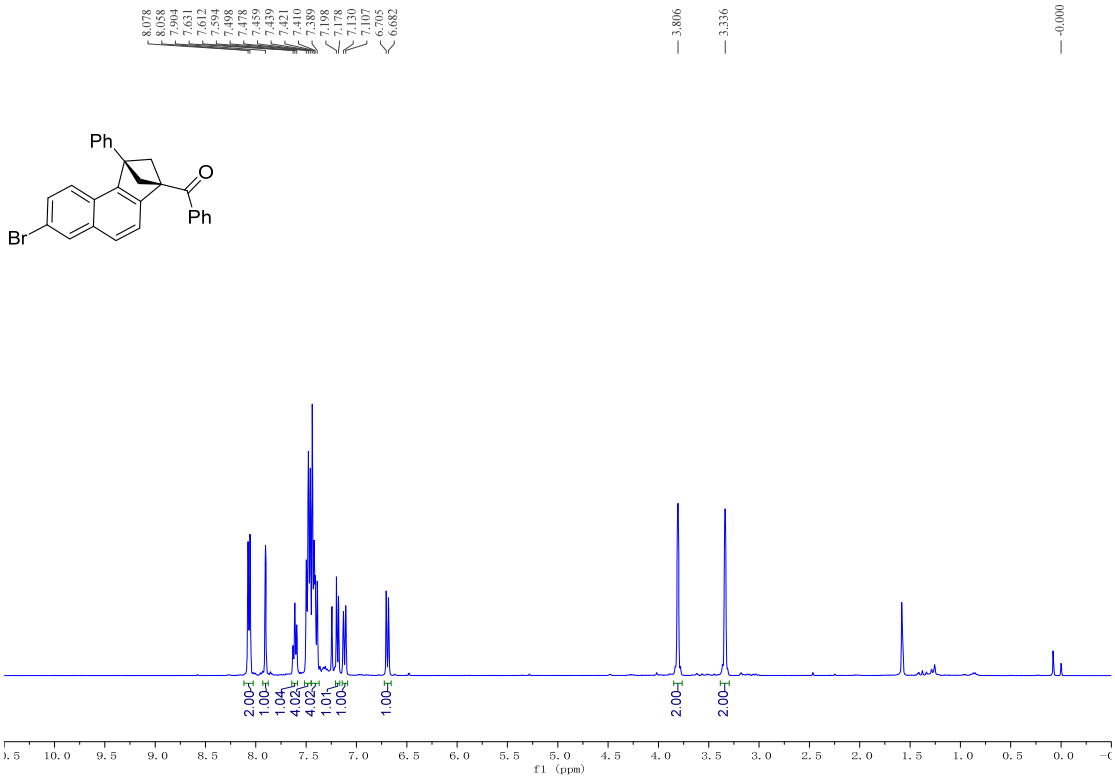


^{13}C NMR (100 MHz, $CDCl_3$)

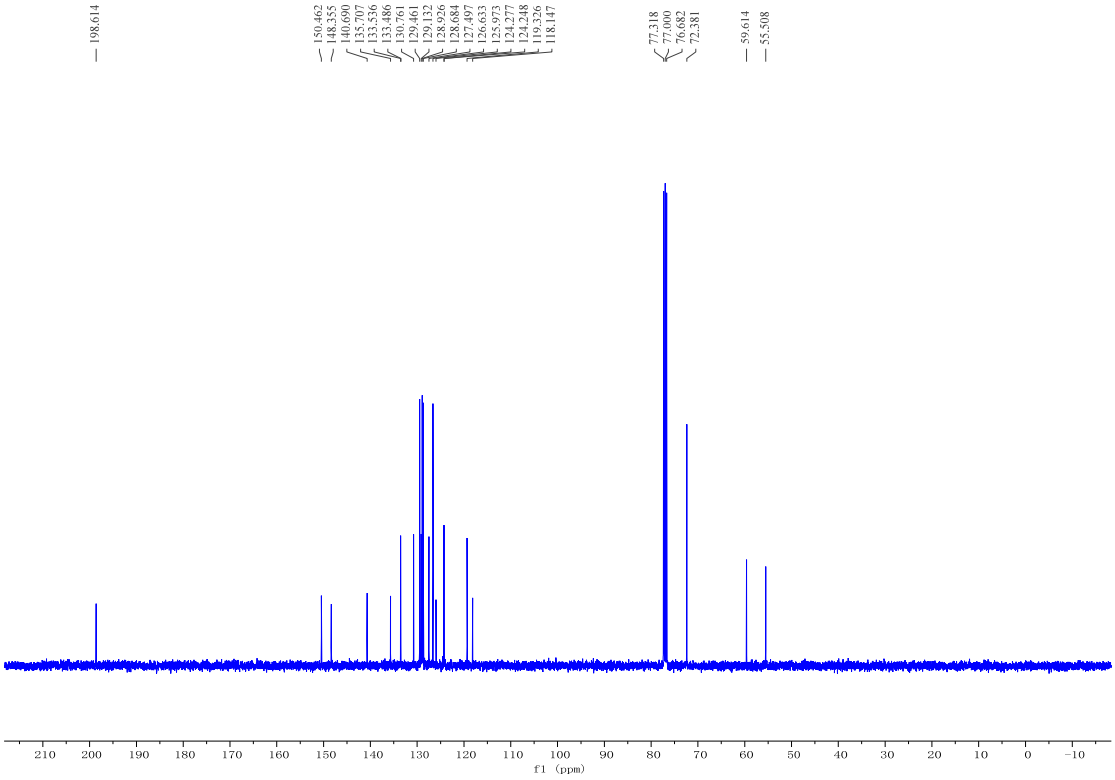


^{1}H and ^{13}C NMR Spectra for Compound 3am

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

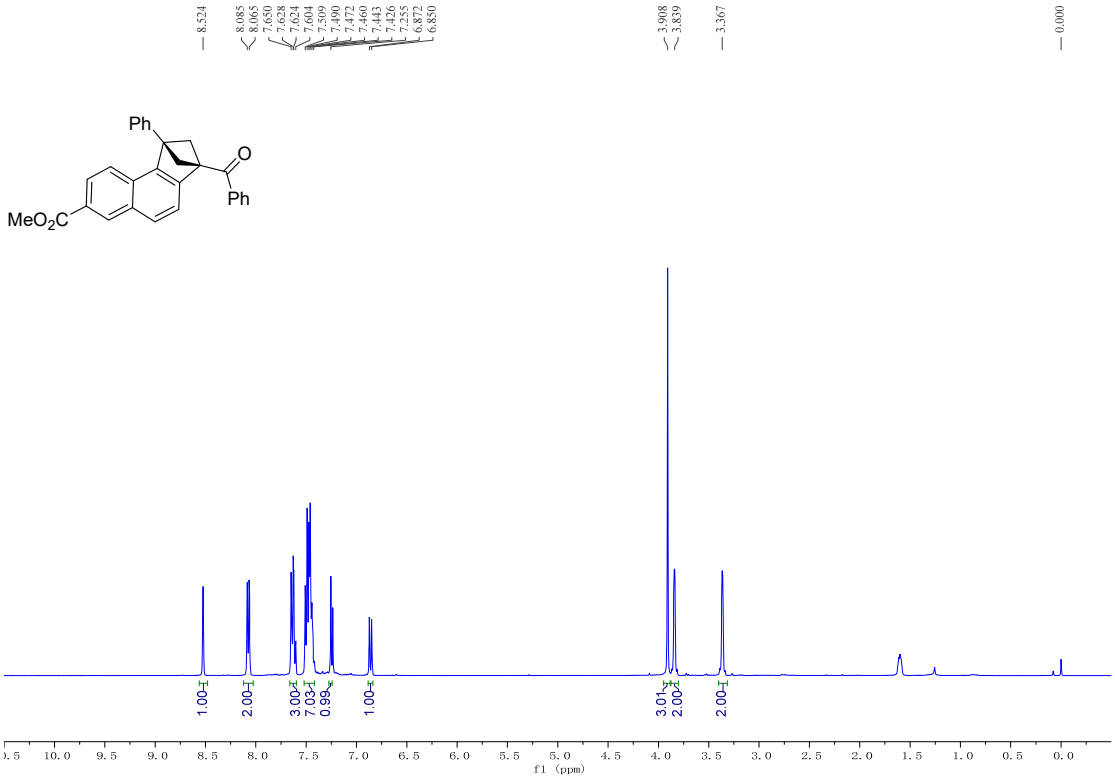


^{13}C NMR (100 MHz, $CDCl_3$)

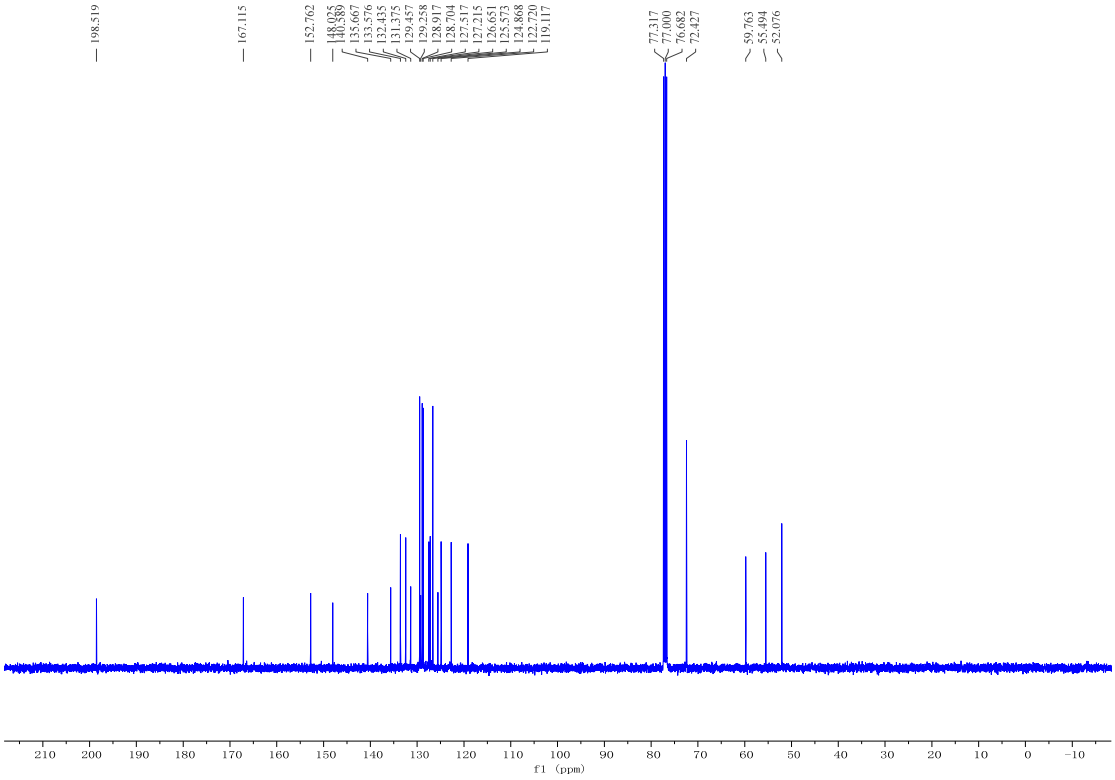


^{1}H and ^{13}C NMR Spectra for Compound 3an

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

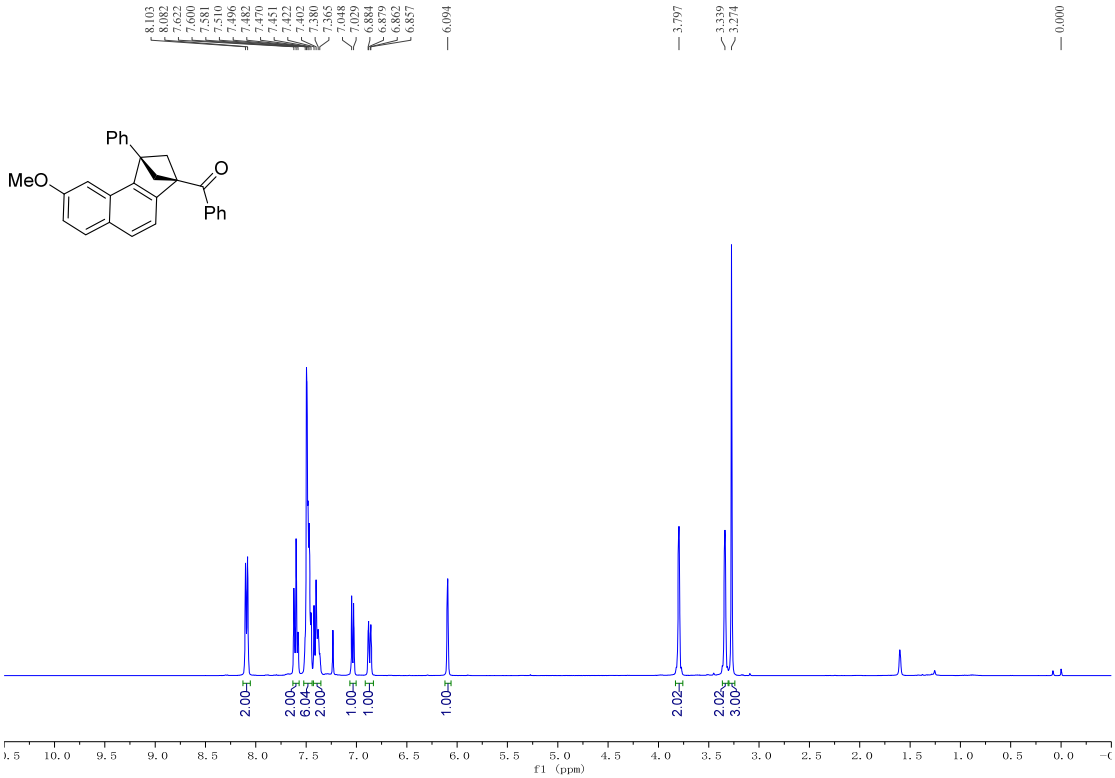


^{13}C NMR (100 MHz, $CDCl_3$)

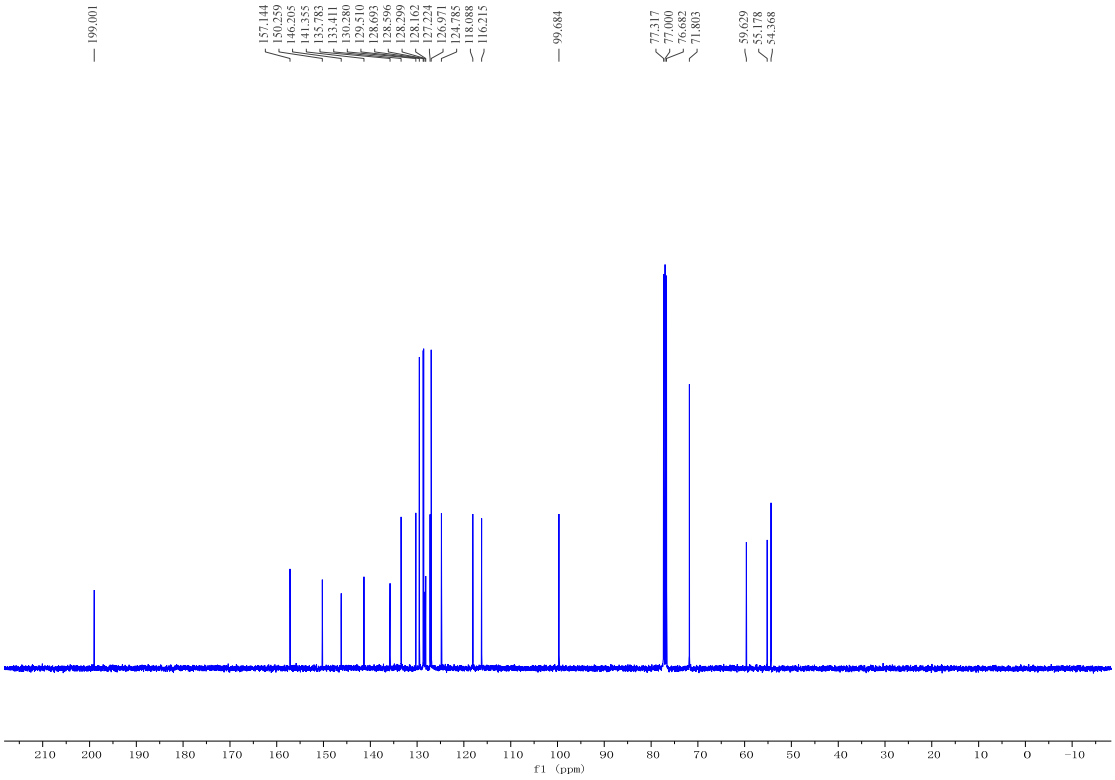


^{1}H and ^{13}C NMR Spectra for Compound 3ao

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

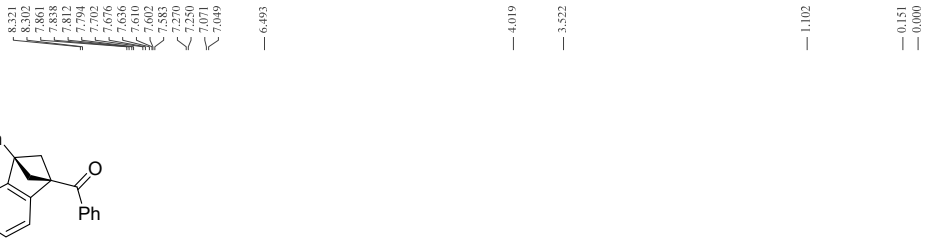


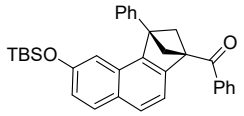
^{13}C NMR (100 MHz, $CDCl_3$)

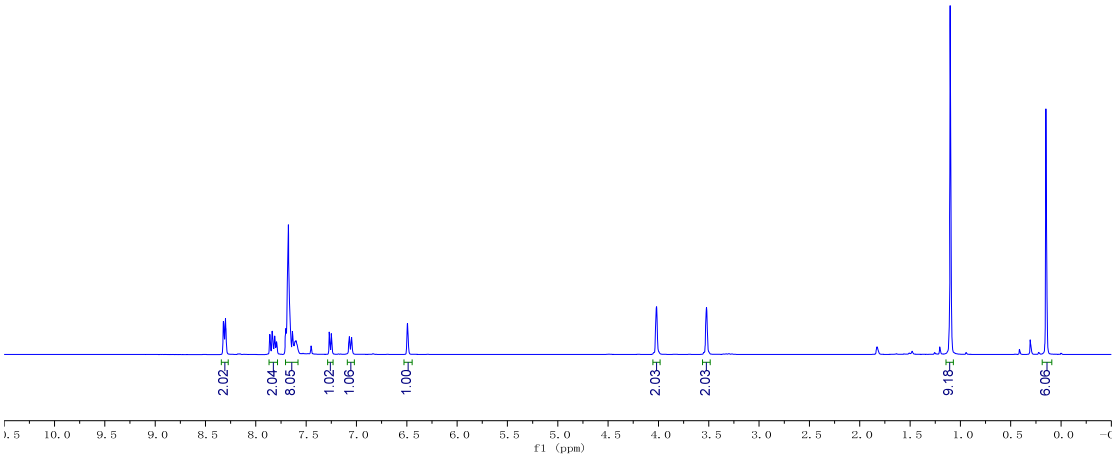


^{1}H and ^{13}C NMR Spectra for Compound 3ap

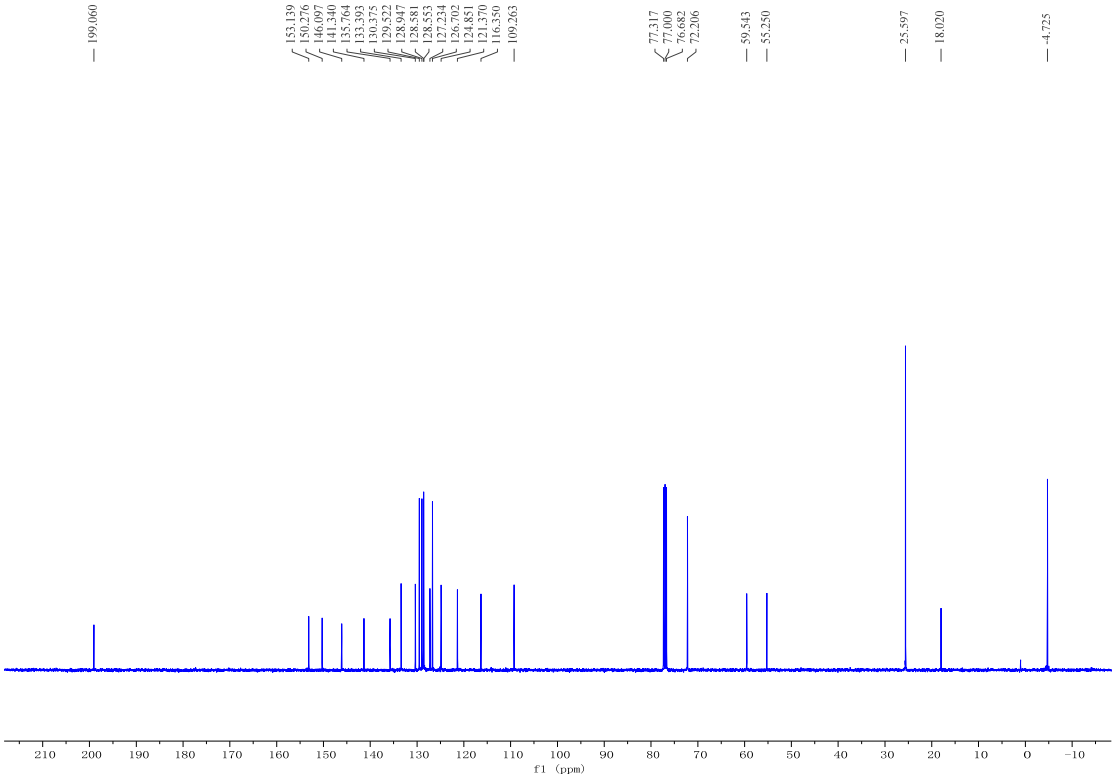
^{1}H NMR (400 MHz, $CDCl_3$)





