C(sp²)−H Cyclobutylation of hydroxyarenes enabled by silver-π-acid catalysis: diastereocontrolled synthesis of 1,3-difunctionalized cyclobutanes

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Supporting Information

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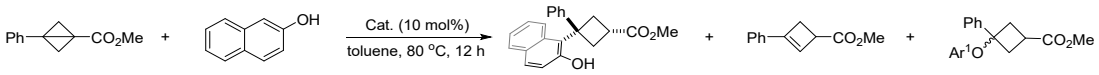
1 General Information

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%, *Jun Ding*) was purchased from commercial suppliers and used as received. Other commercially available reagents were purchased from *Sigma-Adrich*, *Leyan*, *Energy Chemical* and *Bide* Chemical Company. Chlorobenzene (PhCl) were purchased from *Energy Chemical* (99%, Extra Dry) 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; acetone-d_6: δ = 2.05 ppm for ^1H NMR and acetone-d_6 δ = 29.8 ppm for ^{13}C NMR; MeOH-d_4: δ = 3.31 ppm for ^1H NMR and MeOH-d_4: δ = 49.0 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 Study

Table S1. Screening of catalysts for the C(sp²)-H cyclobutylation[a]

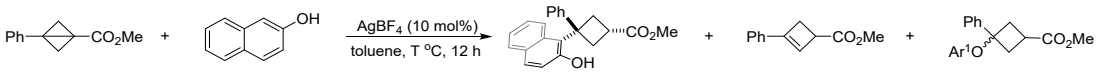


1a (1.1 equiv) **2a** (1.0 equiv) ***cis*-3aa** **4a** **5aa**
Ar^1 = 2-naphthyl

entry	Catalyst	*cis*-**3aa** Yield [%][b] (d.r. = *cis*/*trans*)	Yield of **4a** [%][b]	Yield of **5a** [%][b]
1	$Bi(OTf)_3$	<5 (-)[c]	0	0
2	$Ga(OTf)_3$	37 (77:23)[c][d]	0	0
3	$Cu(OTf)_2$	0	0	0
4	$Sc(OTf)_3$	0	0	0
5	$Zn(OTf)_2$	9 (62:38)[c][d]	31	63
6	$FeCl_3$	35 (84:16)[c][d]	8	0
7	$AlCl_3$	49 (82:18)	15	0
8[e]	$AlCl_3$	34 (45:55)	17	0
9	$Ni(ClO_4)_2{\cdot}6H_2O$	69 (90:10)	-[c]	-[c]
10	$AgClO_4$	69 (85:15)	23	0
11	$AgNO_3$	0	58	19
12	Ag_2CO_3	0	0	0
13	AgOTf	61 (83:17)	18	0
14	$AgSbF_6$	35 (74:26)	5	0
15	$AgPF_6$	21 (43:57)	39	10
16	$AgNTf_2$	55 (90:10)	31	0
17	**$AgBF_4$**	**84 (89:11)**	**16**	**0**
18[f]	$AgBF_4$	79 (90:10)	11	0
19	$BF_3{\cdot}Et_2O$	72 (85:15)	-[c]	0
20	$B(C_6F_5)_3$	24 (52:48)	54	0
21	$TsOH{\cdot}H_2O$	75 (77:23)	8	0
22[e]	$TsOH{\cdot}H_2O$	40 (45:55)	6	0
23	CF_3COOH	0	62	17
24	CF_3SO_3H	0	0	0

[a] Reaction conditions: **1a** (0.22 mmol, 1.1 equiv), **2a** (0.20 mmol, 1.0 equiv) and catalyst (10.0 mol%), toluene (2 mL), 80 °C, under N_2 for 12 h. [b] NMR yield with CH_2Br_2 as an internal standard. The d.r. value was determined by ^{1}HNMR spectroscopic analysis of the crude reaction mixture. [c] The reaction afforded a complex reaction mixture and some unknown side products have the same chemical shift as the aimed product. So the d.r. value (or NMR yield) cannot be determined by ^{1}HNMR spectroscopic analysis of the crude reaction mixture. [d] The d.r. value was determined by ^{1}HNMR spectroscopic analysis of the crude reaction product after short column chromatography. [e] Run at 25 °C. [f] **1a** (0.2 mmol, 1.0 equiv) and **2a** (0.30 mmol, 1.5 equiv) were used.

Table S2. Screening of temperature for the C(sp^2)-H cyclobutylation[a]

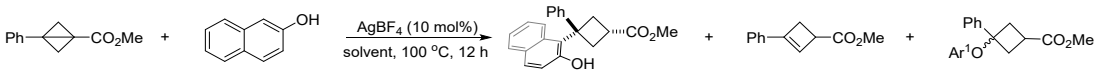


1a (1.1 equiv) **2a** (1.0 equiv) *cis*-**3aa** **4a** **5aa**
Ar^1 = 2-naphthyl

entry	T °C	*cis*-**3aa** Yield [%][b] (d.r. = *cis*/*trans*)	Yield of **4a** [%][b]	Yield of **5a** [%][b]
1	25	23 (50:50)	9	53
2	40	36 (62:38)	11	35
3	60	76 (85:15)	18	0
4	80	84 (89:11)	16	0
5	**100**	**78 (91:9)**	**17**	**0**

[a] Reaction conditions: **1a** (0.22 mmol, 1.1 equiv), **2a** (0.20 mmol, 1.0 equiv) and $AgBF_4$ (10.0 mol%), toluene (2 mL), at T °C under N_2 for 12 h. [b] NMR yield with CH_2Br_2 as an internal standard.

Table S3. Screening of solvent for the C(sp^2)-H cyclobutylation[a]



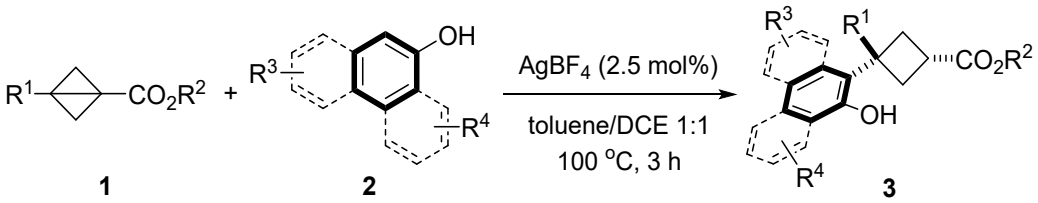
1a (1.1 equiv) **2a** (1.0 equiv) *cis*-**3aa** **4a** **5aa**
Ar^1 = 2-naphthyl

entry	solvent	*cis*-**3aa** Yield [%][b] (d.r. = *cis*/*trans*)	Yield of **4a** [%][b]	Yield of **5a** [%][b]
1	Toluene	78 (91:9)	17	0
2	Chlorobenzene	46 (90:10)	12	0
3	Anisole	33 (87:13)	8	0
4	$MeNO_2$	0	0	0
5	HFIP	36 (55:45)	21	4
6	EtOAc	43 (60:40)	11	0

7	DCE	51 (94.5:5.5)	9	0
8	$CHCl_3$	68 (92:8)	8	0
9	CCl_4	40 (58:42)	23	7
10	MeCN	25 (48:52)	15	20
11	THF	22 (40:60)	12	27
12	*n*-Hexane	36 (57:43)	24	15
13	Toluene/DCE(1:1, v/v)	73 (94:6)	14	0
14[c]	**Toluene/DCE(1:1**, v/v**)**	**85 (95:5)**	**11**	**0**
15	Toluene/DCE(1:4, v/v)	63 (94:6)	16	0
16	Toluene/DCE(4:1, v/v)	69 (92:8)	16	0
17	Toluene/DCE(10:1, v/v)	61 (90:10)	16	0

[a] Reaction conditions: **1a** (0.22 mmol, 1.1 equiv), **2a** (0.20 mmol, 1.0 equiv), $AgBF_4$ (10.0 mol%), toluene (2 mL), 100 °C, under N_2 for 12 h. HFIP = 1,1,1,3,3,3-Hexafluoro-2-propanol; DCE = 1,2-dichloroethane; [b] NMR yield with CH_2Br_2 as an internal standard. [c] **1a** (0.36 mmol, 1.2 equiv), **2a** (0.3 mmol, 1.0 equiv) and $AgBF_4$ (2.5 mol%) in toluene/1,2-dichloroethane(DCE) (1:1, v/v, 2 mL) at 100 °C for 3 h under N_2.

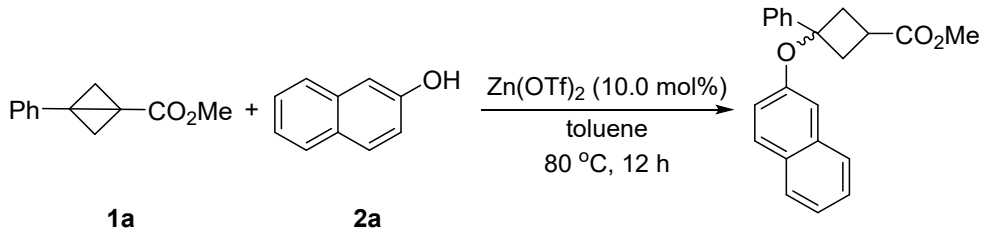
3 General Procedure for C(sp²)−H Cyclobutylation of Hydroxyarenes (GP)



1 **2** **3**

To a flame-dried Schlenk tube is added BCB **1** (0.36 mmol, 1.2 equiv), hydroxyarene **2** (0.3 mmol, 1.0 equiv), and $AgBF_4$ (1.5 mg, 7.5 μmol, 2.5 mol%). The tube is evacuated and backfilled with N_2 (3 times) followed by the addition of toluene/DCE (2.0 mL, 1/1, v/v). The reaction mixture is stirred at 100 °C for 3 h. Upon complete consumption of **2**, the solvent is removed under reduced pressure, and the residue is purified by chromatography on a short silica gel column to afford the desired 1,3-difunctionalized cyclobutane **3**.

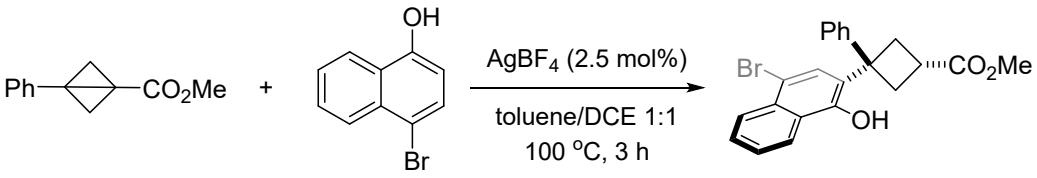
4 Procedure for the Synthesis of 5aa



1a 1.1 equiv | **2a** 1.0 equiv | *cis/trans*-**5aa**

To a flame-dried Schlenk tube is added methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate **1a** (41.4 mg, 0.22 mmol, 1.1 equiv), naphthalen-2-ol **2a** (28.8 mg, 0.2 mmol, 1.0 equiv) and $Zn(OTf)_2$ (7.3 mg, 20.0 μmol, 10.0 mol%). The tube is evacuated and backfilled with N_2 (3 times) followed by the addition of toluene (2.0 mL). The reaction mixture is stirred at 80 °C for 12 h. Upon complete consumption of **2a**, the solvent is removed under reduced pressure, and the residue is purified by flash chromatography on silica gel using petroleum ether/EtOAc (50/1) to afford the desired **5aa** as a white solid (63% NMR yield, d.r. = 1:1): major isomer (21.3 mg, 32% yield), minor isomer (20.6 mg, 31% yield).

5 Scale-Up Experiment

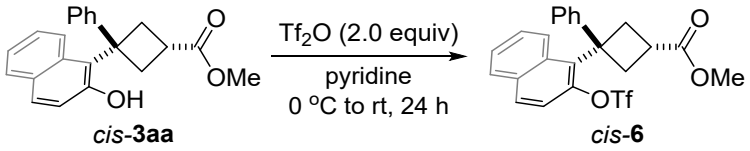


1a 1.2 mmol | **2m** 1.0 mmol | *cis*-**3am** 0.334 g, 81%, d.r. > 98:2

To a flame-dried Schlenk tube is added methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate **1a** (225.9 mg, 1.2 mmol, 1.2 equiv), 4-bromonaphthalen-1-ol **2m** (223.1 mg, 1.0 mmol, 1.0 equiv) and $AgBF_4$ (4.9 mg, 0.025 mmol, 2.5 mol%). The tube is evacuated and backfilled with N_2 (3 times) followed by the addition of toluene/DCE (6.6 mL, 1/1, v/v). The reaction mixture is stirred at 100 °C for 3 h. Upon complete consumption of **2m**, the solvent is removed under reduced pressure, and the residue is purified by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to

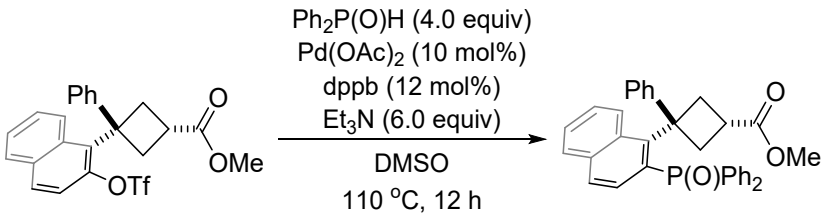
5/1) to afford the desired 1,3-difunctionalized cyclobutane *cis*-**3am** as a white solid (0.334 g, 81% yield, d.r. > 98:2).

6 Synthetic Transformations



cis-**3aa** *cis*-**6**

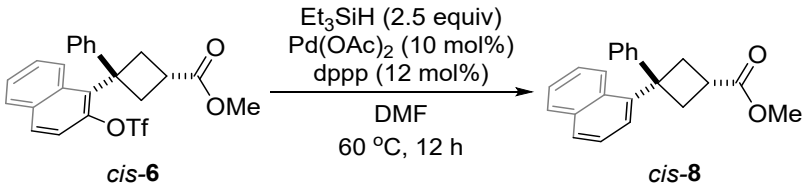
Synthesis of (6)[3]**:** The *cis*-**3aa** (332 mg, 1 mmol, 1.0 equiv) is dissolved in freshly distilled pyridine (5 mL). The reaction mixture is cooled at 0 °C and trifluoromethanesulfonic anhydride (564 mg, 2.0 mmol, 2.0 equiv) is added dropwise. The resulting solution is then stirred at room temperature for 24 h. After addition of water (4 mL), the reaction mixture is extracted with Et_2O (3 × 10 mL). The combined organic layer is washed successively with water (2 × 15 mL), 10% aqueous HCl solution (2 × 15 mL), brine (2 × 15 mL), dried over $MgSO_4$, filtered, concentrated in vacuum and purified by chromatography on silica gel (petroleum ether/EtOAc = 10/1) to give the product *cis*-**6** (410 mg, 88%) as a white solid.



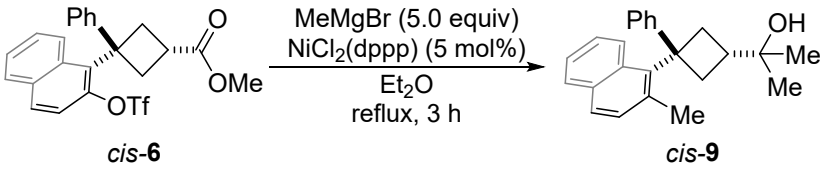
cis-**6** *cis*-**7**

Synthesis of (7)[3]**:** Compound *cis*-**6** (46.4 mg, 0.1 mmol, 1.0 equiv) is dissolved in DMSO (3 mL, pre-deoxygenized by ultrasonic). Then $Ph_2P(O)H$ (80.9 mg, 0.4 mmol, 4.0 equiv), $Pd(OAc)_2$ (2.2 mg, 10 umol, 10 mol%), and dppb (5.1 mg, 12 umol, 12 mol%) are added to the solution. NEt_3 (60.7 mg, 0.6 mmol, 6.0 equiv) is added and the reaction mixture is heated to 110 °C for 12 h. After completion of the reaction, dichloromethane is added and the reaction quenched by hydrochloric acid (1 M). The resulting mixture is extracted with dichloromethane and the organic layer successively washed by saturated $NaHCO_3$ aqueous solution and saturated NaCl aqueous solution, and finally dried with anhydrous Na_2SO_4. Solvents are removed in *vacuo* and purified

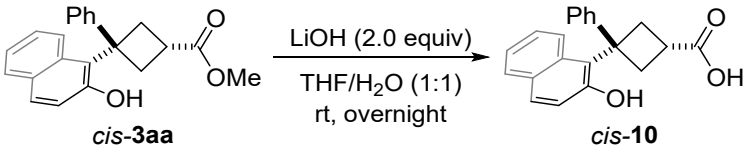
by flash column chromatography (petroleum ether/EtOAc = 2/1) to afford compound *cis*-**7** (38.5 mg, 74%) as a white solid.



Synthesis of (8) [3]**:** To a mixture of *cis*-**6** (46.4 mg, 0.1 mmol, 1.0 equiv), $Pd(OAc)_2$ (2.2 mg, 10 umol, 10 mol%) and dppp (4.9 mg, 12 umol, 12 mol%) in 2 mL of DMF at 60 °C, Et_3SiH (29.1 mg, 0.25 mmol, 2.5 equiv) is added *via* syringe. After 12 h, the mixture is diluted with Et_2O successively washed with water, sat.*aq.* $NaHCO_3$ and sat.*aq.* NaCl, dried over Na_2SO_4, concentrated in vacuum and purified by chromatography (petroleum ether/EtOAc = 10/1) on silica gel to give the product *cis*-**8** (31.2 mg, 99%) as a white solid.

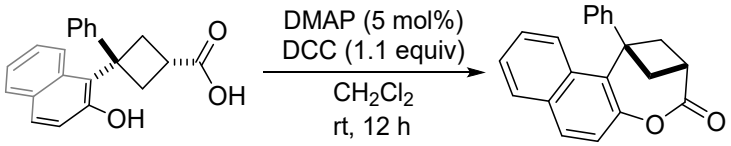


Synthesis of (9) [3]**:** To a mixture of *cis*-**6** (56.2 mg, 0.1 mmol, 1.0 equiv), $NiCl_2$(dppp) (2.7 mg, 5 umol, 5 mol%) in 1 mL of Et_2O at 0 °C, methyl magnesiumbromide (0.167 mL, 3.0 M in Et_2O, 0.5 mmol, 5.0 equiv) was added via syringe. The reaction mixture is heated to reflux for 3 h. At this point the reaction is quenched by addition of MeOH (0.2 mL) slowly at 0 °C. Solvents are removed in *vacuo* and purified by flash column chromatography (petroleum ether/EtOAc = 10/1) to afford compound *cis*-**9** (30.1 mg, 91%) as a white solid.



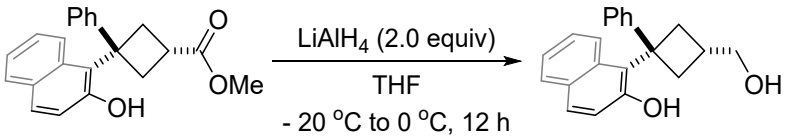
Synthesis of (10) [1a]**:** A Schlenk tube is charged with *cis*-**3aa** (166.2 mg, 0.5 mmol, 1.0 equiv) and LiOH (24.0 mg, 1.0 mmol, 2 equiv). The solids are dissolved in a 1:1 v/v

THF/H_2O mixture (5.0 mL). The reaction mixture is stirred at room temperature overnight. The mixture is then concentrated under reduced pressure. The resulting residue is dissolved in water (5.0 mL) and acidified with 1 M HCl to adjust the pH to 4-6. Once the solution reached the desired pH range, the aqueous phase is extracted with CH_2Cl_2 (5 mL). The organic layer is dried using anhydrous $MgSO_4$, followed by filtration and evaporation of the solvent to give compound *cis*-**10** (150.0 mg, 94%) as a white solid.



cis-**10** **11**

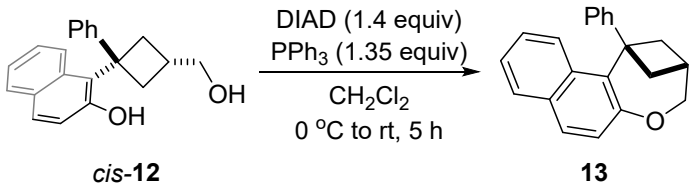
Synthesis of (11) [4]**:** Acid *cis*-**10** (0.15 mmol, 47.8 mg, 1.0 equiv) is dissolved in CH_2Cl_2 (6 mL) and a solution of DMAP (0.92 mg, 7.5 umol, 5 mol%) and DCC (34.0 mg, 0.165 mmol, 1.1 equiv) in CH_2Cl_2 (3 mL) is added. The reaction is stirred at room temperature for 12 hours before being quenched with water. The mixture is separated and the aqueous layer is extracted with CH_2Cl_2. The combined organic extracts are washed with brine and dried ($MgSO_4$) followed by filtration and evaporation of the solvent. The residue is purified by flash column chromatography (petroleum ether/EtOAc = 20/1) to afford **11** as a white solid. (28.9 mg, 64% yield).



cis-**3aa** *cis*-**12**

Synthesis of (12) [5]**:** To a suspension of $LiAlH_4$ (30 mg, 0.8 mmol, 2.0 equiv) in anhydrous THF (20 mL), a solution of *cis*-**3aa** (132.7 mg, 0.4 mmol, 1.0 equiv) in anhydrous THF (5 mL) is added dropwise at -20 °C. Then the reaction mixture is stirred at 0 °C for 12 h. The reaction is quenched with ice water and saturated aqueous sodium potassium tartrate is added, and the solution is stirred for another 30 min, then the aqueous layer is extracted with EtOAc for three times, the combined organic layers are

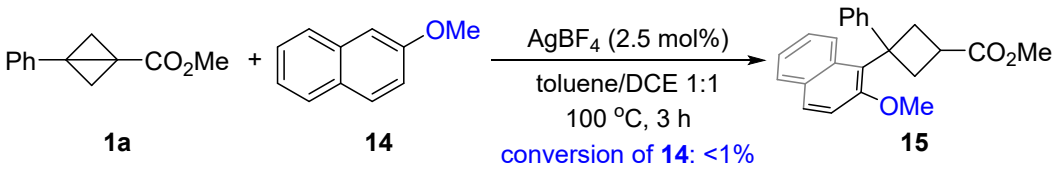
dried and concentrated under reduced pressure. The crude product is purified by silica gel column chromatography (petroleum ether/EtOAc = 2:1) to afford the corresponding product *cis*-**12** (115.0 mg, 94% yield) as a white solid.



cis-**12** **13**

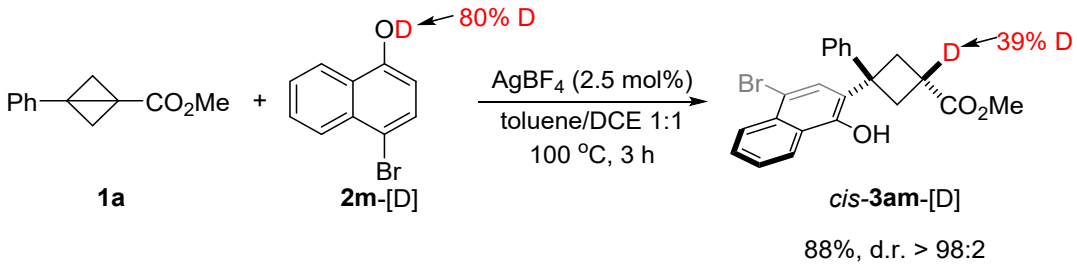
Synthesis of (13) [5]**:** To a solution of *cis*-**12** (57.5 mg, 0.19 mmol, 1.0 equiv) and PPh_3 (67.1 mg, 0.256 mmol, 1.35 equiv) in anhydrous CH_2Cl_2 (8.0 mL) at 0 °C is added diisopropyl azodicarboxylate (69.8 mg, 0.266 mmol, 1.4 equiv) slowly under N_2 atmosphere. The reaction is stirred at 0 °C for 30 min, then at room temperature for another 5 h. After evaporation, the residue is purified by column chromatography on silica gel (petroleum ether/EtOAc = 100:1) to afford the desired product **13** (21.1 mg, 39% yield) as a white solid.

7 Procedure for the Control Experiments



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

To a flame-dried Schlenk tube is added **1a** (67.8 mg, 0.36 mmol, 1.2 equiv), 2-methoxynaphthalene (47.5 mg, 0.3 mmol, 1.0 equiv) and $AgBF_4$ (1.5 mg, 7.5 μmol, 2.5 mol%). The tube is evacuated and backfilled with N_2 (3 times) followed by the addition of toluene/DCE (2.0 mL, 1/1, v/v). The reaction mixture is stirred at 100 °C for 3 h. Then the solvent is removed under reduced pressure, and the residue is dissolved in $CDCl_3$ (0.5 mL). The conversion of **14** (< 1%) is determined by ^1H NMR analysis with CH_2Br_2 as the internal standard. *(The desired reaction did not occur when 2-methoxynaphthalene was employed.)*

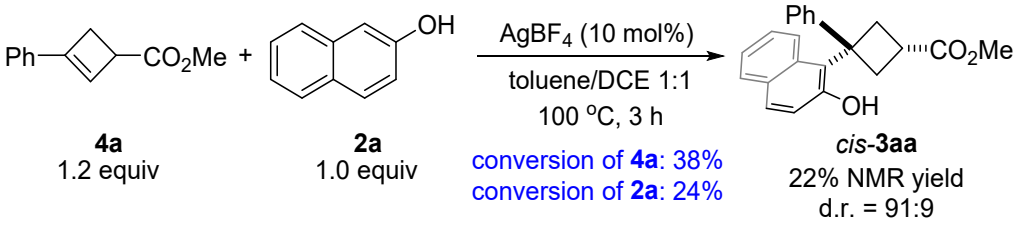


1a **2m**-[D] *cis*-**3am**-[D]

88%, d.r. > 98:2

In a glove box, to a flame-dried Schlenk tube is charged with **1a** (67.8 mg, 0.36 mmol, 1.2 equiv), deuterated 4-bromonaphthalen-1-ol **2m**-[D] (67.2 mg, 0.30 mmol, 1.0 equiv),[6] and $AgBF_4$ (1.5 mg, 7.5 μmol, 2.5 mol %). The tube is removed from the glove box and evacuated and backfilled with N_2 (3 times) followed by the addition of toluene/DCE (2.0 mL, 1/1, v/v). The reaction mixture is stirred at 100 °C for 3 h. Evaporation of the solvent under reduced pressure afforded the crude title compound. The yield of product *cis*-**3am**-[D] is determined by ^{1}H NMR analysis with CH_2Br_2 as the internal standard.

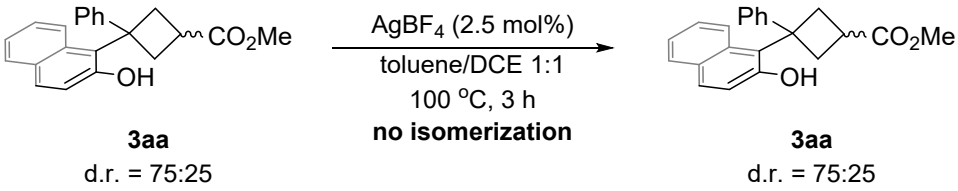
When deuterated 4-bromonaphthalen-1-ol **2m**-[D] was used under standard conditions, the reaction gave *cis*-**3am**-[D] in 88% NMR yield with 39% deuterium incorporation. The above deuterium labeling experiment confirmed the critical role of hydroxyl group of phenols in the current transformation.