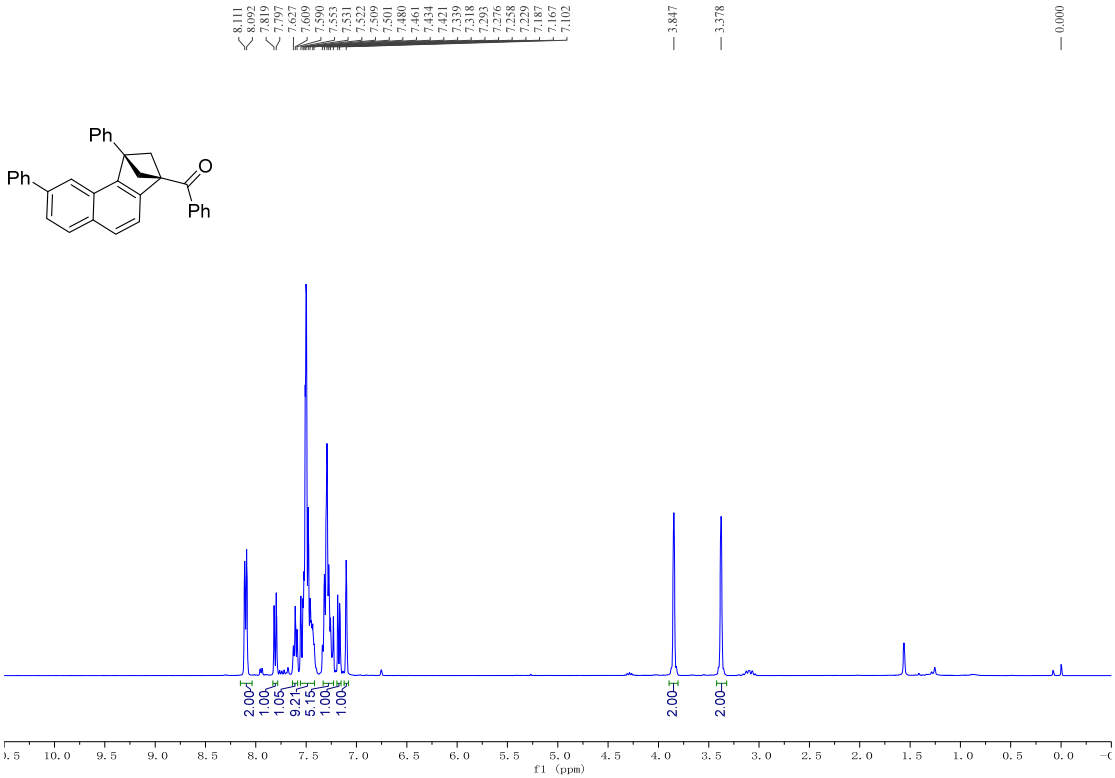


^{13}C NMR (100 MHz, $CDCl_3$)

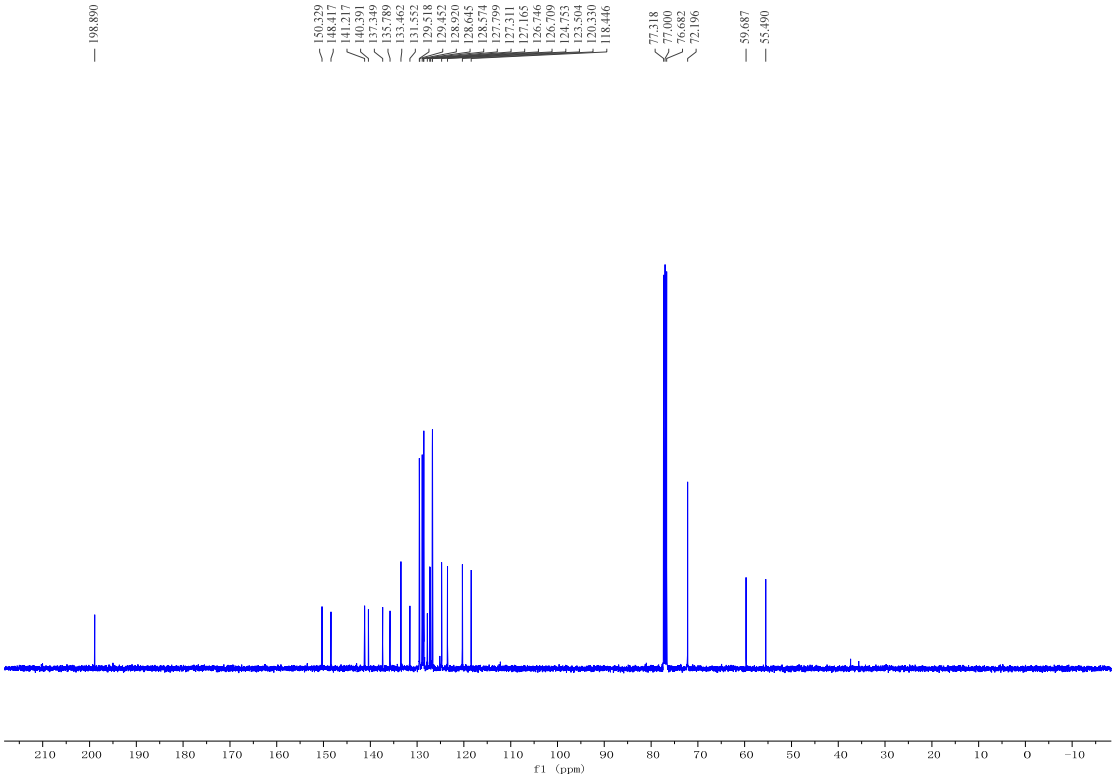


^{1}H and ^{13}C NMR Spectra for Compound 3aq

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

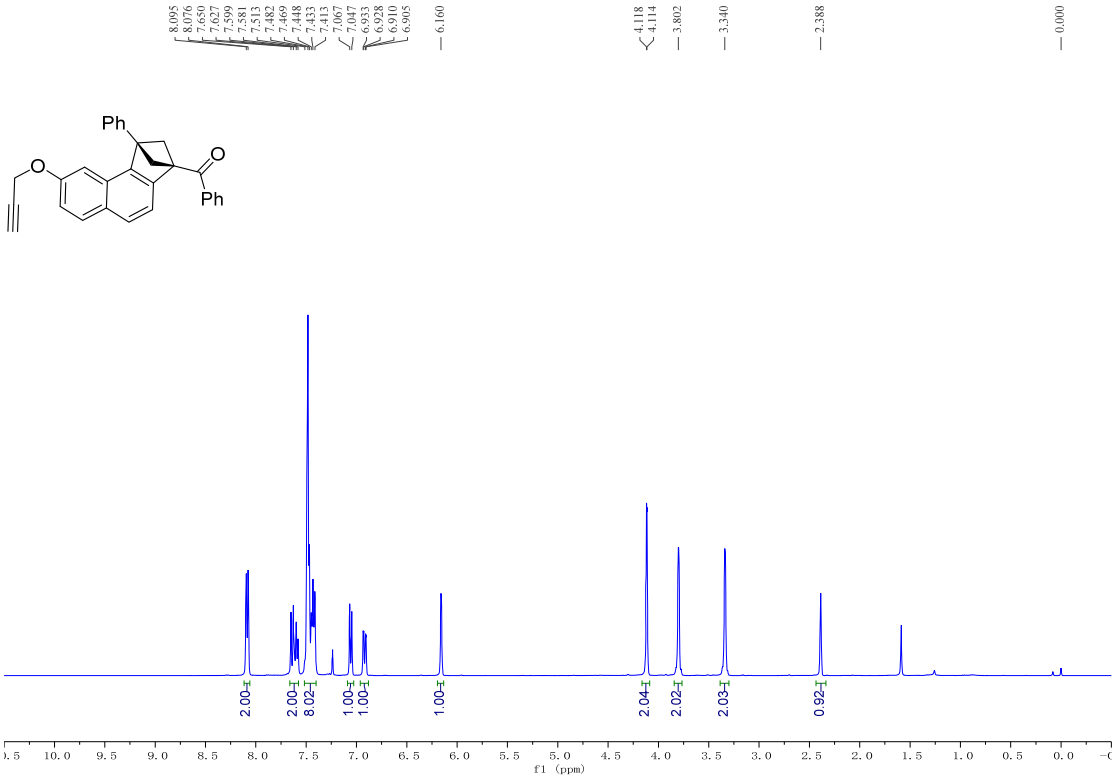


^{13}C NMR (100 MHz, $CDCl_3$)

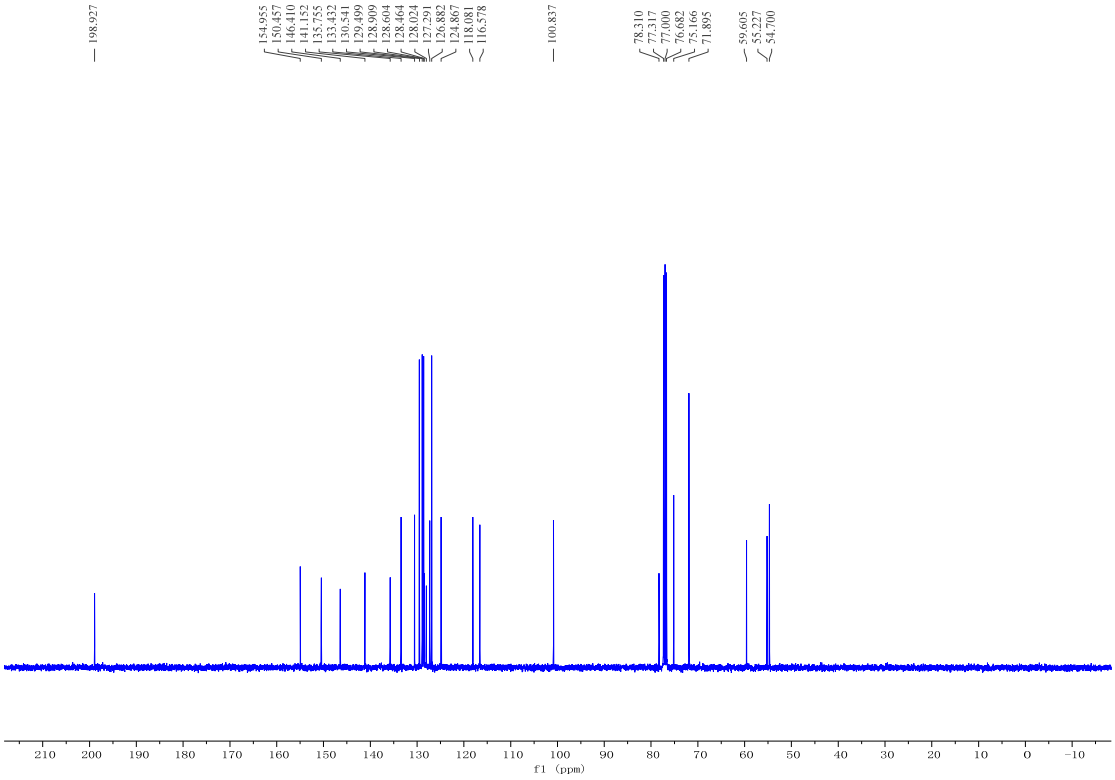


^{1}H and ^{13}C NMR Spectra for Compound 3ar

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

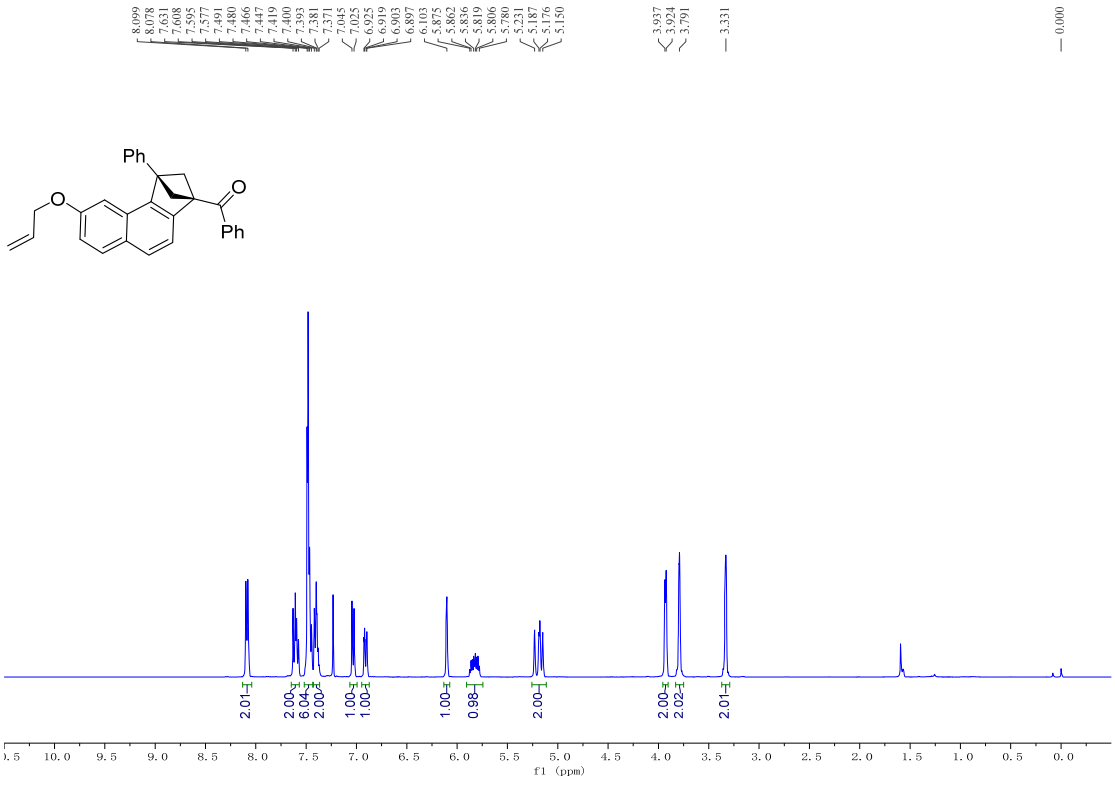


^{13}C NMR (100 MHz, $CDCl_3$)

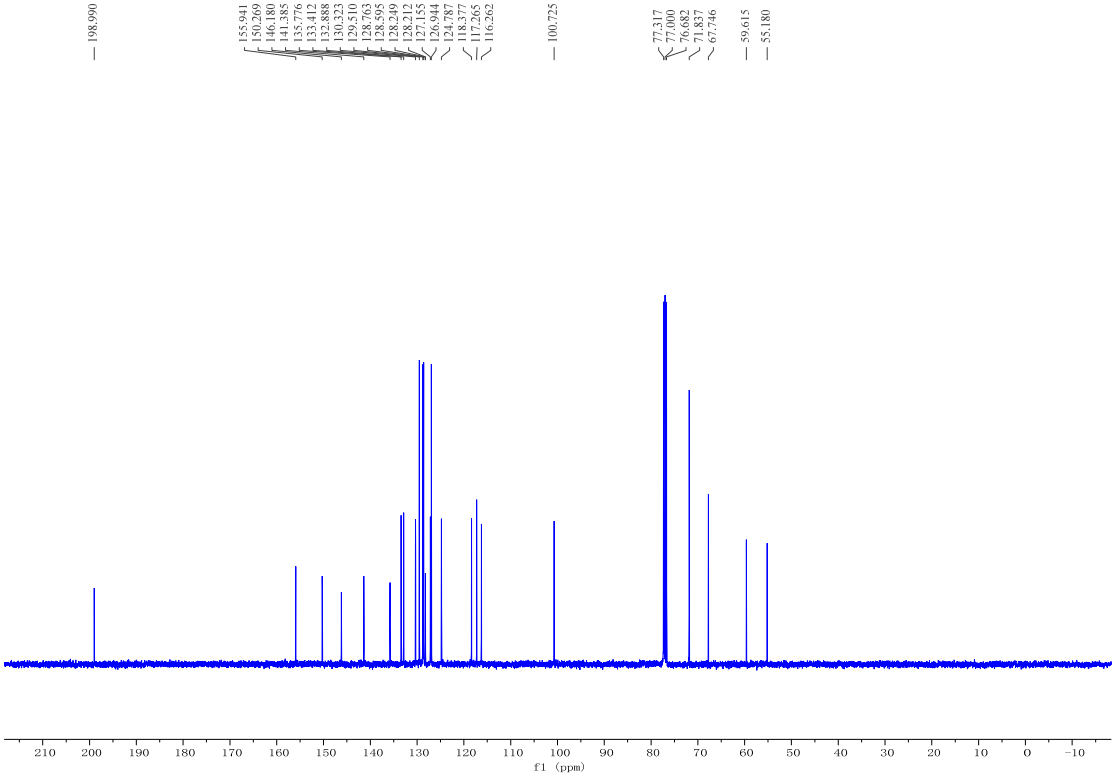


^{1}H and ^{13}C NMR Spectra for Compound 3as

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

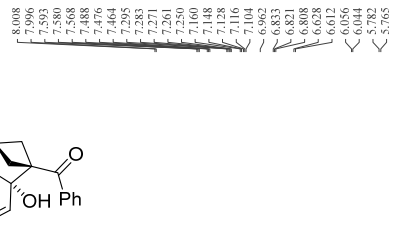


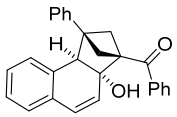
^{13}C NMR (100 MHz, $CDCl_3$)

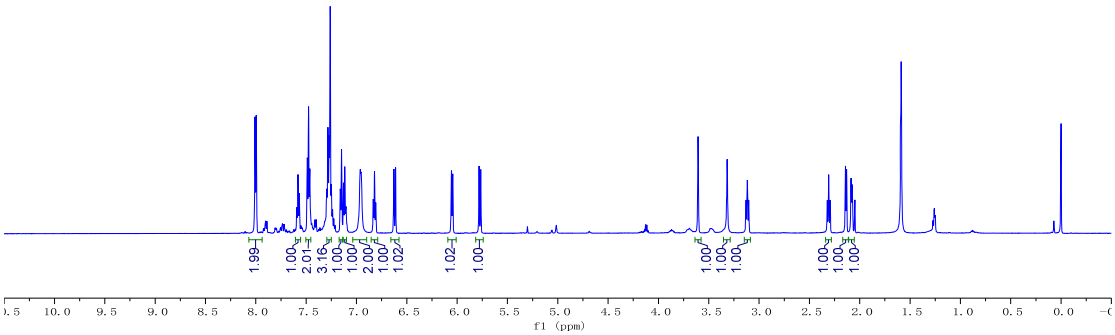


^{1}H and ^{13}C NMR Spectra for Compound 4

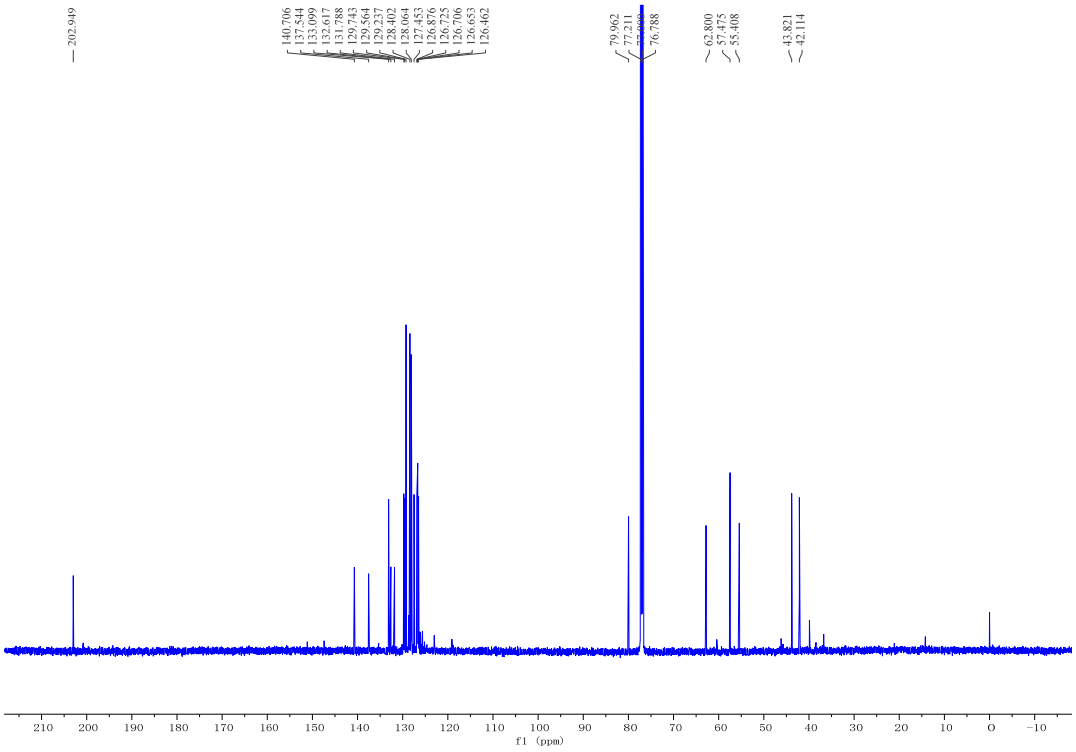
^{1}H NMR (600 MHz, $CDCl_3$)