4a 1.2 equiv **2a** 1.0 equiv *cis*-**3aa** 22% NMR yield d.r. = 91:9

To a flame-dried Schlenk tube is added methyl 3-phenylcyclobut-2-ene-1-carboxylate **4a** (17.8 mg, 0.095 mmol, 1.2 equiv), naphthalen-2-ol **2a** (11.4 mg, 0.079 mmol, 1.0 equiv), and $AgBF_4$ (1.5 mg, 7.9 μmol, 10 mol%). The tube is evacuated and backfilled with N_2 (3 times) followed by the addition of toluene/DCE (1.5 mL, 1/1, v/v). The reaction mixture is stirred at 100 °C for 3 h. Then the solvent is removed under reduced pressure, and the residue is dissolved in $CDCl_3$ (0.5 mL). The conversion of **4a** (38%) and **2a** (24%) and the NMR yield of *cis*-**3aa** (22%) are determined by ^{1}H NMR analysis

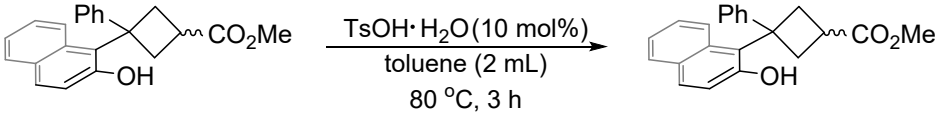
with CH_2Br_2 as the internal standard. *(Treatment of **4a** with standard conditions gave **3aa** in 22% NMR yield. However, cyclobutene **4a** was far less reactive than bicyclobutane **1a**).*



3aa
d.r. = 75:25

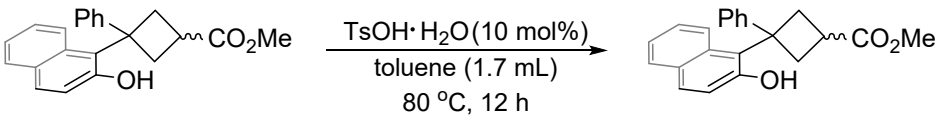
3aa
d.r. = 75:25

To a flame-dried Schlenk tube is added methyl 3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate **3aa** (66.5 mg, 0.2 mmol, d.r = 75:25) and $AgBF_4$ (1.0 mg, 5 μmol, 2.5 mol%). The tube is evacuated and backfilled with N_2 (3 times) followed by the addition of toluene/DCE (1.67 mL, 1/1, v/v). The reaction mixture is stirred at 100 °C for 3 h. Then the solvent is removed under reduced pressure, and the residue is dissolved in $CDCl_3$ (0.5 mL). The diastereoisomer ratio of **3aa** is determined by ^1H NMR analysis with CH_2Br_2 as the internal standard. *(When **3aa** with 75:25 d.r. was applied under the standard conditions, no change in diastereoselectivity of **3aa** was found. This result suggests that high diastereoselectivity might not be able to obtain via an isomerization pathway (trans- to cis-**3aa**). However, high diastereoselectivity can be obtain via a keto-enol tautomerism in the presence of TsOH.*



3aa (0.2 mmol)
d.r. = 44:56 (*cis/trans*)

3aa
d.r. = 57:43 (*cis/trans*)

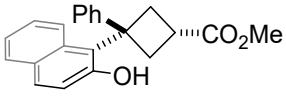


3aa (0.17 mmol)
d.r. = 57:43 (*cis/trans*)

3aa
d.r. = 82:18 (*cis/trans*)

To a flame-dried Schlenk tube is added methyl 3-(4-bromo-1-hydroxynaphthalen-2-yl)-3-phenylcyclobutane-1-carboxylate **3am** (123.4 mg, 0.3 mmol, *d.r* > 98:2) and $AgBF_4$ (1.5 mg, 7.5 μmol, 2.5 mol%). The tube is evacuated and backfilled with N_2 (3 times), Then CD_3OD (10.8 mg, 0.3 mmol, 1.0 equiv) is add to the Schlenk tube followed by the addition of toluene/DCE (2 mL, 1/1, v/v). The reaction mixture is stirred at 100 °C for 3 h. Then the solvent is removed under reduced pressure, and the residue is dissolved in $CDCl_3$ (0.5 mL). The conversion of *cis*-**3am** is determined by ^1H NMR analysis. *(When cis-**3am** with >98:2 d.r. was applied under the standard conditions in the presence of CD_3OD, no change in diastereoselectivity of **3am** was found and no deuterium-labeled **3am** was observed. This result again suggests that high diastereoselectivity might not be able to obtain via an isomerization.*

8 Characterization Data of the Products



cis-**3aa**

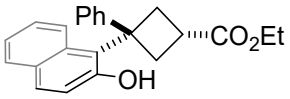
$C_{22}H_{20}O_3$

M = 332.40 g/mol

(*cis*)-Methyl-3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3aa**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3aa** as a white solid (79.4 mg, 80% yield, d.r. = 95:5).

cis-**3aa**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.66-7.63 (m, 3H), 7.57-7.53 (m, 1H), 7.36-7.25 (m, 4H), 7.20-7.17

(m, 1H), 6.97 (dd, *J* = 8.8 and 1.6 Hz, 1H), 5.41-5.30 (m, 1H), 3.65 (s, 3H), 3.43-3.26 (m, 5H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.6, 150.6, 146.5, 132.1, 129.6, 128.7, 128.6, 128.5, 126.4, 126.3, 126.2, 125.7, 124.4, 122.6, 118.7, 51.9, 46.0, 40.5, 34.3 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{22}H_{19}O_3$: 331.1334; found: 331.1312.



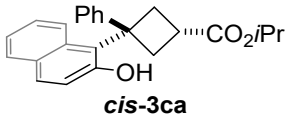
***cis*-3ba**

$C_{23}H_{22}O_3$

M = 346.43 g/mol

(*cis*)-Ethyl-3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ba**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and ethyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1b**, 72.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ba** as a white solid (82.8 mg, 80% yield, d.r. = 93:7)

cis-**3ba**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$) 7.70-7.64 (m, 4H), 7.45-7.42 (m, 1H), 7.35-7.23 (m, 4H), 7.18-7.15 (m, 1H), 6.93 (d, *J* = 8.8 Hz, 1H), 6.05 (broad s, 1H), 4.13 (q, *J* = 7.2 Hz, 2H), 3.42-3.25 (m, 5H), 1.23 (t, *J* = 7.2 Hz, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.0, 150.6, 146.5, 132.1, 129.7, 128.7, 128.6, 128.5, 126.3, 126.2, 125.7, 124.4, 122.6, 118.7, 60.8, 46.0, 40.5, 34.5, 14.2 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{21}O_3$: 345.1491; found: 345.1456.



***cis*-3ca**

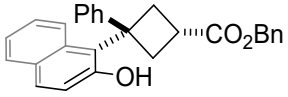
$C_{24}H_{24}O_3$

M = 360.45 g/mol

(*cis*)-Isopropyl-3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ca**): Prepared from naphthalen-2-ol (**2a,** 43.3 mg, 0.3 mmol) and isopropyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1c**, 77.9 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum

ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ca** as a white solid (82.2 mg, 76% yield, d.r. = 90:10)

cis-**3ca**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.67-7.65 (m, 4H), 7.37-7.21 (m, 5H), 7.17-7.13 (m, 1H), 6.91 (d, *J* = 8.8 Hz, 1H), 6.52-6.50 (m, 1H), 5.05-4.99 (m, 1H), 3.34-3.23 (m, 5H), 1.21 (d, *J* = 6.4 Hz, 6H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.0, 150.8, 146.6, 132.2, 129.6, 128.7, 128.5, 128.4, 126.4, 126.3, 126.1, 125.6, 124.4, 122.5, 118.7, 68.2, 46.0, 40.4, 34.8, 21.8 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{24}H_{23}O_3$: 359.1647; found: 359.1620.



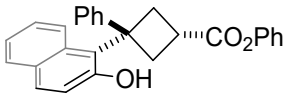
***cis*-3da**

$C_{28}H_{24}O_3$

M = 408.50 g/mol

(*cis*)-Benzyl-3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3da**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and benzyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1d**, 95.2 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3da** as a white solid (94.7 mg, 77% yield, d.r. = 93:7)

cis-**3da**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1).**^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.69-7.64 (m, 4H), 7.46-7.41 (m, 1H), 7.33-7.23 (m, 9H), 7.18-7.14 (m, 1H), 6.91 (d, *J* = 8.8 Hz, 1H), 6.12-5.70 (m, 1H), 5.12 (s, 2H), 3.48-3.29 (m, 5H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.0, 150.6, 146.4, 135.7, 132.1, 129.7, 128.7, 128.63, 128.56, 128.5, 128.3, 128.2, 126.3, 126.2, 125.7, 124.4, 122.6, 118.7, 66.6, 46.1, 40.5, 34.5 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{28}H_{23}O_3$: 407.1647; found: 407.1616 .



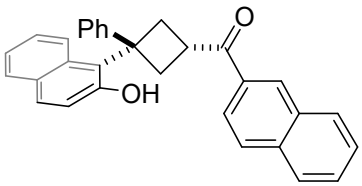
***cis*-3ea**

$C_{27}H_{22}O_3$

M = 394.47 g/mol

(*cis*)-Phenyl-3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ea**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and phenyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1e**, 90.1 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ea** as a white solid (76.1 mg, 64% yield, d.r. = 81:19).

cis-**3ea**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.71-7.68 (m, 4H), 7.48 (d, *J* = 8.8 Hz, 1H), 7.36-7.27 (m, 6H), 7.20-7.16 (m, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 1H), 5.60 (s, 1H), 3.63-3.56 (m, 1H), 3.38 (broad s, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 174.1, 150.6, 150.4, 146.2, 132.1, 129.8, 129.4, 128.77, 128.75, 128.6, 126.6, 126.5, 126.33, 126.29, 125.9, 124.4, 122.8, 121.4, 118.7, 46.1, 40.5, 34.7 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{27}H_{21}O_3$: 393.1491; found: 393.1461.



***cis*-3fa**

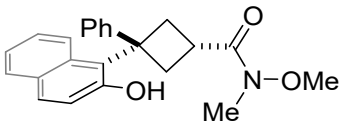
$C_{31}H_{24}O_2$

M = 428.53 g/mol

(*cis*)-(3-(2-hydroxynaphthalen-1-yl)-3-phenylcyclobutyl)(naphthalen-2-yl)methanone ((*cis*)-**3fa**) Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and naphthalen-2-yl(3-phenylbicyclo[1.1.0]butan-1-yl)methanone (**1f**, 102.4 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (10/1 to 5/1) afforded *cis*-**3fa** as a pale yellow solid (64.7 mg,

50% yield, d.r. = 86:14) together with trace amount of *trans*-**3fa**, which cannot be separated by chromatography.

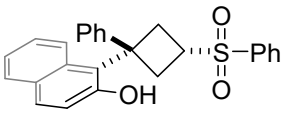
cis-**3fa**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.43 (s, 1H), 8.00 (d, *J* = 8.8 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.87-7.80 (m, 3H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.59-7.45 (m, 4H), 7.39-7.35 (m, 2H), 7.32-7.28 (m, 1H), 7.25-7.20 (m, 2H), 6.96 (d, *J* = 8.4 Hz, 1H), 6.10 (broad s, 1H), 4.37-4.28 (m, 1H), 3.56-3.27 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 201.9, 150.7, 147.1, 135.7, 132.9, 132.5, 132.2, 130.2, 129.7, 129.6, 128.7, 128.6, 128.5, 128.4, 127.8, 126.8, 126.4, 126.3, 125.7, 125.6, 124.5, 124.2, 122.6, 118.8, 45.9, 40.8, 40.0, 38.7 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{31}H_{24}O_2Na$: 451.1669; found: 451.1161.



***cis*-3ga**
$C_{23}H_{23}NO_3$
M = 361.44 g/mol

(*cis*)-3-(2-hydroxynaphthalen-1-yl)-N-methoxy-N-methyl-3-phenylcyclobutane-1-carboxamide ((*cis*)-**3ga**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and *N*-methoxy-*N*-methyl-3-phenylbicyclo[1.1.0]butane-1-carboxamide (**1g**, 78.2 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (5/1 to 2/1) afforded *cis*-**3ga** as a white solid (86.2 mg, 80% yield, d.r. > 98:2).

cis-**3ga**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 2/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.23 (s, 1H), 7.74 (d, *J* = 7.6 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 1H), 7.30-7.25 (m, 3H), 7.23-7.12 (m, 2H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.86 (d, *J* = 8.8 Hz, 1H), 3.76-3.63 (m, 1H), 3.70 (s, 3H), 3.55-2.88 (m, 4H) 3.22 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.6, 151.6, 147.3, 132.1, 129.2, 128.6, 128.3, 128.2, 126.4, 125.9, 125.8, 125.1, 124.1, 121.8, 118.7, 61.7, 46.2, 40.1, 32.4, 32.3 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{23}H_{23}NO_3Na$: 384.1570; found: 384.1564.



***cis*-3ha**

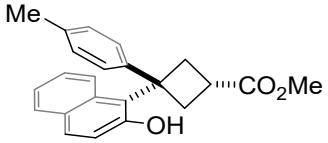
$C_{26}H_{22}O_3S$

M = 414.52 g/mol

(*cis*)-1-(1-phenyl-3-(phenylsulfonyl)cyclobutyl)naphthalen-2-ol ((*cis*)-**3ha**)

Prepared from naphthalen-2-ol (**2a**, 28.8 mg, 0.2 mmol) and 1-phenyl-3-(phenylsulfonyl)bicyclo[1.1.0]butane (**1h**, 64.9 mg, 0.24 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (10/1 to 3/1) afforded *cis/trans*-**3ha** as a white solid (46.6 mg, 56% yield, d.r. = 67:33), which cannot be separated by chromatography.

R_f = 0.30 (petroleum ether/EtOAc = 3/1). *cis*-**3ha**: **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.88 (d, *J* = 8.0 Hz, 2H), 7.72-7.69 (m, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.61-7.58 (m, 2H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.24-7.11 (m, 5H), 7.07 (d, *J* = 8.0 Hz, 1H), 3.79-3.59 (m, 2H), 3.58-3.36 (m, 2H), 3.25 (broad s, 1H) ppm. *trans*-**3ha**: **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.86 (d, *J* = 8.8 Hz, 2H), 7.72-7.69 (m, 1H), 7.65-7.58 (m, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.34-7.30 (m, 1H), 7.24-7.11 (m, 7H), 6.98 (d, *J* = 8.4 Hz, 1H), 3.99-3.90 (m, 1H), 3.79-3.59 (m, 2H), 3.58-3.36 (m, 2H) ppm. *cis/trans*-**3ha**: **^{13}C NMR** (100 MHz, $CDCl_3$): δ 152.3, 150.6, 147.3, 145.4, 138.2, 138.0, 133.7, 132.7, 131.8, 130.1, 129.7, 129.6, 129.34, 129.30, 129.1, 128.9, 128.8, 128.6, 128.5, 128.2, 128.1, 126.6, 126.5, 126.4, 126.2, 126.0, 125.6, 125.5, 125.1, 123.8, 122.8, 122.7, 121.0, 119.2, 118.7, 54.3, 52.8, 45.1, 45.0, 37.9, 37.5 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{26}H_{22}O_3SNa$: 437.1182; found: 437.1172.



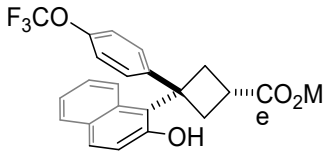
***cis*-3ia**

$C_{23}H_{22}O_3$

M = 346.43 g/mol

(*cis*)-Methyl-3-(2-hydroxynaphthalen-1-yl)-3-(*p*-tolyl)cyclobutane-1-carboxylate (*cis*-**3ia**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and methyl 3-(*p*-tolyl)bicyclo[1.1.0]butane-1-carboxylate (**1i**, 72.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ia** as a white solid (78.9 mg, 76% yield, d.r. > 98:2)

cis-**3ia**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 8.4 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.43 (d, *J* = 8.8 Hz, 1H), 7.34-7.30 (m, 1H), 7.26-7.22 (m, 1H), 7.09 (d, *J* = 7.6 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 1H), 5.98 (s, 1H), 3.66 (s, 3H), 3.43-3.25 (m, 5H), 2.27 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.5, 150.6, 143.5, 135.7, 132.1, 129.7, 129.2, 128.7, 128.5, 126.6, 126.1, 125.7, 124.4, 122.6, 118.7, 51.9, 45.6, 40.6, 34.4, 20.9 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{21}O_3$: 345.1491; found: 345.1466.



***cis*-3ja**

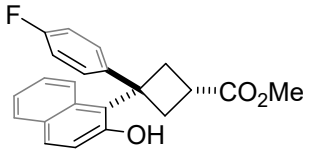
$C_{23}H_{19}F_3O_4$

M = 416.40 g/mol

(*cis*)-methyl-3-(2-hydroxynaphthalen-1-yl)-3-(4-(trifluoromethoxy)phenyl)cyclobutane-1-carboxylate (*cis*-**3ja**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and methyl 3-(4-(trifluoromethoxy)phenyl)bicyclo[1.1.0]butane-1-carboxylate (**1j**, 97.9 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ja** as a white solid (92.4 mg, 74% yield, d.r. = 92:8).

cis-**3ja**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.71-7.66 (m, 3H), 7.61 (d, *J* = 8.8 Hz, 1H), 7.51-7.44 (m, 1H), 7.37-7.33 (m, 1H), 7.26 (d, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 1H), 5.94 (broad s, 1H), 3.67 (s, 3H), 3.37-3.26 (m, 5H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.8, 150.7, 147.5,

145.3, 131.9, 129.6, 128.9, 127.8, 125.9, 125.8, 124.3, 124.0, 122.7, 120.8, 120.4 (q, *J* = 255.3 Hz), 118.6, 52.1, 45.7, 40.5, 34.3 ppm.**^{19}F NMR** (376 MHz, $CDCl_3$): δ -57.81 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{18}F_3O_4$: 415.1163; found: 415.1160.



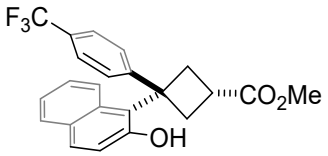
***cis*-3ka**

$C_{22}H_{19}FO_3$

M = 350.39 g/mol

(*cis*)-Methyl-3-(4-fluorophenyl)-3-(2-hydroxynaphthalen-1-yl)cyclobutane-1-carboxylate (*cis*-**3ha**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and methyl 3-(4-fluorophenyl)bicyclo[1.1.0]butane-1-carboxylate (**1k**, 74.2 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ka** as a white solid (84.6 mg, 80% yield, d.r. > 98:2)

cis-**3ka**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.67-7.58 (m, 4H), 7.35-7.31 (m, 2H), 7.26-7.22 (m, 1H), 6.96-6.88 (m, 3H), 6.60 (s, 1H), 3.68 (s, 3H), 3.48-3.25 (m, 5H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.9, 161.3 (d, *J* = 243.1 Hz), 150.6, 142.2 (d, *J* = 3.2 Hz), 131.9, 129.5, 128.8, 128.7, 127.9 (d, *J* = 7.8 Hz), 126.1, 125.8, 124.0, 122.6, 118.6, 115.0 (d, *J* = 20.9 Hz), 52.1, 45.6, 40.6, 34.3 ppm.**^{19}F NMR** (376 MHz, $CDCl_3$): δ -117.25 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{22}H_{18}FO_3$: 349.1240; found: 349.1212.



***cis*-3la**

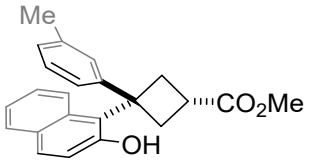
$C_{23}H_{19}F_3O_3$

M = 400.40 g/mol

(*cis*)-Methyl-3-(2-hydroxynaphthalen-1-yl)-3-(4(trifluoromethyl)phenyl)cyclobutane-1-carboxylate (*cis*-**3ia**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and methyl 3-(4-(trifluoromethyl)phenyl)bicyclo[1.1.0]butane-1-carboxylate (**1l**, 92.2 mg,

0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3la** as a white solid (29.5 mg, 25% yield, d.r. > 98:2)

cis-**3la**: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 5/1) **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.76-7.73 (m, 3H), 7.65 (d, *J* = 8.4Hz, 1H), 7.53-7.47 (m, 3H), 7.35-7.25 (m, 2H), 7.00 (d, *J* = 8.8 Hz, 1H), 5.75 (broad s, 1H), 3.67 (s, 3H), 3.59-3.54 (m, 2H), 3.40-3.37 (m, 2H), 3.14-3.08 (m, 1H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.6, 151.6, 150.9, 132.2, 130.0, 129.3, 128.9, 128.1 (q, *J* = 32.2 Hz), 126.9, 125.9, 125.2 (q, *J* = 3.8 Hz), 124.7, 124.2 (q, *J* = 270.2 Hz), 123.0, 118.9, 52.0, 47.7, 39.7, 33.7 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -62.38 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{18}F_3O_3$: 399.1208; found: 399.1178.

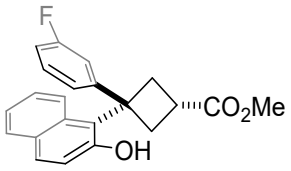


***cis*-3ma**
$C_{23}H_{22}O_3$
M = 346.43 g/mol

(*cis*)-Methyl-3-(2-hydroxynaphthalen-1-yl)-3-(*m*-tolyl)cyclobutane-1-carboxylate (*cis*-**3ma**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and methyl 3-(m-tolyl)bicyclo[1.1.0]butane-1-carboxylate (**1m**, 72.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ma** as a white solid (78.2 mg, 75% yield, d.r. > 98:2).

cis-**3ma**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1).**^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.45-7.41 (m, 3H), 7.34-7.30 (m, 1H), 7.26-7.22 (m, 1H), 7.19-7.15 (m, 1H), 6.99 (d, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 8.8 Hz, 1H), 6.01-5.94 (m, 1H), 3.66 (s, 3H), 3.44-3.25 (m, 5H), 2.30 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.5, 150.6, 146.4, 138.0, 132.2, 129.7, 128.7, 128.6, 128.4, 127.1,

126.9, 126.6, 125.7, 124.5, 123.3, 122.6, 118.7, 51.9, 45.9, 40.5, 34.4, 21.8 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{21}O_3$: 345.1491; found: 345.1465.



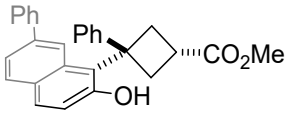
***cis*-3na**

$C_{22}H_{19}FO_3$

M = 350.39 g/mol

(*cis*)-Methyl-3-(3-fluorophenyl)-3-(2-hydroxynaphthalen-1-yl)cyclobutane-1-carboxylate (*cis*-**3na**): Prepared from naphthalen-2-ol (**2a**, 43.3 mg, 0.3 mmol) and methyl 3-(3-fluorophenyl)bicyclo[1.1.0]butane-1-carboxylate (**1n**, 74.2 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis/trans*-**3na** as a white solid (80 mg, 76% yield, d.r. = 80:20), which cannot be separated by chromatography.

$\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). *cis*-**3na**: **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.67 (d, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 8.8 Hz, 1H), 7.46-7.16 (m, 6H), 6.91-6.79 (m, 2H), 6.47 (s, 1H), 3.68 (s, 3H), 3.53-3.05 (m, 5H) ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -112.99 ppm. *trans*-**3na**: **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.46-7.16 (m, 6H), 7.00-6.97 (m, 1H), 6.91-6.79 (m, 1H), 6.00 (s, 1H), 3.68 (s, 3H), 3.53-3.05 (m, 5H) ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -113.15 ppm. *cis/trans*-**3na**: **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.8, 176.7, 163.1 (d, *J* = 243.2 Hz), 162.9 (d, *J* = 243.2 Hz), 150.9, 150.8, 150.2 (d, *J* = 6.7 Hz), 149.4 (d, *J* = 6.6 Hz), 132.3, 132.0, 129.9, 129.8, 129.7, 129.6, 129.5, 129.0, 128.8 (d, *J* = 3.1 Hz), 125.9, 125.7 (d, *J* = 3.9 Hz), 124.9, 124.8, 124.1, 122.8,122.6, 122.0 (d, *J* = 2.6 Hz), 121.7 (d, *J* = 2.6 Hz), 118.9, 118.6, 113.8 (d, *J* = 22.1 Hz), 113.7 (d, *J* = 21.9 Hz), 113.0 (d, *J* = 21.0 Hz), 112.9 (d, *J* = 20.9 Hz), 52.0, 47.8, 46.0, 40.4, 34.3, 33.8 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{22}H_{18}FO_3$: 349.1240; found: 349.1213.



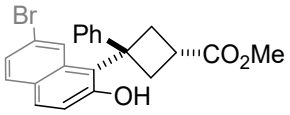
***cis*-3ab**

$C_{28}H_{24}O_3$

M = 408.50 g/mol

(*cis*)-Methyl-3-(2-hydroxy-7-phenylnaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ab**): Prepared from 7-phenylnaphthalen-2-ol (**2b**, 66.1 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ab** as a white solid (113.0 mg, 92% yield, d.r. > 98:2).

cis-**3ab**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, Acetone-d_6): δ 8.87-8.86 (m, 1H), 7.97-7.96 (m, 1H), 7.85-7.82 (m, 3H), 7.71-7.66 (m, 3H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.49-7.45 (m, 2H), 7.36-7.25 (m, 4H), 7.15-7.12 (m, 1H), 3.58 (s, 3H), 3.30-3.05 (m, 5H) ppm. **^{13}C NMR** (100 MHz, Acetone-d_6): δ 175.6, 153.0, 148.1, 142.2, 138.7, 133.4, 130.2, 129.8, 129.6, 129.2, 129.0, 128.1, 127.9, 127.8, 127.2, 126.8, 123.1, 122.6, 120.1, 51.7, 47.1, 41.5, 34.9 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{28}H_{23}O_3$: 407.1647; found: 407.1614.



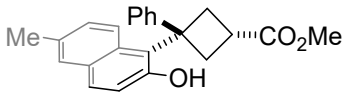
***cis*-3ac**

$C_{22}H_{19}BrO_3$

M = 411.30 g/mol

(*cis*)-Methyl-3-(7-bromo-2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ac**): Prepared from 7-bromonaphthalen-2-ol (**2c**, 66.9 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis/trans*-**3ac** as a white solid (90.4 mg, 73% yield, d.r. = 78:22), which cannot be separated by chromatography.

R_f = 0.35 (petroleum ether/EtOAc = 5/1). *cis*-**3ac: ^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (s, 1H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.48 (d, *J* = 8.8 Hz, 1H), 7.31-7.12 (m, 5H), 6.88 (d, *J* = 8.8 Hz, 1H), 6.78 (s, 1H), 3.70 (s, 3H), 3.51-3.04 (m, 5H) ppm. *trans*-**3ac**: **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (s, 1H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.55 (d, *J* = 4.0 Hz, 1H), 7.31-7.12 (m, 5H), 7.00 (d, *J* = 8.8 Hz, 1H), 6.08 (s, 1H), 3.66 (s, 3H), 3.51-3.04 (m, 5H) ppm. *cis/trans*-**3ka**: **^{13}C NMR** (100 MHz, $CDCl_3$): δ 177.0, 176.7, 151.8, 151.5, 146.6, 145.9, 133.6, 133.3, 130.3, 128.7, 128.6, 128.44, 128.42, 128.2, 127.9, 127.2, 126.5, 126.43, 126.36, 126.24, 126.20, 126.1, 125.8, 125.6, 125.0, 120.1, 119.3, 119.0, 52.14, 52.05, 47.6, 45.8, 40.4, 39.7, 34.3, 33.9 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{22}H_{18}BrO_3$: 409.0440; found: 409.0409.



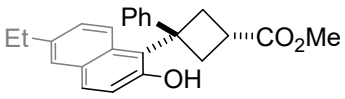
***cis*-3ad**

$C_{23}H_{22}O_3$

M = 346.43 g/mol

(*cis*)-Methyl-3-(2-hydroxy-6-methylnaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ad**): Prepared from 6-methylnaphthalen-2-ol (**2d**, 47.5 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ad** as a white solid (79.7 mg, 77% yield, d.r. = 92:8).

cis-**3ad**: **R_f** = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.63 (d, *J* = 7.2 Hz, 2H), 7.55 (d, *J* = 8.8 Hz, 1H), 7.46 (s, 1H), 7.42-7.39 (m, 1H), 7.29-7.25 (m, 2H), 7.17-7.12 (m, 2H), 6.90 (d, *J* = 8.4 Hz, 1H), 5.67 (broad s, 1H), 3.65 (s, 3H), 3.41-3.22 (m, 5H), 2.41 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.3, 150.0, 146.5, 132.0, 130.3, 130.0, 128.5, 127.98, 127.96, 127.8, 126.5, 126.3, 126.2, 124.3, 118.8, 51.8, 46.0, 40.5, 34.4, 21.1 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{21}O_3$: 345.1491; found: 345.1465.



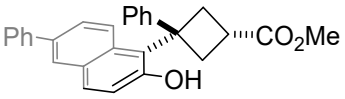
***cis*-3ae**

$C_{24}H_{24}O_3$

M = 360.45 g/mol

(*cis*)-Methyl-3-(6-ethyl-2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ae**): Prepared from 6-ethylnaphthalen-2-ol (**2e**, 51.7 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ae** as a white solid (83.2 mg, 77% yield, d.r. = 91:9).

cis-**3ae**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.64 (d, *J* = 7.2 Hz, 2H), 7.58 (d, *J* = 9.2 Hz, 1H), 7.47 (s, 1H), 7.40 (dd, *J* = 8.8 and 2.8 Hz, 1H), 7.29-7.25 (m, 2H), 7.23-7.14 (m, 2H), 6.91-6.88 (m, 1H), 5.94-5.86 (m, 1H), 3.65 (s, 3H), 3.40-3.26 (m, 5H), 2.72 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.4, 150.0, 146.5, 138.3, 130.5, 129.9, 128.5, 128.1, 126.9, 126.4, 126.3, 126.1, 124.4, 118.7, 51.9, 46.0, 40.5, 34.4, 28.4, 15.4 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{24}H_{23}O_3$: 359.1647; found: 359.1618.



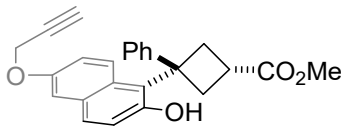
***cis*-3af**

$C_{28}H_{24}O_3$

M = 408.50 g/mol

(*cis*)-Methyl-3-(2-hydroxy-6-phenylnaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3af**): Prepared from 6-phenylnaphthalen-2-ol (**2f**, 51.7 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3af** as a white solid (92.8 mg, 76% yield, d.r. = 88:12).

cis-**3af**: $\mathbf{R_f}$ = 0.40 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.82 (s, 1H), 7.73-7.59 (m, 6H), 7.45-7.41 (m, 2H), 7.37-7.33 (m, 2H), 7.30-7.27 (m, 2H), 7.16 (t, *J* = 7.6 Hz, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 6.37 (s, 1H), 3.68 (s, 3H), 3.44-3.31 (m, 5H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.8, 150.8, 146.4, 140.9, 135.0, 131.3, 129.9, 128.9, 128.8, 128.5, 127.02, 126.96, 126.6, 126.29, 126.28, 126.2, 125.2, 124.8, 119.1, 52.0, 46.0, 40.5, 34.4 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{28}H_{23}O_3$: 407.1647; found: 407.1616.



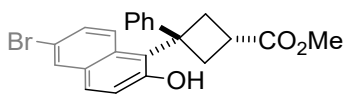
***cis*-3ag**

$C_{25}H_{22}O_4$

M = 386.45 g/mol

(*cis*)-Methyl-3-(2-hydroxy-6-(prop-2-yn-1-yloxy)naphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ag**): Prepared from 6-(prop-2-yn-1-yloxy)naphthalen-2-ol (**2g**, 59.5 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ag** as a yellow solid (49.8 mg, 43% yield, d.r. = 93:7).

cis-**3ag**: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 7.6 Hz, 2H), 7.57 (d, *J* = 9.2 Hz, 1H), 7.41-7.36 (m, 1H), 7.30-7.24 (m, 2H), 7.18-7.13 (m, 2H), 7.06 (d, *J* = 9.2 Hz, 1H), 6.91 (d, *J* = 9.2 Hz, 1H), 5.82-5.64 (m, 1H), 4.74 (s, 2H), 3.66 (s, 3H), 3.40- 3.24 (m, 5H), 2.53 (s, 1H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.3, 153.0, 149.4, 146.4, 130.4, 128.5, 127.8, 127.5, 126.9, 126.2, 126.0, 119.3, 118.1, 108.9, 78.7, 75.5, 55.8, 51.9, 46.0, 40.5, 34.3 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{25}H_{21}O_4$: 385.1440; found: 385.1411.



***cis*-3ah**

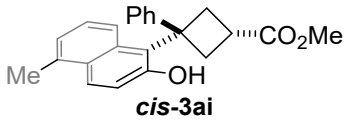
$C_{22}H_{19}BrO_3$

M = 411.30 g/mol

(*cis*)-Methyl-3-(6-bromo-2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate

(*cis*-**3ah**): Prepared from 6-bromonaphthalen-2-ol (**2h**, 66.9 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ah** as a white solid (89.4 mg, 73% yield, d.r. = 93:7).

cis-**3ah**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (s, 1H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.49 (d, *J* = 9.2 Hz, 1H), 7.37 (dd, *J* = 9.2 Hz and 2.4 Hz, 1H), 7.30-7.24 (m, 2H), 7.20-7.15 (m, 2H), 6.90 (d, *J* = 8.8 Hz, 1H), 6.58 (s, 1H), 3.69 (s, 3H), 3.45-3.25 (m, 5H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.9, 151.0, 146.1, 130.8, 130.58, 130.56, 128.8, 128.6, 127.6, 126.6, 126.3, 126.2, 126.0, 119.7, 116.2, 52.1, 45.9, 40.4, 34.3 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{22}H_{18}BrO_3$: 409.0440; found: 409.0406.



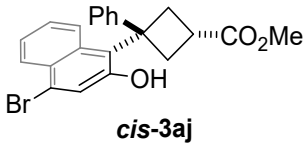
***cis*-3ai**

$C_{23}H_{22}O_3$

M = 346.43 g/mol

(*cis*)-Methyl-3-(2-hydroxy-5-methylnaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate ((*cis*)-**3ai**): Prepared from 5-methylnaphthalen-2-ol (**2i**, 66.9 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ai** as a white solid (81.3 mg, 78% yield, d.r. = 93:7).

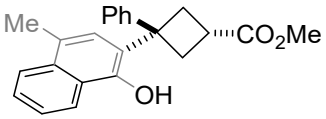
cis-**3ai**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.66-7.62 (m, 3H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.29-7.25 (m, 2H), 7.23-7.16 (m, 2H), 7.08 (d, *J* = 6.8 Hz, 1H), 6.97 (d, *J* = 8.8 Hz, 1H), 6.19-6.07 (m, 1H), 3.66 (s, 3H), 3.43-3.26 (m, 5H), 2.57 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.5, 150.5, 146.6, 134.8, 132.3, 128.6, 128.5, 127.0, 126.3, 126.1, 125.5, 124.6, 123.7, 123.0, 118.3, 51.9, 46.1, 40.6, 34.4, 19.9 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{21}O_3$: 345.1491; found: 345.1465.



***cis*-3aj**
$C_{22}H_{19}BrO_3$
M = 411.30 g/mol

(cis)-methyl-3-(4-bromo-2-hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate ((*cis*)-**3aj**): Prepared from 4-bromonaphthalen-2-ol (**2j**, 66.9 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3aj** as a white solid (83.2 mg, 82% yield, d.r. > 98:2).

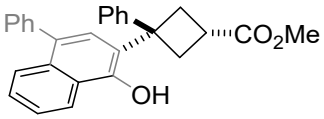
cis-**3aj**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, Acetone-d_6): δ 9.11 (s, 1H), 8.10 (d, *J* = 8.4 Hz, 1H), 7.77-7.74 (m, 3H), 7.65 (s, 1H), 7.42-7.35 (m, 2H), 7.32-7.28 (m, 2H), 7.18-7.14 (m, 1H), 3.59 (s, 3H), 3.32-3.23 (m, 2H), 3.14-3.06 (m, 3H) ppm. **^{13}C NMR** (100 MHz, Acetone-d_6): δ 175.5, 152.4, 147.6, 134.0, 129.2, 128.3, 128.2, 128.1, 127.3, 127.1, 126.9, 125.8, 124.7, 123.7, 122.0, 51.7, 46.8, 41.2, 34.7 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{22}H_{18}BrO_3$: 409.0440; found: 409.0439.



***cis*-3ak**
$C_{23}H_{22}O_3$
M = 346.43 g/mol

(*cis*)-methyl-3-(1-hydroxy-4-methylnaphthalen-2-yl)-3-phenylcyclobutane-1-carboxylate ((*cis*)-**3ak**): Prepared from 4-methylnaphthalen-1-ol (**2k**, 47.5 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3ak** as a white solid (79.4 mg, 76% yield, d.r. = 88:12).

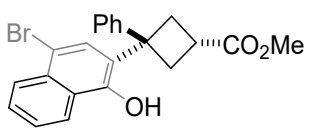
cis-**3ak**: $\mathbf{R_f}$ = 0.55 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 7.6 Hz, 2H), 7.46-7.38 (m, 2H), 7.31-7.27 (m, 2H), 7.25 (s, 1H), 7.22-7.16 (m, 1H), 4.93 (s, 1H), 3.64 (s, 3H), 3.31-3.22 (m, 1H), 3.07 (d, *J* = 8.8 Hz, 4H), 2.64 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 175.2, 145.9, 145.5, 132.2, 128.8, 128.7, 126.54, 126.49, 126.2, 125.5, 125.4, 125.2, 125.1, 124.2, 121.1, 51.8, 45.1, 37.5, 33.4, 19.1 ppm.. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{23}H_{21}O_3$: 345.1491; found: 345.1489.



***cis*-3al**
$C_{28}H_{24}O_3$
M = 408.50 g/mol

(*cis*)-methyl-3-(1-hydroxy-4-phenylnaphthalen-2-yl)-3-phenylcyclobutane-1-carboxylate ((*cis*)-**3al**): Prepared from 4-phenylnaphthalen-1-ol (**2l**, 66.1 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3al** as a white solid (85.4 mg, 70% yield, d.r. = 89:11).

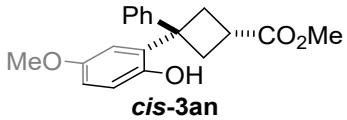
cis-**3al**: $\mathbf{R_f}$ = 0.50 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.54-7.47 (m, 6H), 7.43-7.39 (m, 3H), 7.37-7.29 (m, 3H), 7.21-7.18 (m, 1H), 5.14 (s, 1H), 3.64 (s, 3H), 3.32-3.23 (m, 1H), 3.10 (d, *J* = 8.8 Hz, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 175.1, 147.1, 145.2, 140.8, 133.0, 131.3, 130.3, 128.8, 128.6, 128.2, 127.0, 126.6, 126.2, 126.0, 125.84, 125.78, 125.3, 125.2, 120.8, 51.8, 45.2, 37.5, 33.4 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{28}H_{23}O_3$: 407.1647; found: 407.1646.



***cis*-3am**
$C_{22}H_{19}BrO_3$
M = 411.30 g/mol

(*cis*)-Methyl-3-(4-bromo-1-hydroxynaphthalen-2-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3am**): Prepared from 4-bromonaphthalen-1-ol (**2m**, 66.9 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 5/1) afforded *cis*-**3am** as a white solid (93.6 mg, 76.0% yield, d.r. > 98:2).

cis-**3am**: $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 8.11 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 7.73 (s, 1H), 7.54-7.42 (m, 4H), 7.35-7.31 (m, 2H), 7.24-7.20 (m, 1H), 5.08 (s, 1H), 3.67 (s, 3H), 3.32-3.23 (m, 1H), 3.10-3.01 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 174.9, 147.5, 144.6, 131.5, 130.0, 129.0, 128.3, 127.2, 127.1, 126.9, 126.4, 126.2, 126.1, 121.2, 113.7, 51.9, 45.0, 37.3, 33.3 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{22}H_{18}BrO_3$: 409.0440; found: 409.0406.



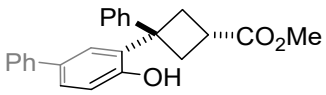
***cis*-3an**

$C_{19}H_{20}O_4$

M = 312.37 g/mol

(*cis*)-Methyl-3-(2-hydroxy-5-methoxyphenyl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3an**): Prepared from 4-methoxyphenol (**2n**, 37.2 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (10/1 to 5/1) afforded *cis*-**3an** as a white solid (39.4 mg, 42% yield, d.r. = 75:25).

cis-**3an**: $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.49-7.47 (m, 2H), 7.32-7.25 (m, 2H), 7.20-7.16 (m, 1H), 6.83 (s, 1H), 6.60-6.54 (m, 2H), 4.65-4.45 (m, 1H), 3.77 (s, 3H), 3.65 (s, 3H), 3.20-3.13 (m, 1H), 3.03-2.96 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 175.5, 153.5, 146.7, 145.4, 136.5, 128.4, 126.4, 126.2, 116.9, 113.3, 111.7, 55.7, 51.8, 45.5, 37.4, 33.3 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{19}H_{19}O_4$: 311.1284; found: 311.1263.



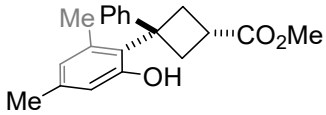
***cis*-3ao**

$C_{24}H_{22}O_3$

M = 358.44 g/mol

(*cis*)-Methyl-3-(4-hydroxy-[1,1'-biphenyl]-3-yl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ao**): Prepared from [1,1'-biphenyl]-4-ol (**2o**, 51.0 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 10/1) afforded *cis*-**3ao** as a white solid (57.3 mg, 53% yield, d.r. = 70:30) together with trace amount of *trans*-**3ao**, which cannot be separated by chromatography.

cis-**3ao**: $\mathbf{R_f}$ = 0.50 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.56-7.51 (m, 4H), 7.47 (s, 1H), 7.43-7.40 (m, 2H), 7.32-7.18 (m, 3H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.20-7.16 (m, 1H), 6.67 (d, *J* = 8.4 Hz, 1H), 5.27 (broad s, 1H), 3.66 (s, 3H), 3.26-3.17 (m, 1H), 3.12-3.01 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): 175.8, 152.5, 145.5, 141.0, 135.6, 133.6, 128.7, 128.4, 126.8, 126.6, 126.5, 126.18, 126.15, 125.7, 116.5, 51.9, 45.5, 37.6, 33.5 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{24}H_{21}O_3$: 357.1491; found: 357.1463.



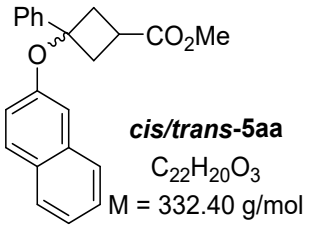
***cis*-3ap**

$C_{20}H_{22}O_3$

M = 310.39 g/mol

(*cis*)-Methyl-3-(2-hydroxy-4,6-dimethylphenyl)-3-phenylcyclobutane-1-carboxylate (*cis*-**3ap**): Prepared from 3,5-dimethylphenol (**2m**, 36.7 mg, 0.3 mmol) and methyl 3-phenylbicyclo[1.1.0]butane-1-carboxylate (**1a**, 67.8 mg, 0.36 mmol) according to the **GP** at 100 °C for 3 h. Purification by flash chromatography on silica gel using petroleum ether/EtOAc (20/1 to 10/1) afforded *cis*-**3ap** as a white solid (56.0 mg, 60% yield, d.r. = 92:8).

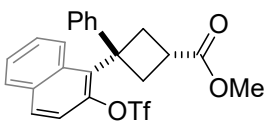
cis-**3ap**: $\mathbf{R_f}$ = 0.50 (petroleum ether/EtOAc = 5/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.57 (d, *J* = 7.2 Hz, 2H), 7.29-7.26 (m, 2H), 7.18-7.14 (m, 1H), 6.44 (s, 1H), 6.39 (s, 1H), 5.61-5.54 (m, 1H), 3.67 (s, 3H), 3.20-3.13 (m, 1H), 3.11-3.01 (m, 4H), 2.16 (s, 3H), 2.08 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 176.3, 153.3, 146.2, 137.1, 136.6, 130.6, 128.3, 126.3, 125.9, 124.5, 114.8, 51.8, 46.1, 39.8, 34.0, 20.62, 20.59 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{20}H_{21}O_3$: 309.1491; found: 309.1470.



***cis/trans*-5aa**
$C_{22}H_{20}O_3$
M = 332.40 g/mol

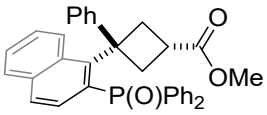
(*cis/trans*)-Methyl-3-(naphthalen-2-yloxy)-3-phenylcyclobutane-1-carboxylate.

Major isomer: white solid. $\mathbf{R_f}$ = 0.3 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.71-7.67 (m, 2H), 7.51-7.47 (m, 3H), 7.35-7.31 (m, 3H), 7.29-7.22 (m, 2H), 7.06 (dd, *J* = 8.8 and 2.4 Hz, 1H), 6.66 (d, *J* = 2.4 Hz, 1H), 3.72 (s, 3H), 3.49-3.40 (m, 1H), 2.97 (d, *J* = 8.4 Hz, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 175.5, 153.0, 142.9, 133.9, 129.2, 128.7, 128.6, 127.4, 127.3, 126.8, 126.1, 125.1, 123.7, 120.1, 112.1, 81.2, 51.9, 37.5, 31.7 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{22}H_{20}O_3Na$: 355.1310; found: 355.1314. **Minor isomer:** white solid. $\mathbf{R_f}$ = 0.25 (petroleum ether/EtOAc = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.69-7.65 (m, 2H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.37-7.30 (m, 3H), 7.27-7.23 (m, 2H), 7.05 (d, *J* = 8.8 Hz, 1H), 6.66 (s, 1H), 3.71 (s, 3H), 3.14-3.06 (m, 1H), 3.04-2.95 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 174.7, 152.7, 142.6, 134.0, 129.2, 128.8, 128.7, 127.5, 127.4, 126.7, 126.0, 124.8, 123.6, 119.9, 111.1, 77.8, 52.0, 39.1, 29.9 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{22}H_{20}O_3Na$: 355.1310; found: 355.1314.



***cis*-6**
$C_{23}H_{19}F_3O_5S$
M = 464.46 g/mol

(*cis*)-Methyl-3-phenyl-3-(2-(((trifluoromethyl)sulfonyl)oxy)naphthalen-1-yl)cyclobutane -1-carboxylate. (*cis*-**6**): $\mathbf{R_f}$ = 0.75 (petroleum ether/EtOAc = 10/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.89-7.83 (m, 2H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.51-7.42 (m, 5H), 7.33-7.30 (m, 2H), 7.25-7.22 (m, 1H), 3.65 (s, 1H), 3.58-3.48 (m, 1H), 3.35-3.16 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 175.1, 145.5, 145.1, 136.3, 133.0, 132.0, 129.9, 129.0, 128.7, 126.9, 126.8, 126.5, 126.3, 126.1, 119.8, 118.3 (q, *J* = 318 Hz), 51.9, 45.9, 41.9, 41.1, 34.1 ppm. **^{19}F NMR** (376 MHz, $CDCl_3$): δ -74.32 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{23}H_{19}F_3O_5SNa$: 487.0803; found: 487.0769.

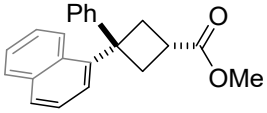


cis-**7**

$C_{34}H_{29}O_3P$

M = 516.58 g/mol

(*cis*)-Methyl-3-(2-(diphenylphosphoryl)naphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate. (*cis*-**7**): $\mathbf{R_f}$ = 0.2 (petroleum ether/EtOAc = 2/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.93-7.88 (m, 2H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.64-7.52 (m, 7H), 7.47-7.27 (m, 9H), 7.25-7.21 (m, 2H), 3.43-3.30 (m, 6H), 3.26-3.19 (m, 1H), 2.89-2.84 (m, 1H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 175.4, 155.4 (d, *J* = 5.4 Hz), 148.1, 137.2 (d, *J* = 5.4 Hz), 135.2 (d, *J* = 2.5 Hz), 133.5 (d, *J* = 98.9 Hz), 132.1, 131.97 (d, *J* = 11.7 Hz), 131.96, 131.8, 131.7, 131.1 (d, *J* = 2.7 Hz), 130.1 (d, *J* = 14.2 Hz), 128.6 ((d, *J* = 12.0 Hz), 128.5, 128.3, 128.2, 127.7, 127.29, 127.26, 126.5, 126.3, 126.0, 125.9, 125.6 (d, *J* = 13.5 Hz), 51.4, 49.0 (d, *J* = 3.6 Hz), 44.1, 43.6, 33.3 ppm. **^{31}P NMR** (162 MHz, $CDCl_3$) δ 32.77 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{34}H_{30}O_3P$: 517.1932; found: 517.1896.

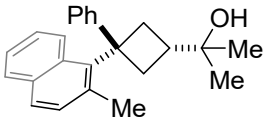


cis-**8**

$C_{22}H_{20}O_2$

M = 316.40 g/mol

(*cis*)-Methyl-3-(naphthalen-1-yl)-3-phenylcyclobutane-1-carboxylate. (*cis*-**8**): $\mathbf{R_f}$ = 0.75 (petroleum ether/EtOAc = 10/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.60-7.55 (m, 2H), 7.52-7.45 (m, 3H), 7.36-7.33 (m, 1H), 7.29-7.24 (m, 3H), 7.15-7.12 (m, 1H), 3.64 (s, 3H), 3.47-3.38 (m, 1H), 3.18-3.15 (m, 4H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 175.1, 146.5, 144.8, 134.4, 130.3, 128.8, 128.5, 127.3, 126.01, 125.95, 125.4, 125.2, 125.0, 124.3, 51.7, 47.5, 38.8, 33.1 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{22}H_{20}O_2Na$: 339.1361; found: 339.1336.

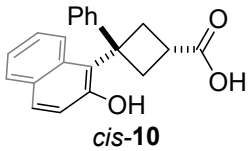


cis-**9**

$C_{24}H_{26}O$

M = 330.47 g/mol

(*cis*)-2-(-3-(2-Methylnaphthalen-1-yl)-3-phenylcyclobutyl)propan-2-ol. (*cis*-**9**): $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 10/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.67-7.62 (m, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.36-7.32 (m, 1H), 7.31-7.23 (m, 4H), 7.21-7.17 (m, 1H), 3.06-3.00 (m, 1H), 2.88-2.66 (m, 4H), 2.35 (s, 3H), 1.10 (s, 3H), 1.08 (s, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 147.8, 143.6, 134.0, 133.0, 131.9, 130.3, 128.5, 126.6, 126.3, 126.2, 125.9, 124.7, 124.1, 70.4, 46.4, 40.7, 40.4, 39.6, 26.8, 26.7, 22.4 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{24}H_{26}ONa$: 353.1882; found: 353.1880.



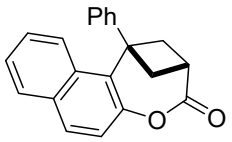
cis-**10**

$C_{21}H_{18}O_3$

M = 318.37 g/mol

(*cis*)-3-(2-Hydroxynaphthalen-1-yl)-3-phenylcyclobutane-1-carboxylic acid. (*cis*-**10**): $\mathbf{R_f}$ = 0.20 (DCM/MeOH = 50/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.0 Hz, 1H), 7.63-7.59 (m, 3H), 7.55-7.52 (m, 1H), 7.33-7.22 (m, 4H), 7.17-7.14 (m, 1H), 6.90-6.87 (m, 1H), 3.37-3.16 (m, 5H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 180.9, 150.2, 146.2, 132.1, 129.8, 128.8, 128.7, 128.6, 126.6, 126.3, 126.2, 125.9, 124.5, 122.9,

118.7, 45.9, 40.3, 34.2 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{21}H_{17}O_3$: 317.3642; found: 317.3628.

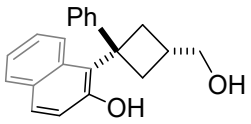


11

$C_{21}H_{16}O_2$

M = 300.36 g/mol

1-Phenyl-2,3-dihydro-1,3-methanonaphtho[2,1-b]oxepin-4(1H)-one (**11**): $\mathbf{R_f}$ = 0.60 (petroleum ether/EtOAc = 10/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.73-7.69 (m, 2H), 7.42 (d, *J* = 8.8 Hz, 1H), 7.37-7.34 (m, 2H), 7.30-7.26 (m, 1H), 7.21-7.17 (m, 3H), 6.90 (d, *J* = 9.2 Hz, 1H), 6.86-6.82 (m, 1H), 3.60 (t, *J* = 8.4 Hz, 1H), 3.19-3.12 (m, 2H), 2.72 (d, *J* = 11.2 Hz, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 172.8, 150.4, 149.3, 131.9, 131.6, 129.4, 129.1, 128.2, 127.5, 126.6, 126.4, 125.6, 124.6, 124.1, 121.1, 49.1, 37.1, 34.3 ppm. **HRMS** (ESI) *m/z*: $[M+Na]^+$ calcd. for $C_{21}H_{16}O_2Na$: 323.1048; found: 323.1025.

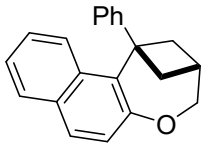


cis-**12**

$C_{21}H_{20}O_2$

M = 304.39 g/mol

(*cis*)-1-(-3-(Hydroxymethyl)-1-phenylcyclobutyl)naphthalen-2-ol. (*cis*-**12**): $\mathbf{R_f}$ = 0.30 (petroleum ether/EtOAc = 2/1). **^{1}H NMR** (400 MHz, Methanol-d_4): δ 7.70-7.65 (m, 4H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.24-7.20 (m, 3H), 7.16-7.12 (m, 1H), 7.11-7.06 (m, 2H), 3.48 (d, *J* = 5.2 Hz, 2H), 3.11 (s, 2H), 2.62-2.56 (m, 3H) ppm. **^{13}C NMR** (100 MHz, Methanol-d_4): δ 153.2, 149.8, 133.9, 130.8, 129.5, 129.1, 129.0, 128.8, 127.7, 126.5, 126.0, 125.9, 123.1, 120.0, 68.1, 47.6, 42.1, 34.1 ppm. **HRMS** (ESI) *m/z*: $[M-H]^-$ calcd. for $C_{21}H_{19}O_2$: 303.1385; found: 303.1365.



13

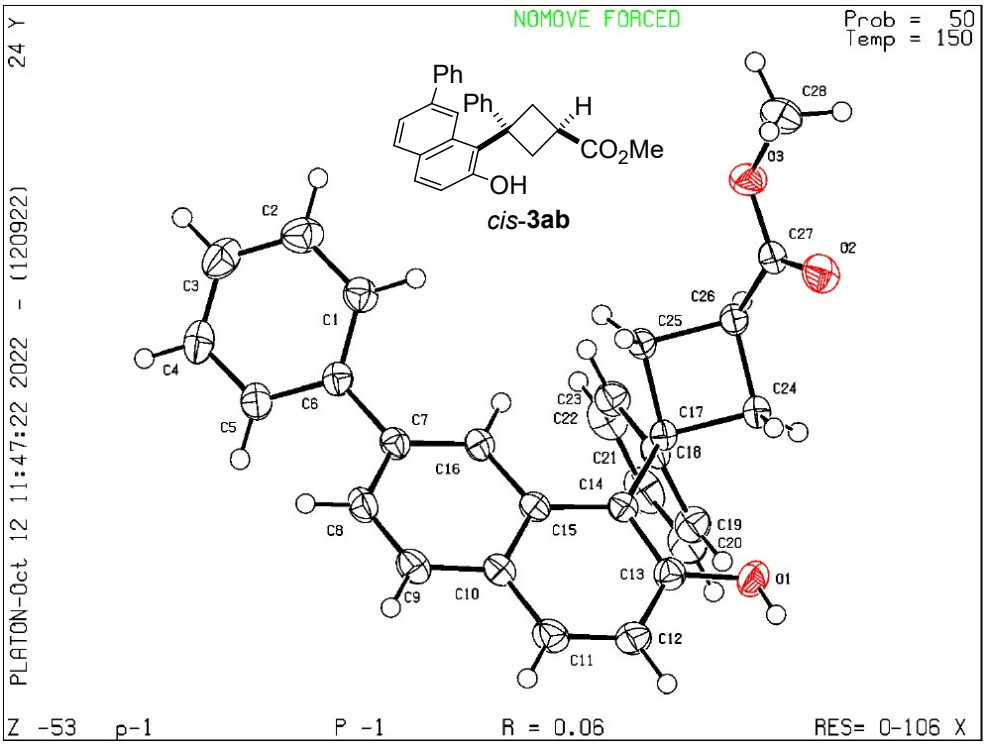
$C_{21}H_{18}O$

M = 286.37 g/mol

1-Phenyl-1,2,3,4-tetrahydro-1,3-methanonaphtho[2,1-b]oxepine (**13**): $\mathbf{R_f}$ = 0.35 (petroleum ether/EtOAc = 100/1). **^{1}H NMR** (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.0 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.27-7.21 (m, 3H), 7.18-7.16 (m, 1H), 7.12-7.10 (m, 4H), 6.87-6.84 (m, 1H), 4.34 (d, *J* = 4.0 Hz, 2H), 2.86-2.77 (m, 3H), 2.68-2.66 (m, 2H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$): δ 157.3, 150.8, 132.5, 131.4, 129.4, 128.6, 128.03, 128.01, 126.5, 125.2, 125.0, 124.0, 123.0, 122.3, 75.5, 52.2, 38.4, 31.6 ppm. **HRMS** (ESI) *m/z*: $[M+H]^+$ calcd. for $C_{21}H_{19}O$: 287.1436; found: 287.1435.