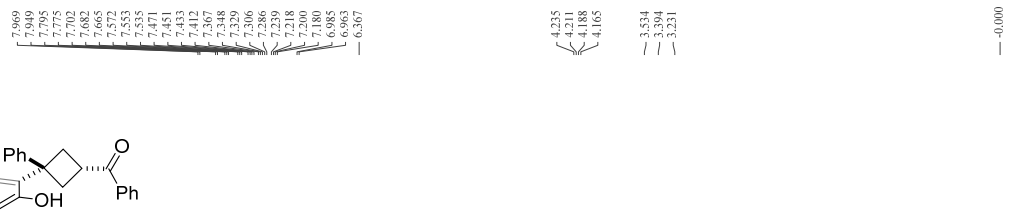


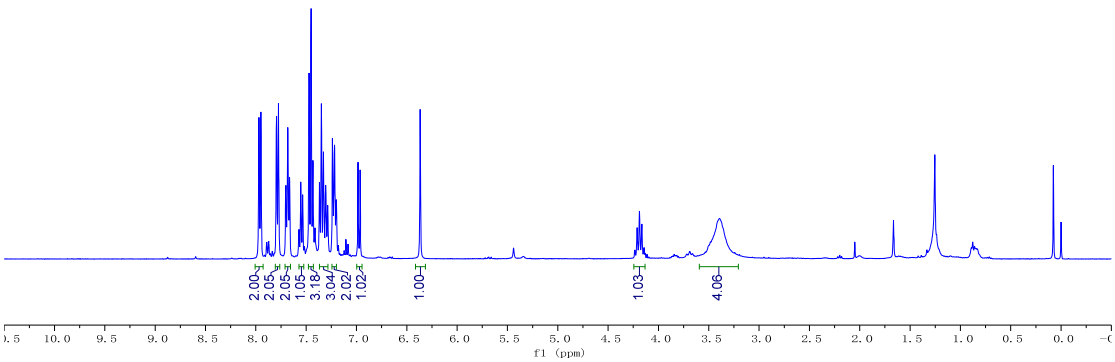
^{13}C NMR (150 MHz, $CDCl_3$)



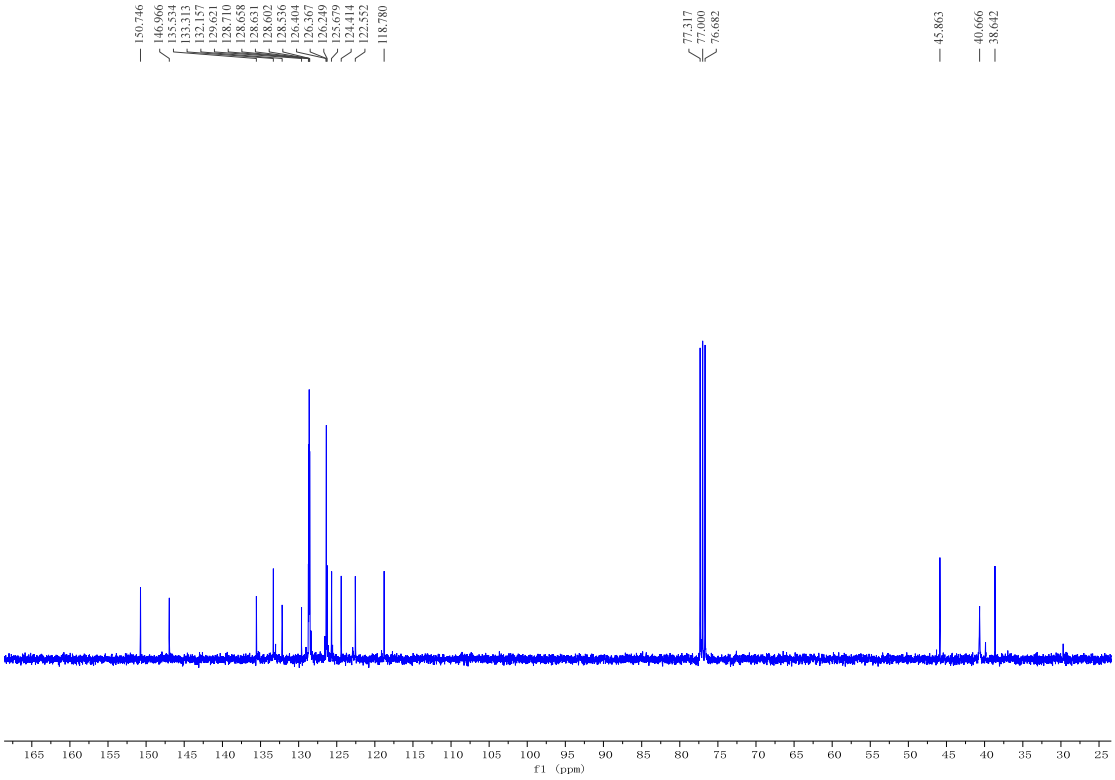
^{1}H and ^{13}C NMR Spectra for Compound 5

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



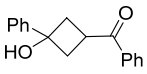


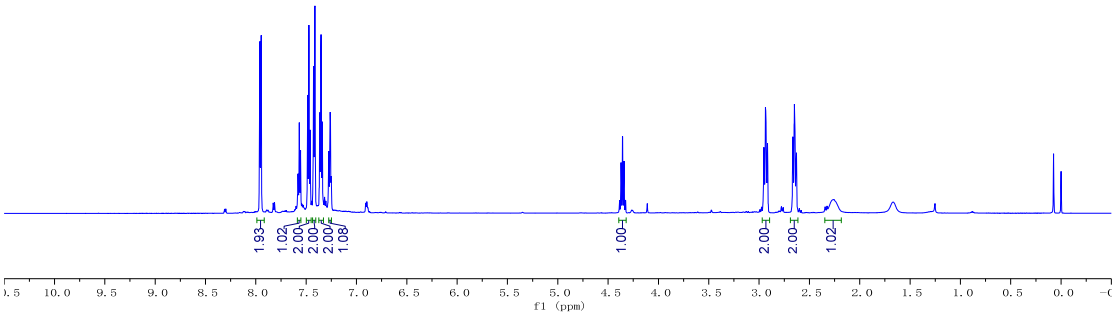
^{13}C NMR (100 MHz, $CDCl_3$)



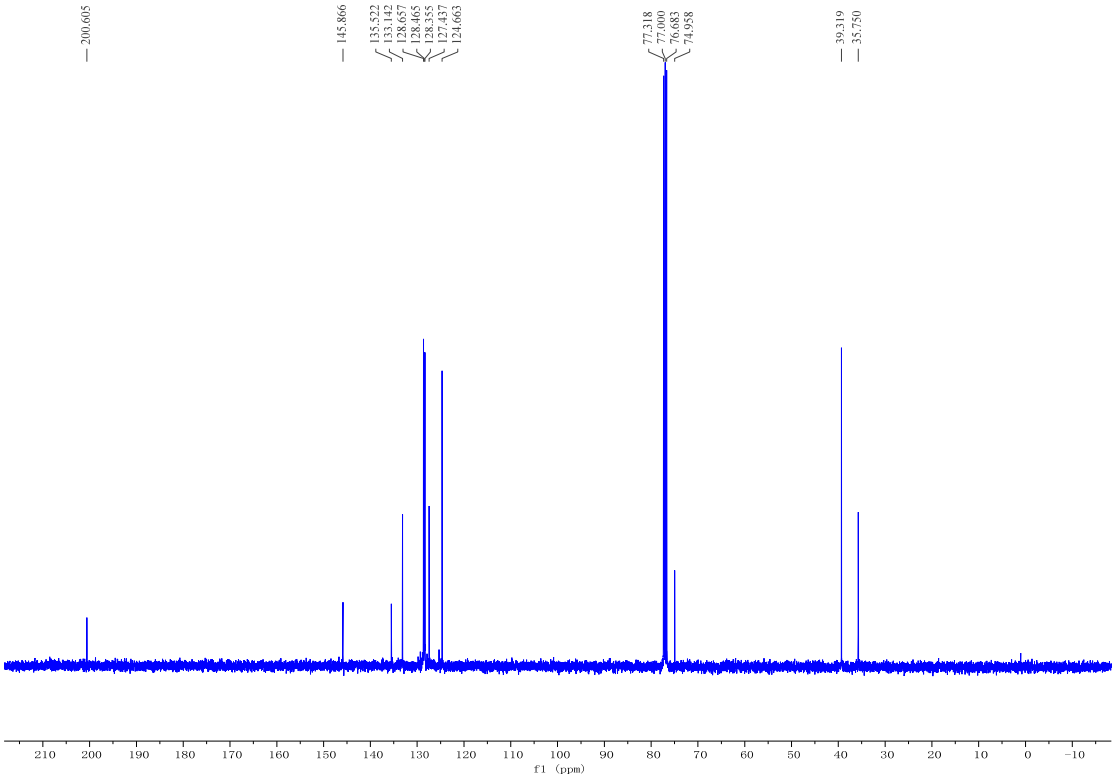
^{1}H and ^{13}C NMR Spectra for Compound 6

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



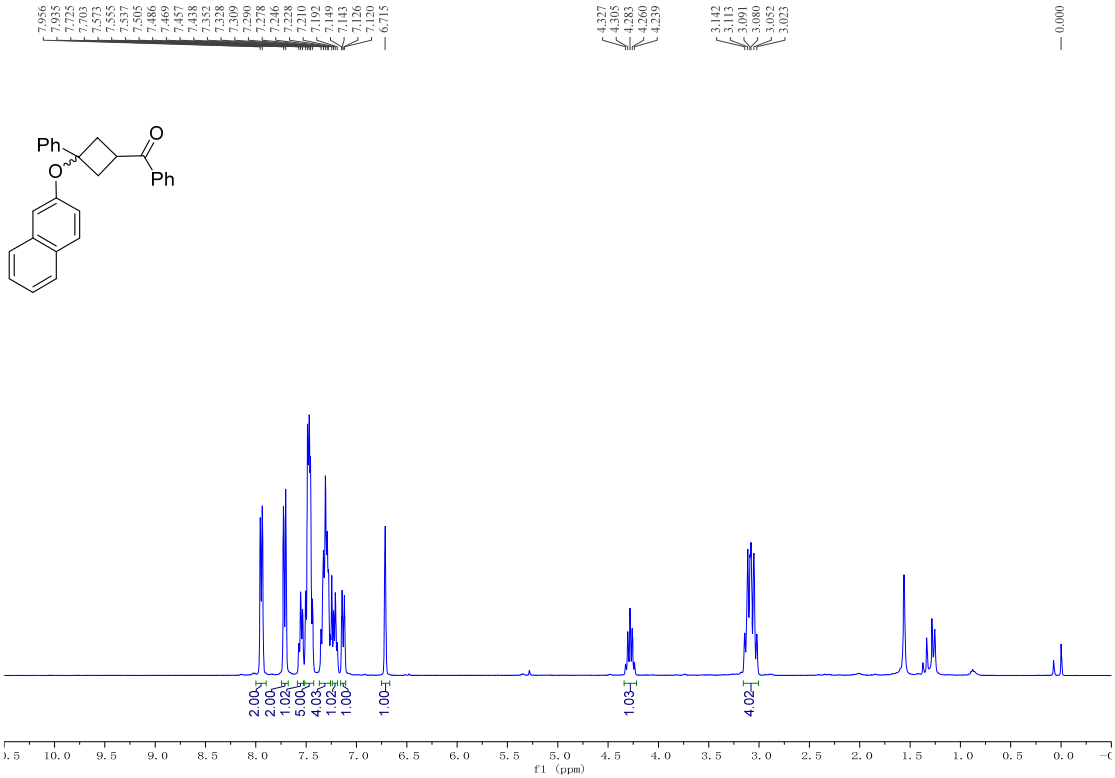


^{13}C NMR (100 MHz, $CDCl_3$)

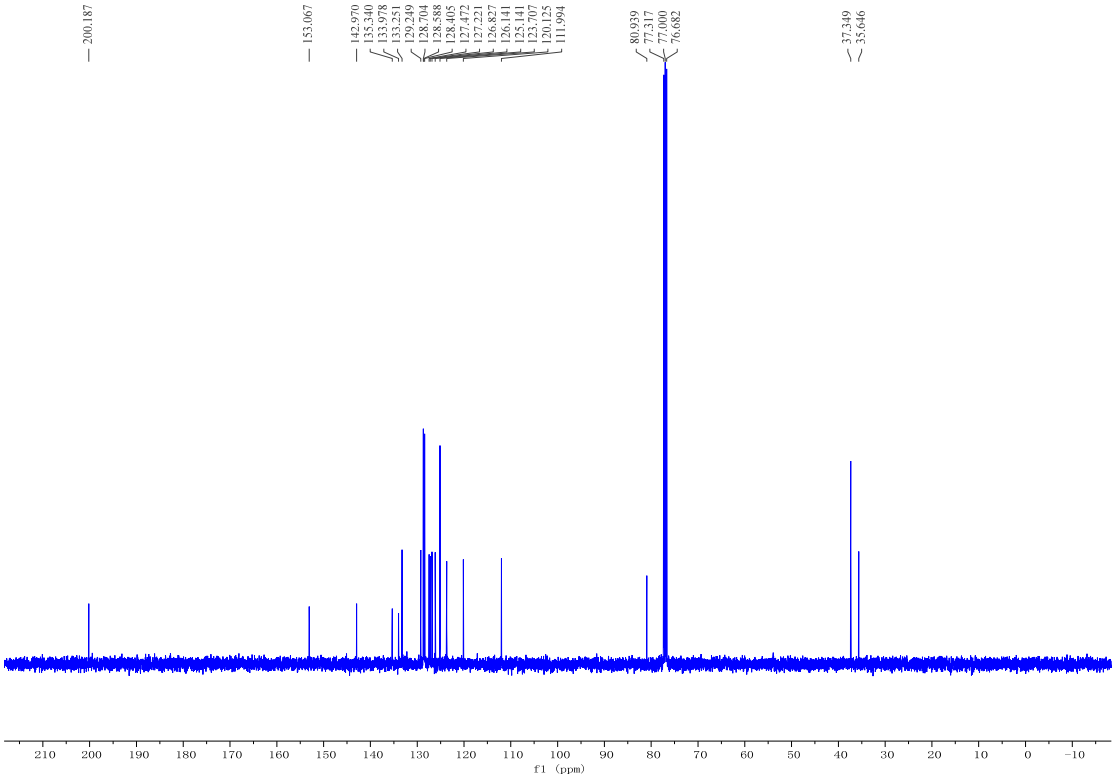


^{1}H and ^{13}C NMR Spectra for Compound 7

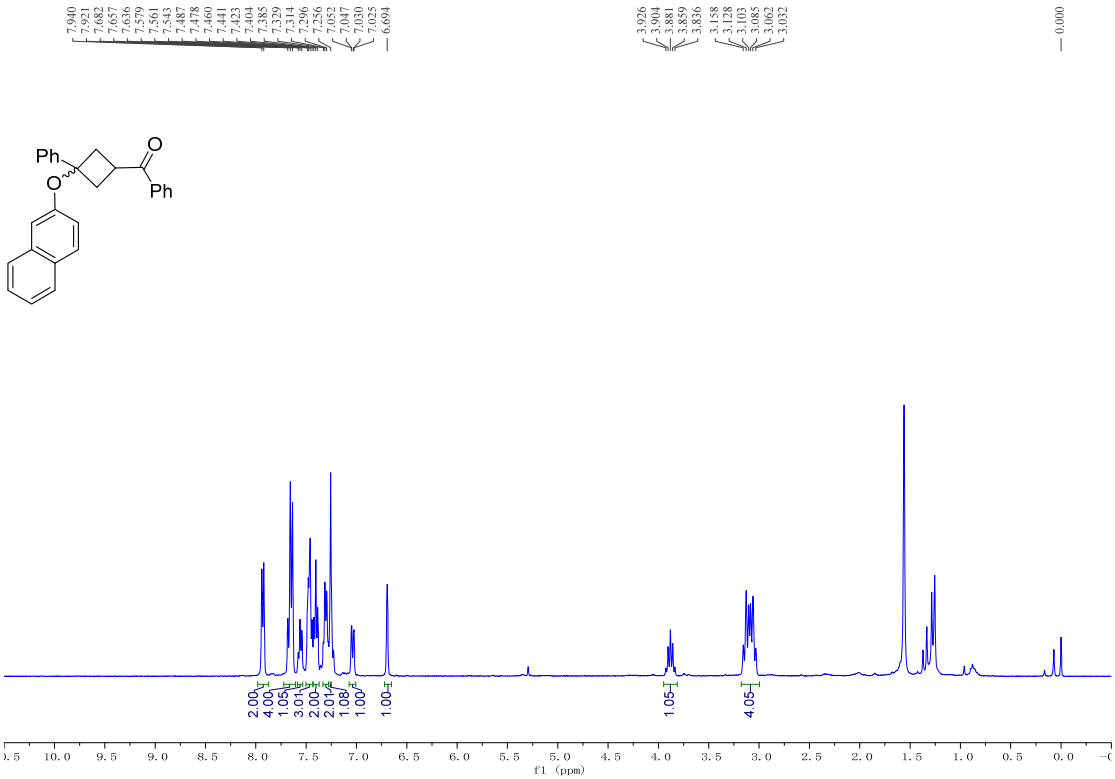
^{1}H NMR (400 MHz, $CDCl_3$) for **major isomer:**



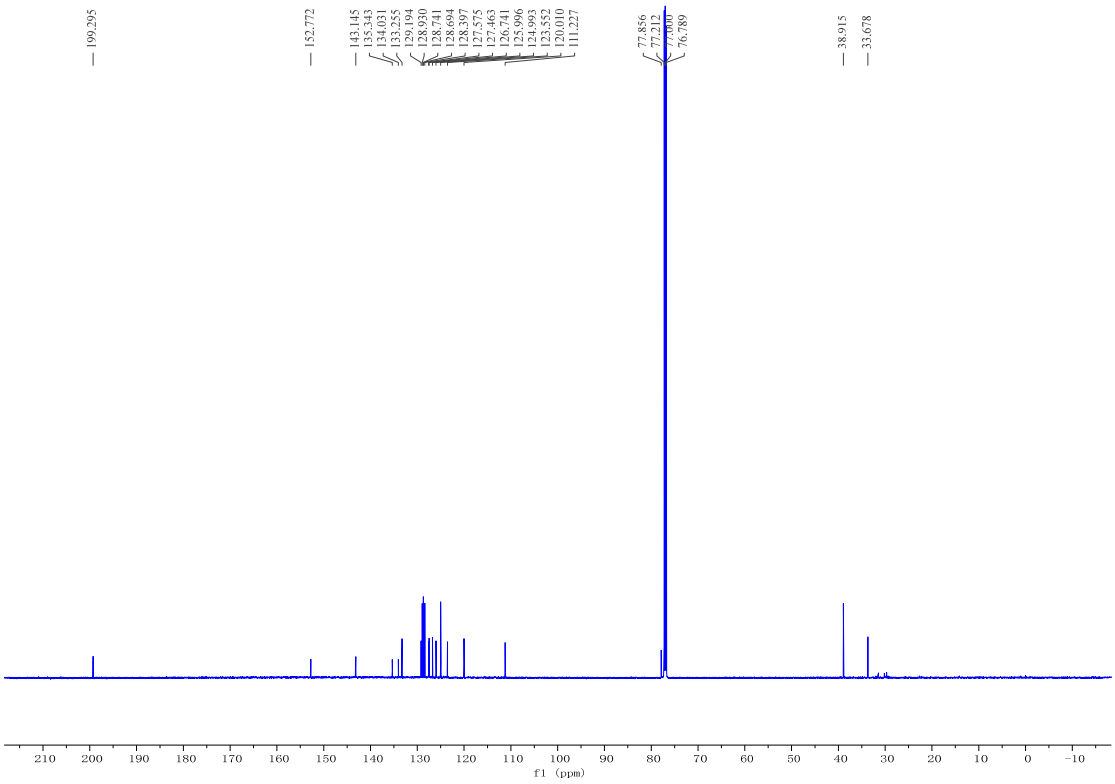
^{13}C NMR (100 MHz, $CDCl_3$) for **major isomer:**



^{1}H NMR (400 MHz, $CDCl_3$) for **minor isomer:**

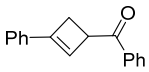


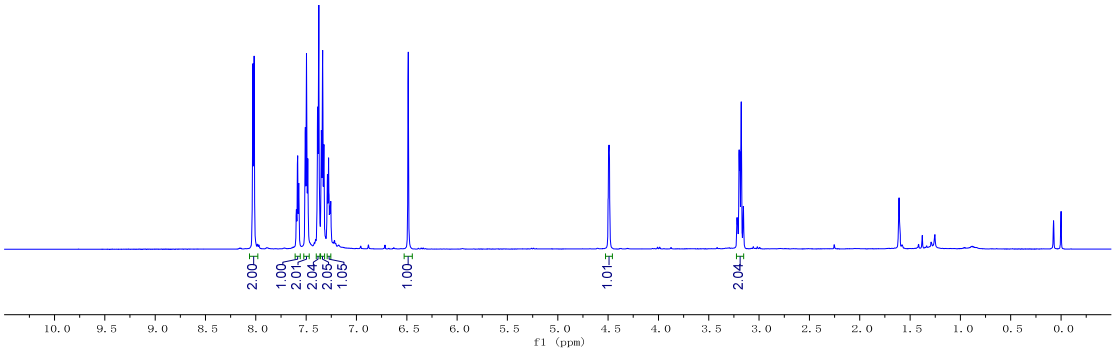
^{13}C NMR (150 MHz, $CDCl_3$) for **minor isomer:**



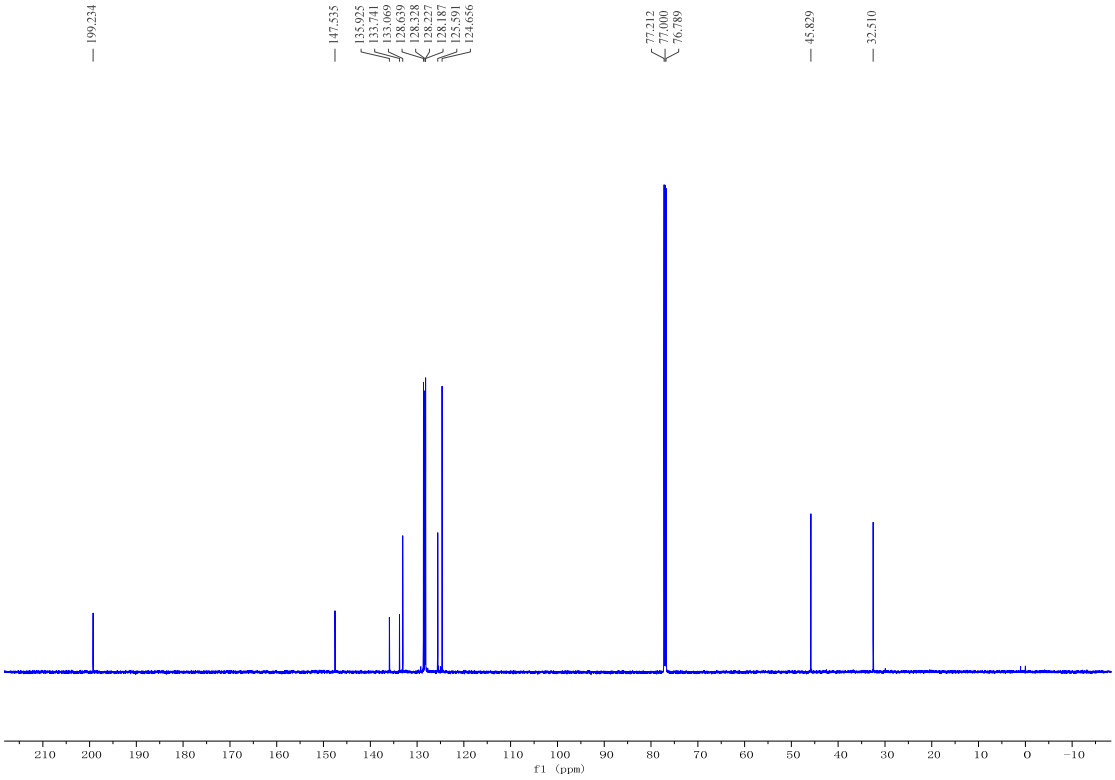
^{1}H and ^{13}C NMR Spectra for Compound 8

^{1}H NMR (600 MHz, $CDCl_3$)



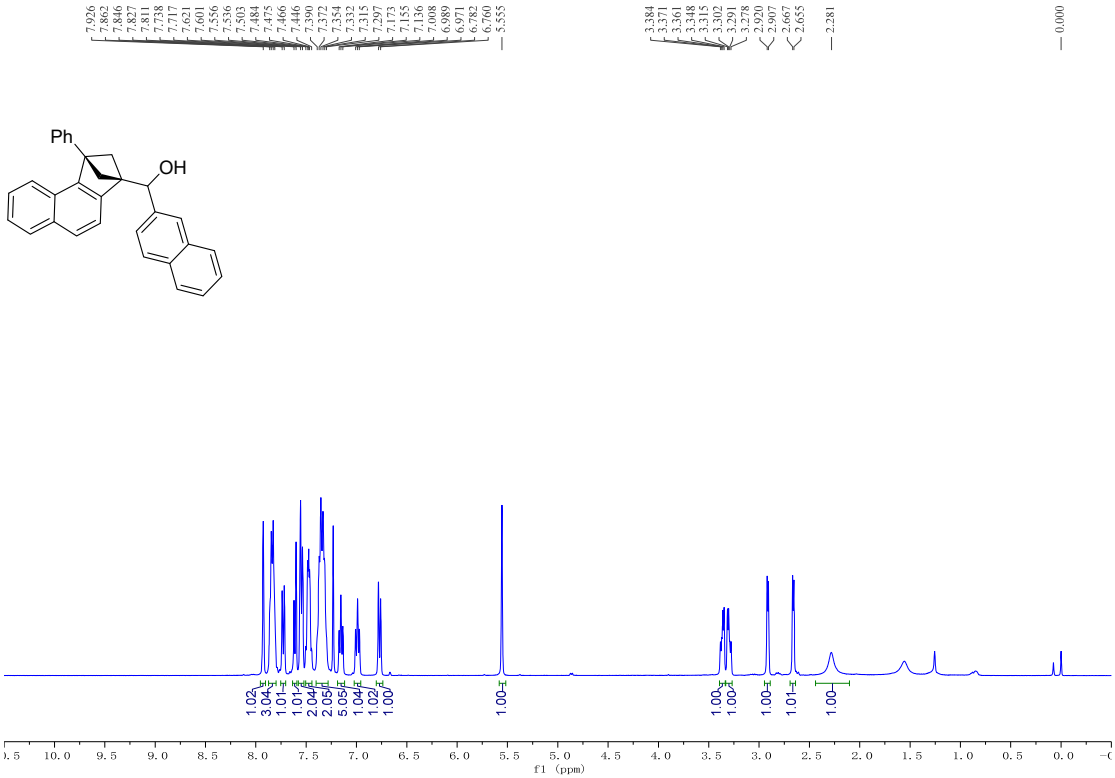


^{13}C NMR (150 MHz, $CDCl_3$)

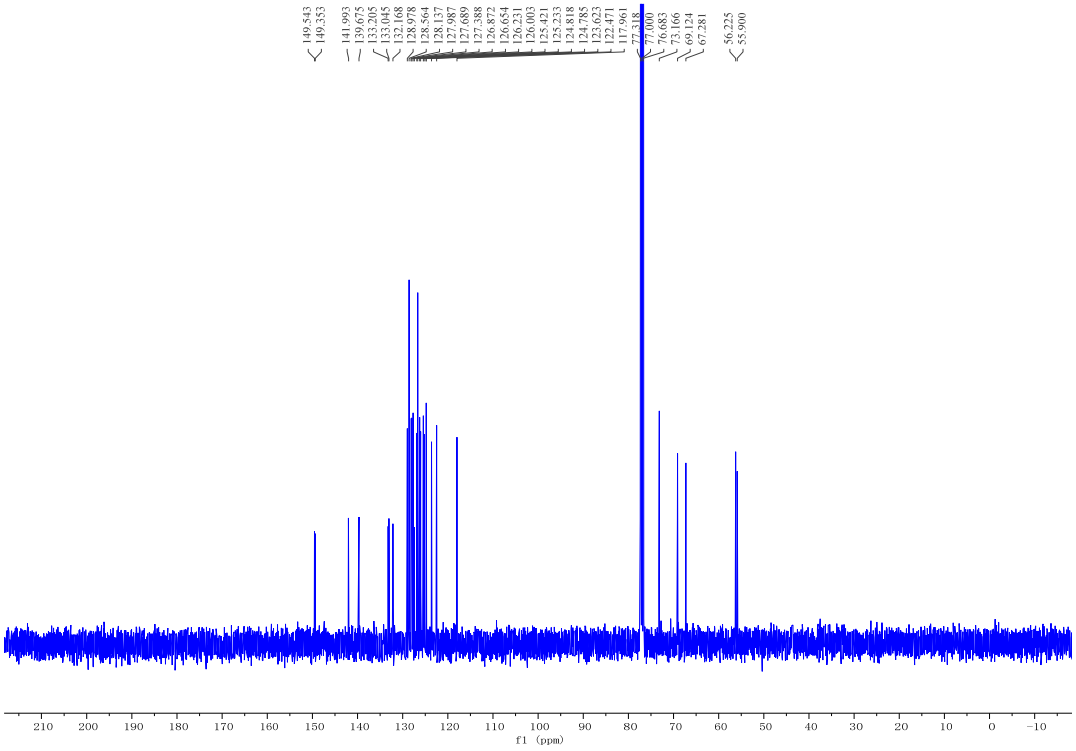


^{1}H and ^{13}C NMR Spectra for Compound 9

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

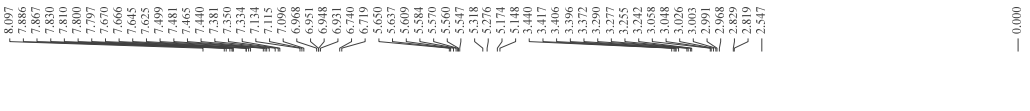


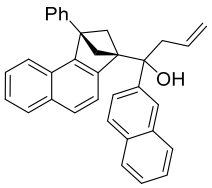
^{13}C NMR (100 MHz, $CDCl_3$)

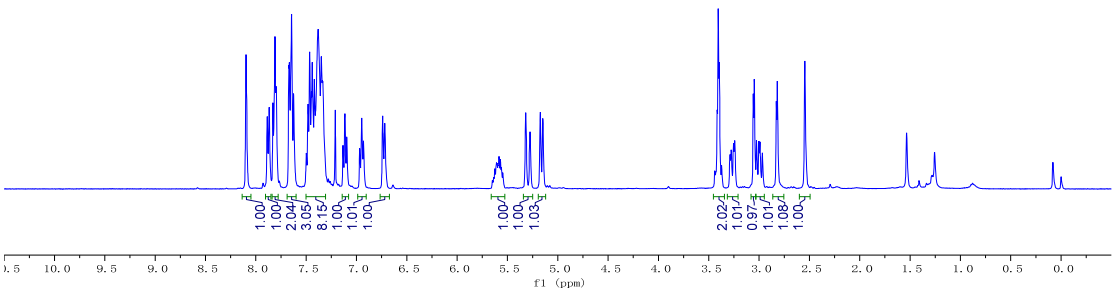


^{1}H and ^{13}C NMR Spectra for Compound 10

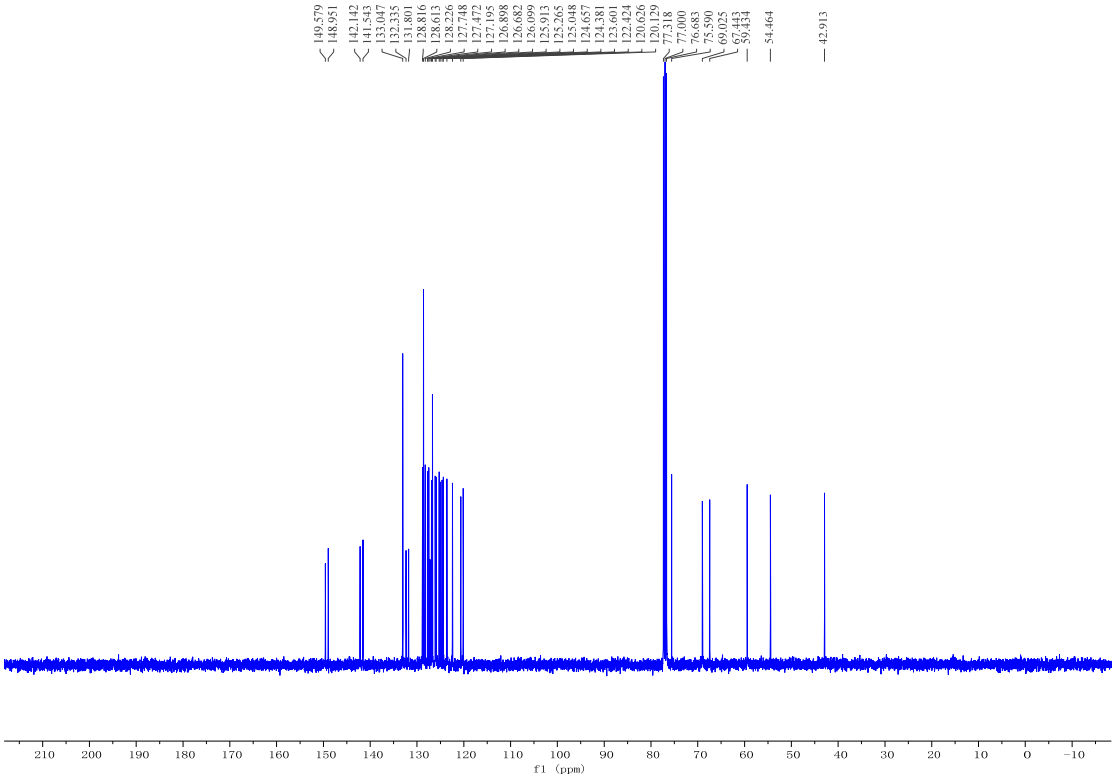
^{1}H NMR (400 MHz, $CDCl_3$)





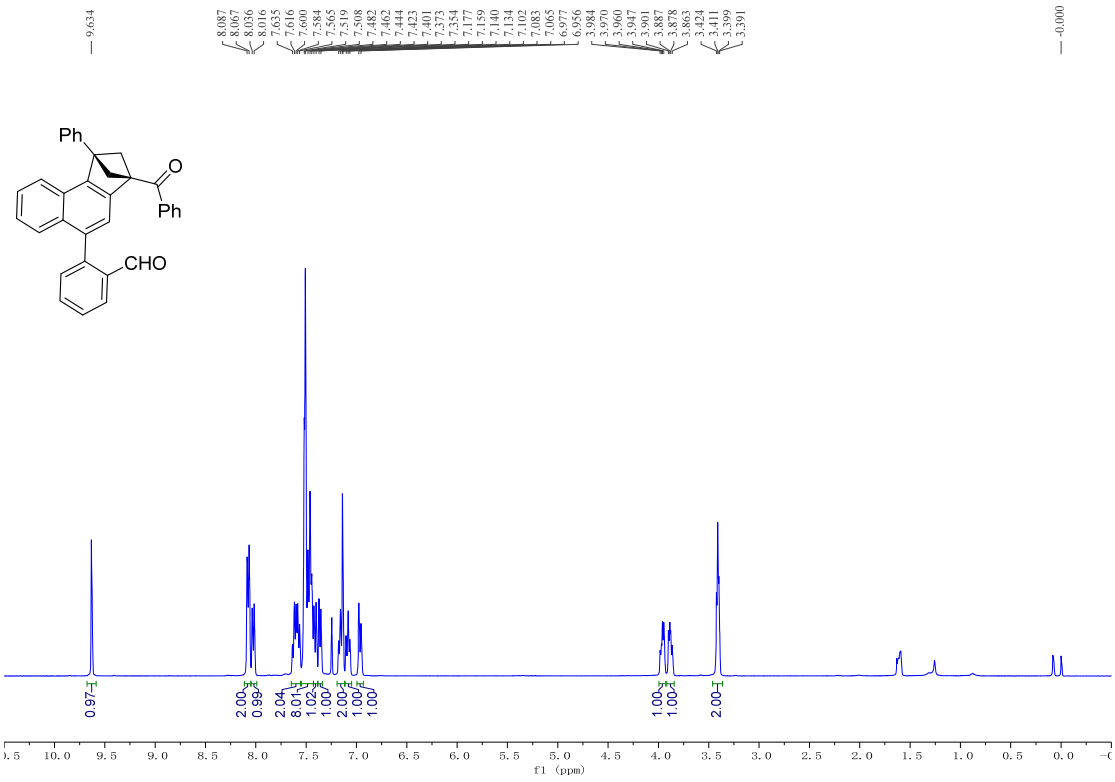


^{13}C NMR (100 MHz, $CDCl_3$)

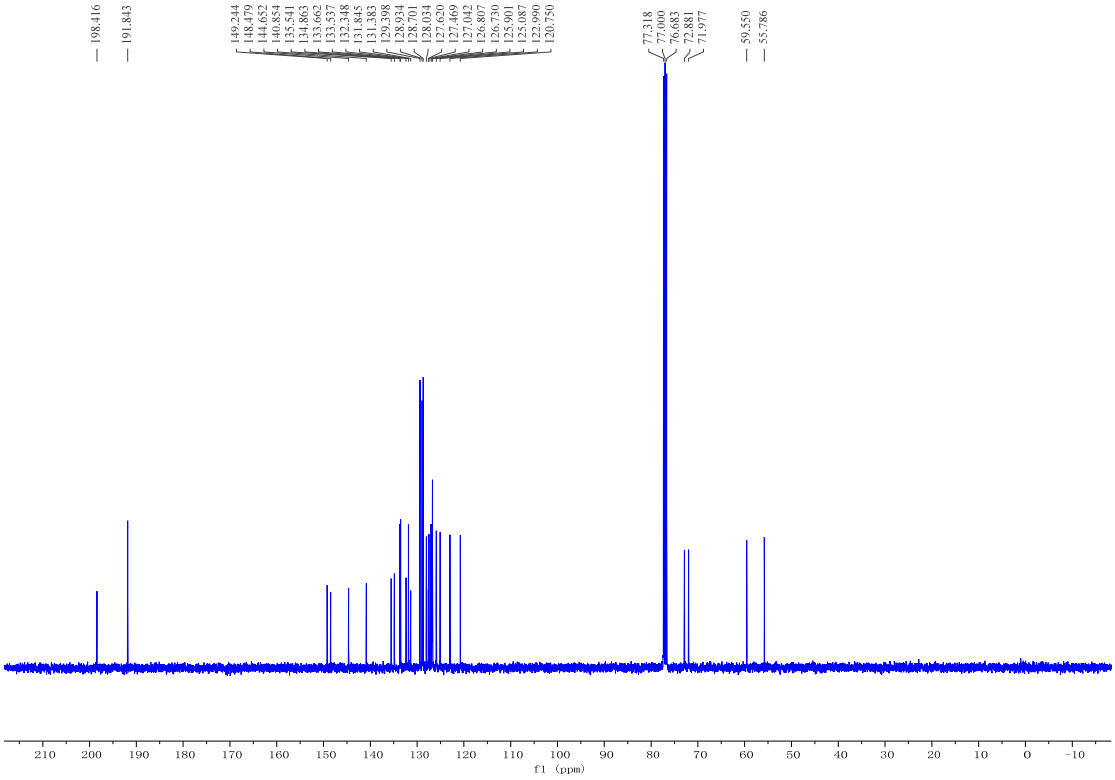


^{1}H and ^{13}C NMR Spectra for Compound 11

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

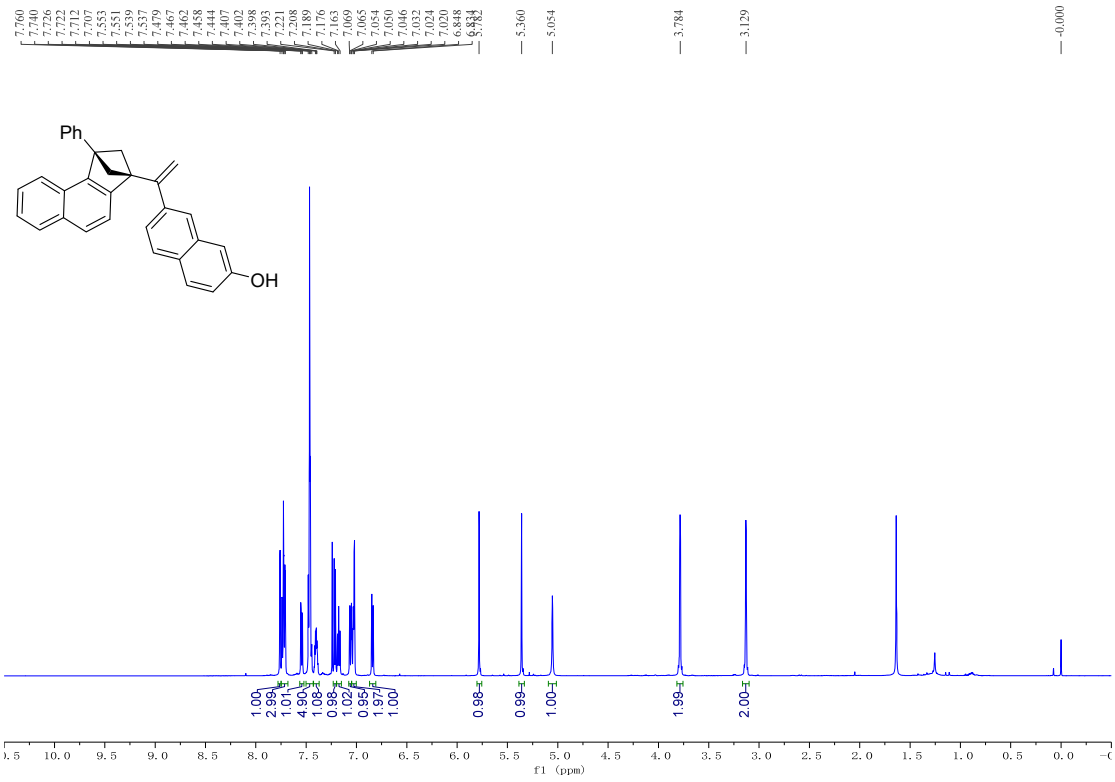


^{13}C NMR (100 MHz, $CDCl_3$)

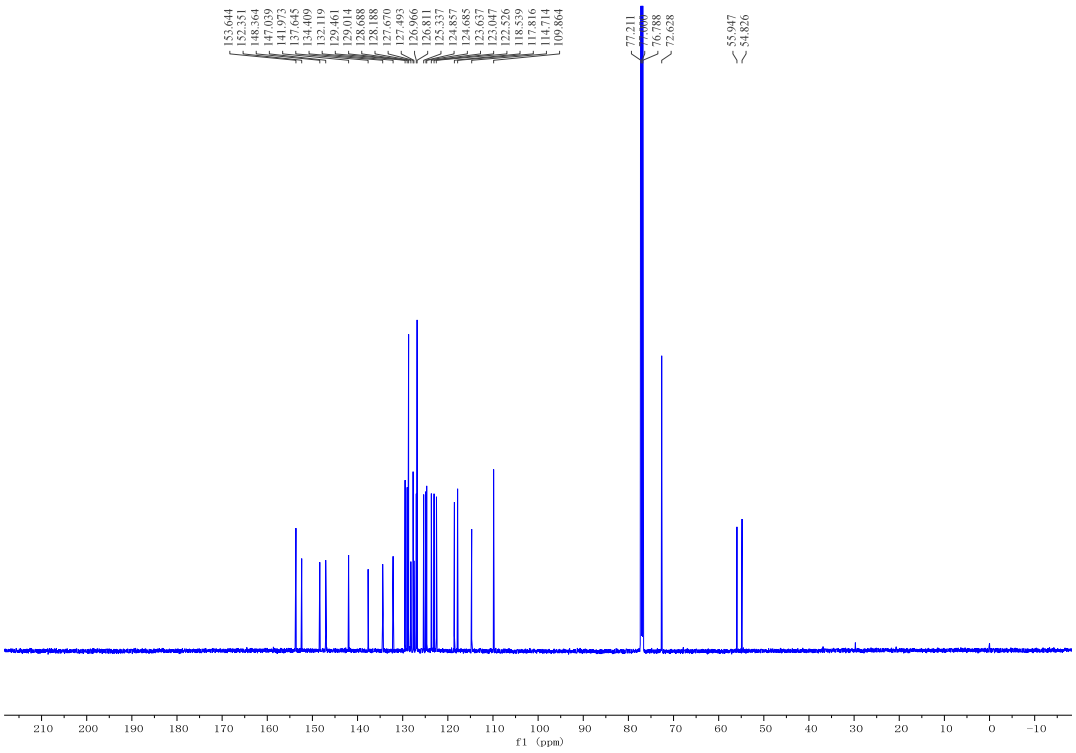


^{1}H and ^{13}C NMR Spectra for Compound 12

^{1}H NMR (600 MHz, $CDCl_3$)