9 Crystal Structure of *cis*-3ab

Note: The thermal ellipsoids are 50% probability level. The crystals are grown by slow solvent (EtOAc/*n*-Hexane) evaporation at room temperature. CCDC number of ***cis*-3ab** is 2262933.



Datablock: p-1

Bond precision: C-C = 0.0028 A Wavelength=0.71073

Cell: a=9.7676(15) b=10.6234(16) c=12.9739(16)
alpha=74.896(6) beta=74.919(6) gamma=77.645(6)
Temperature: 150 K

	Calculated	Reported
Volume	1239.4(3)	1239.4(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H24 O3 [+ solvent]	C28 H24 O3
Sum formula	C28 H24 O3 [+ solvent]	C28 H24 O3
Mr	408.47	408.47
Dx,g cm-3	1.094	1.094
Z	2	2
Mu (mm-1)	0.070	0.070
F000	432.0	432.0
F000'	432.20	
h,k,lmax	13,14,17	13,14,17
Nref	6165	6151
Tmin,Tmax	0.983,0.986	0.679,0.746
Tmin'	0.983	

Correction method= # Reported T Limits: Tmin=0.679 Tmax=0.746
AbsCorr = ?

Data completeness= 0.998 Theta(max)= 28.304

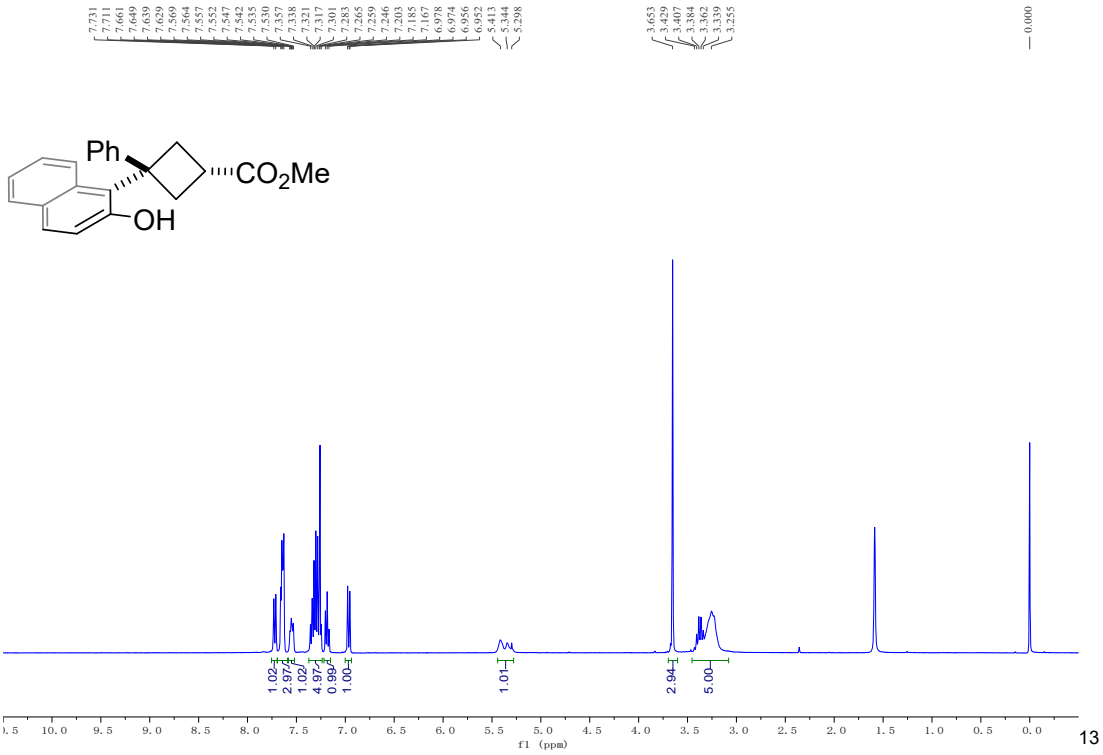
R(reflections)= 0.0585(4807) wR2(reflections)= 0.1861(6151)

S = 1.064 Npar= 282

10 NMR Spectra

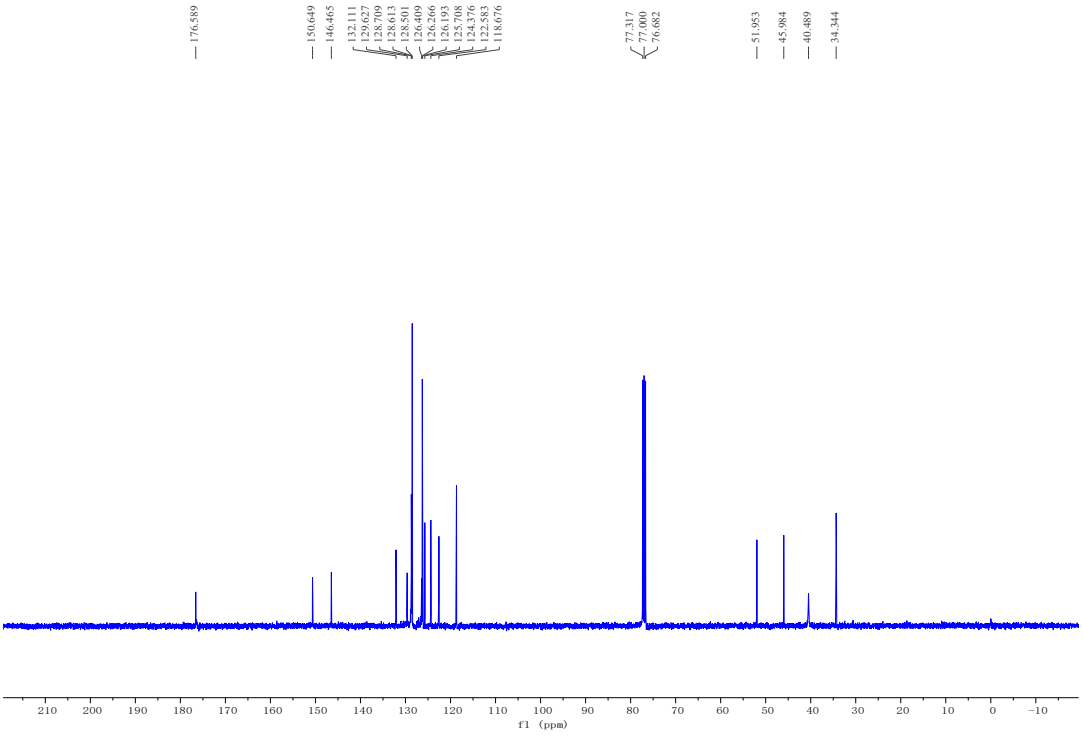
^{1}H and ^{13}C NMR Spectra for Compound *cis*-3aa:

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



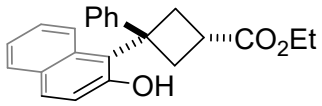
13

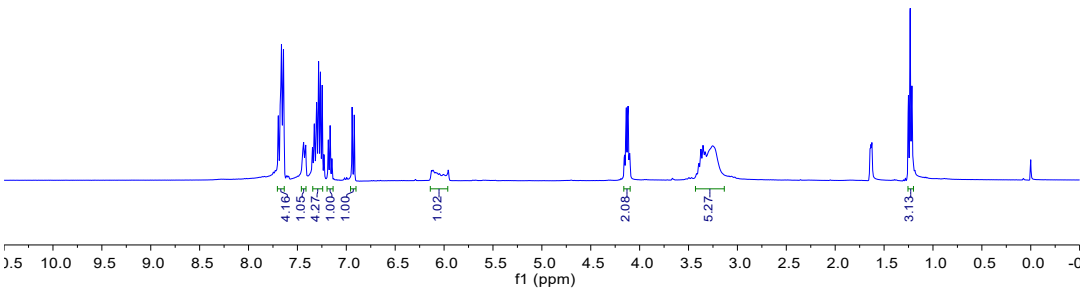
C NMR (100 MHz, $CDCl_3$)



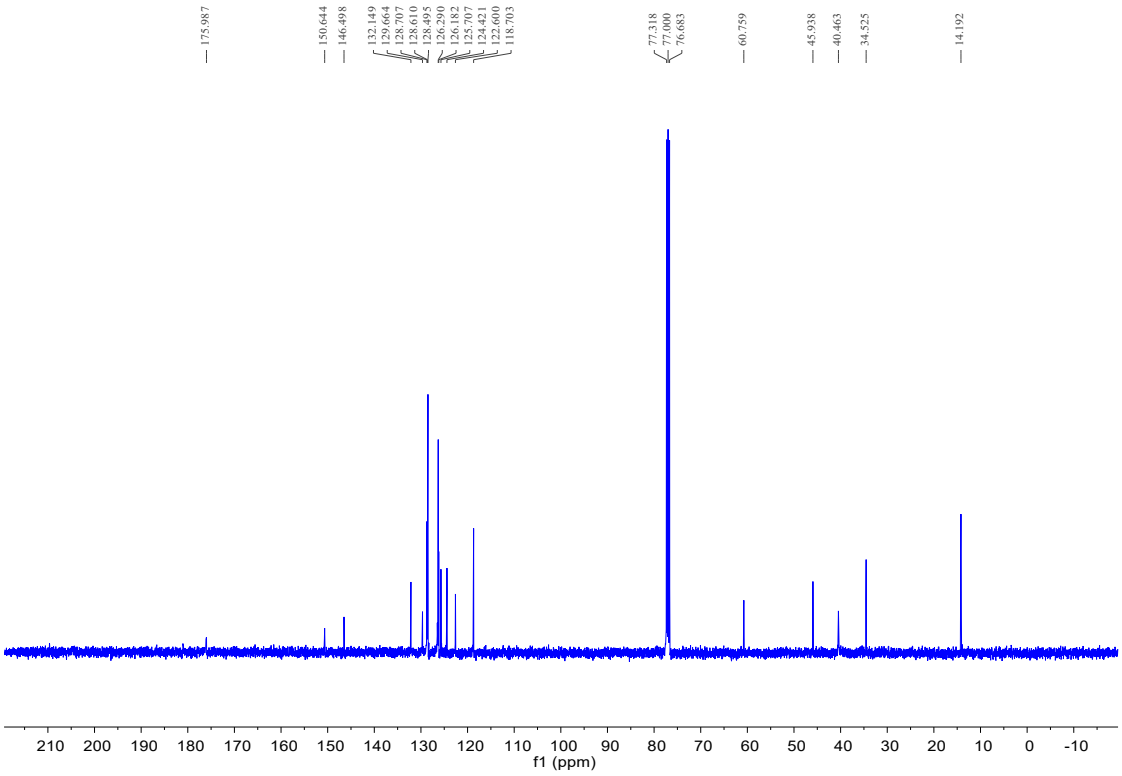
^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ba:

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



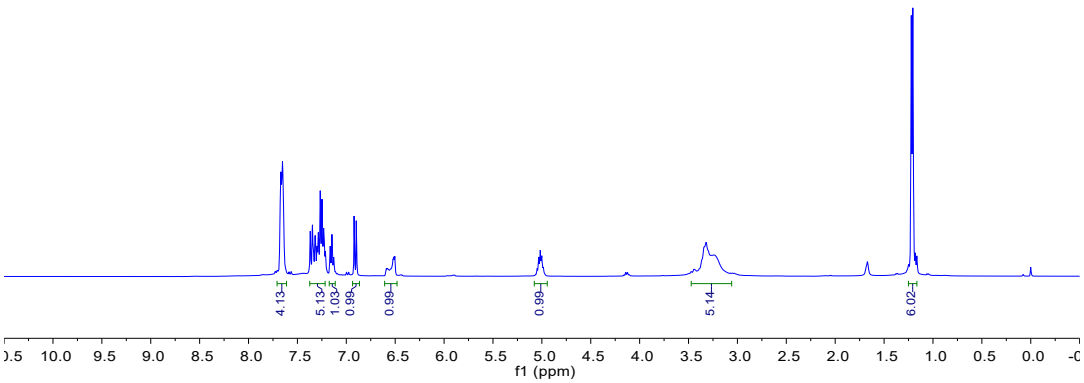


^{13}C NMR (100 MHz, $CDCl_3$)

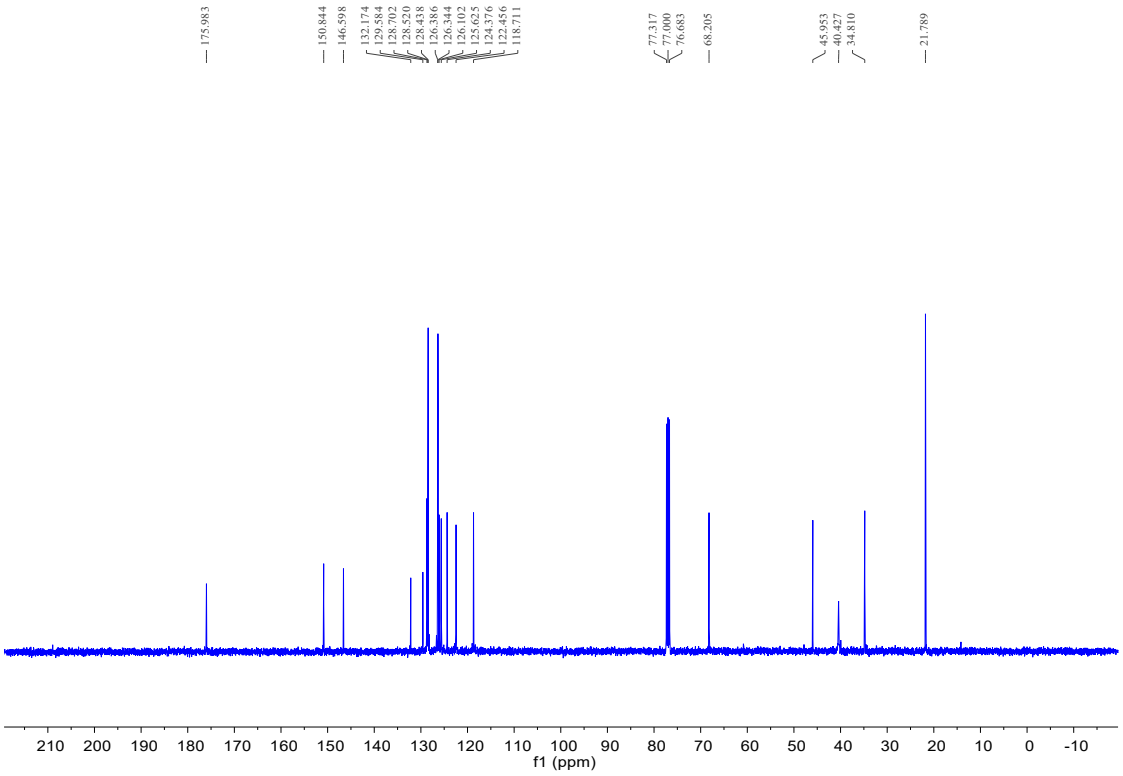


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ca:

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

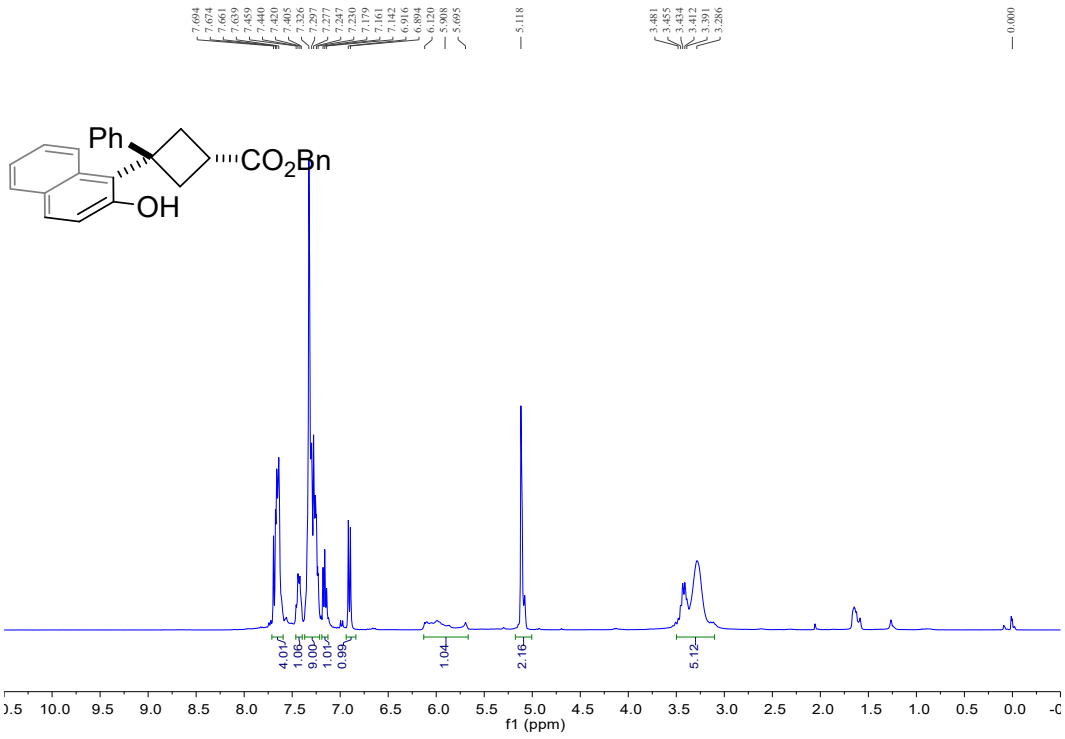


^{13}C NMR (100 MHz, $CDCl_3$)

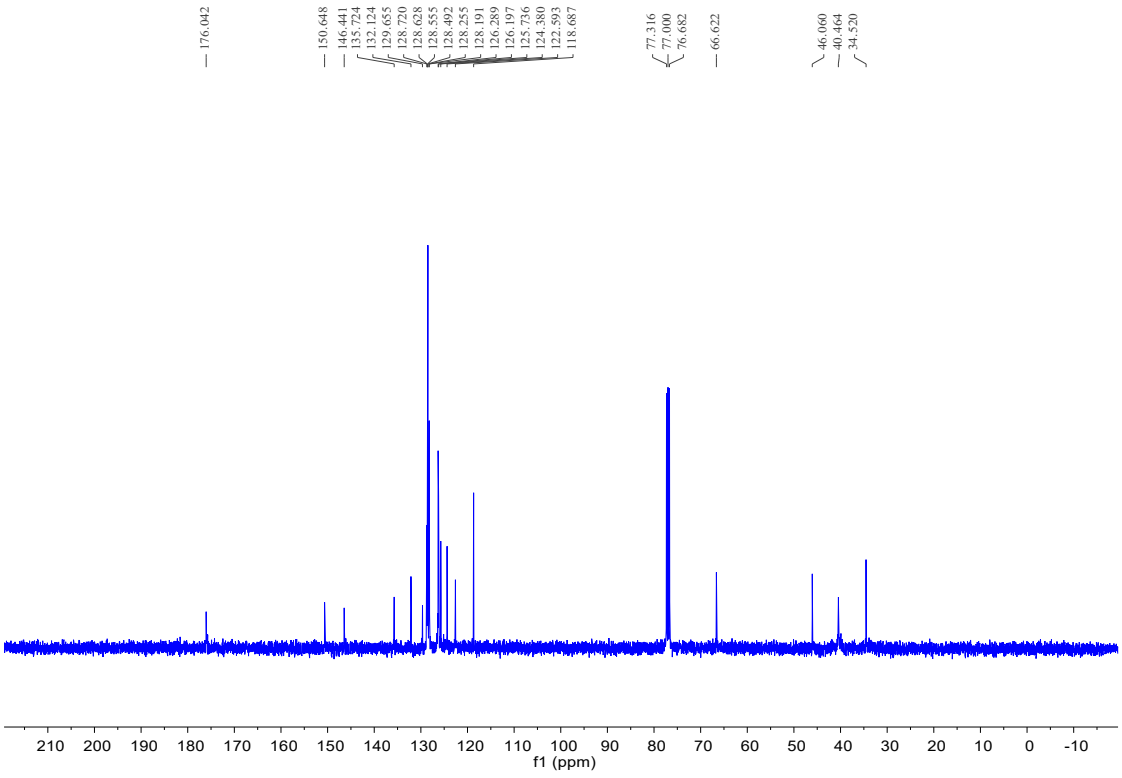


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3da:

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

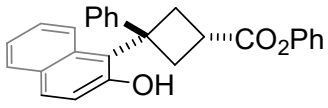


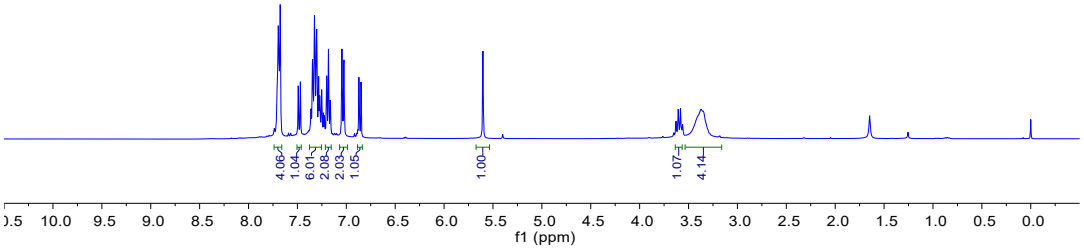
^{13}C NMR (100 MHz, $CDCl_3$)



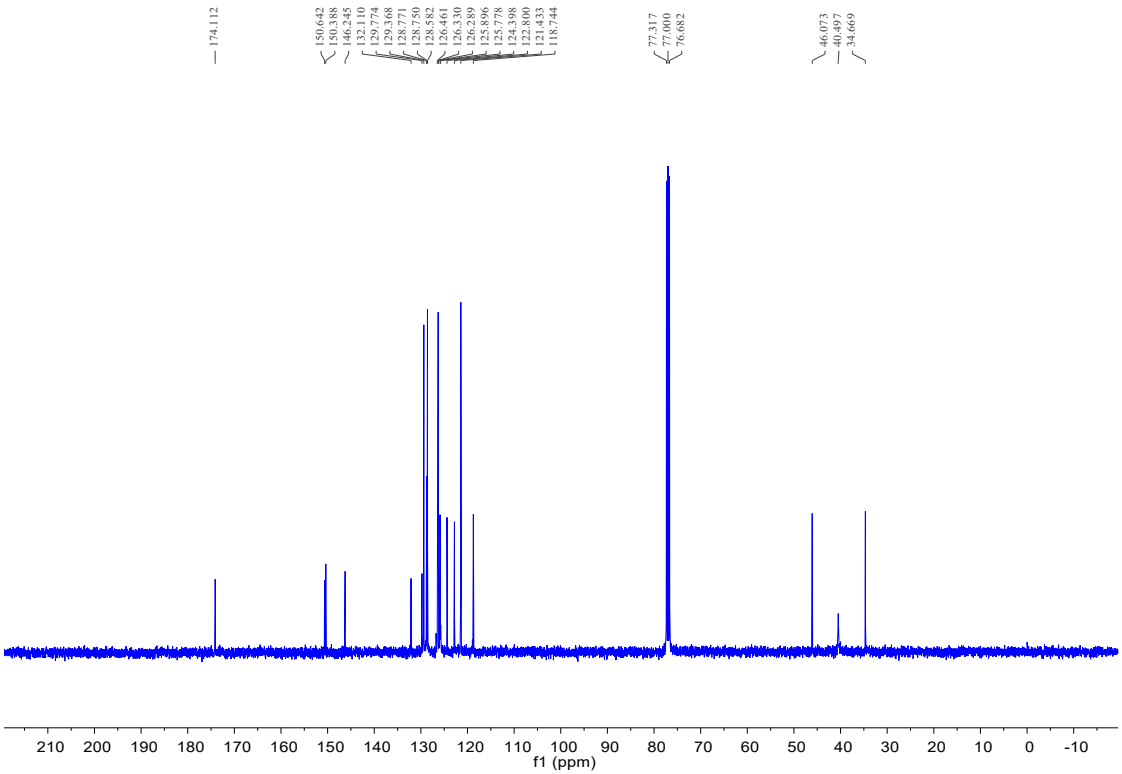
^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ea:

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



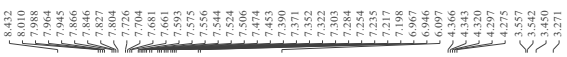


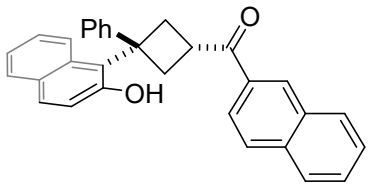
^{13}C NMR (100 MHz, $CDCl_3$)

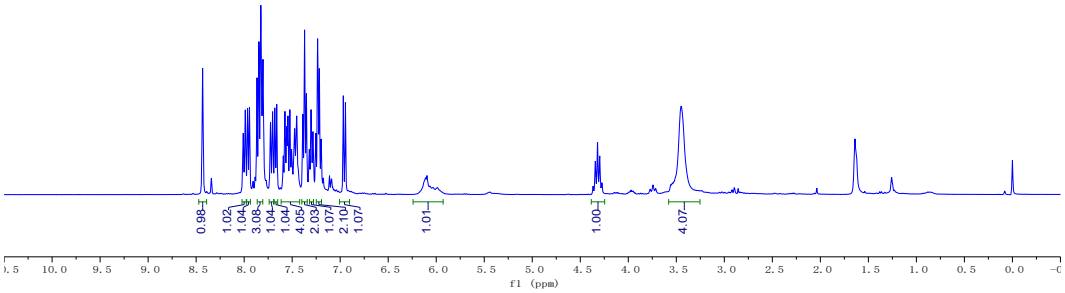


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3fa

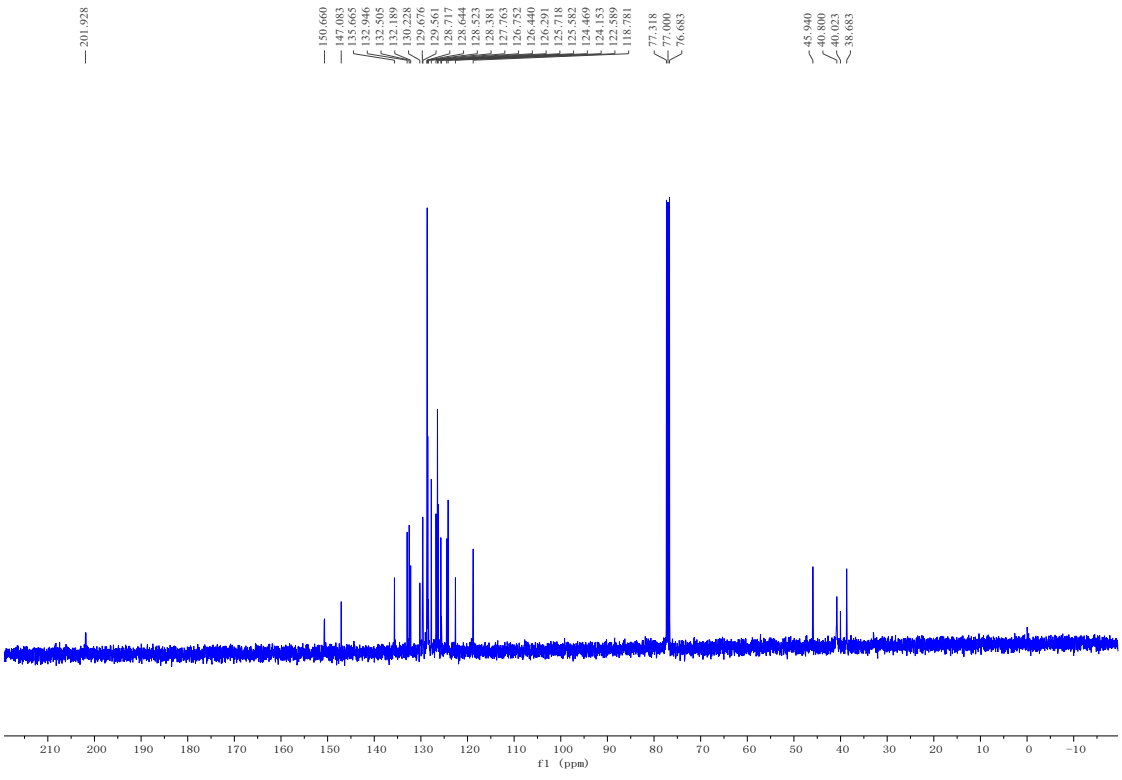
^{1}H NMR (400 MHz, $CDCl_3$)