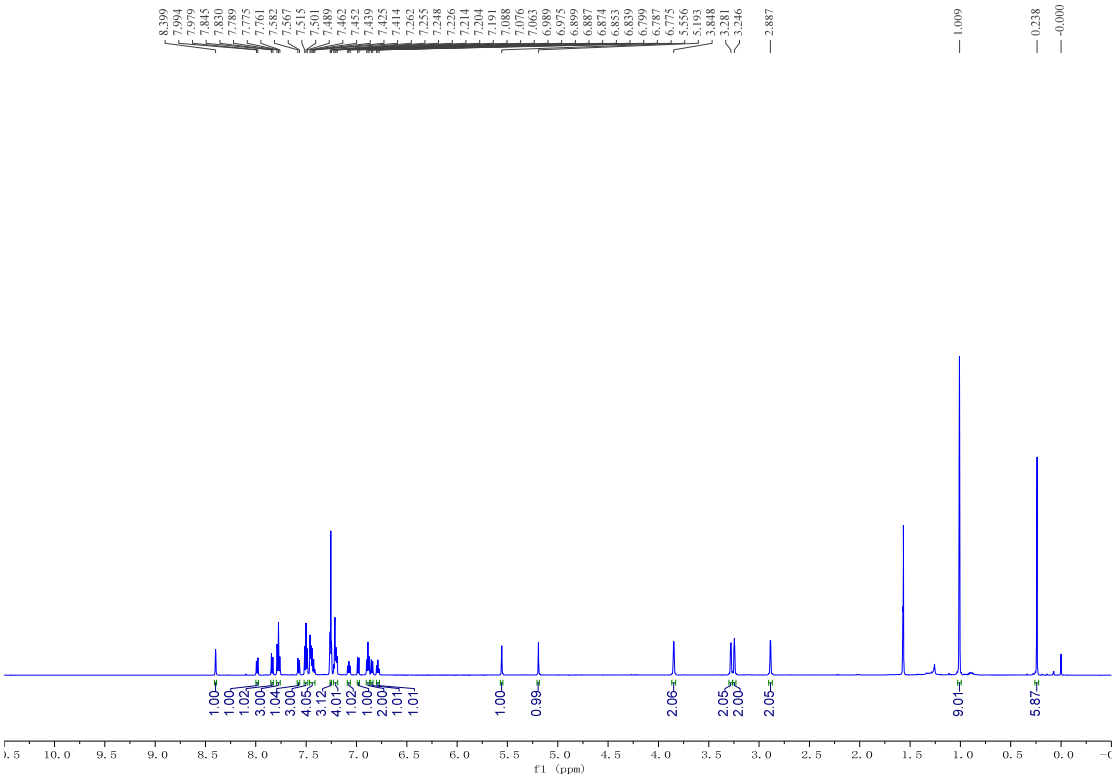


^{13}C NMR (150 MHz, $CDCl_3$)

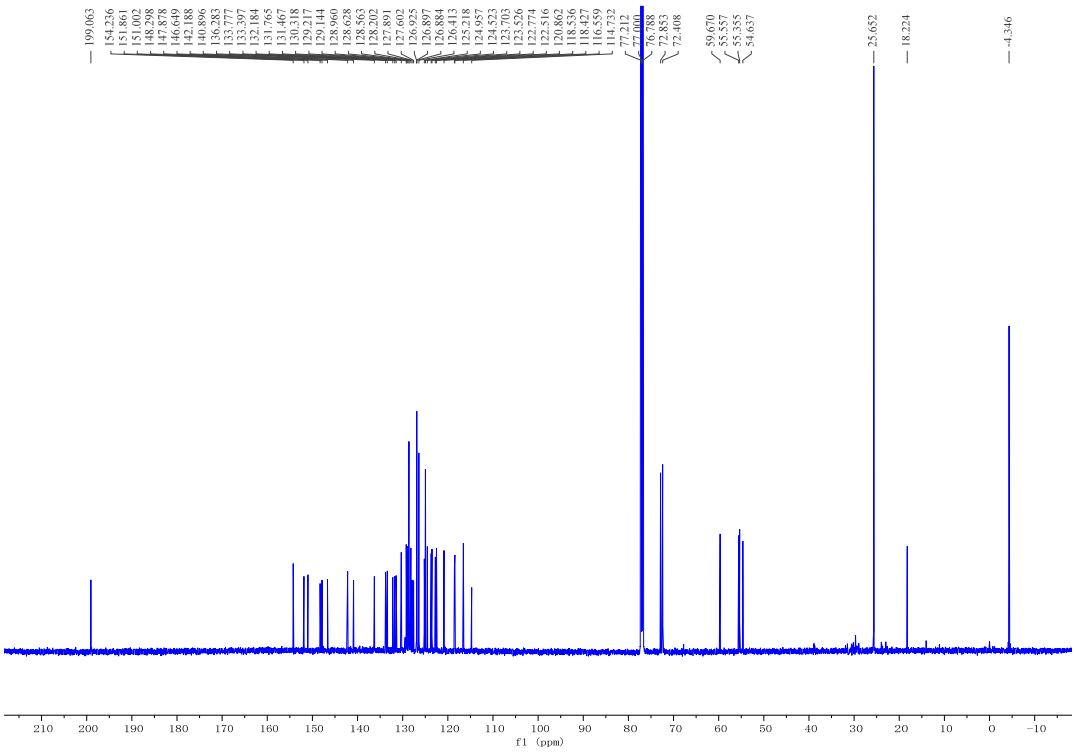


^{1}H and ^{13}C NMR Spectra for Compound 13:

^{1}H NMR (600 MHz, $CDCl_3$):

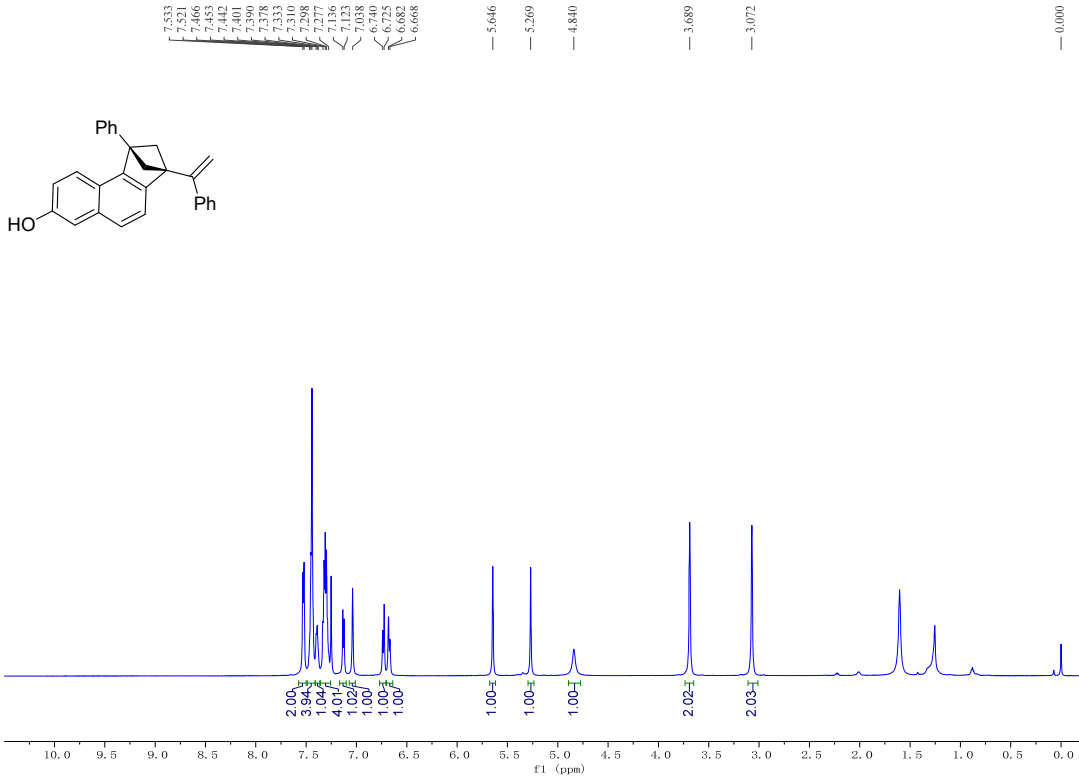


^{13}C NMR (150 MHz, $CDCl_3$)

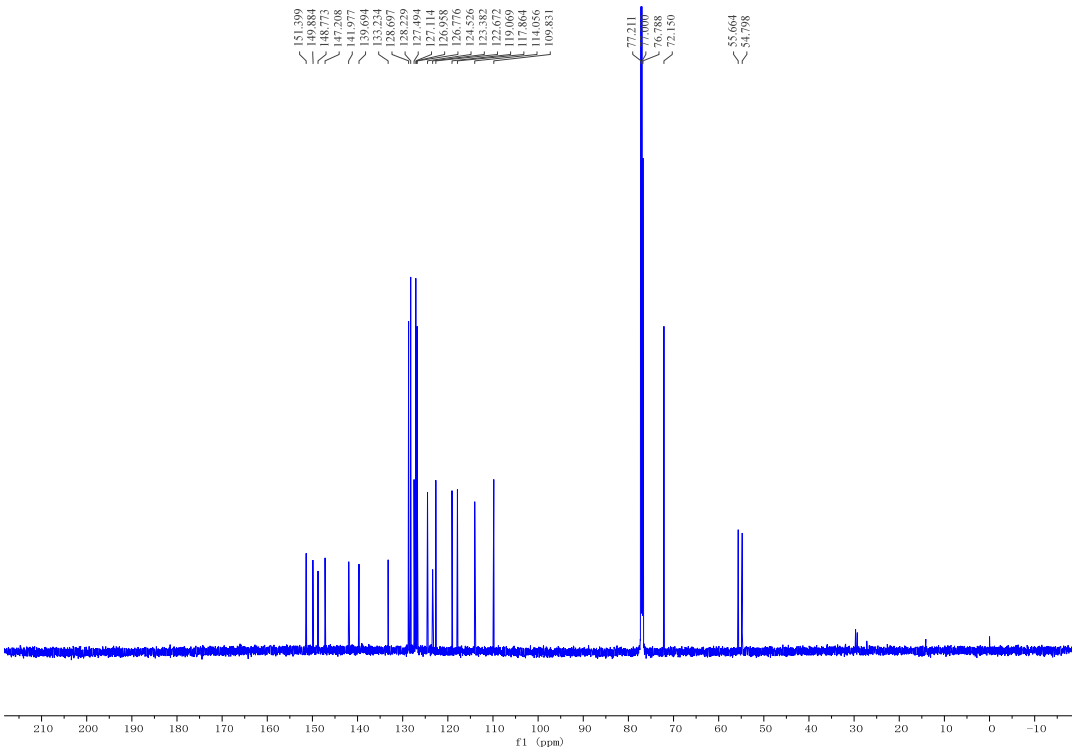


^{1}H and ^{13}C NMR Spectra for Compound 14

^{1}H NMR (600 MHz, $CDCl_3$)

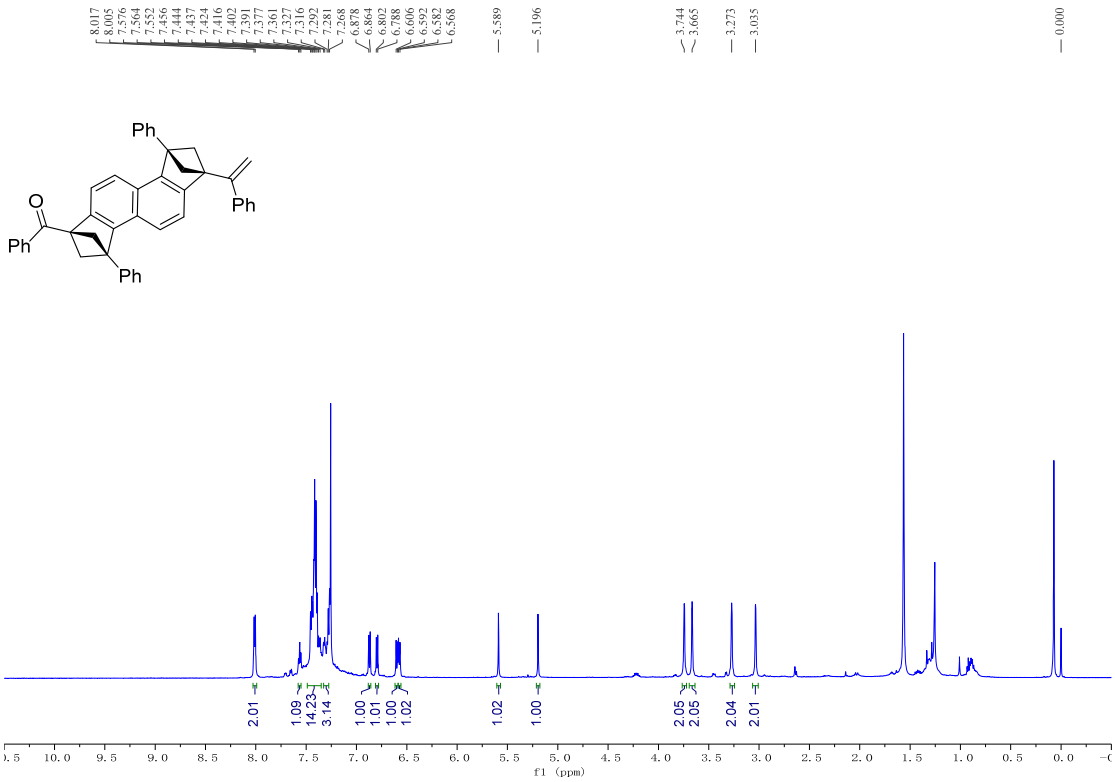


^{13}C NMR (150 MHz, $CDCl_3$)

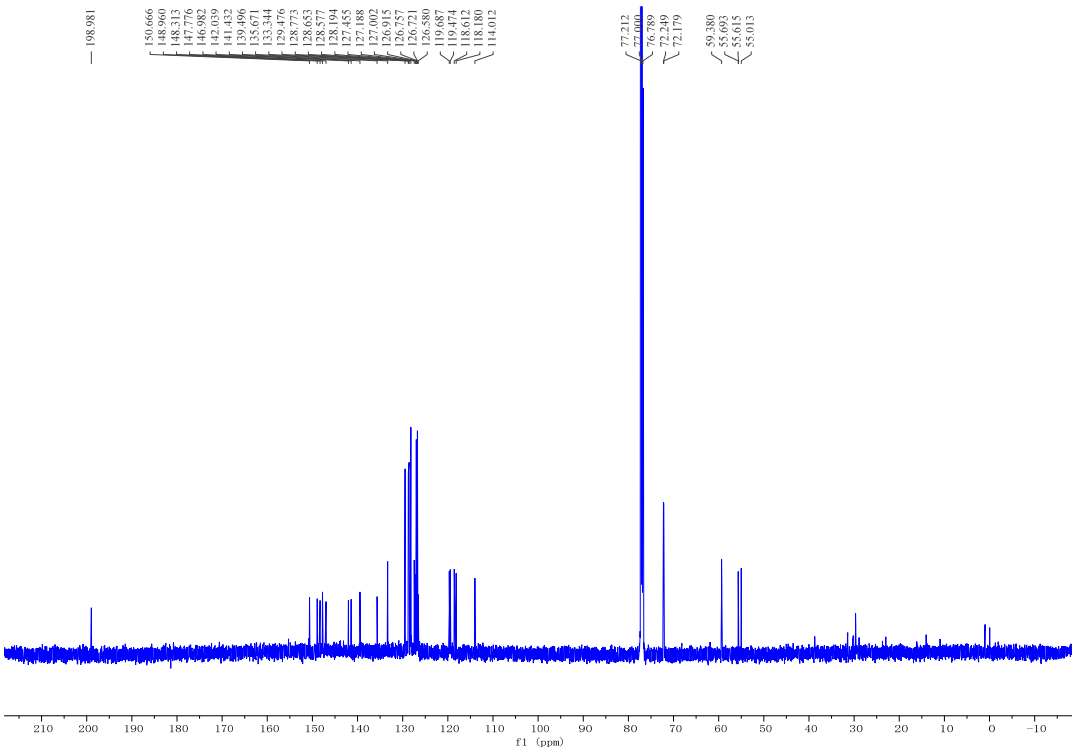


^{1}H and ^{13}C NMR Spectra for Compound 15

^{1}H NMR (600 MHz, $CDCl_3$)

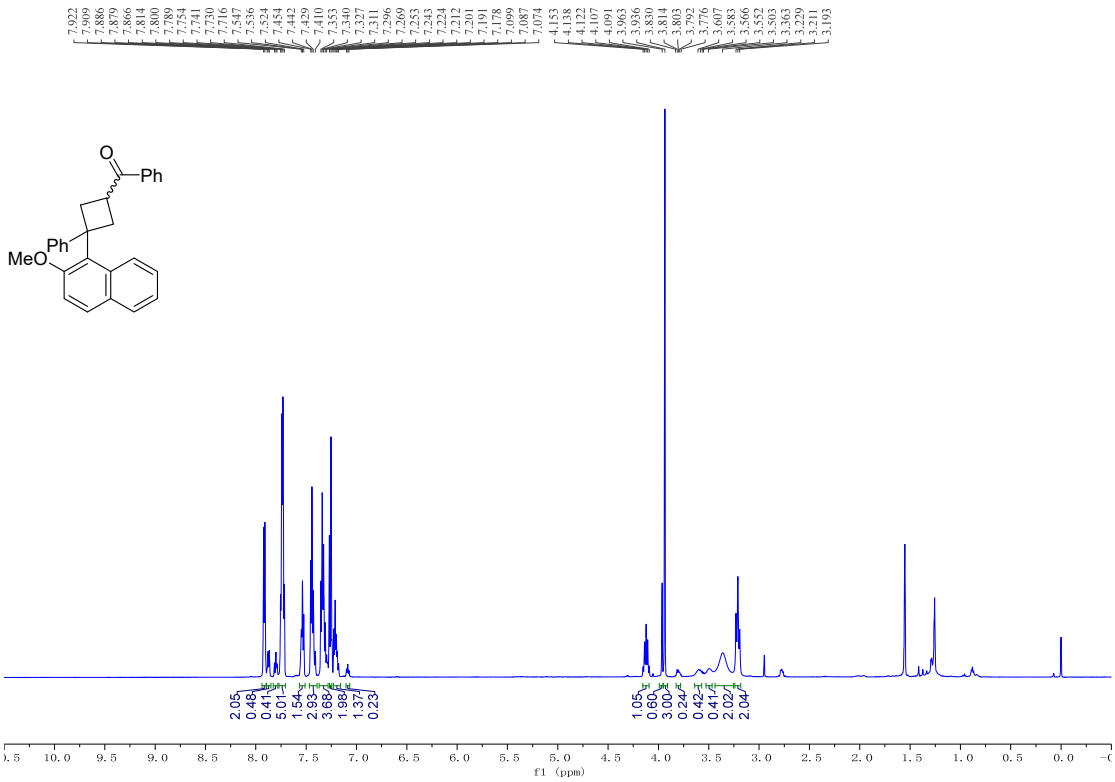


^{13}C NMR (150 MHz, $CDCl_3$)

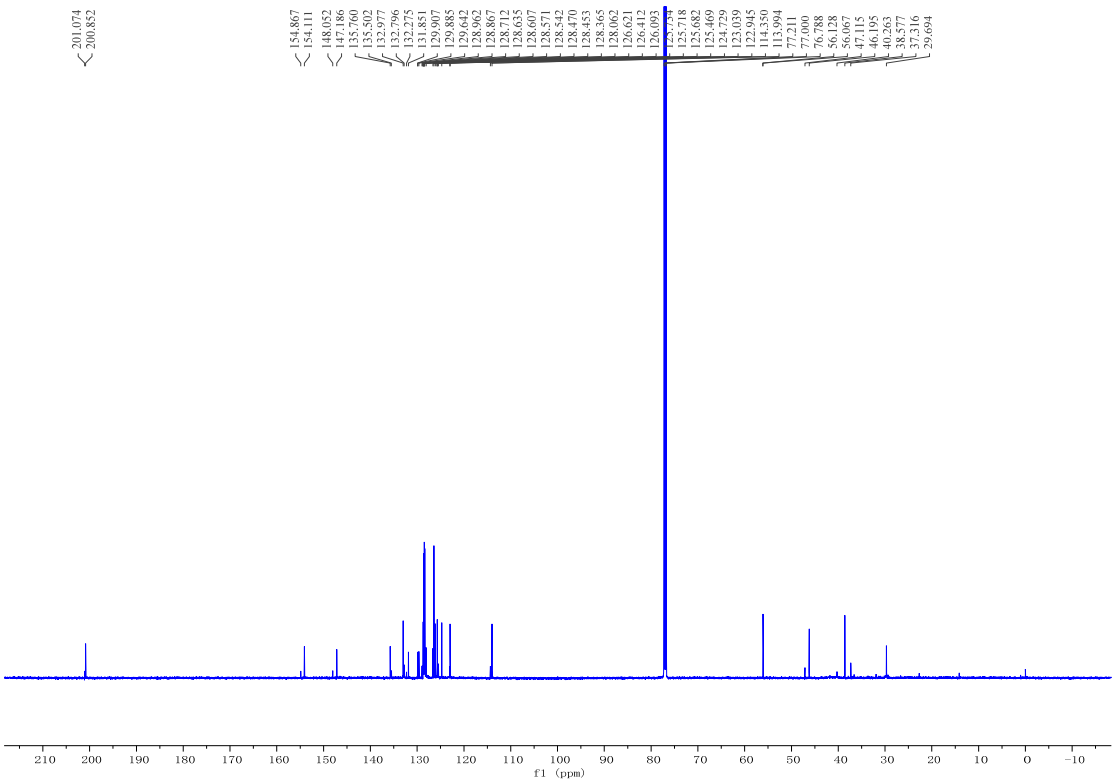


^{1}H and ^{13}C NMR Spectra for Compound 17

^{1}H NMR (600 MHz, $CDCl_3$)

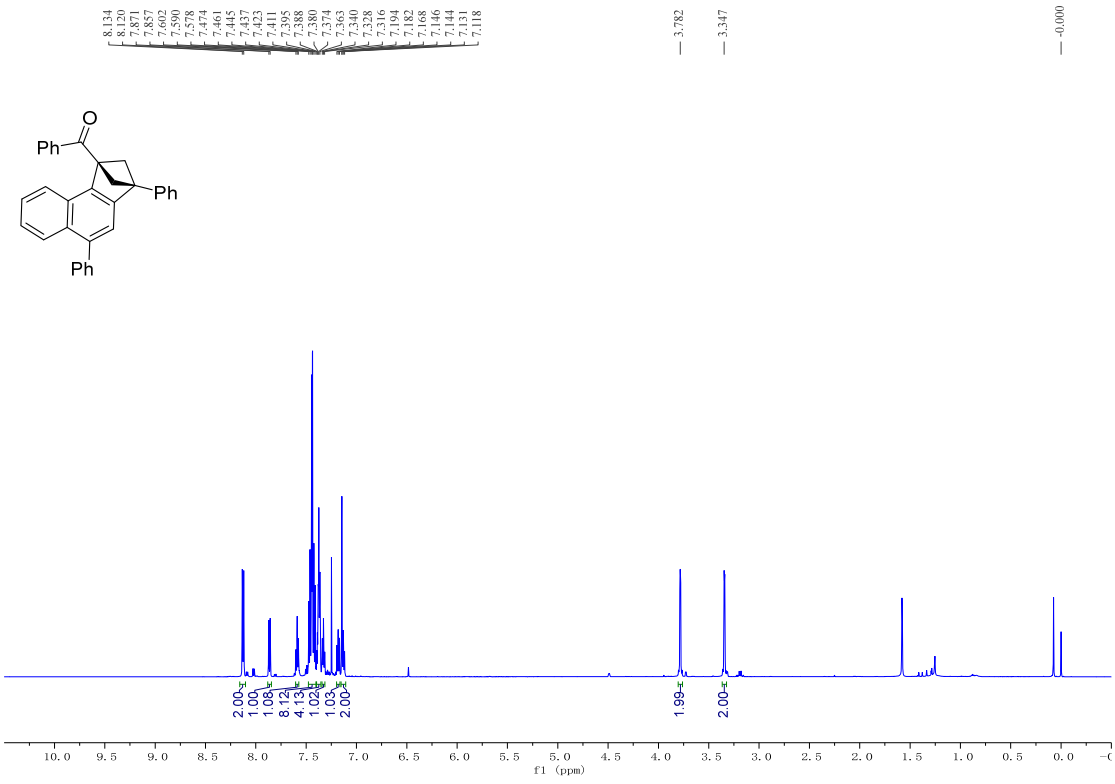


^{13}C NMR (150 MHz, $CDCl_3$)

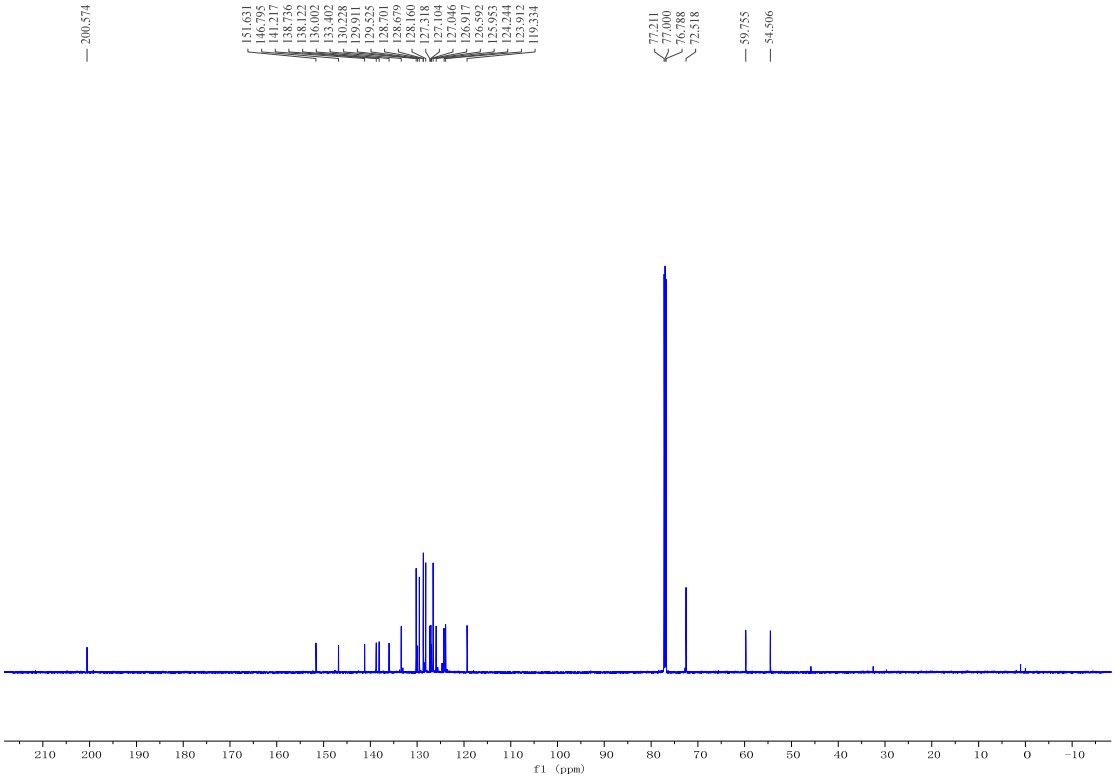


^{1}H and ^{13}C NMR Spectra for Compound 3az

^{1}H NMR (600 MHz, $CDCl_3$)

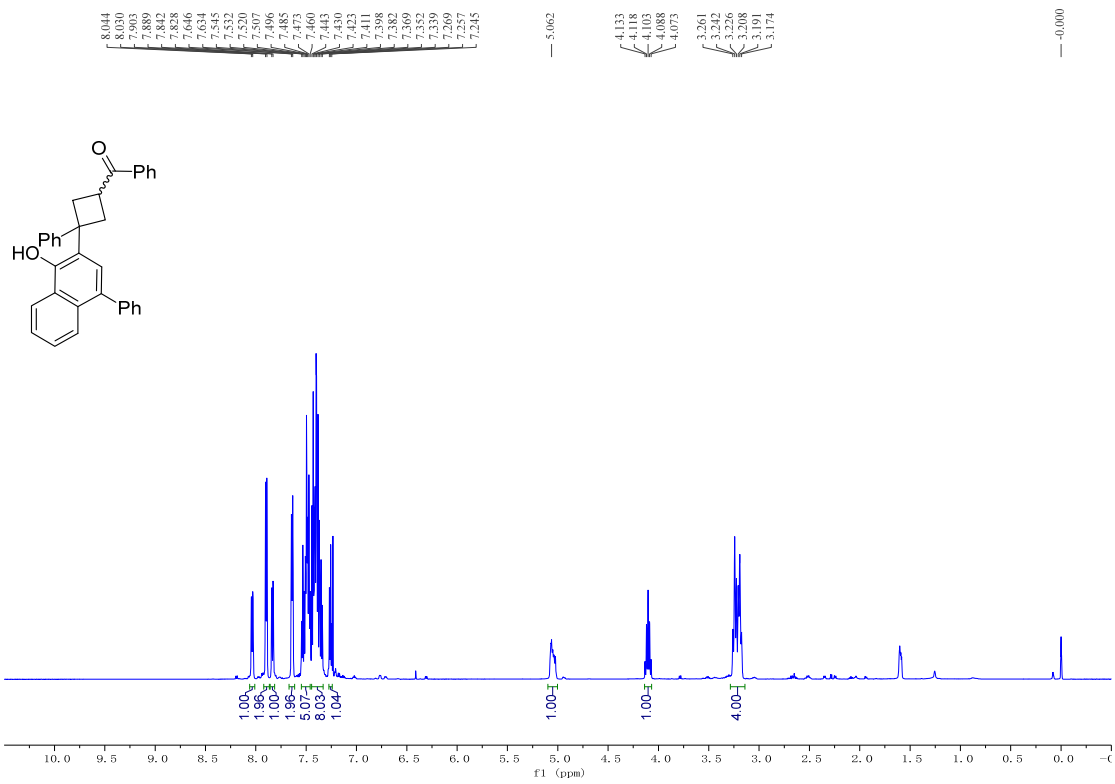


^{13}C NMR (150 MHz, $CDCl_3$)

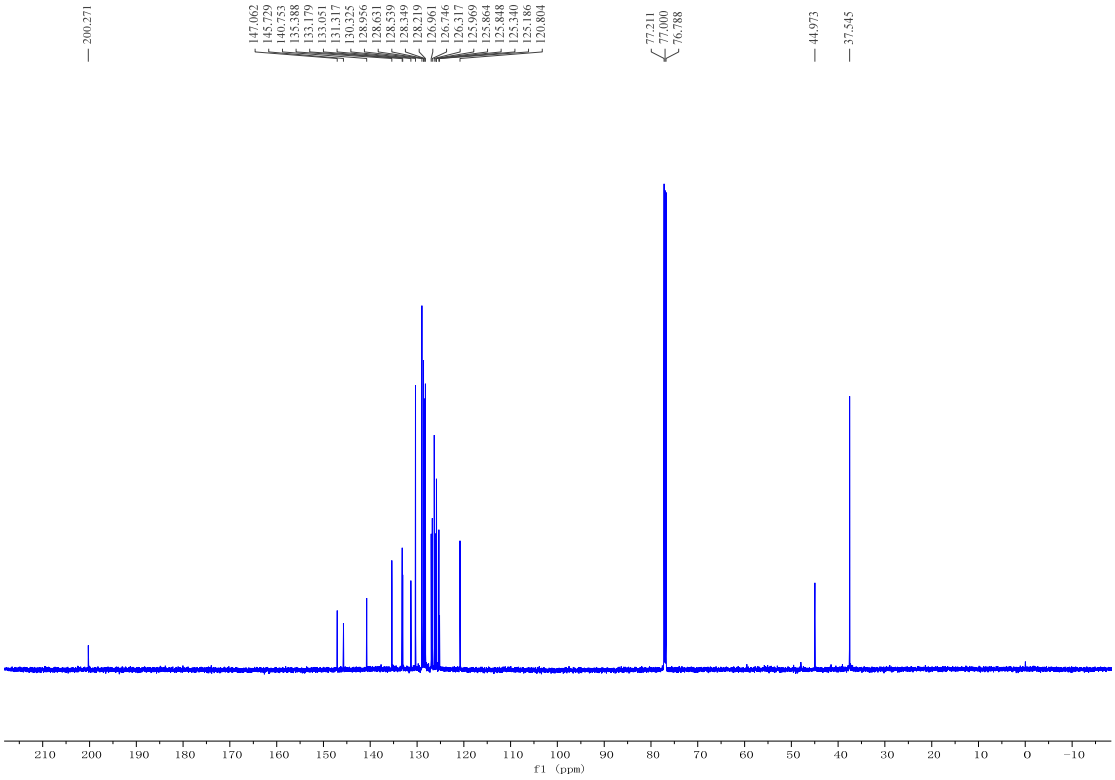


^{1}H and ^{13}C NMR Spectra for Compound 18

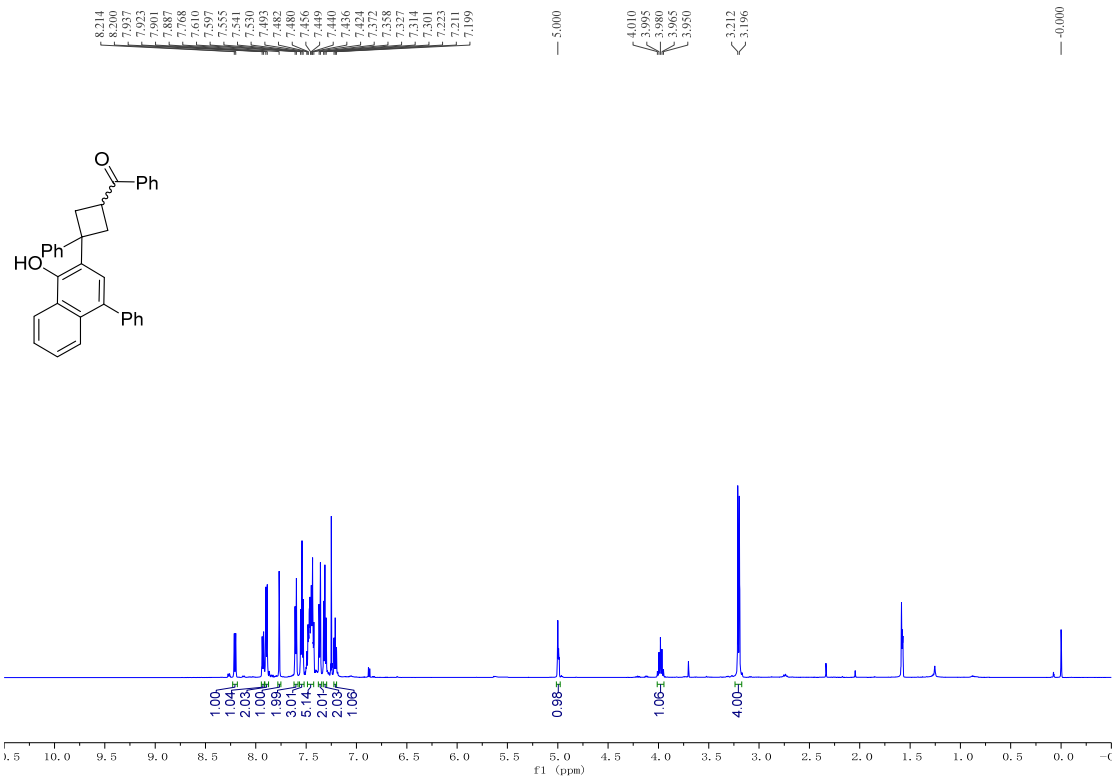
^{1}H NMR (600 MHz, $CDCl_3$) for the **major isomer:**



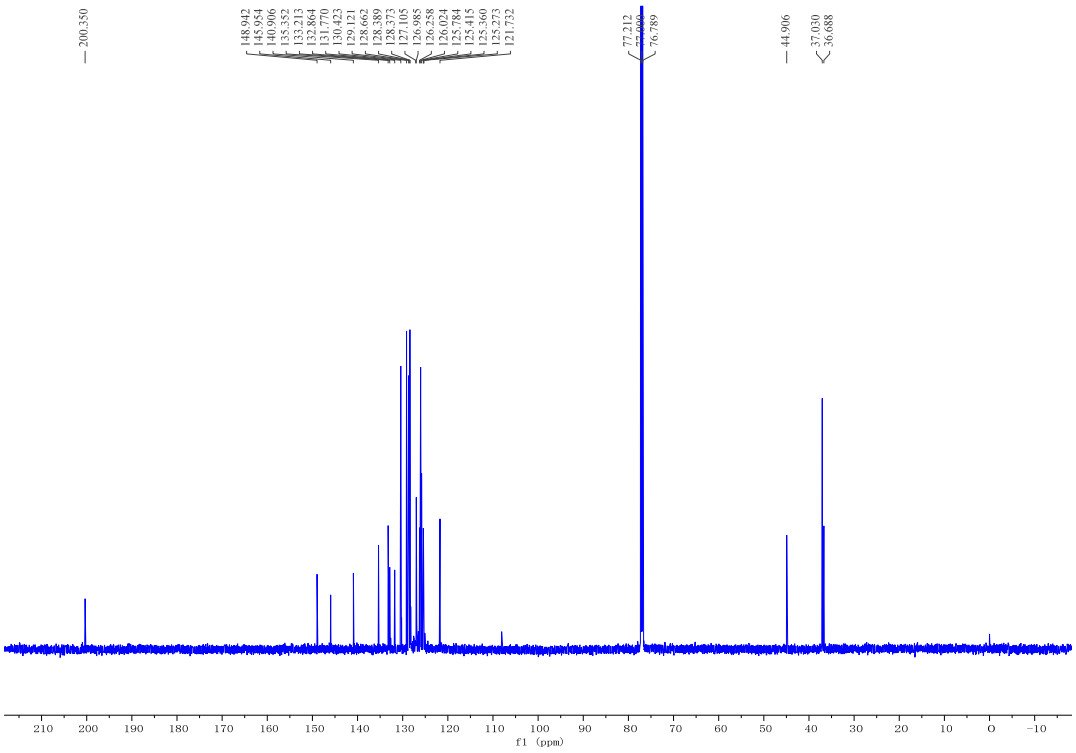
^{13}C NMR (150 MHz, $CDCl_3$) for the **major isomer:**



^{1}H NMR (600 MHz, $CDCl_3$) for the **minor isomer:**



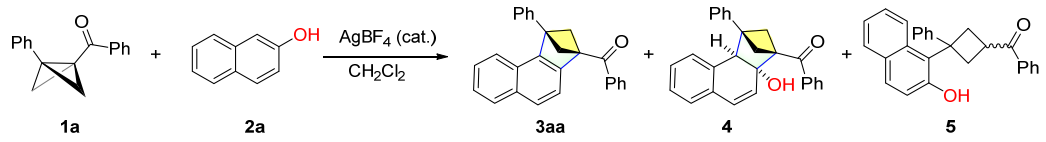
^{13}C NMR (150 MHz, $CDCl_3$) for the **minor isomer:**



11. Computational Data

11.1 Computational details

All density functional theory (DFT) calculations were performed using the Gaussian 16 package (A03 version) [3]. 3D structures were visualized using CYLview software.[4] Geometry optimization and vibrational frequency calculations for all stationary points were conducted at B3LYP-D3(BJ) [5,6] /def2-SVP level of theory [7]. Single-point energies were computed at B3LYP-D3/def2-TZVP level with the polarizable continuum model (PCM [8], dichloromethane) for all species along the reaction pathway. Activation barriers are defined as the free energy difference between the transition state and the lowest-energy stationary point before it along the reaction pathway. The reaction between 1,3-disubstituted BCB ketone **1a** and 2-naphthol **2a** was selected as the model substrate. In addition to the pathway leading to the formation of the desired [2π+2σ] cycloadduct **3aa**, the competitive formation of dearomative [2π+2σ] cycloadduct **4** and C-cyclobutylation of naphthol (leading to byproduct **5**) were also investigated theoretically (Scheme 1). Nucleus independent chemical shifts (NICS), specifically NICS(0) and NICS(1) were calculated for the cycloaddition/rearomatization products **3aa** and its derivatives **15** at B3LYP/6-311+G(d,p) level of theory [9]. The NICS probes (bq's) were placed at the geometric centers of the systems, with NICS(0) calculated at the center of the molecular plane (0.0 Å) and NICS(1) calculated 1.0 Å above the plane along the line perpendicular to it.



Scheme S3. Model reaction.

11.2 Results of the DFT Calculations

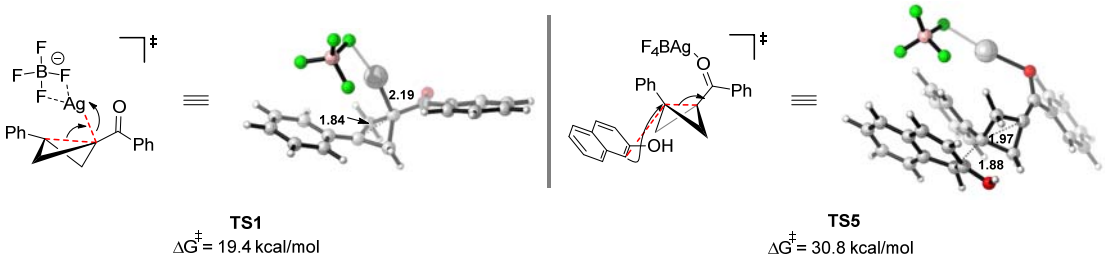


Figure S2. Key transition states for the ring-opening of BCB **1a**: Left: via 1,3-silver cation migration (**TS1**); Right: via a concerted nucleophilic addition/ring-opening transition state (**TS5**) (energies are relative to **IM1**).