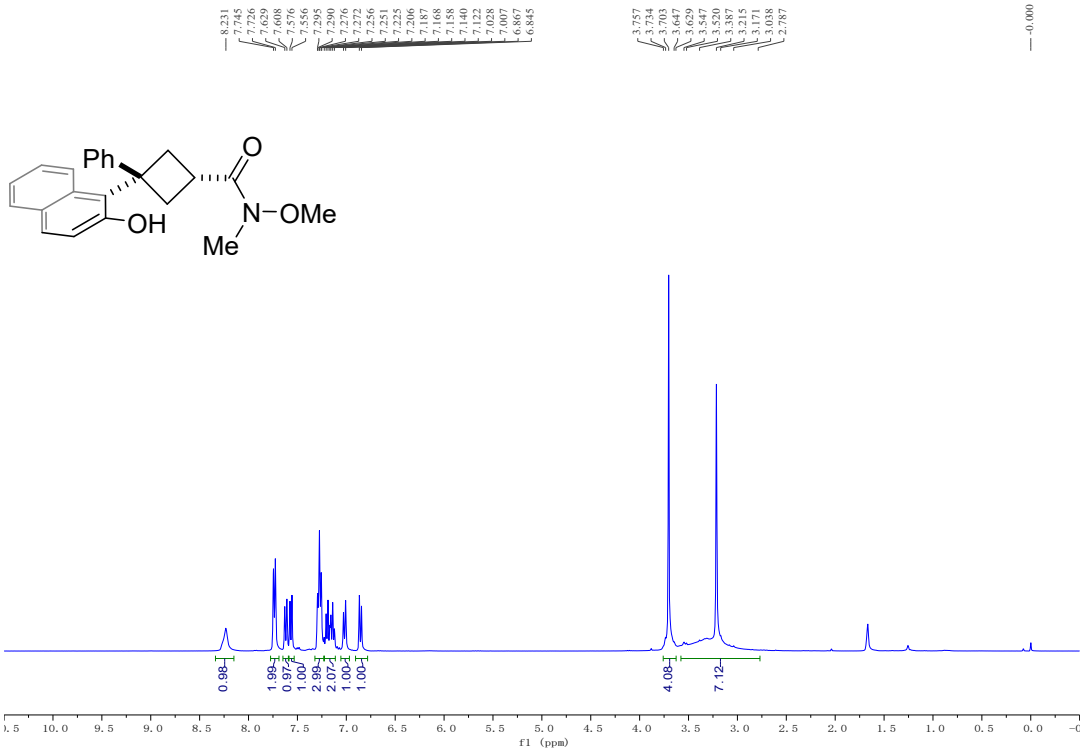


^{13}C NMR (100 MHz, $CDCl_3$)

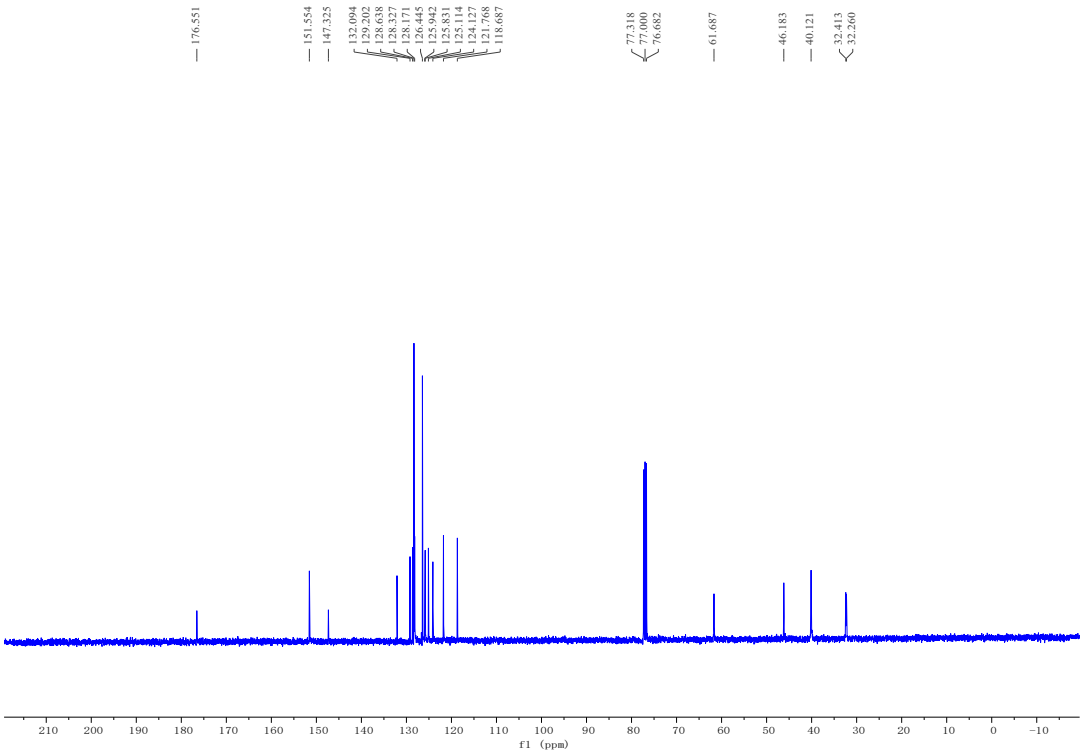


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ga

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

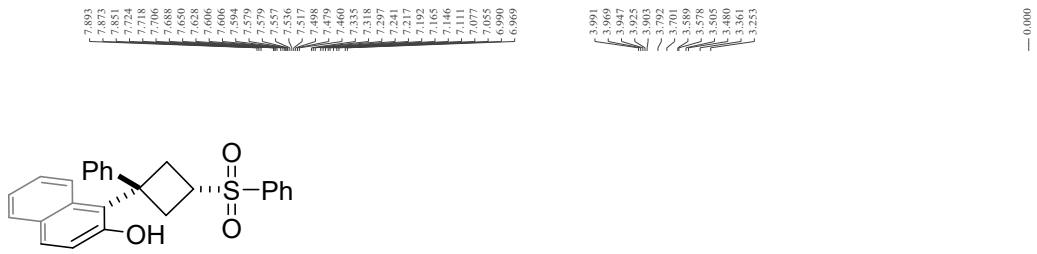


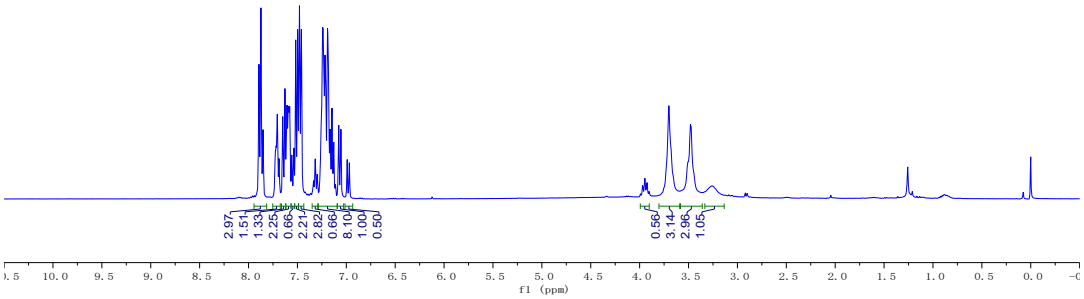
^{13}C NMR (100 MHz, $CDCl_3$)



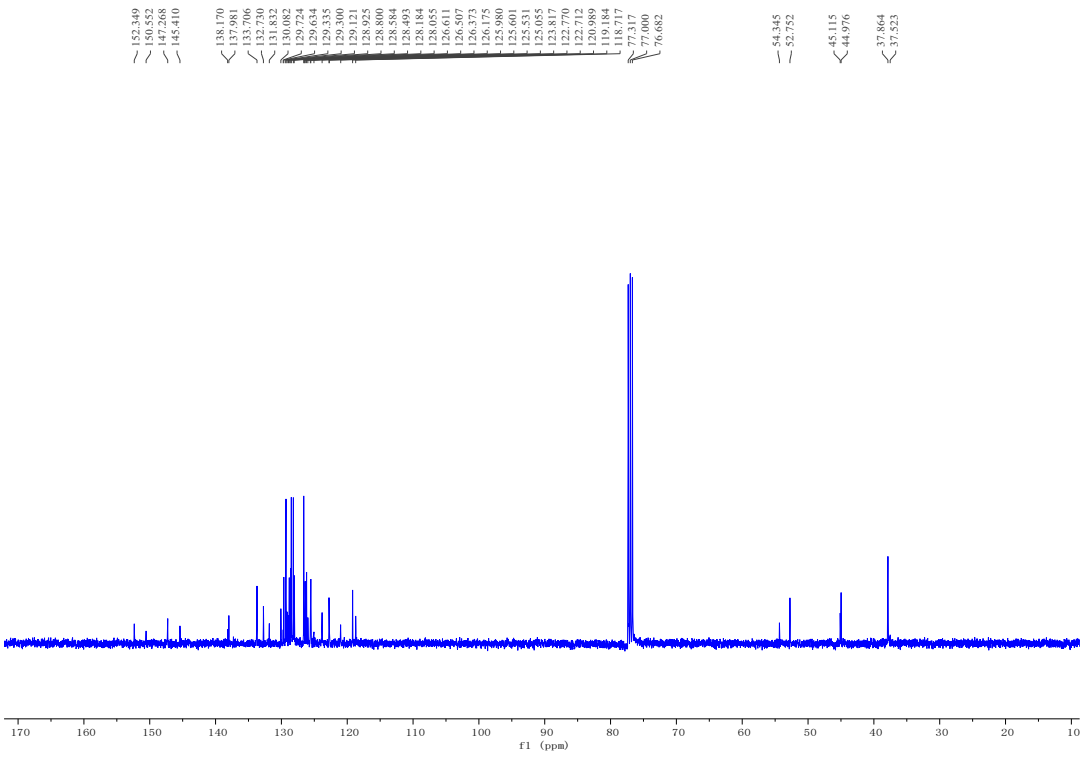
^{1}H and ^{13}C NMR Spectra for Compound 3ha

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



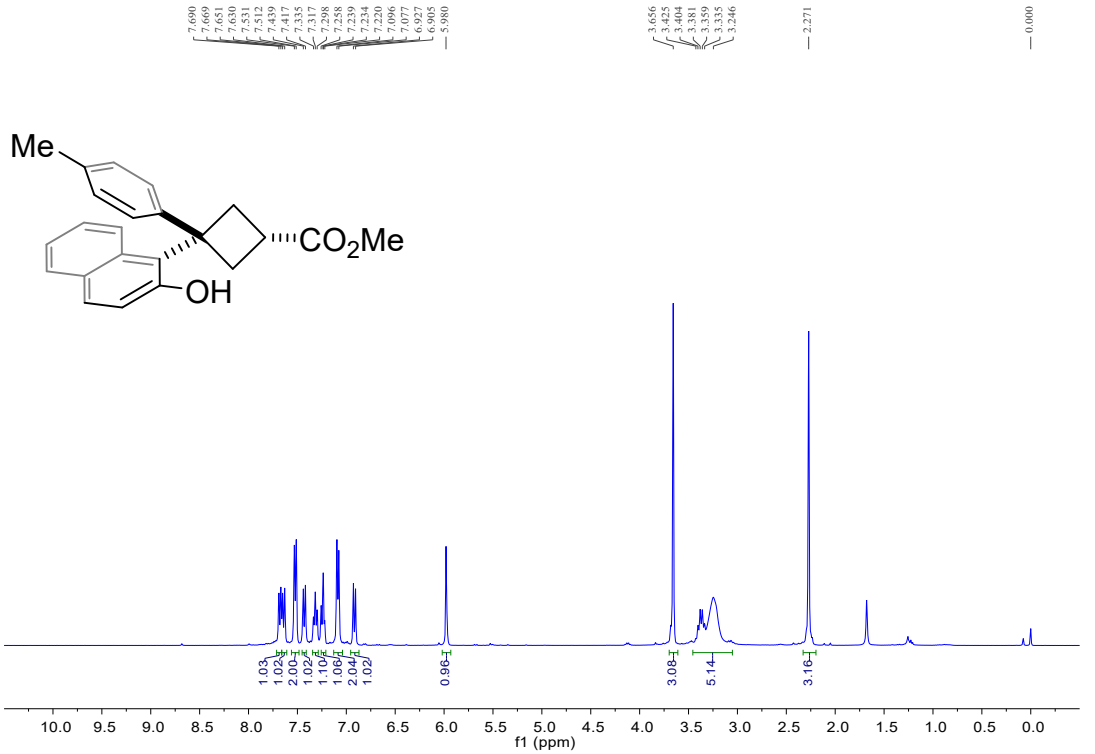


^{13}C NMR (100 MHz, $CDCl_3$)

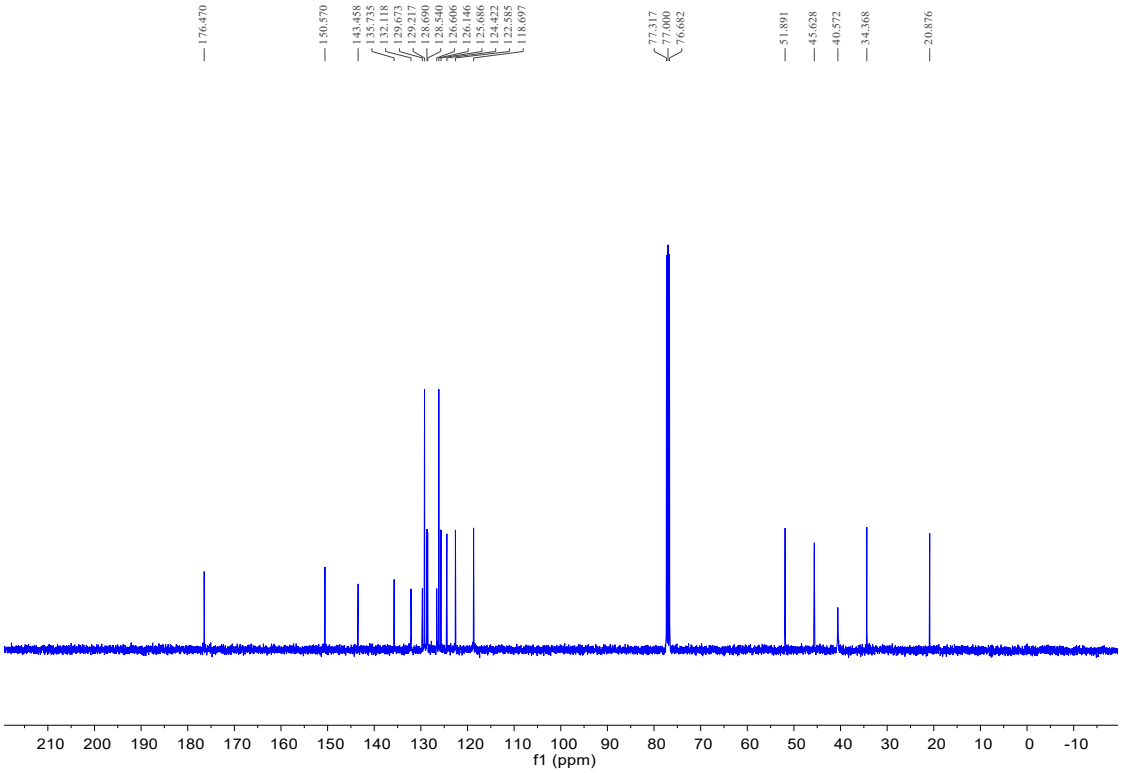


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ia:

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

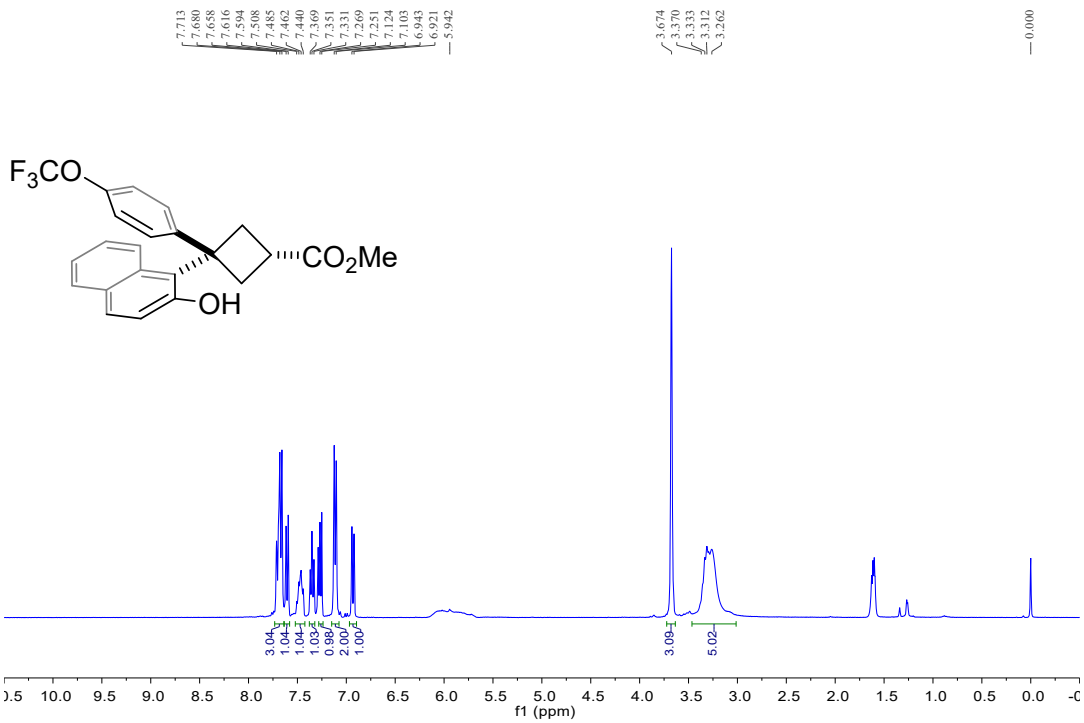


^{13}C NMR (100 MHz, $CDCl_3$)

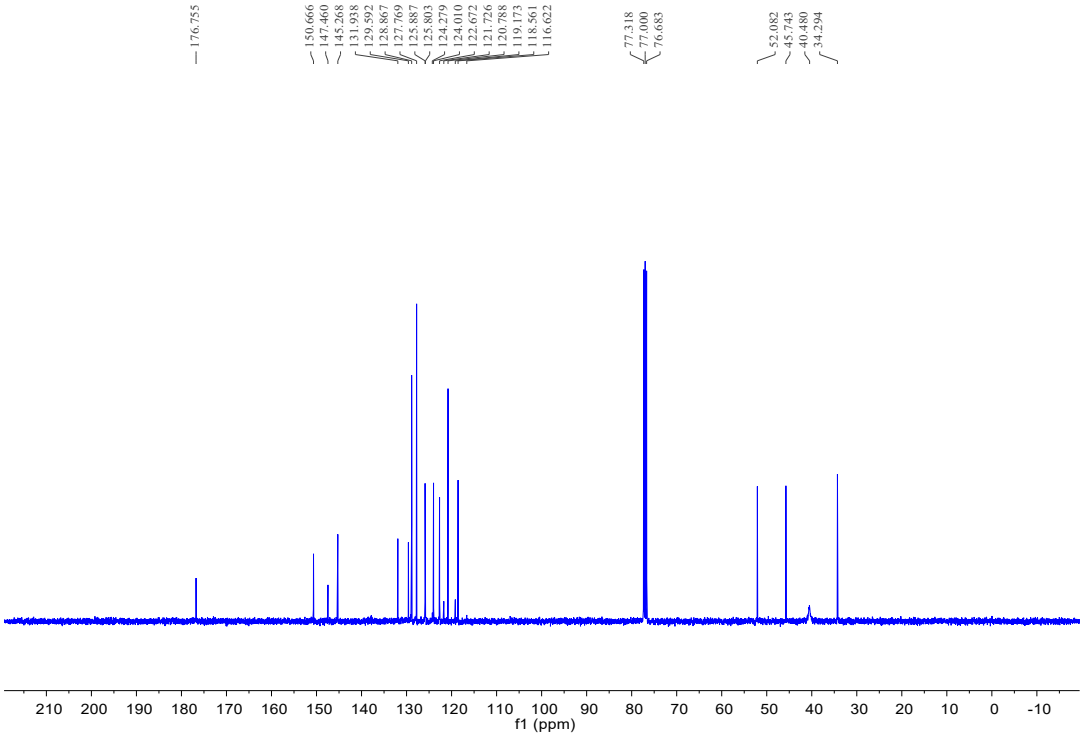


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound *cis*-3ja:

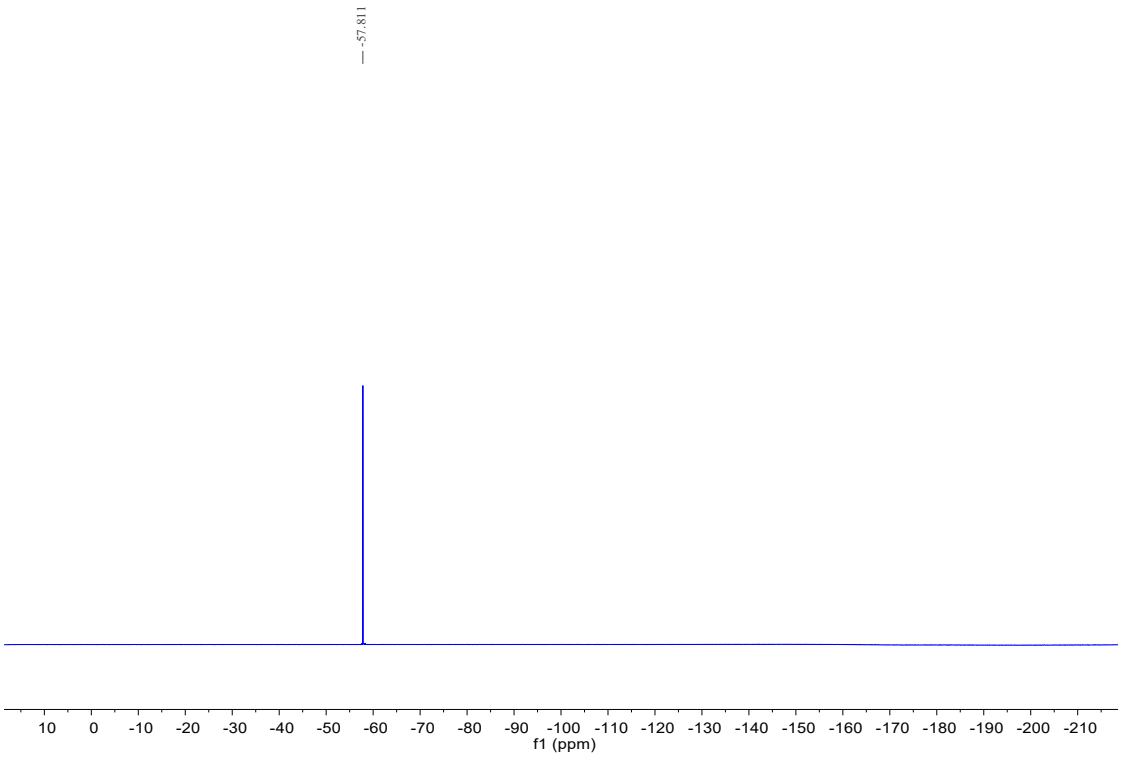
^{1}H NMR (400 MHz, $CDCl_3$)



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

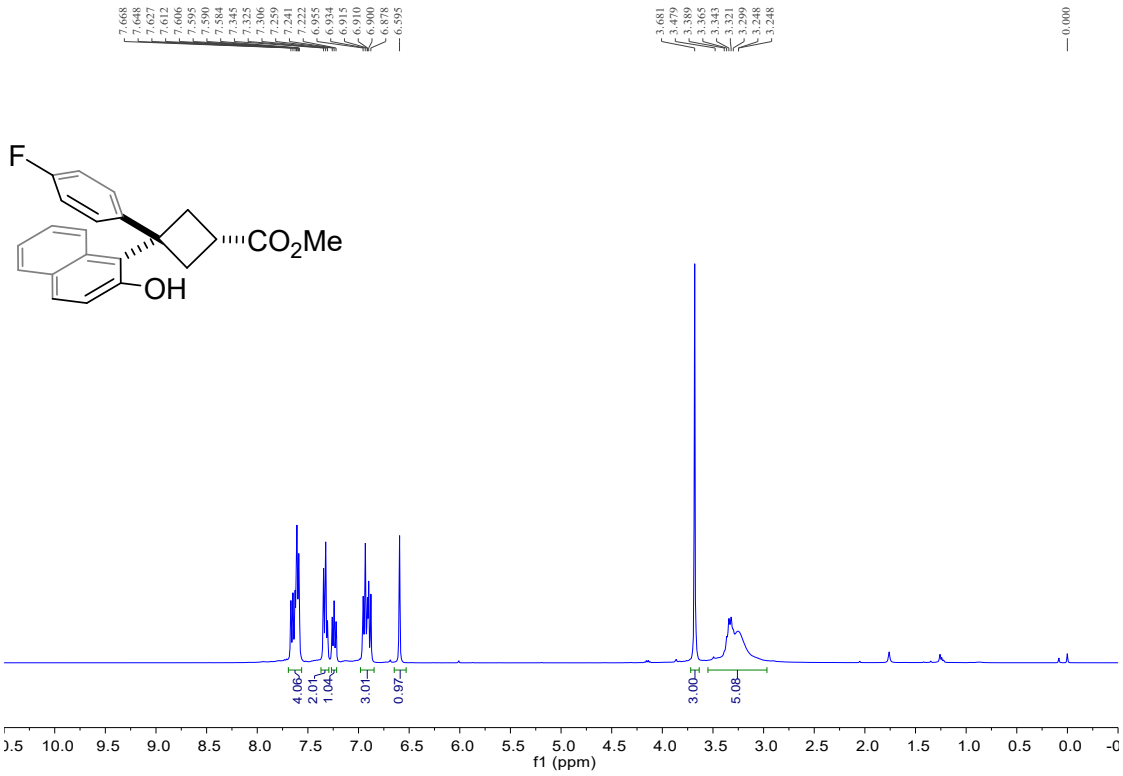


^{19}F NMR (376 MHz, $CDCl_3$)