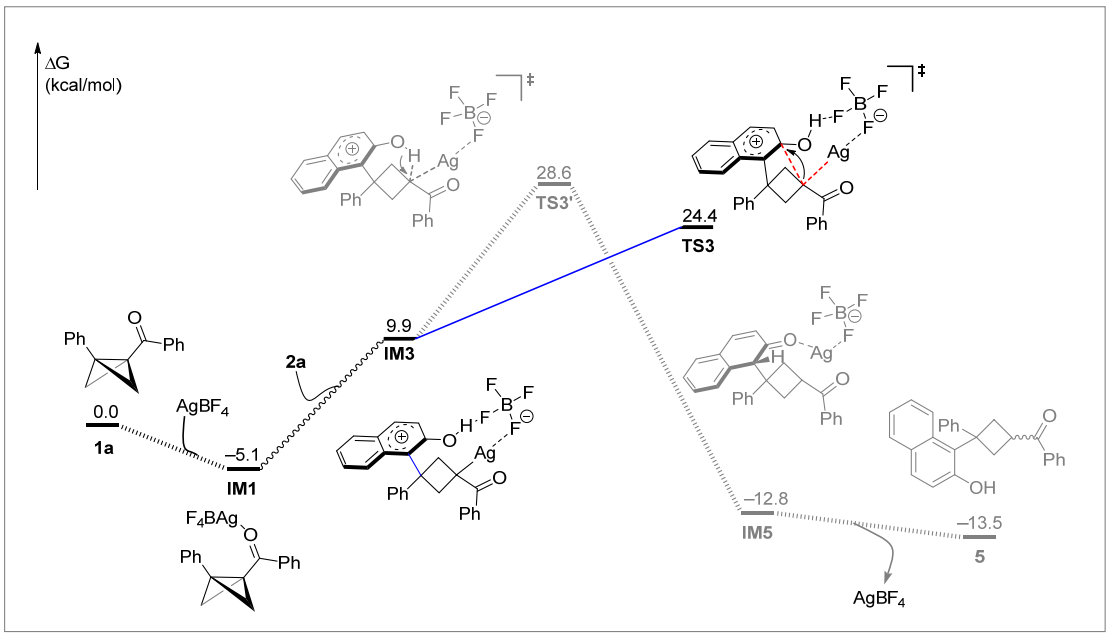
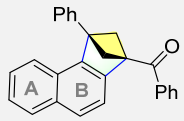
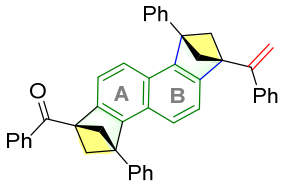
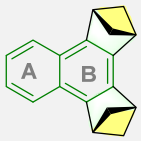


Figure S3. Gibbs free energy profile for the dearomative C-cyclobutylation of naphthol **2a** (in kcal/mol). Computed at B3LYP-D3/def2-TZVP (PCM, dichloromethane)//B3LYP-D3(BJ)/def2-SVP (PCM, dichloromethane) level of theory.

11.3 Aromaticity of the Selected Cycloadducts with Nucleus-Independent Chemical Shifts (NICS) as a Criterion

Table S3. NICS(total) B3LYP/6-311+G** Values for Selected Benzobicyclo[2.1.1]hexenes[a]

	NICS(0) A ring	NICS(0) B ring	NICS(1) A ring	NICS(1) B ring
Naphthalene	-8.57		-10.65	
 **3aa**	-7.90	-9.57	-10.19	-10.88
 **15**	-8.98	-9.01	-9.91	-10.31
 **16**	-6.2	-9.85	-8.52	-10.82

[a]Computed based on the structures optimized at B3LYP-D3(BJ) /def2-SVP level.

11.4 Cartesian Coordinates of the Optimized Stationary Points

1a

C	0.14930600	1.82160100	-1.52180500
C	-0.04062100	1.94126600	-0.03270500
C	1.23271900	2.67931100	0.27575600
C	1.31779400	1.50909400	-0.64429400
H	-0.33348300	0.98144500	-2.02771200
H	0.16455700	2.75163600	-2.10619700
H	1.62273500	2.55504600	1.28887900
H	1.34623300	3.68590300	-0.14794100
C	-0.71009000	1.05181000	0.92861100
O	-0.29919900	0.96920400	2.08186000
C	-1.84168900	0.19805200	0.45319600
C	-2.69524700	0.58383100	-0.59362800
C	-2.06900000	-1.02254700	1.11206200
C	-3.75347700	-0.24291300	-0.97865500
H	-2.54973100	1.54351500	-1.09095400
C	-3.11377800	-1.85484100	0.71459300
H	-1.40678000	-1.30209900	1.93316900
C	-3.95854600	-1.46566500	-0.33237700
H	-3.27509900	-2.80895100	1.22167700
C	2.00176800	0.22350000	-0.44957400
C	2.84086000	0.01631400	0.66056200
C	1.80949700	-0.83611700	-1.35542000

C	3.45241700	-1.22105800	0.86803900
H	3.01955600	0.83029000	1.36425100
C	2.42339900	-2.07174400	-1.14582500
H	1.17885000	-0.68961200	-2.23403000
C	3.24489500	-2.27145200	-0.03149100
H	4.09848600	-1.36420000	1.73745900
H	2.26188000	-2.88282000	-1.85988500
H	3.72708500	-3.23820200	0.13055000
H	-4.78087200	-2.11535700	-0.64141100
H	-4.42105600	0.06912300	-1.78499800

2a

C	1.04002200	-1.11562100	-0.00100000
C	2.11171000	-0.24024600	-0.00088500
C	-0.29264900	-0.62851400	-0.00062800
C	0.59881700	1.65905900	-0.00048700
C	-2.93072500	0.39986000	0.00082300
C	-1.86306300	1.27270900	0.00038800
C	-2.70273700	-1.00103000	0.00035100
C	-1.41804000	-1.50239100	-0.00035000
C	-0.52540900	0.78882700	-0.00035300
C	1.88419700	1.16379500	-0.00070100
H	2.74056500	1.84437500	-0.00016400
H	0.43219200	2.73918000	-0.00048300
H	-2.02950800	2.35321400	0.00104300

H	-3.95425300	0.78175500	0.00125100
H	-3.55478700	-1.68527400	0.00070200
H	-1.24476100	-2.58158400	-0.00039400
H	1.23009800	-2.19094600	-0.00112400
O	3.36907000	-0.75104100	0.00147500
H	4.01515600	-0.03107700	0.00442600

$AgBF_4$

Ag	-1.36578200	0.00005900	0.00014600
B	1.61476500	0.00035900	-0.00017100
F	0.73864400	0.02832000	-1.13927700
F	2.37576800	1.14880000	0.02908400
F	2.37900200	-1.14618100	-0.03027300
F	0.74191500	-0.03144900	1.13979900

IM1

C	-3.01664100	0.36659800	-1.16348800
C	-3.43055000	-0.86558800	-1.92206800
C	-3.31874200	-0.99932000	-0.43812900
H	-3.76478200	0.69618700	0.92237900
H	-5.07615800	0.36877600	-0.32779500
H	-2.66428100	-1.34360500	-2.53635700
H	-4.43604100	-0.85971300	-2.36009500
C	-1.63812600	0.79005700	-1.05616000
O	-0.80469900	0.37381300	-1.88695200

C	-1.23240500	1.60055500	0.12162100
C	-1.91669400	2.78012300	0.45794100
C	-0.14920200	1.17370000	0.91157500
C	-1.49179400	3.54575200	1.54500700
H	-2.76403900	3.10749100	-0.14780900
C	0.26483300	1.93786900	2.00349500
H	0.34648600	0.22052800	0.71461300
C	-0.40079600	3.12736800	2.31560700
H	1.11296800	1.59342900	2.59655100
C	-2.33564200	-1.76205600	0.34512600
C	-1.39249700	-2.59044500	-0.29215300
C	-2.27074300	-1.61071500	1.74186100
C	-0.39186600	-3.22075700	0.44712800
H	-1.43537900	-2.73515500	-1.37226400
C	-1.27150300	-2.24909600	2.47769500
H	-3.00343800	-0.98576600	2.25479000
C	-0.32368500	-3.04851100	1.83284700
H	0.34512500	-3.84419700	-0.06299300
H	-1.23013000	-2.11523200	3.56095900
H	0.46699200	-3.53554100	2.40724300
H	-0.07295100	3.72891900	3.16651100
H	-2.01220000	4.47399600	1.79054900
Ag	1.38866700	0.39404500	-1.57767900
B	3.32069300	-0.39925900	0.59944800
F	3.43809900	0.45522900	-0.57150100

F	3.10940200	0.40317400	1.70944000
F	4.46245900	-1.16076400	0.71107800
F	2.18918500	-1.21487300	0.36532800

TS1

O	2.80501900	-1.71930000	-1.78961600
C	2.41935400	-1.15842000	-0.77471600
C	0.75106200	-1.80498300	1.22944700
H	0.63278200	-1.04916700	2.01110000
H	1.39430900	-2.63899400	1.55355300
C	-1.81326800	-1.85083700	0.63547800
C	0.28182000	-2.65599900	-0.75317100
H	0.88707400	-3.56906000	-0.62467400
H	-0.24035800	-2.63912100	-1.71449100
C	-0.44217300	-2.21704800	0.46020500
C	-2.76105700	-2.13586700	-0.37885900
H	-2.44511000	-2.65329600	-1.28534300
C	-2.23367000	-1.19318100	1.81591200
H	-1.51093800	-0.97532900	2.60224800
C	-3.55886800	-0.80816100	1.96283800
H	-3.87873600	-0.28674200	2.86633300
C	-4.08298800	-1.74556400	-0.22280700
H	-4.81150900	-1.95464600	-1.00801800
C	-4.47957400	-1.07456100	0.94288000
H	-5.51799800	-0.75572700	1.05517100

C	3.33365000	-0.25858100	0.00773900
C	4.70715300	-0.32515500	-0.27860600
C	2.88416500	0.63779500	0.99035400
C	5.61405700	0.48054000	0.40975500
H	5.04354500	-1.01919000	-1.05024700
C	3.79019300	1.44996000	1.67397000
H	1.81922400	0.72525700	1.21221500
C	5.15732600	1.37027800	1.38808100
H	3.42680300	2.15041800	2.42899500
H	5.86573700	2.00532100	1.92516300
H	6.68052700	0.41772000	0.18153100
Ag	-0.01989700	0.43570700	-0.81845200
B	-2.29750000	2.30176000	-0.22947300
F	-3.48928100	1.64386200	-0.46749700
F	-1.61762900	1.72599600	0.86369500
F	-2.46808200	3.65706800	-0.04804100
F	-1.42468400	2.09607200	-1.38477500
C	1.03852300	-1.39305900	-0.25723600

IM2

O	2.74817500	-0.81492000	-2.31250800
C	2.44458500	-0.65854900	-1.13664000
C	0.79749500	-1.91566800	0.51672000
H	0.69773200	-1.58235200	1.55473400
H	1.48883800	-2.77184100	0.44268100

C	1.05335400	-0.89711800	-0.66769300
C	-1.78572300	-1.96529100	0.13433200
C	0.17995400	-1.80917600	-1.59453300
H	0.79319200	-2.64151300	-1.98274800
H	-0.44402200	-1.38539200	-2.38795300
C	-0.43844100	-2.08336100	-0.28078800
C	-2.81441400	-1.73737200	-0.81716200
H	-2.56457900	-1.65444000	-1.87446500
C	-2.11692800	-2.05731600	1.51326800
H	-1.32990900	-2.23413800	2.24699500
C	-3.43398100	-1.92747300	1.92003800
H	-3.69280400	-1.99788500	2.97767600
C	-4.12707800	-1.59552700	-0.39805500
H	-4.91627700	-1.39875300	-1.12476800
C	-4.43454000	-1.68791400	0.96606200
H	-5.47025200	-1.56902000	1.29265600
C	3.48064600	-0.24442200	-0.12789100
C	4.82926700	-0.31977800	-0.51346800
C	3.16506100	0.20536700	1.16445400
C	5.84259400	0.03720900	0.37603300
H	5.06082200	-0.66401800	-1.52262100
C	4.17861300	0.56738800	2.05349300
H	2.12296700	0.29847300	1.47331300
C	5.51917500	0.48164100	1.66266200
H	3.92086500	0.92392100	3.05326800

H	6.31112300	0.76573000	2.35969100
H	6.88812800	-0.02893000	0.06608000
Ag	0.07687400	0.99534600	-0.38460600
B	-2.69786000	1.97137100	0.03898900
F	-3.01577200	1.35533500	-1.16673400
F	-2.50450000	1.02083900	1.04452300
F	-3.62951000	2.91928300	0.40140700
F	-1.40720100	2.64516200	-0.14785600

TS2

O	-0.99986800	2.23263100	-2.49838900
C	-1.25913100	1.98143200	-1.31686700
C	0.03577500	1.22679300	0.82928900
H	-0.29004700	0.60335100	1.67296900
H	-0.03349700	2.27977000	1.14894300
C	-0.56776900	0.91204100	-0.58127500
C	2.60767100	1.67281500	0.51123600
C	0.84844900	0.57255100	-1.11324000
H	1.20017300	1.25728200	-1.90249900
H	1.03060200	-0.45161300	-1.47105500
C	1.39961400	0.91785900	0.24892600
C	3.61195000	1.78329200	-0.47347800
H	3.47712900	1.29149400	-1.43742000
C	2.80003500	2.30654800	1.76013200
H	2.03304200	2.21945500	2.53257400

C	3.95774600	3.03369900	2.00859500
H	4.09999500	3.52011600	2.97570500
C	4.76378800	2.52991100	-0.22641500
H	5.53023100	2.61775000	-0.99881800
C	4.94016500	3.15084400	1.01244600
H	5.84525900	3.73022500	1.20807800
C	-2.30235000	2.81028300	-0.60200700
C	-2.71345900	4.00684300	-1.21067500
C	-2.87435300	2.44945800	0.63031600
C	-3.66248100	4.82972400	-0.60282300
H	-2.26930700	4.27133100	-2.17157400
C	-3.82846900	3.26832500	1.23795400
H	-2.59421500	1.51163600	1.11197400
C	-4.22322200	4.46234100	0.62509600
H	-4.26996500	2.96984100	2.19172800
H	-4.96992000	5.10207800	1.10174500
H	-3.96909400	5.75964300	-1.08802900
Ag	-1.99936200	-0.68047900	-0.63144000
B	-3.10599100	-3.32543700	0.60855300
F	-3.45118200	-2.39062100	-0.43421900
F	-2.43850900	-2.55920800	1.62247700
F	-2.22064500	-4.25635800	0.09156900
F	-4.24263500	-3.88973500	1.11912300
C	2.04793000	-1.03455300	1.21454000
C	0.83095200	-1.75739600	1.14197200

C	3.13539700	-1.39647000	0.34263000
C	1.57042300	-2.83699800	-0.88526400
C	5.17530600	-2.01840600	-1.50380300
C	3.90557300	-2.54287600	-1.68831400
C	5.44165600	-1.19788400	-0.39045800
C	4.43785900	-0.88796200	0.51892500
C	2.87101300	-2.25243600	-0.76852800
C	0.58185200	-2.62970500	0.05021700
H	-0.36437300	-3.16805000	-0.01021000
H	1.37503600	-3.50628100	-1.72668500
H	3.69108000	-3.19376900	-2.53898300
H	5.97214400	-2.24780300	-2.21400200
H	6.44644200	-0.79676400	-0.24144800
H	4.65261600	-0.25312000	1.37984300
H	2.26341200	-0.52175100	2.15179700
O	-0.05749900	-1.56453300	2.10285000
H	-0.91264600	-2.02704100	1.91928700

IM3

O	-0.97830200	2.19238400	-2.51844400
C	-1.21840200	1.96240600	-1.32828200
C	0.10575800	1.22976600	0.81651800
H	-0.33298200	0.75762400	1.70415000
H	0.18436800	2.30875100	1.01744200
C	-0.49395600	0.92313000	-0.58052400

C	2.64341800	1.60582000	0.54643300
C	0.90338100	0.56151800	-1.11046900
H	1.29044500	1.34128700	-1.78134200
H	1.03822900	-0.40102900	-1.62315300
C	1.47520600	0.66832900	0.32885000
C	3.53431300	1.93485000	-0.48288200
H	3.38404500	1.52533300	-1.48252400
C	2.87462300	2.13290900	1.82756500
H	2.19079800	1.88902000	2.64498200
C	3.96936500	2.96229400	2.07457200
H	4.13217100	3.36246200	3.07807600
C	4.62996000	2.76958200	-0.24110800
H	5.31433900	3.01224500	-1.05737600
C	4.85370500	3.28338100	1.03791800
H	5.71070000	3.93355500	1.22832100
C	-2.26059000	2.79605500	-0.61650200
C	-2.70186300	3.96944300	-1.24858100
C	-2.80334800	2.46019000	0.63570000
C	-3.65316400	4.79320100	-0.64528700
H	-2.27938800	4.21468200	-2.22426200
C	-3.76002700	3.27929800	1.23892300
H	-2.49593200	1.54215400	1.13782100
C	-4.18571300	4.44994300	0.60198900
H	-4.17834800	3.00010400	2.20890200
H	-4.93387400	5.09039500	1.07543100

H	-3.98357300	5.70494000	-1.14909900
Ag	-1.95659900	-0.65217500	-0.62917000
B	-3.10947000	-3.30478600	0.65218300
F	-3.43067700	-2.34675500	-0.37072600
F	-2.41174000	-2.57231800	1.68184800
F	-2.24778300	-4.25054900	0.12256600
F	-4.25392700	-3.84391600	1.16622800
C	1.88629300	-0.76478400	0.99205500
C	0.70873100	-1.67212700	1.01633400
C	3.05752700	-1.32716600	0.23621600
C	1.51766000	-2.87189100	-0.89656200
C	5.17238500	-2.24661900	-1.38904500
C	3.88460500	-2.72270600	-1.60412900
C	5.40997000	-1.34266800	-0.34477700
C	4.36101800	-0.88282000	0.45837400
C	2.82195300	-2.28302900	-0.78547100
C	0.49751500	-2.62429300	-0.00411800
H	-0.41766600	-3.21689300	-0.02222700
H	1.35784700	-3.61785700	-1.67950600
H	3.68428700	-3.45271500	-2.39126300
H	5.99702100	-2.58837100	-2.01719000
H	6.42510500	-0.98890000	-0.15264900
H	4.56525800	-0.17697000	1.26328100
H	2.15119200	-0.52734800	2.03097700
O	-0.10055800	-1.52197700	2.01642100

H	-0.95047300	-2.04178000	1.91594800

TS3

O	-1.55836900	1.19530500	-2.44457000
C	-1.36919200	1.53730400	-1.21680800
C	0.49096700	1.67228400	0.72968700
H	0.07812600	1.40839300	1.71360800
H	0.67464300	2.76054200	0.72270100
C	-0.18886200	1.18926200	-0.53161400
C	3.07556500	1.65970500	0.38033700
C	1.11935900	0.74648500	-1.13800300
H	1.51488100	1.47888800	-1.86189100
H	1.18068000	-0.24411000	-1.62166600
C	1.77301400	0.90864100	0.26726400
C	3.98982400	1.71590200	-0.67949000
H	3.75266800	1.22712600	-1.62587000
C	3.41311300	2.27931300	1.59414300
H	2.71154700	2.24557400	2.43195200
C	4.63595000	2.93509200	1.74655300
H	4.88189900	3.41210600	2.69825000
C	5.21397200	2.37497700	-0.53226700
H	5.91570500	2.40615000	-1.36904700
C	5.54260500	2.98375100	0.68138500
H	6.49990900	3.49702000	0.79820600
C	-2.43037500	2.36267000	-0.54286500

C	-3.26720900	3.15167900	-1.34967200
C	-2.63760600	2.35721600	0.84746100
C	-4.26732200	3.94050200	-0.77934000
H	-3.11548300	3.12862000	-2.42975200
C	-3.64901100	3.13402200	1.41609500
H	-2.02976100	1.71742800	1.48655200
C	-4.46136500	3.93514400	0.60634200
H	-3.80801100	3.10831000	2.49679000
H	-5.24912000	4.54622200	1.05342300
H	-4.90339900	4.55842100	-1.41804500
Ag	-1.98177100	-0.77734200	-1.08779600
B	-3.18660400	-2.63133200	1.19230200
F	-3.21222500	-2.55799200	-0.24161200
F	-2.62435600	-1.37170600	1.63370000
F	-2.32203500	-3.63959600	1.57116400
F	-4.45165800	-2.77497200	1.68559500
C	1.92195700	-0.50938900	1.02721300
C	0.59002300	-1.18096300	1.09733900
C	2.97236900	-1.33127100	0.33094500
C	1.17802800	-2.63040300	-0.73787600
C	4.89476400	-2.70533000	-1.20301600
C	3.54220900	-2.94579600	-1.41984800
C	5.28915100	-1.80831300	-0.20162900
C	4.33305900	-1.12384300	0.55632400
C	2.56943300	-2.27738400	-0.64598600

C	0.22756300	-2.16653600	0.15066900
H	-0.73904900	-2.66414000	0.22617700
H	0.88744900	-3.39258200	-1.46501500
H	3.22010400	-3.66721400	-2.17400400
H	5.64641700	-3.22687400	-1.79884600
H	6.35040900	-1.63583300	-0.01071100
H	4.65296200	-0.41927300	1.32462100
H	2.22736700	-0.25873800	2.05236500
O	-0.15448400	-0.85017200	2.11303900
H	-1.09026700	-1.18525300	2.02764900

IM4

O	-0.77924000	-1.29204500	2.81978800
C	-0.85253900	-1.49260700	1.61773900
C	0.92426900	-1.88943600	-0.44397200
H	0.51025100	-1.70482400	-1.44379300
H	1.00334300	-2.96659200	-0.24486900
C	0.32878900	-1.10686200	0.76066200
C	3.56999500	-1.59645500	-0.47808800
C	1.72854300	-1.22755200	1.41483700
H	1.88727100	-2.22513200	1.84551500
H	2.03103300	-0.45101700	2.12877800
C	2.21858100	-1.12819700	-0.04932500
C	4.64565800	-1.59912500	0.42056800
H	4.48244700	-1.28869000	1.45475200

C	3.79677300	-1.99021300	-1.80602000
H	2.96665500	-1.99216300	-2.51711000
C	5.07268600	-2.37066800	-2.22797400
H	5.23476300	-2.67393100	-3.26523500
C	5.92345500	-1.98011500	0.00169300
H	6.75254600	-1.97364200	0.71343000
C	6.14141100	-2.36464100	-1.32443800
H	7.14005100	-2.66158400	-1.65356300
C	-2.11056500	-2.07763400	1.04272000
C	-3.16352900	-2.36134800	1.93092900
C	-2.29495500	-2.33490800	-0.33962300
C	-4.37275900	-2.87645900	1.46579500
H	-3.00677300	-2.16000000	2.99109400
C	-3.52597600	-2.83682600	-0.80474700
H	-1.46580900	-2.23078900	-1.03783500
C	-4.56239100	-3.10295600	0.09811800
H	-3.65220700	-3.04748900	-1.86836700
H	-5.51270800	-3.49713000	-0.26731100
H	-5.17771800	-3.09330700	2.17092500
Ag	-2.97658600	-0.04884900	-0.67038600
B	-2.86064300	2.92055200	-0.77012100
F	-3.40953600	2.05011200	-1.76621700
F	-1.48583900	3.07622800	-1.04738300
F	-3.00544000	2.24286500	0.46516100
F	-3.51325700	4.12457700	-0.76286700

C	1.81631600	0.34822500	-0.39990900
C	0.37308300	0.36865500	0.22441400
C	2.78380700	1.39751700	0.08483700
C	1.10676300	2.21295900	1.73465500
C	4.64982000	3.29240000	1.01702200
C	3.39503100	3.18934100	1.61651000
C	4.96615500	2.46875900	-0.06800700
C	4.03394800	1.53582800	-0.53056200
C	2.45063500	2.25426200	1.15745100
C	0.14633500	1.38077300	1.30419700
H	-0.86273300	1.42604300	1.71821900
H	0.88372500	2.93124800	2.52858100
H	3.12738200	3.84780100	2.44699100
H	5.37470800	4.02204800	1.38531000
H	5.94006700	2.55080300	-0.55610500
H	4.28572400	0.89810400	-1.37950700
H	1.71284400	0.43413700	-1.49180700
O	-0.61453100	0.53403700	-0.79940200
H	-0.71131200	1.49300800	-0.97758700

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O	3.65282400	2.70340800	8.35831100
C	3.15493500	1.92101700	9.15569700
C	3.44234900	1.28995800	11.79218200
H	3.01003100	0.31806000	12.06088100

H	2.77996800	2.10874100	12.10457100
C	3.97708200	1.49110700	10.34760900
C	5.32207900	1.98801100	13.54501100
C	4.96487000	2.52051900	10.95445200
H	4.47471000	3.48124700	11.16175100
H	5.92131900	2.68316400	10.44122600
C	4.92182000	1.56205200	12.17107000
C	6.28604300	2.98813800	13.73388500
H	6.72075000	3.48545700	12.86420000
C	4.77781400	1.35289000	14.67217800
H	4.02448300	0.57222300	14.53880400
C	5.19393400	1.70373700	15.95853300
H	4.76151500	1.19998900	16.82660200
C	6.70364900	3.34272100	15.01968200
H	7.45805600	4.12249500	15.14992000
C	6.16101200	2.69962500	16.13603800
H	6.48724300	2.97508800	17.14180100
C	1.75127400	1.44225900	8.97340700
C	0.91858600	2.16765400	8.10153400
C	1.24391700	0.30119400	9.61720400
C	-0.40083700	1.77331900	7.89175000
H	1.33051000	3.04496600	7.59999300
C	-0.07509400	-0.10056100	9.39385600
H	1.89603100	-0.29523600	10.25150900
C	-0.90090100	0.63681100	8.54005000

H	-0.45977500	-0.99570700	9.88803400
H	-1.93505700	0.32457400	8.37538500
H	-1.04374200	2.34870700	7.22157100
C	5.61582800	0.28246300	11.57901200
C	4.90751100	0.24592500	10.17327300
C	7.12239000	0.31603100	11.58963200
C	7.15590000	0.50400800	9.10717600
C	9.93698000	0.45798000	11.65796800
C	9.25836800	0.55568300	10.44361700
C	9.21376900	0.26166700	12.83884600
C	7.81888500	0.18505700	12.79760700
C	7.85514600	0.47890600	10.39262900
C	5.82367200	0.38211000	8.99416800
H	5.34291300	0.37230000	8.01287200
H	7.77118600	0.59873200	8.20769200
H	9.81594700	0.68358400	9.51202000
H	11.02728800	0.52249700	11.68320300
H	9.73473400	0.16986800	13.79474100
H	7.25988100	0.03084700	13.72217300
H	5.27429500	-0.59336600	12.15163900
O	4.08632500	-0.90423100	10.01118500
H	4.66490100	-1.66298700	9.84956300

TS4

O	1.03056500	4.11112200	-1.69706400

C	0.36185200	3.42038400	-0.94414500
C	1.94216400	2.09483100	0.81357200
H	1.45214600	1.91035400	1.77727000
H	2.59957600	2.97223500	0.84345000
C	1.00366000	2.13238200	-0.43916700
C	3.97816400	0.41451200	0.43142200
C	2.29877800	1.65351500	-1.23572400
H	2.94794300	2.51531800	-1.42582400
H	2.14186000	1.07383200	-2.15648600
C	2.61083400	0.89669700	0.07630200
C	4.95072800	0.22357600	-0.55869000
H	4.71652000	0.45825800	-1.59938500
C	4.29287800	0.10598300	1.76432700
H	3.54102600	0.25023500	2.54434100
C	5.55284200	-0.39354500	2.09779600
H	5.78523900	-0.63195700	3.13835700
C	6.21332900	-0.27723400	-0.22653300
H	6.96144700	-0.42509600	-1.00887400
C	6.51651700	-0.58950300	1.10134500
H	7.50215000	-0.98216900	1.36170500
C	-1.00345800	3.85237400	-0.53509300
C	-1.51756300	5.02794500	-1.11741200
C	-1.78403300	3.14739100	0.39419000
C	-2.78847300	5.48359800	-0.78003500
H	-0.89883200	5.56667000	-1.83626100

C	-3.05862800	3.60906900	0.73209300
H	-1.40456400	2.23424900	0.85293900
C	-3.56355000	4.77314200	0.14704700
H	-3.65898600	3.05277300	1.45585900
H	-4.56203400	5.13000300	0.41078900
H	-3.18187700	6.39371000	-1.23836600
Ag	-2.28980000	-0.74919000	1.26927400
B	-3.22569900	-3.21477900	-0.27665400
F	-3.86042800	-2.05496000	0.34099800
F	-1.96052400	-3.32449200	0.31554700
F	-3.10432200	-2.96061900	-1.64181500
F	-4.00189600	-4.32446500	-0.02820500
C	1.42671000	-0.13142400	0.10365300
C	0.34708500	0.79112900	-0.39167500
C	1.48010300	-1.47669500	-0.55946100
C	-0.72756200	-0.98628800	-1.57339200
C	1.35267400	-4.08646600	-1.63543000
C	0.29947000	-3.20712400	-1.84391800
C	2.46240300	-3.66952400	-0.88572800
C	2.51820600	-2.38545500	-0.33575200
C	0.35647200	-1.89520500	-1.32513300
C	-0.73244700	0.33023100	-1.15843600
H	-1.51767700	1.01241400	-1.48492700
H	-1.56496200	-1.36147700	-2.16478200
H	-0.59401100	-3.51569200	-2.38858300

H	1.31350000	-5.09929500	-2.04066200
H	3.29372200	-4.35835900	-0.71884200
H	3.37601300	-2.09475600	0.26906200
O	-0.67972900	0.53801600	1.69515700
H	1.15720400	-0.33530100	1.15741700
H	-0.85338000	1.15781600	2.41959800

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C	0.76914600	0.47853700	-0.25580000
C	-0.57933200	0.65326900	-0.55506900
C	-2.53009900	-1.08260000	-0.99266700
C	1.64160200	1.57841200	-0.11186600
C	-0.31972500	3.02705100	-0.60601400
C	-5.78238600	0.26138200	1.47975200
C	-6.02482600	-0.46249900	0.30534000
C	0.90466300	-1.05561000	-0.18523900
C	3.23750100	3.90446600	0.14277600
C	1.89991900	4.03541700	-0.15600300
C	-0.38758000	-1.39609700	0.63553500
C	3.80642600	2.61483700	0.31990500
C	-4.47015200	0.55587700	1.86146700
C	4.74947200	-2.79097900	0.68587300
C	3.03300800	1.48222000	0.19642800
C	2.22344400	-1.69104900	0.11563500
C	1.05952000	2.89207100	-0.29398100

C	-4.95701500	-0.88847300	-0.48071900
C	2.60778200	-1.94608200	1.44033200
C	-1.09773500	-0.78663100	-0.63090800
C	-3.63260700	-0.59737000	-0.10683700
C	-3.39914500	0.12979400	1.07329700
C	0.05547100	-1.44600400	-1.44788500
C	3.11381500	-2.00772900	-0.92089100
C	4.36962700	-2.55120100	-0.63877900
C	3.86287200	-2.49011500	1.72495700
H	-0.53220000	-0.88706200	1.59809900
H	-0.55050700	-2.47915500	0.73284200
H	-0.06944600	-2.53262100	-1.55505100
H	0.32000500	-0.98109600	-2.40741200
C	-1.14740500	1.92038200	-0.74058400
O	-2.77198400	-1.72700900	-2.00159200
H	-6.61885100	0.59651600	2.09764300
H	-7.04997200	-0.69247400	0.00621900
H	-5.12163100	-1.45408100	-1.39910100
H	-2.38335500	0.37346900	1.38056400
H	-4.27882300	1.12082500	2.77634200
H	1.92139800	-1.70646000	2.25597700
H	4.15018100	-2.68018100	2.76195900
H	5.73135800	-3.21584500	0.90736800
H	5.05466800	-2.78907500	-1.45619500
H	2.82348000	-1.81666400	-1.95665600

H	-2.20604600	2.04006600	-0.97888600
H	-0.72589300	4.03251100	-0.74124300
H	1.45840500	5.02597600	-0.29374600
H	3.86676100	4.79182200	0.24434900
H	4.86921400	2.52296400	0.55660800
H	3.47955700	0.49896200	0.33473300

TS3'

O	-2.01404300	-1.47696000	2.12160600
C	-1.95951200	-1.49078100	0.89060000
C	-0.02772900	-1.60126600	-0.83352600
H	-0.12694500	-1.43577200	-1.91718000
H	-0.13091500	-2.67939800	-0.64894200
C	-0.90182300	-0.75910100	0.14669800
C	2.23466100	-2.02654000	0.33740000
C	0.35107700	-0.35292500	0.94444700
H	0.40286600	-0.87068500	1.91147900
H	0.51060000	0.72081800	1.12475600
C	1.24811800	-0.99806800	-0.16055700
C	2.95930100	-1.80099800	1.51655700
H	2.79535700	-0.88183100	2.08292300
C	2.47308700	-3.20706100	-0.38157600
H	1.92570700	-3.40054200	-1.30684800
C	3.41963800	-4.13485900	0.06089600
H	3.59458600	-5.04741000	-0.51378900

C	3.90258400	-2.72737900	1.96501600
H	4.45880600	-2.53277600	2.88492600
C	4.13874200	-3.89703400	1.23624400
H	4.87738100	-4.62248800	1.58492400
C	-2.95259300	-2.30754500	0.10548700
C	-3.71876700	-3.26048300	0.79572500
C	-3.14986100	-2.14569200	-1.27662200
C	-4.65462700	-4.04357900	0.12034400
H	-3.56154600	-3.36889800	1.87001300
C	-4.09274800	-2.92322300	-1.95206900
H	-2.58052100	-1.39692000	-1.82897700
C	-4.84390300	-3.87624500	-1.25624200
H	-4.24349100	-2.78321300	-3.02487900
H	-5.57941100	-4.48598100	-1.78636100
H	-5.24155200	-4.78548000	0.66696500
Ag	-2.42706400	1.03770600	0.13490000
B	-1.72007900	3.94981400	0.57890900
F	-2.94615500	3.26240100	0.20725100
F	-1.16982800	4.50664800	-0.57036300
F	-0.85908800	2.96318600	1.10317400
F	-2.01335900	4.90424200	1.52759300
C	1.92516900	0.09879800	-1.12171100
C	1.00806000	1.28965000	-1.26514000
C	3.36108800	0.47391300	-0.81222000
C	2.71257000	2.84301100	-0.56831700

C	6.03304600	1.17606000	-0.17455800
C	5.03438300	2.14027200	-0.13349800
C	5.70972800	-0.12308900	-0.58483200
C	4.39339300	-0.46522900	-0.90441400
C	3.70456800	1.80747600	-0.47056400
C	1.43677900	2.61358600	-1.00745500
H	0.69355700	3.40727200	-1.07912800
H	3.00933600	3.86128500	-0.30302200
H	5.26824900	3.17262200	0.13585800
H	7.06151000	1.43393500	0.08508100
H	6.49062300	-0.88302900	-0.65763900
H	4.17828000	-1.48131100	-1.22862300
H	1.92645300	-0.38380600	-2.11655900
O	-0.22128800	1.10891300	-1.60495600
H	-0.74458900	0.32843100	-1.00859900

IM5

O	-0.28228800	3.03263300	-2.24550600
C	-0.78492600	2.41520900	-1.32055600
C	0.60396100	1.51255400	0.70002100
H	0.10940100	1.10827800	1.59101800
H	0.80659600	2.58092000	0.85468000
C	-0.06808000	1.24501500	-0.68078200
C	3.18421700	1.50790400	0.46305300

C	1.31197200	0.87681200	-1.25215000
H	1.73396900	1.72736000	-1.80052800
H	1.37334100	-0.01511800	-1.88709500
C	1.88488300	0.78407000	0.18985900
C	4.13102200	1.72442100	-0.54587000
H	3.92699200	1.38464400	-1.56251600
C	3.47891800	1.93982000	1.76559600
H	2.75116800	1.77982800	2.56582700
C	4.69211600	2.56755100	2.05424000
H	4.90415900	2.89800000	3.07391300
C	5.34654500	2.35437500	-0.26200100
H	6.07434700	2.51082000	-1.06173800
C	5.63274700	2.77548900	1.03884200
H	6.58275500	3.26663500	1.26206500
C	-2.12452900	2.80149300	-0.77641300
C	-2.83505100	3.83364300	-1.41293700
C	-2.69337800	2.16947000	0.34137300
C	-4.09078900	4.21944700	-0.94827800
H	-2.38010200	4.31701400	-2.27905400
C	-3.94873100	2.55822800	0.81081400
H	-2.15481000	1.37607800	0.85641400
C	-4.65081500	3.58056600	0.16504800
H	-4.38151900	2.06006800	1.68119400
H	-5.63625100	3.88056300	0.52927400
H	-4.63879900	5.01836300	-1.45305200

Ag	-2.29339000	-1.53708200	1.60379700
B	-3.59772200	-1.87540300	-1.01034000
F	-4.15951900	-1.79509600	0.33240200
F	-2.88129100	-3.07251800	-1.08402900
F	-2.71667100	-0.79109500	-1.13939000
F	-4.61846900	-1.81980600	-1.92722800
C	2.02018900	-0.71756400	0.74814400
C	0.67145600	-1.39890700	0.72151100
C	3.08840800	-1.46134900	-0.01365400
C	1.30833300	-2.62308600	-1.27528100
C	5.05122600	-2.73193400	-1.58898300
C	3.70148100	-2.94284900	-1.85956200
C	5.42064200	-1.91343600	-0.51556800
C	4.44608400	-1.28159000	0.26327200
C	2.71314300	-2.32607500	-1.06958000
C	0.32736700	-2.20034400	-0.43316600
H	-0.71334500	-2.49353000	-0.58638800
H	1.04472100	-3.26313300	-2.12197400
H	3.39636300	-3.60187300	-2.67573800
H	5.81570900	-3.21484200	-2.20104300
H	6.47686600	-1.76225400	-0.28215100
H	4.74823200	-0.64349500	1.09415300
H	2.30205400	-0.60596500	1.80415700
O	-0.10903500	-1.20613100	1.67554800
H	-0.76027100	0.39250500	-0.64625400

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O	-2.66807100	0.87326600	-1.97124300
C	-2.67088600	-0.07313200	-1.19832600
C	-0.89383500	-0.47205700	0.64715000
H	-0.77382300	-1.37789700	1.25050300
H	-1.51199200	0.24717900	1.20351100
C	-1.38709200	-0.76761300	-0.79553200
C	0.58000200	1.64408200	0.39010600
C	-0.07860000	-0.19546000	-1.35521700
H	-0.22125800	0.67342900	-2.00853400
H	0.52972400	-0.94178000	-1.87647700
C	0.45667200	0.14808100	0.08983600
C	-0.37933100	2.55601900	-0.08881300
H	-1.20086600	2.21118800	-0.71776800
C	1.62276300	2.14568800	1.18502500
H	2.39097500	1.46765100	1.55891100
C	1.70545700	3.50683600	1.49747100
H	2.53066500	3.86763600	2.11645000
C	-0.29749000	3.91487700	0.22090200
H	-1.05495200	4.60084600	-0.16653600
C	0.74524000	4.39907100	1.01786200
H	0.80889500	5.46286700	1.25870400
C	-3.95014000	-0.56033800	-0.59325200
C	-5.14137600	0.10851900	-0.92567400

C	-4.00090800	-1.64945600	0.29400000
C	-6.35803000	-0.30188100	-0.38541600
H	-5.08486600	0.95312500	-1.61415100
C	-5.22034200	-2.05953700	0.83650800
H	-3.09109900	-2.18394300	0.56906800
C	-6.39913000	-1.38807200	0.49766800
H	-5.25074200	-2.90645100	1.52544000
H	-7.35242700	-1.71123800	0.92254400
H	-7.27870200	0.22318900	-0.64993000
C	1.71554800	-0.61842900	0.47858200
C	1.85574400	-1.20376400	1.73435600
C	2.83078200	-0.70496600	-0.42576600
C	3.95906200	-2.24602100	1.13027000
C	5.05689800	-0.92427100	-2.19018600
C	5.03213000	-1.65942300	-1.02357800
C	3.99065100	-0.03931900	-2.47695400
C	2.91052500	0.06579800	-1.62298100
C	3.94644500	-1.55413500	-0.11276100
C	2.95494800	-2.05043500	2.04274700
H	2.97164400	-2.52250200	3.02692400
H	4.79964600	-2.90350200	1.36463200
H	5.86085500	-2.32563000	-0.76949200
H	5.90052800	-1.00640600	-2.87918000
H	4.02488100	0.57553200	-3.37962900
H	2.12364500	0.78019300	-1.85734500

O	0.97836600	-1.02103500	2.76064300
H	-1.50530000	-1.84599400	-0.97498400
H	0.38797300	-0.27929200	2.57397900

TS5

O	2.24045100	-1.51687000	-1.19223500
C	2.56467700	-0.27325800	-1.06696200
C	1.65673000	2.17395500	-0.83855200
H	1.57024900	2.98768800	-1.57183100
H	2.36327500	2.45159100	-0.04795100
C	1.74148600	0.78616600	-1.44502300
C	0.23496800	0.86448400	0.87432700
C	0.25416800	0.72058900	-1.67238800
H	-0.27700700	-0.23759700	-1.61357900
H	-0.07427100	1.25215200	-2.57807600
C	0.27860800	1.62090100	-0.42499400
C	-0.70571600	-0.16824600	1.04292000
H	-1.43713100	-0.37212400	0.26364200
C	1.08435600	1.17524300	1.94595700
H	1.81196000	1.98200100	1.85313800
C	1.01631700	0.45486700	3.14107200
H	1.69625000	0.70464500	3.95889600
C	-0.78445400	-0.88090600	2.24316900
H	-1.54321700	-1.65855200	2.34001600
C	0.08550900	-0.57797200	3.29396400

H	0.03083100	-1.13391400	4.23272800
C	3.88714200	0.01457800	-0.43993300
C	4.38433100	-0.87892500	0.52640200
C	4.65395200	1.14587200	-0.77136900
C	5.59987700	-0.63282700	1.16470700
H	3.79378500	-1.76236300	0.77351700
C	5.87574200	1.38687200	-0.13894400
H	4.30309700	1.82546000	-1.54982300
C	6.34992000	0.50239800	0.83536200
H	6.46491300	2.26510000	-0.41406800
H	7.30474600	0.69289900	1.33130800
H	5.96668700	-1.32903000	1.92301900
Ag	0.38689200	-2.33821700	-0.51046900
B	-2.75085800	-2.63108000	-0.53363400
F	-1.57622300	-3.37091200	-0.09283800
F	-3.33257700	-2.04834000	0.58407500
F	-3.60693200	-3.50531200	-1.16841500
F	-2.29248500	-1.63850100	-1.42066200
C	-1.03519600	2.96633200	-0.34801200
C	-1.40513400	3.13434600	-1.72911100
C	-2.09375800	2.48651600	0.54627300
C	-3.34097400	1.73249000	-1.42419600
C	-3.98462700	1.24378300	2.22719900
C	-4.11496100	1.12528500	0.85497900
C	-2.93136700	2.00730900	2.76883400

C	-1.99626100	2.61585400	1.94010100
C	-3.18765800	1.76106800	-0.00672400
C	-2.50632100	2.44323900	-2.26585300
H	-2.69371100	2.47527800	-3.34167500
H	-4.17237500	1.16538200	-1.84842500
H	-4.92646700	0.53935700	0.42005200
H	-4.69633100	0.74936200	2.89102000
H	-2.84001700	2.11091800	3.85218700
H	-1.16484100	3.17684700	2.36982100
H	-0.40640800	3.76661300	0.05263300
O	-0.59718300	3.87996000	-2.47589100
H	-0.86398200	3.86269100	-3.40995800

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