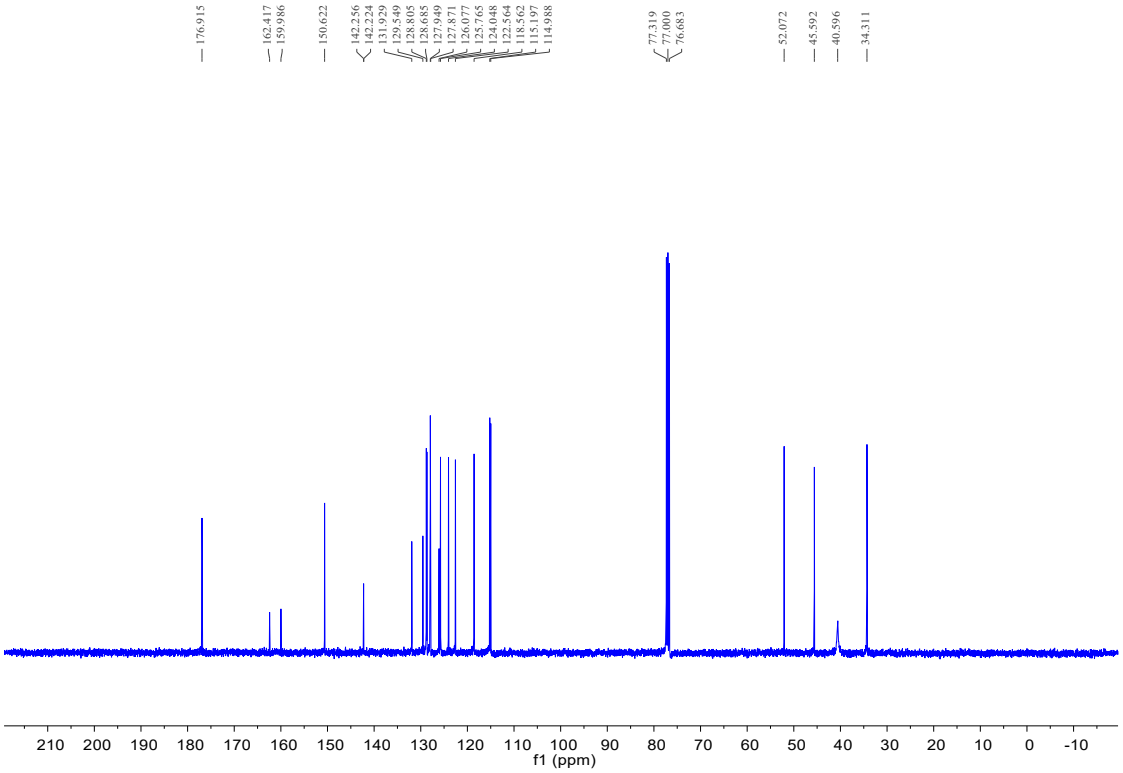


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound *cis*-3ka:

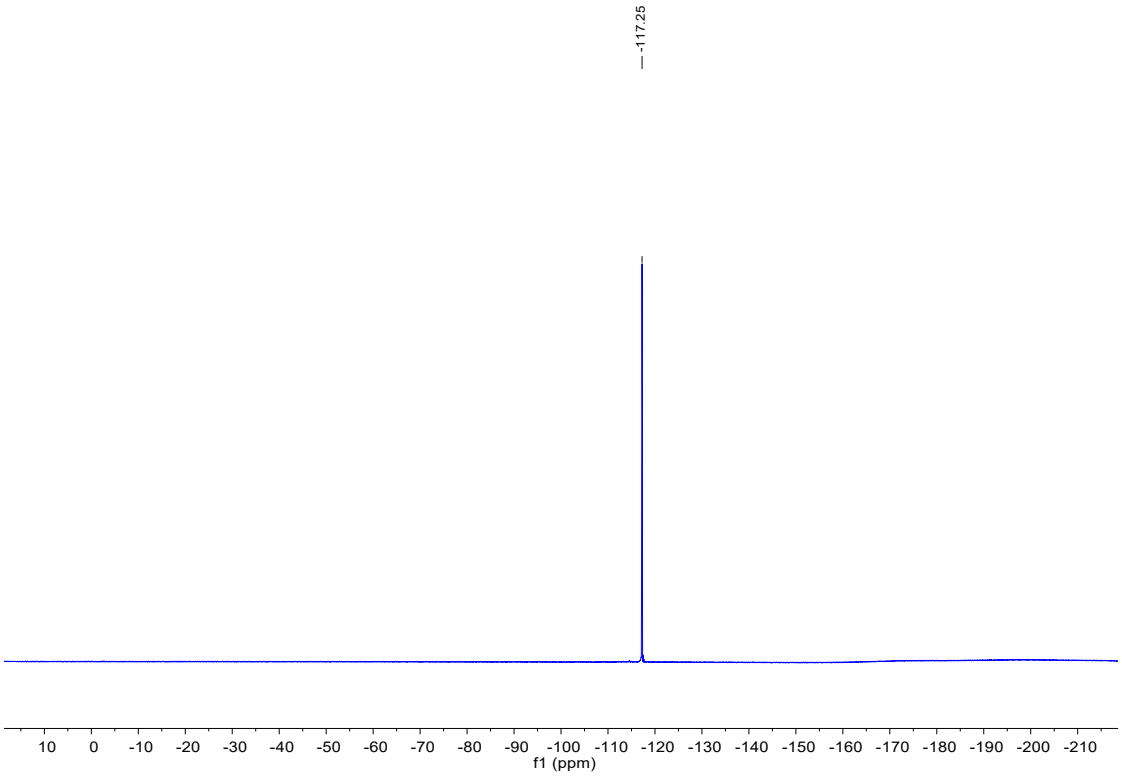
^{1}H NMR (400 MHz, $CDCl_3$)



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

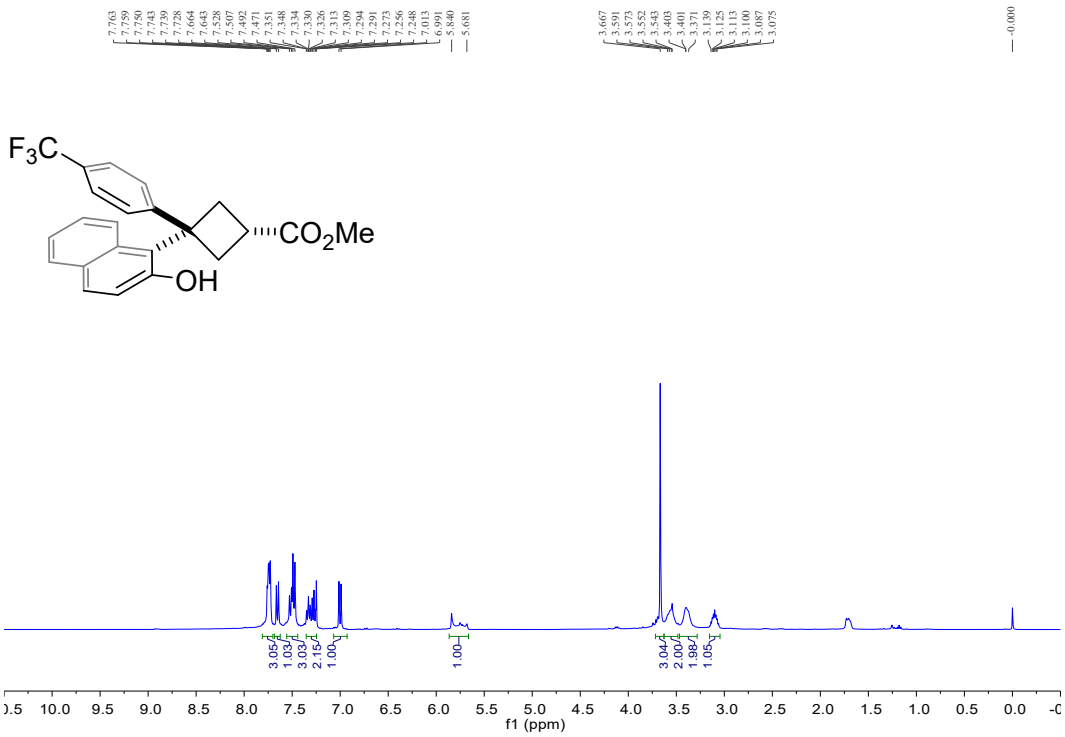


^{19}F NMR (376 MHz, $CDCl_3$)

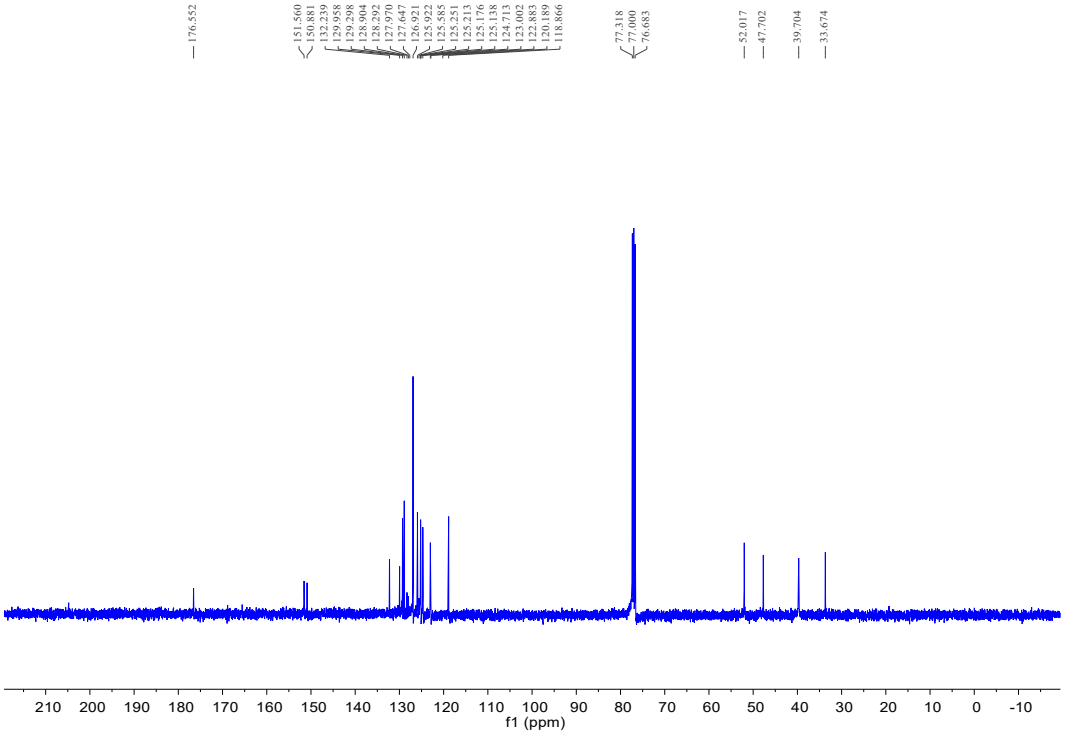


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound *cis*-3la:

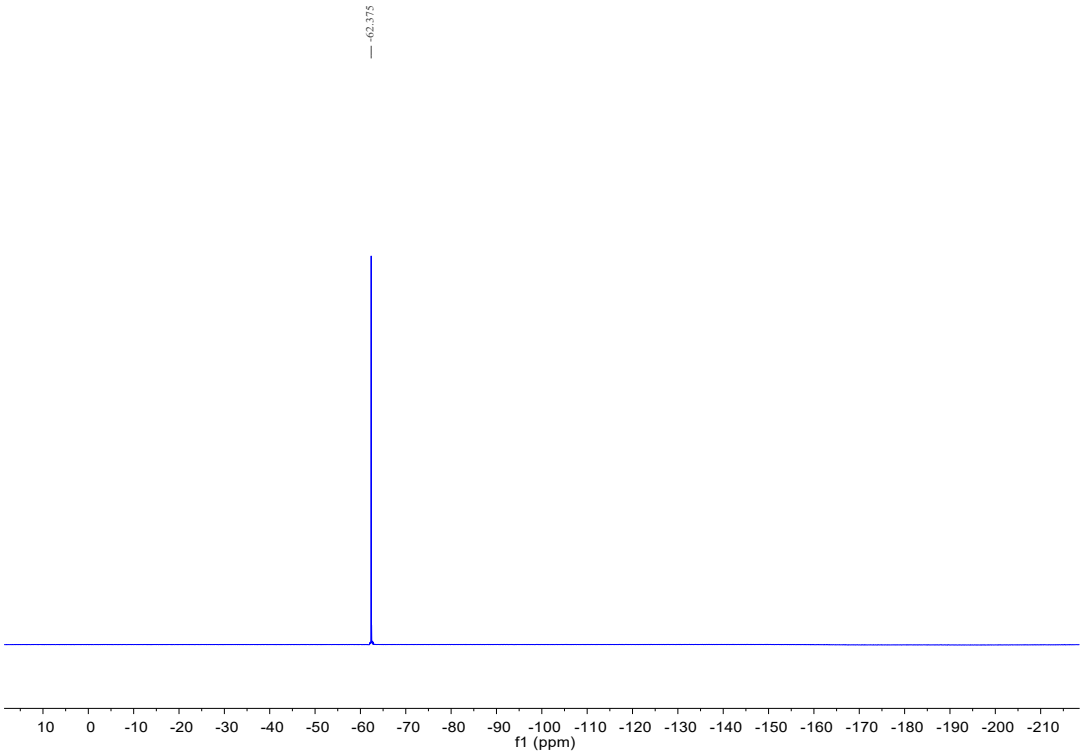
^{1}H NMR (400 MHz, $CDCl_3$)



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

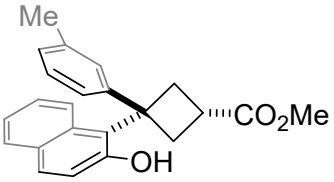


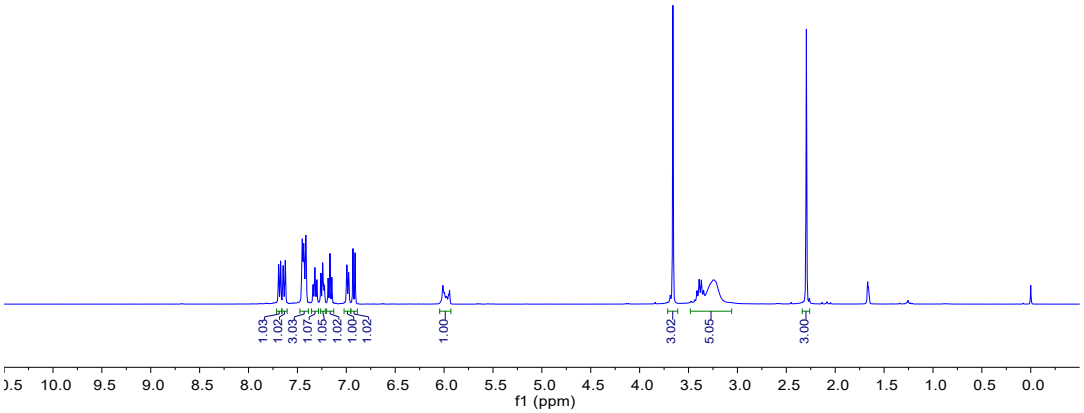
^{19}F NMR (376 MHz, $CDCl_3$)



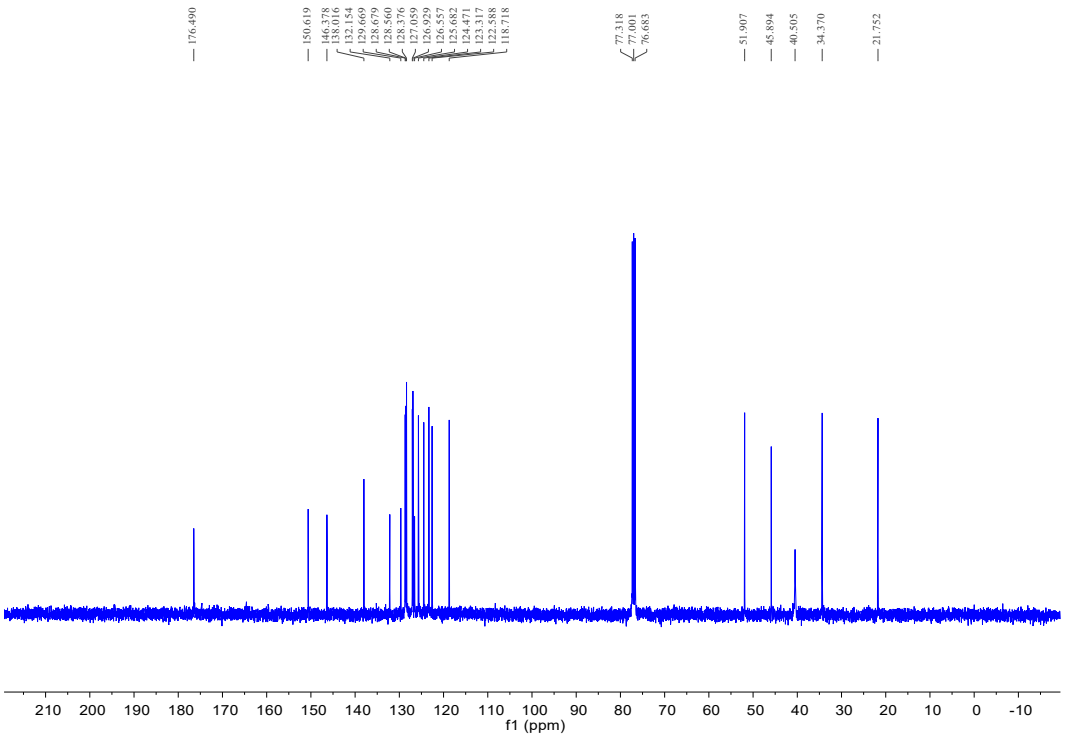
^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ma

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



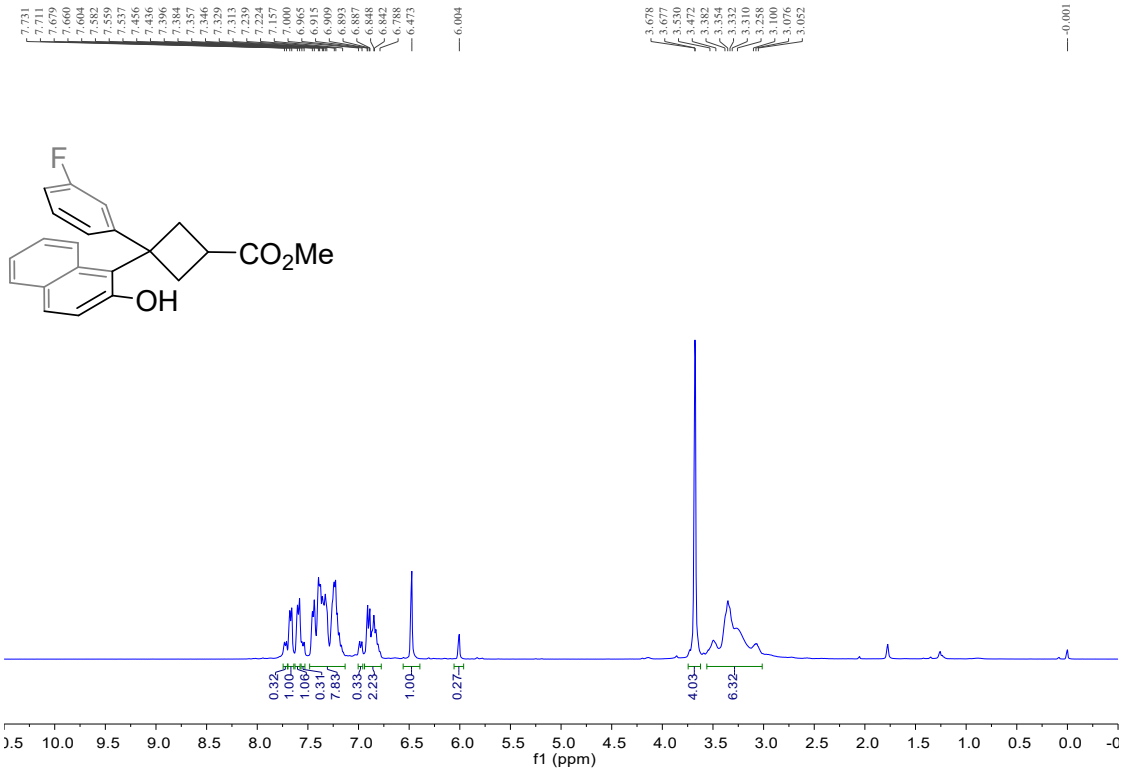


^{13}C NMR (100 MHz, $CDCl_3$)

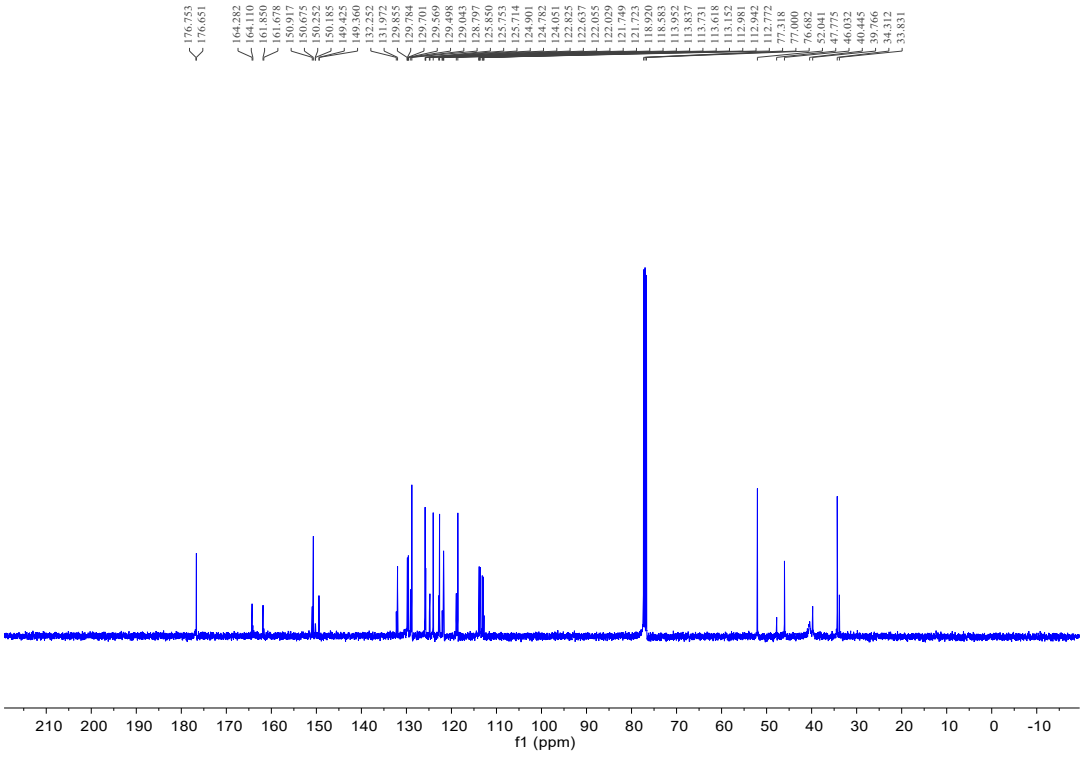


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound 3na

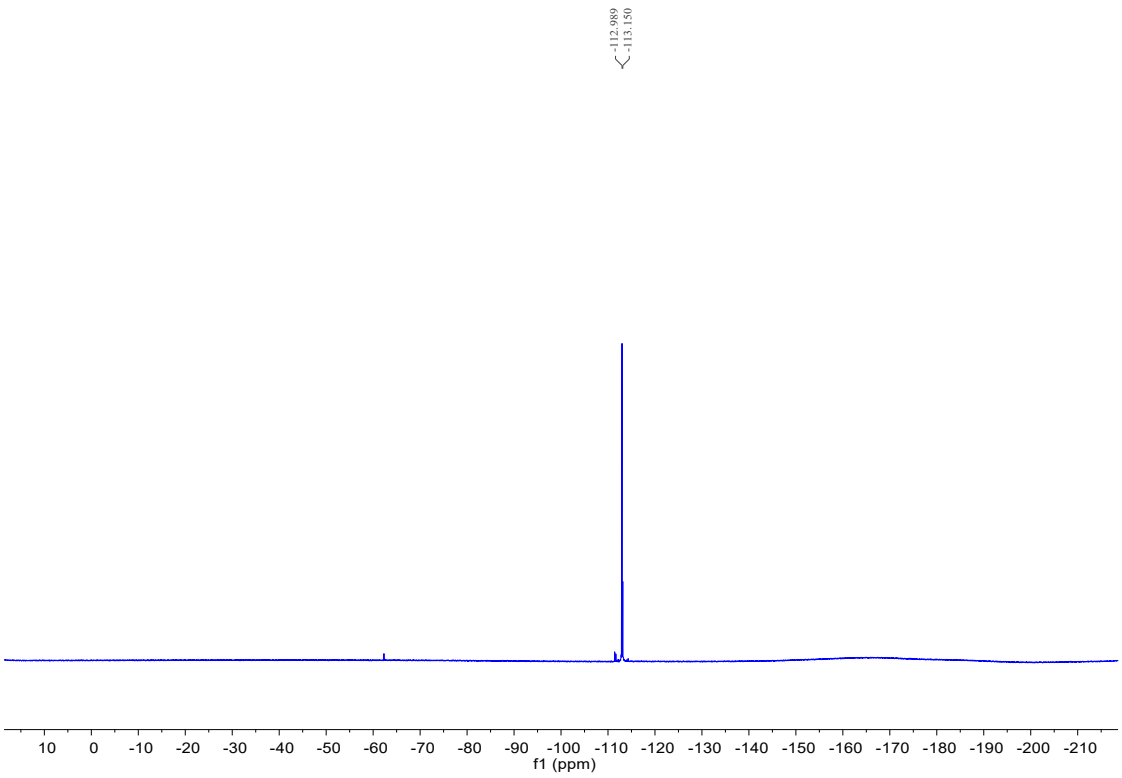
^{1}H NMR (400 MHz, $CDCl_3$)



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

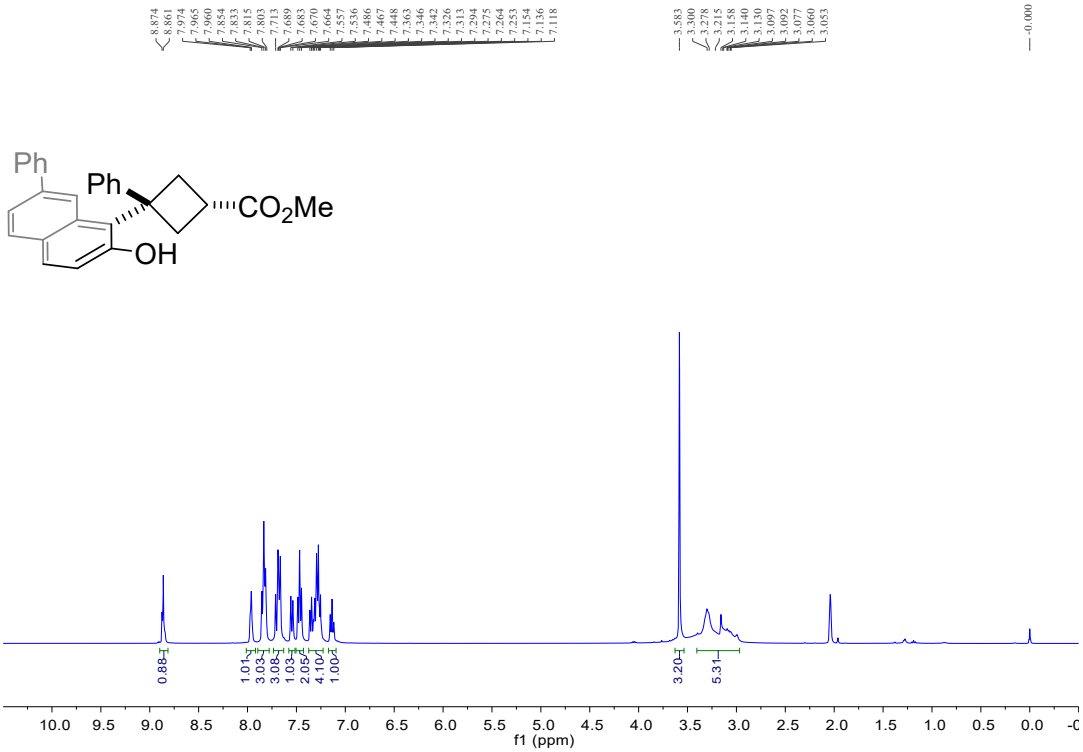


^{19}F NMR (376 MHz, $CDCl_3$)

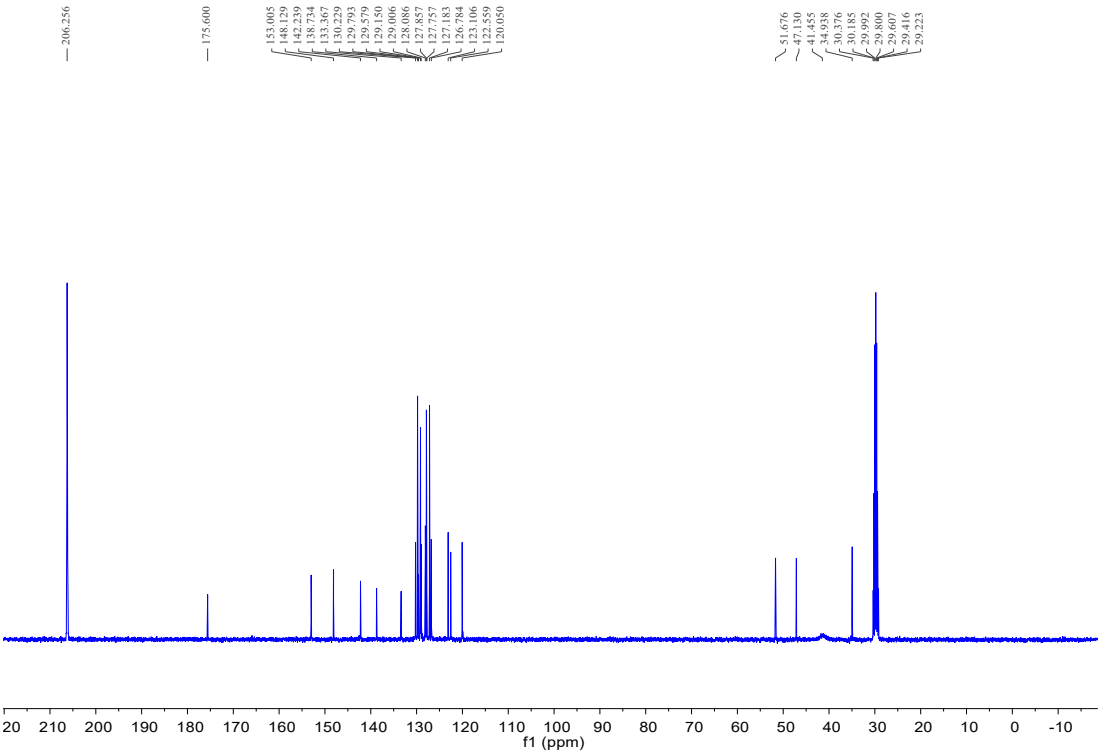


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ab

^{1}H NMR (400 MHz, Acetone-d_6)

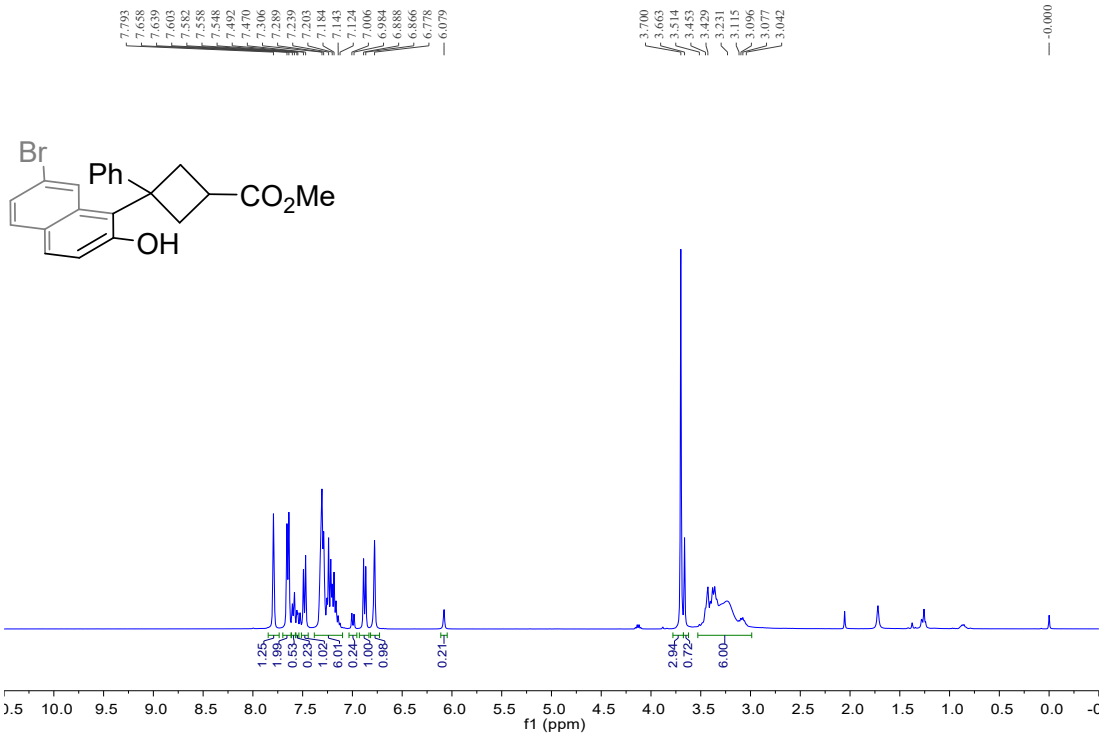


^{13}C NMR (100 MHz, Acetone-d_6)

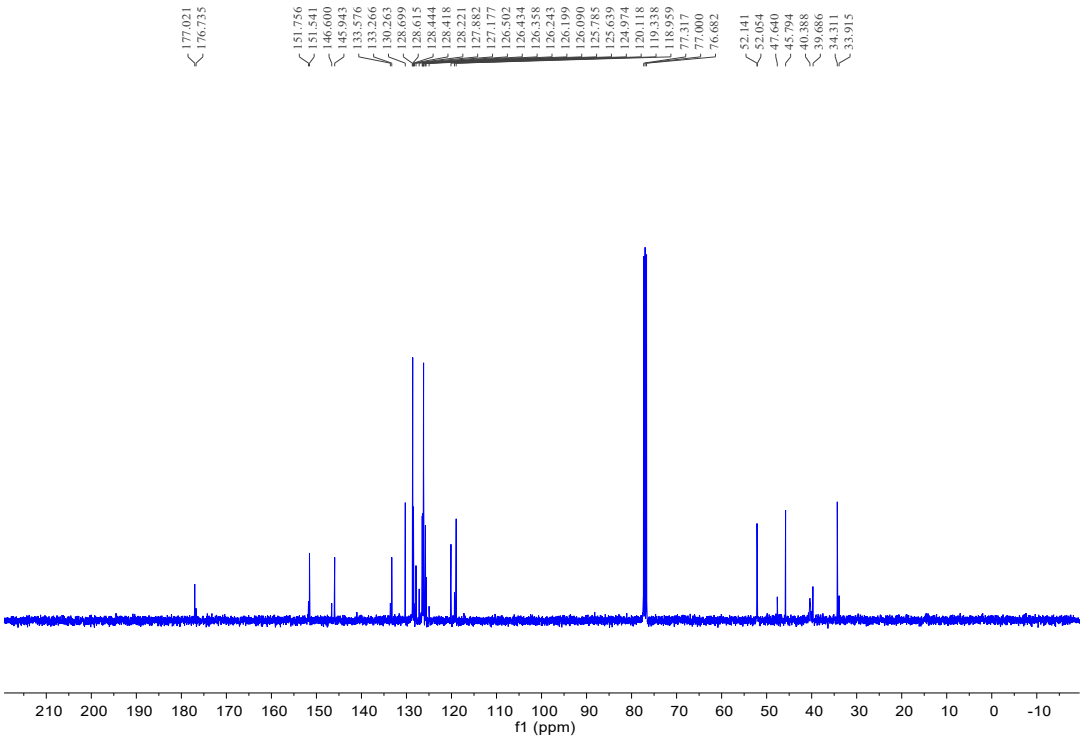


^{1}H and ^{13}C NMR Spectra for Compound 3ac

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

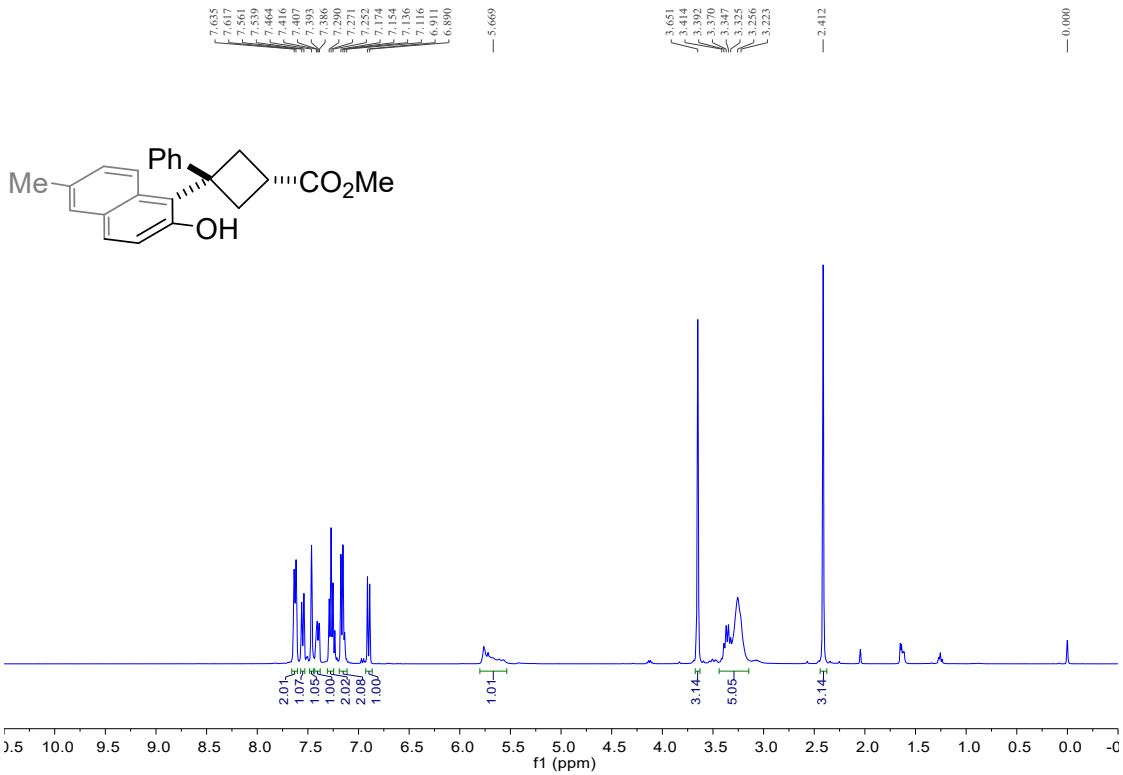


^{13}C NMR (100 MHz, $CDCl_3$)

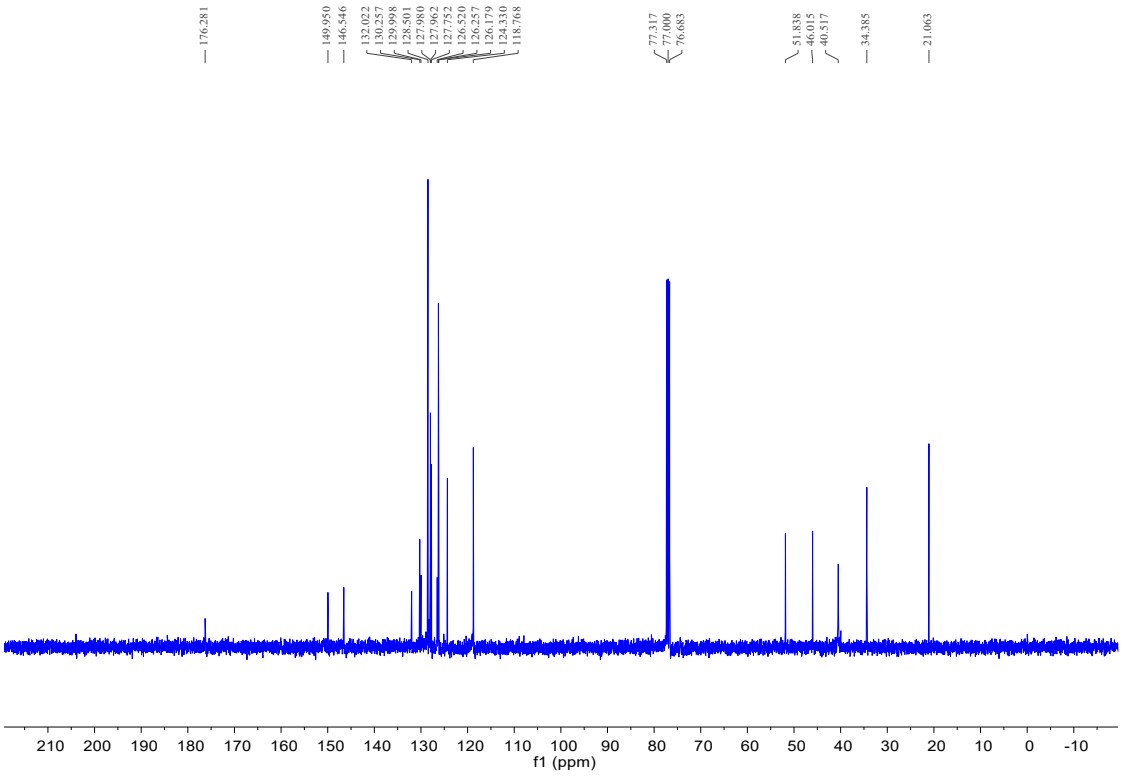


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ad

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

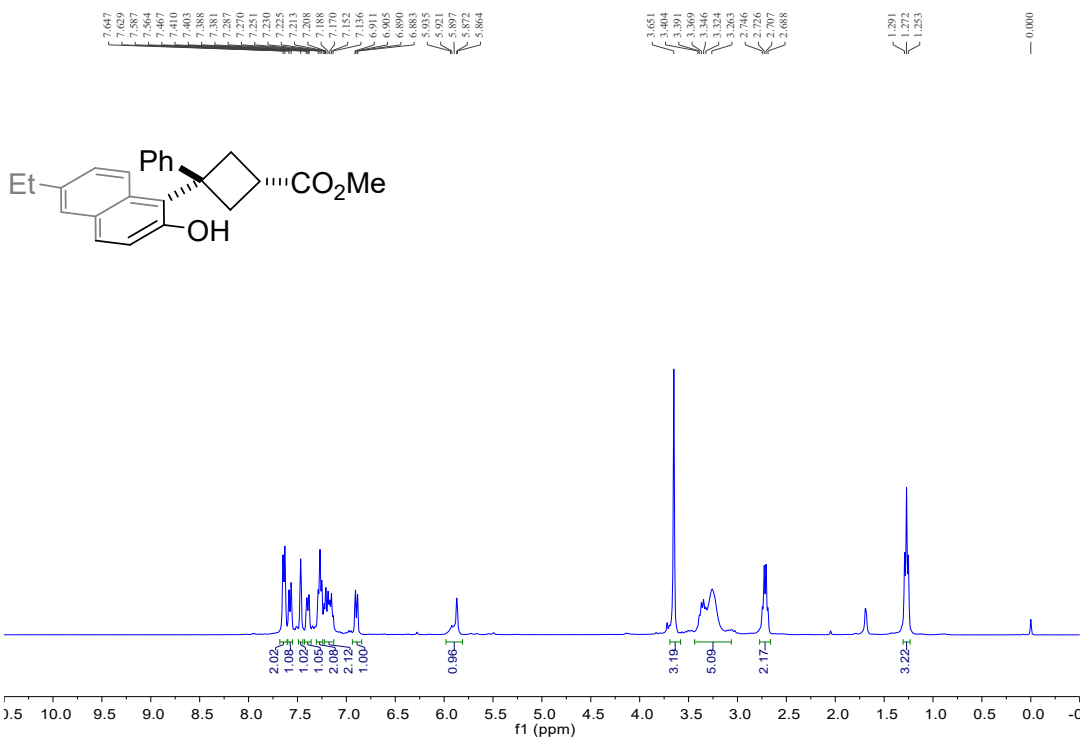


^{13}C NMR (100 MHz, $CDCl_3$)

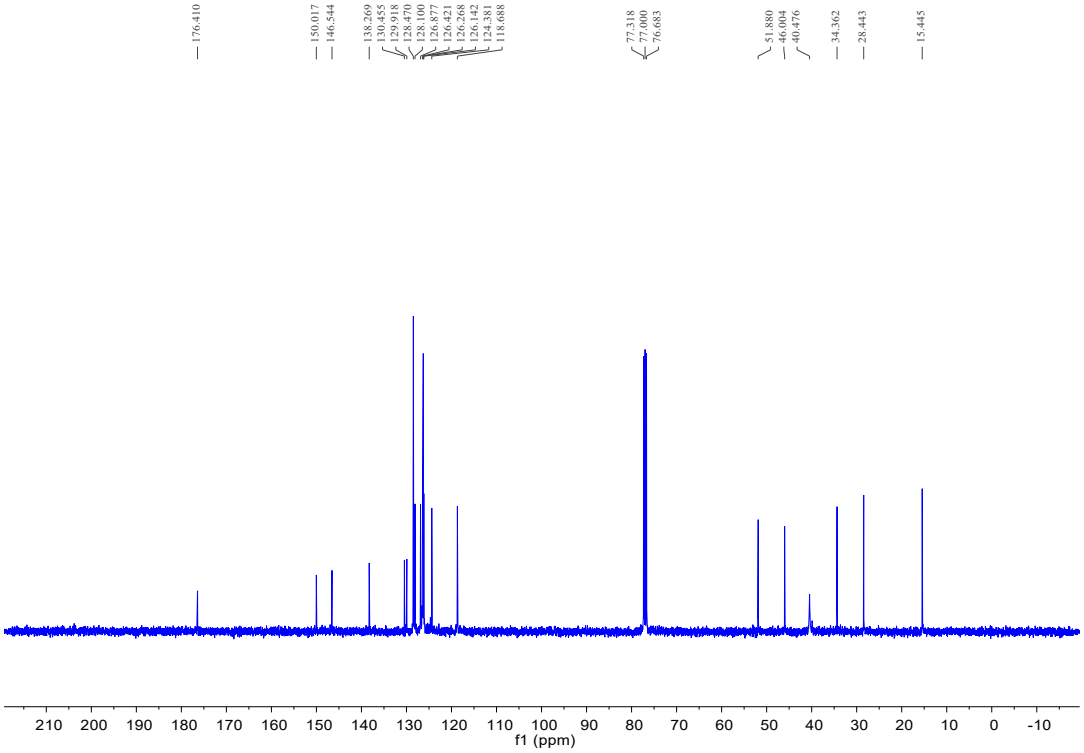


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ae

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

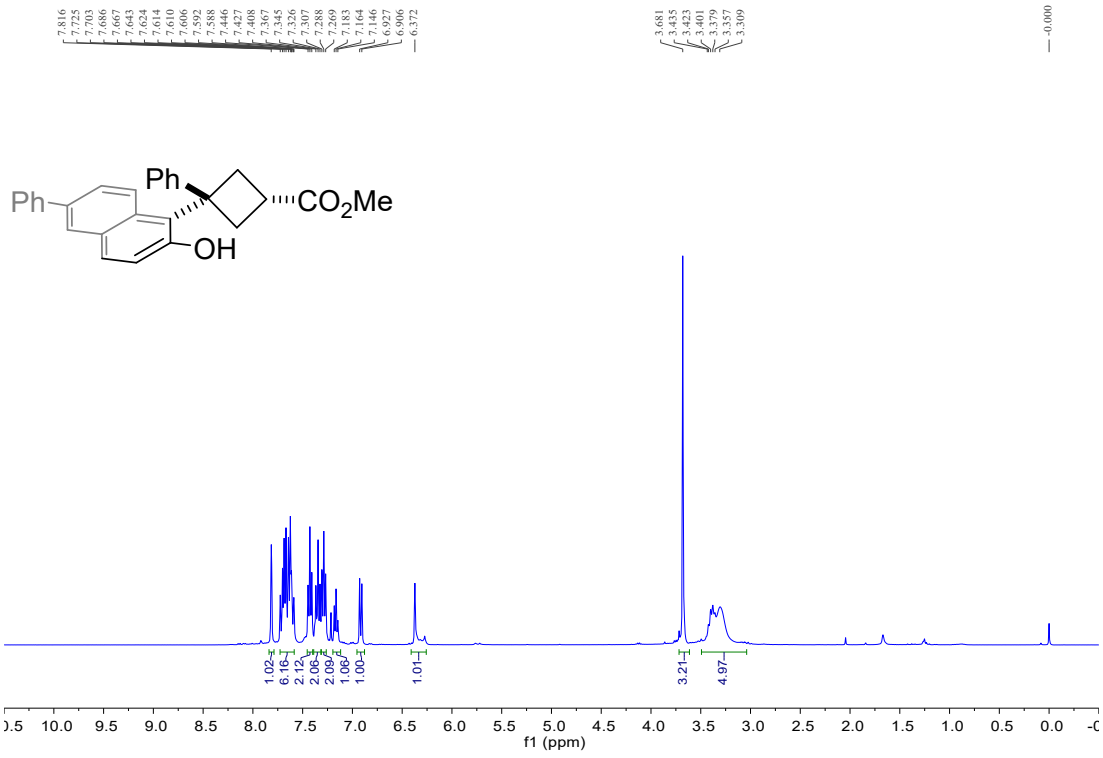


^{13}C NMR (100 MHz, $CDCl_3$)

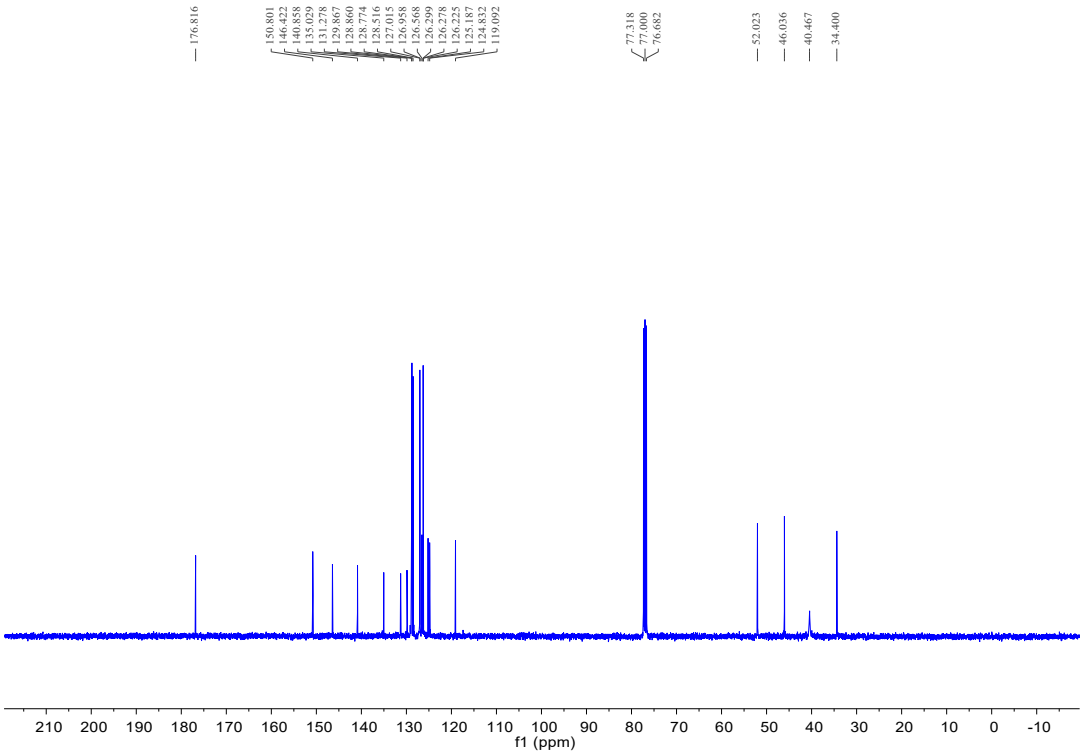


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3af

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

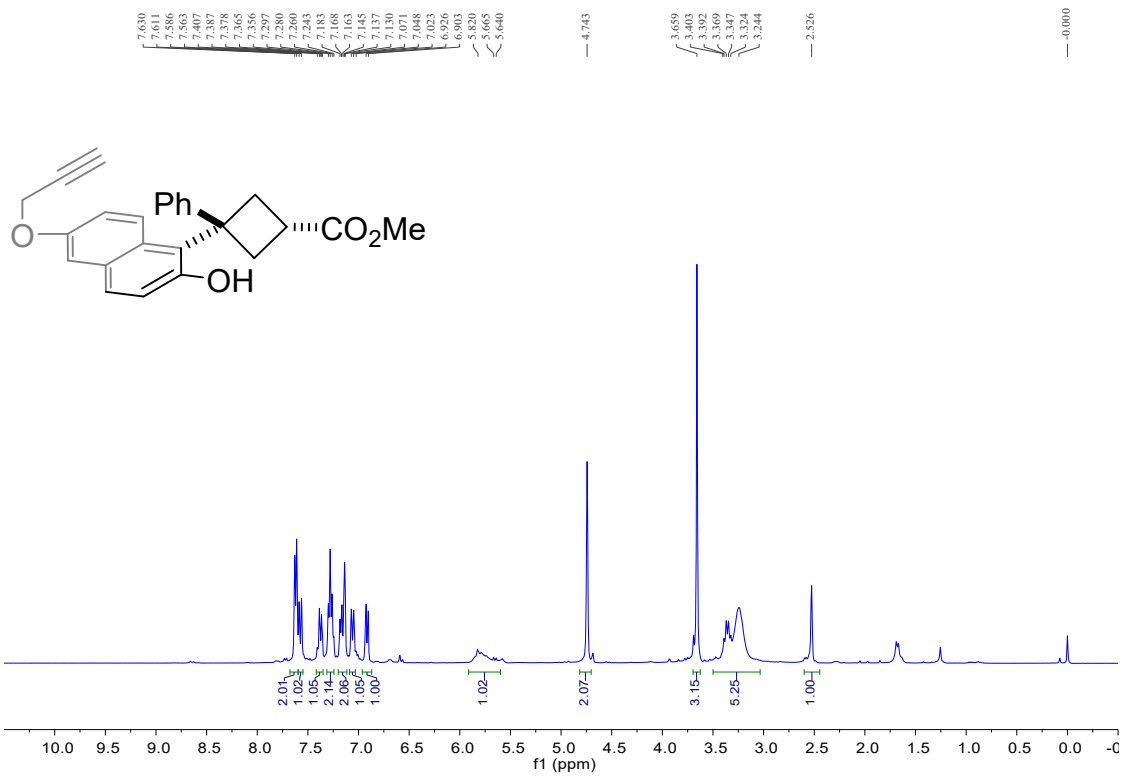


^{13}C NMR (100 MHz, $CDCl_3$)

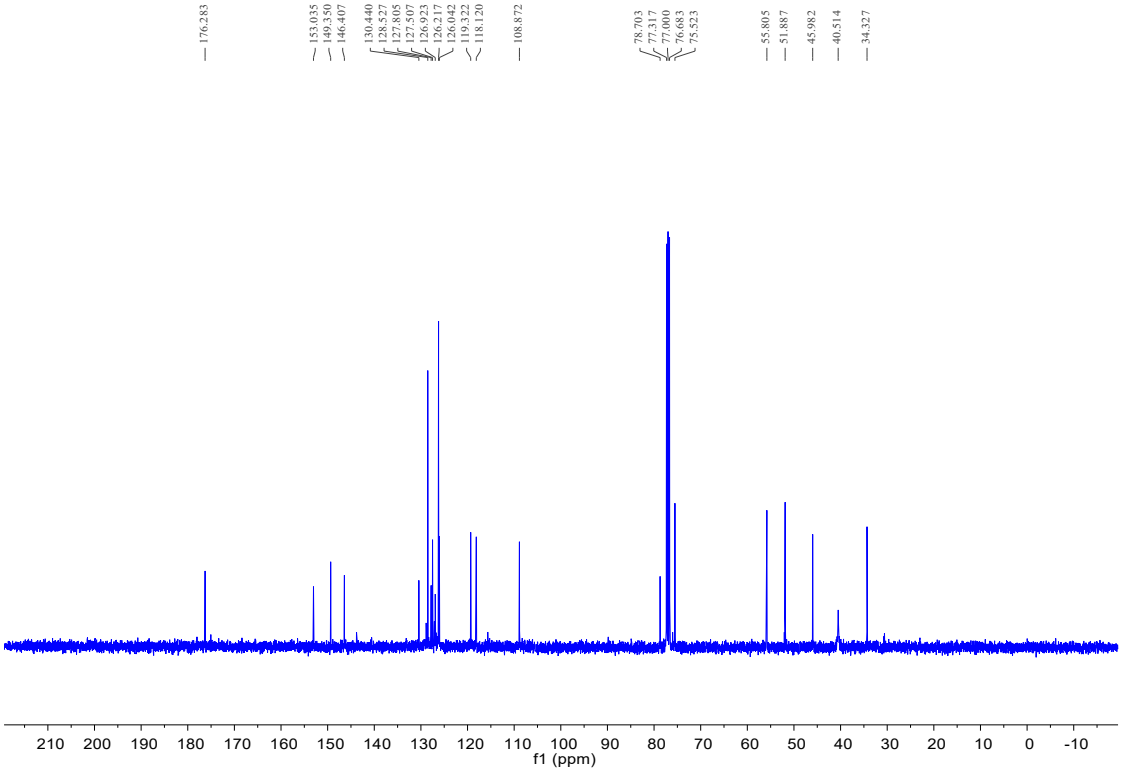


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ag

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

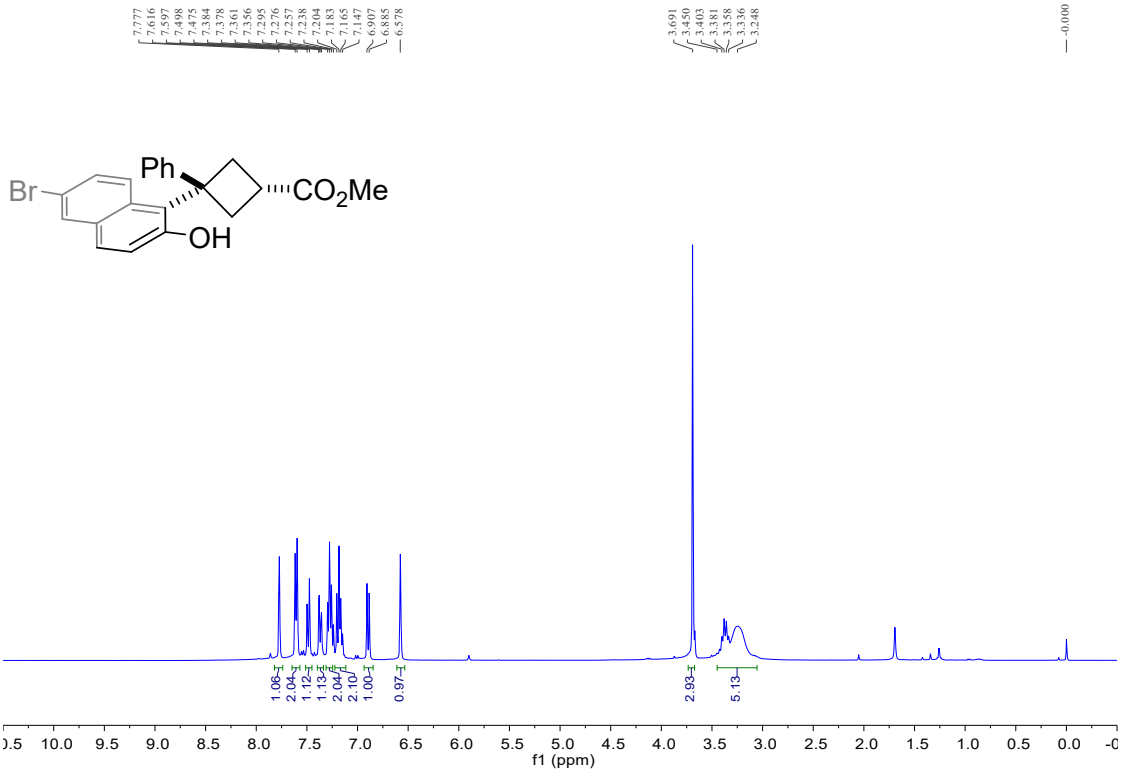


^{13}C NMR (100 MHz, $CDCl_3$)

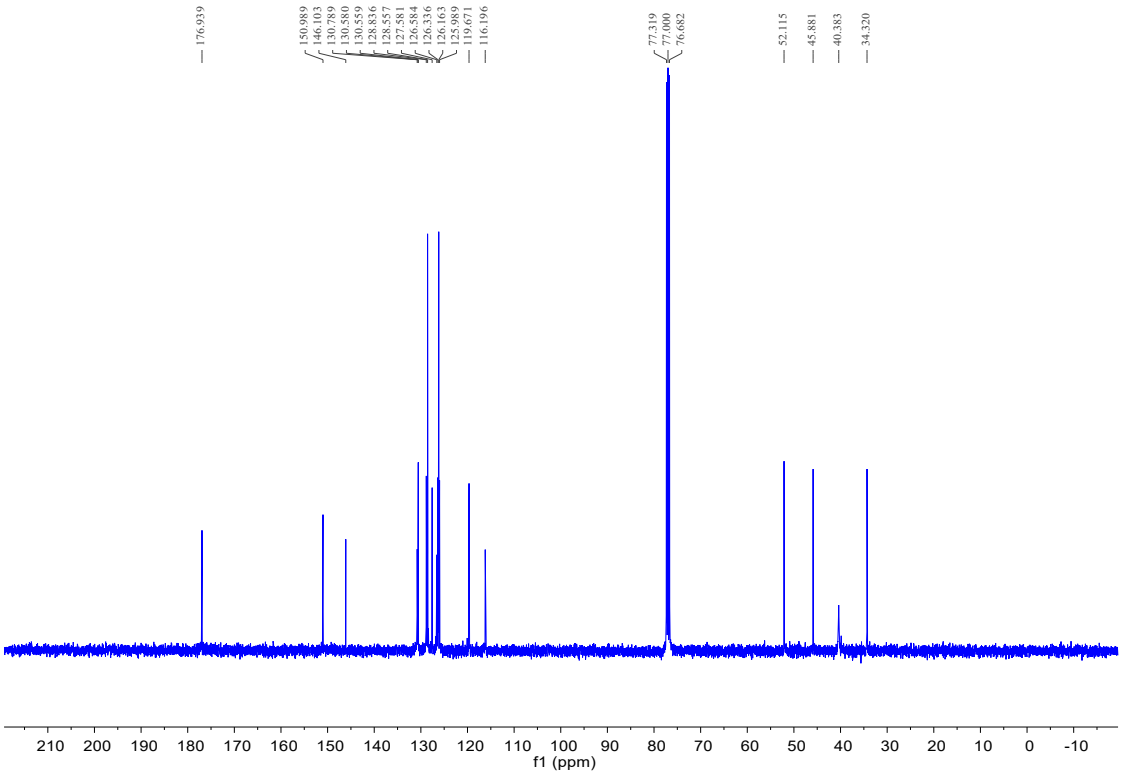


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ah

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

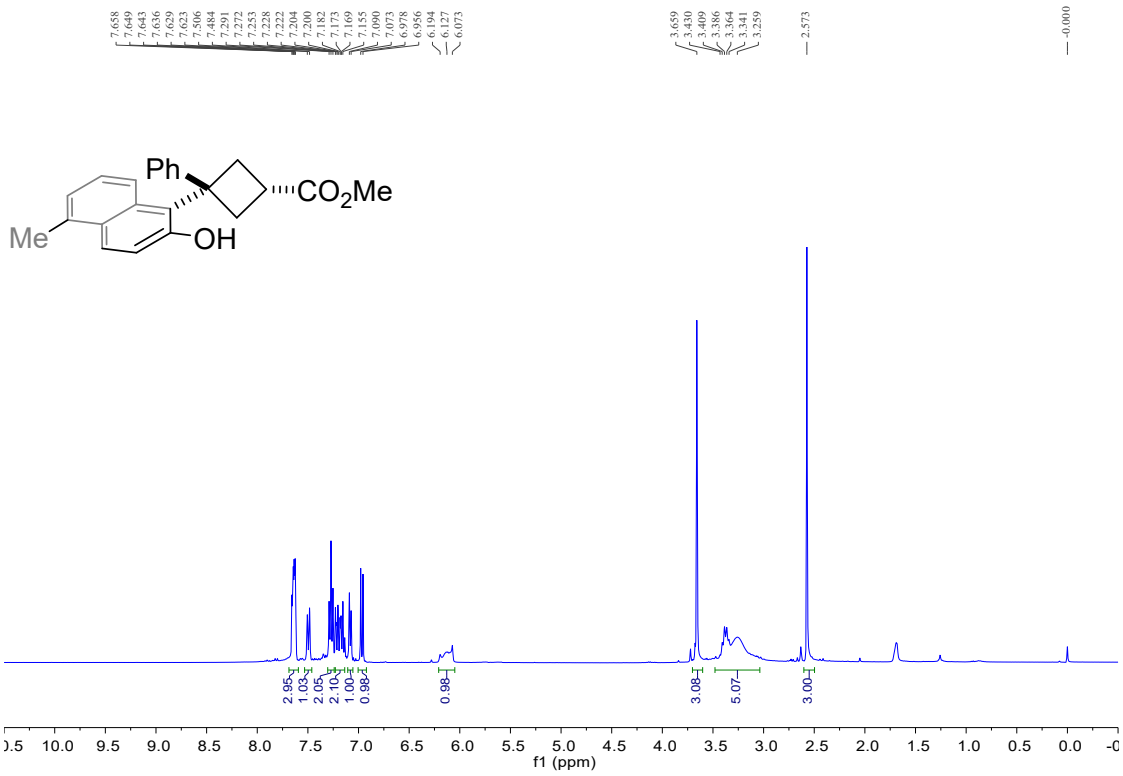


^{13}C NMR (100 MHz, $CDCl_3$)

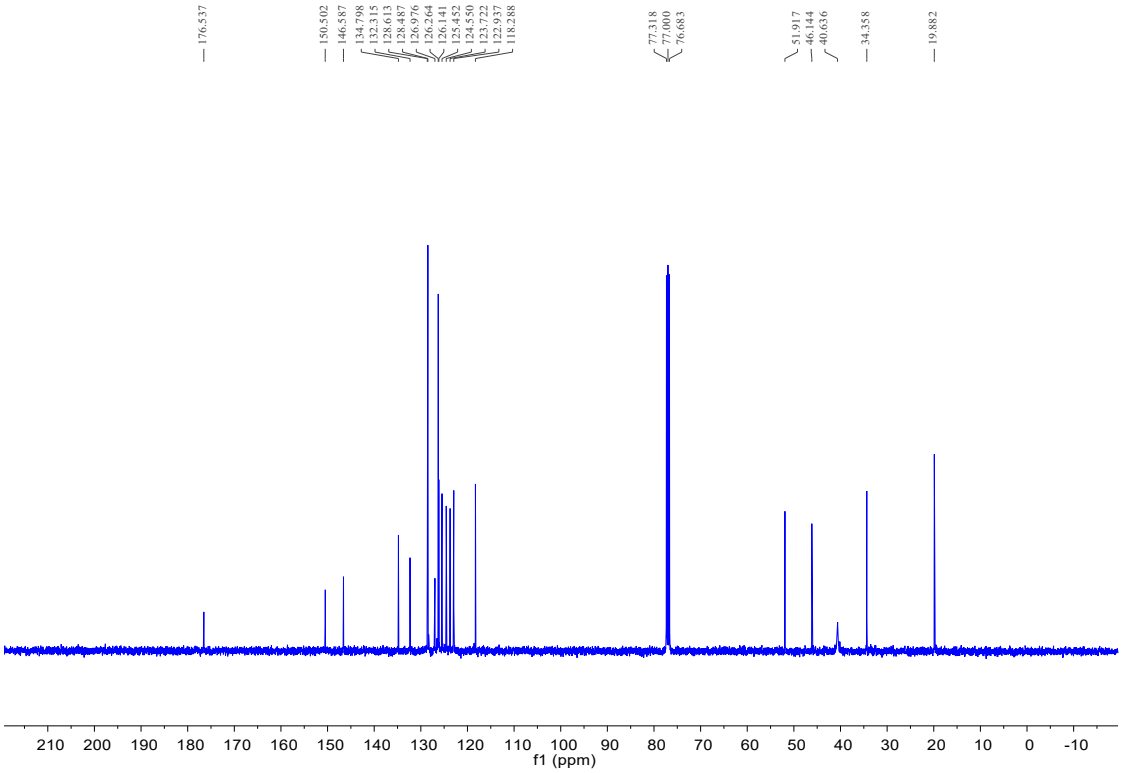


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ai

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

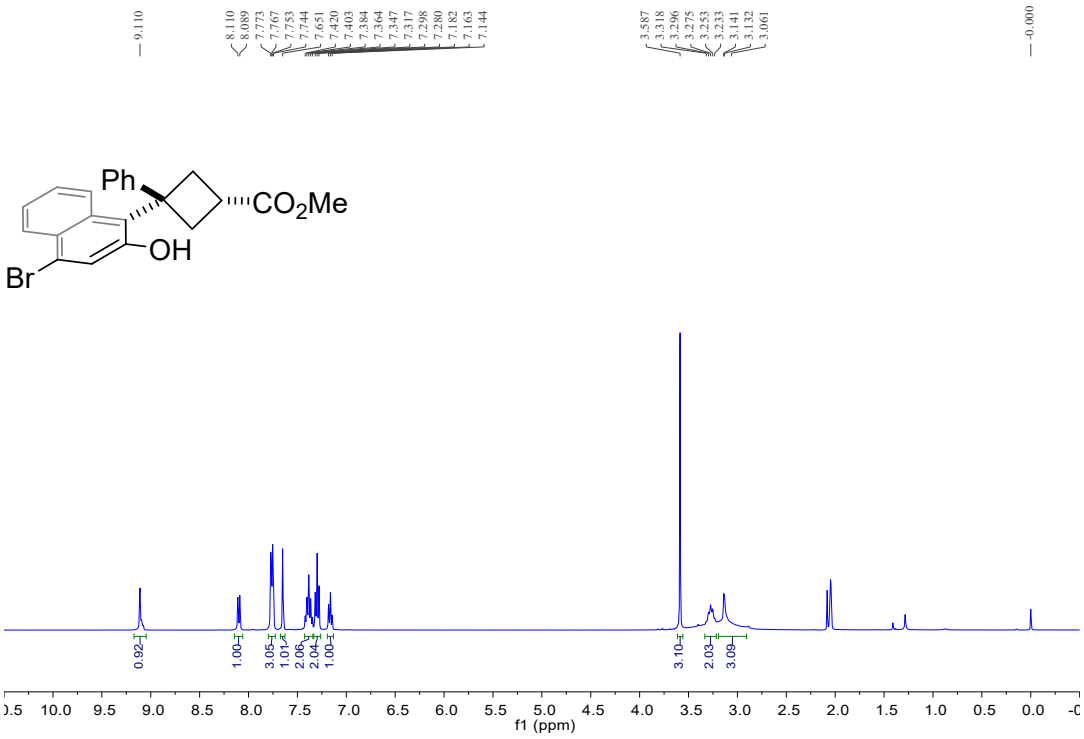


^{13}C NMR (100 MHz, $CDCl_3$)

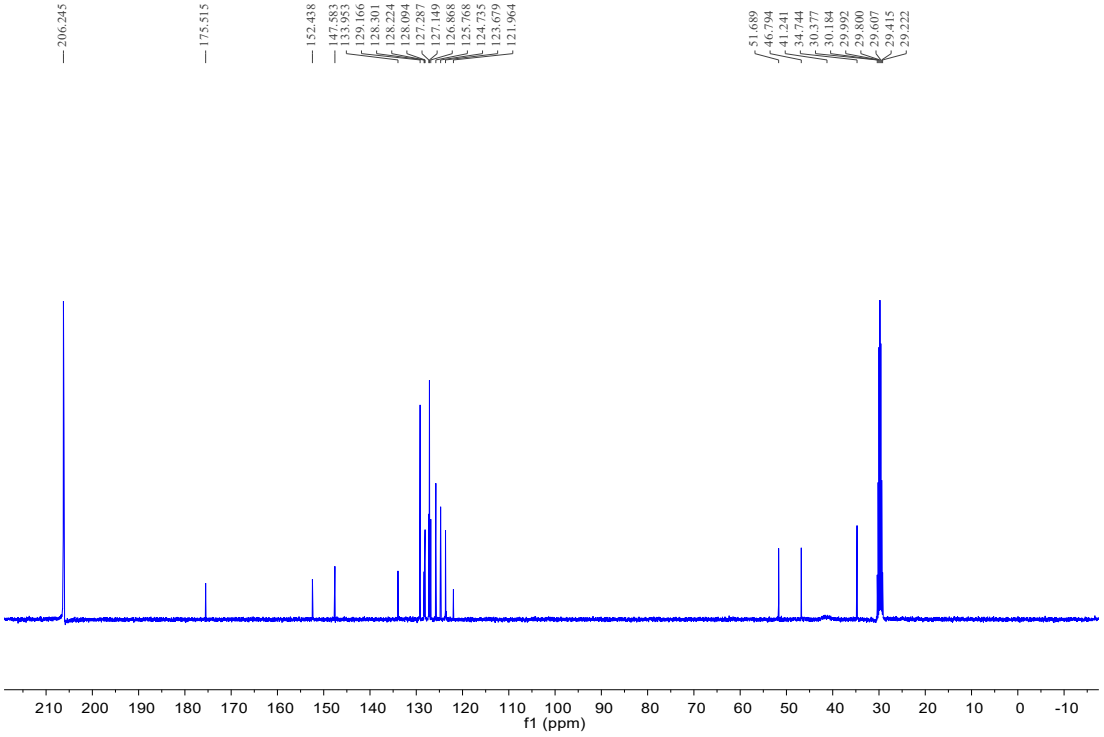


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3aj

^{1}H NMR (400 MHz, Acetone-d_6)

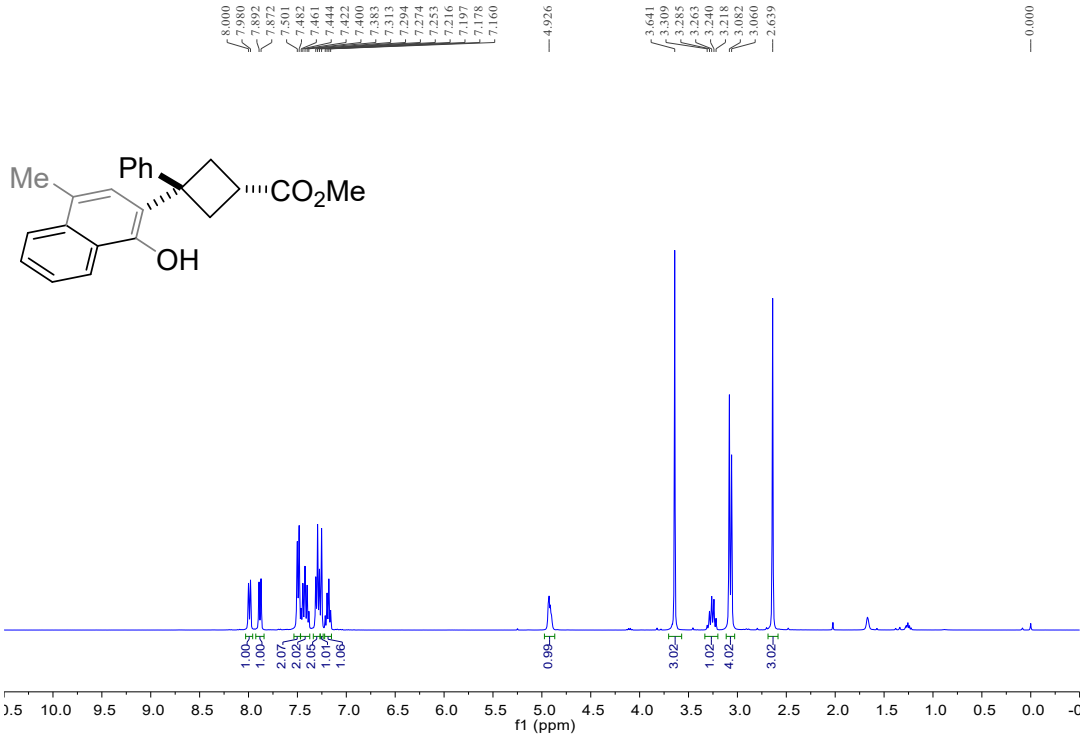


^{13}C NMR (100 MHz, Acetone-d_6)

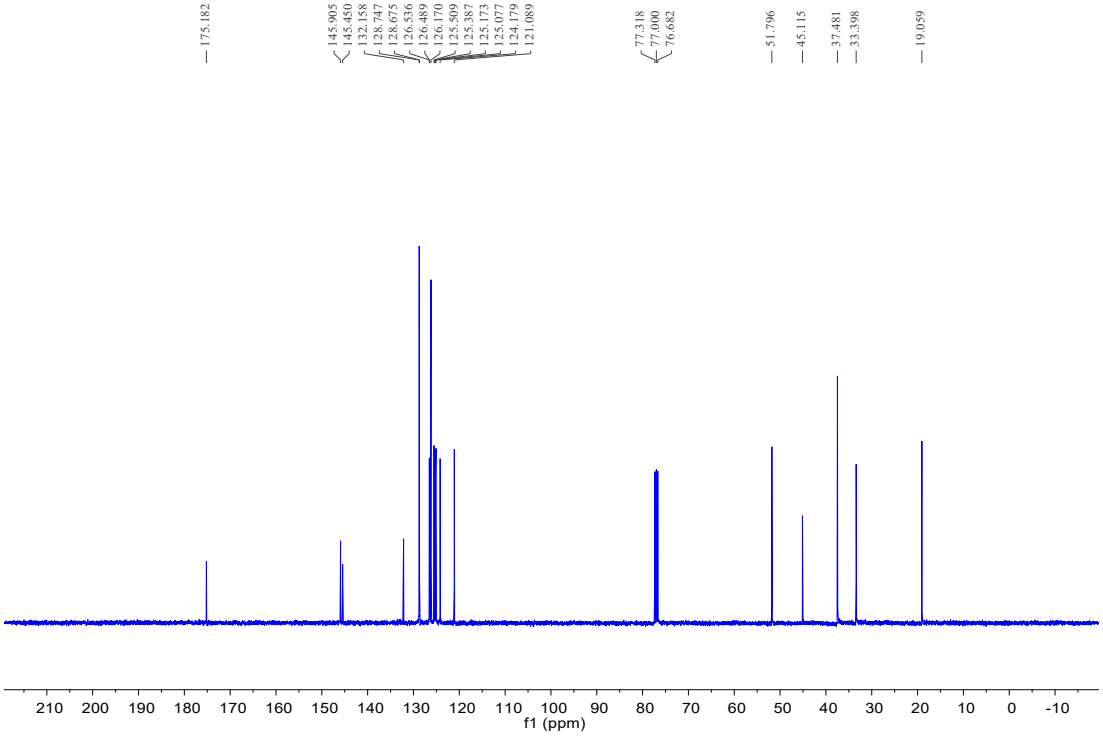


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ak

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

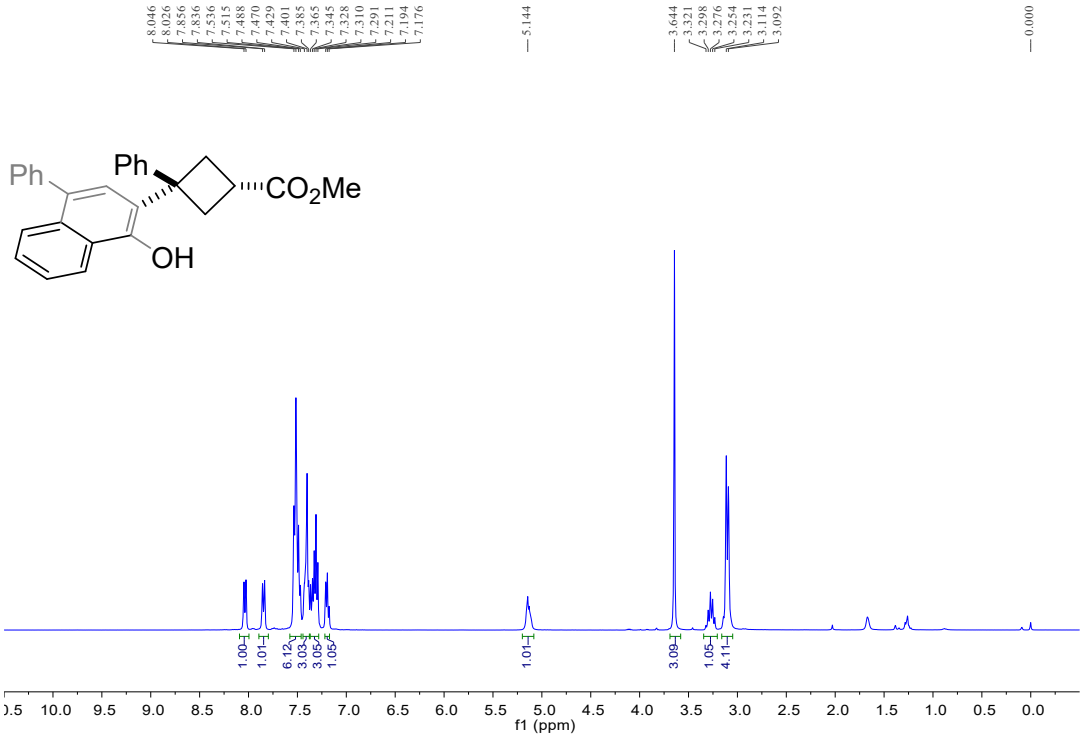


^{13}C NMR (100 MHz, $CDCl_3$)

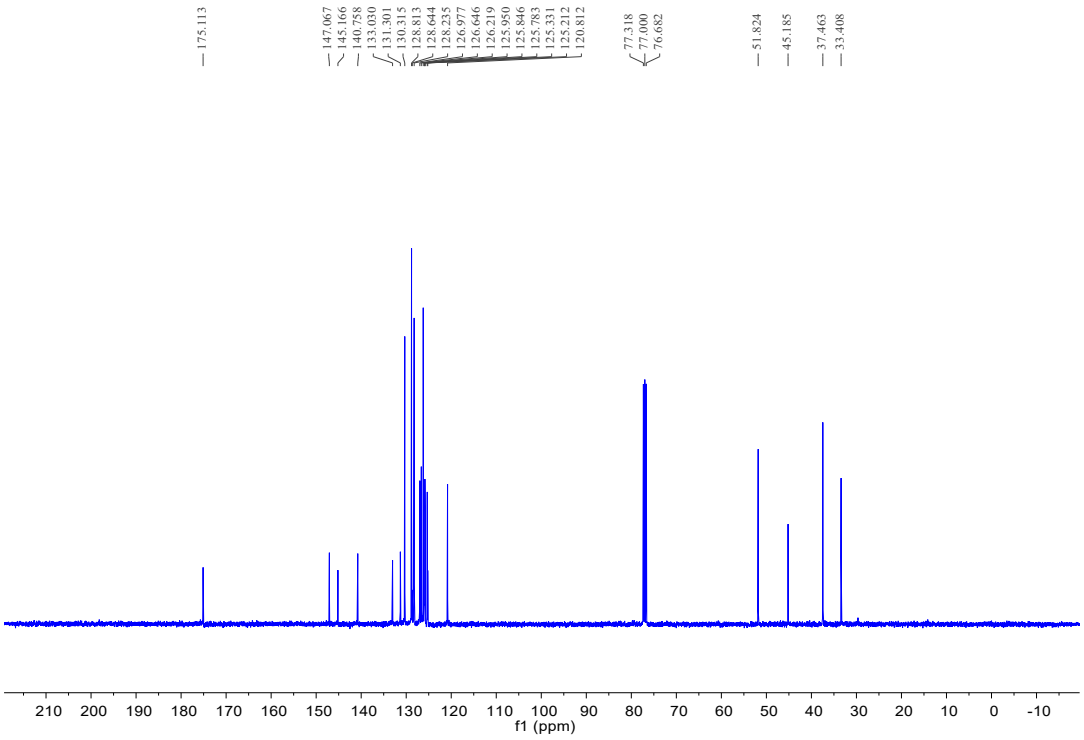


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3al

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

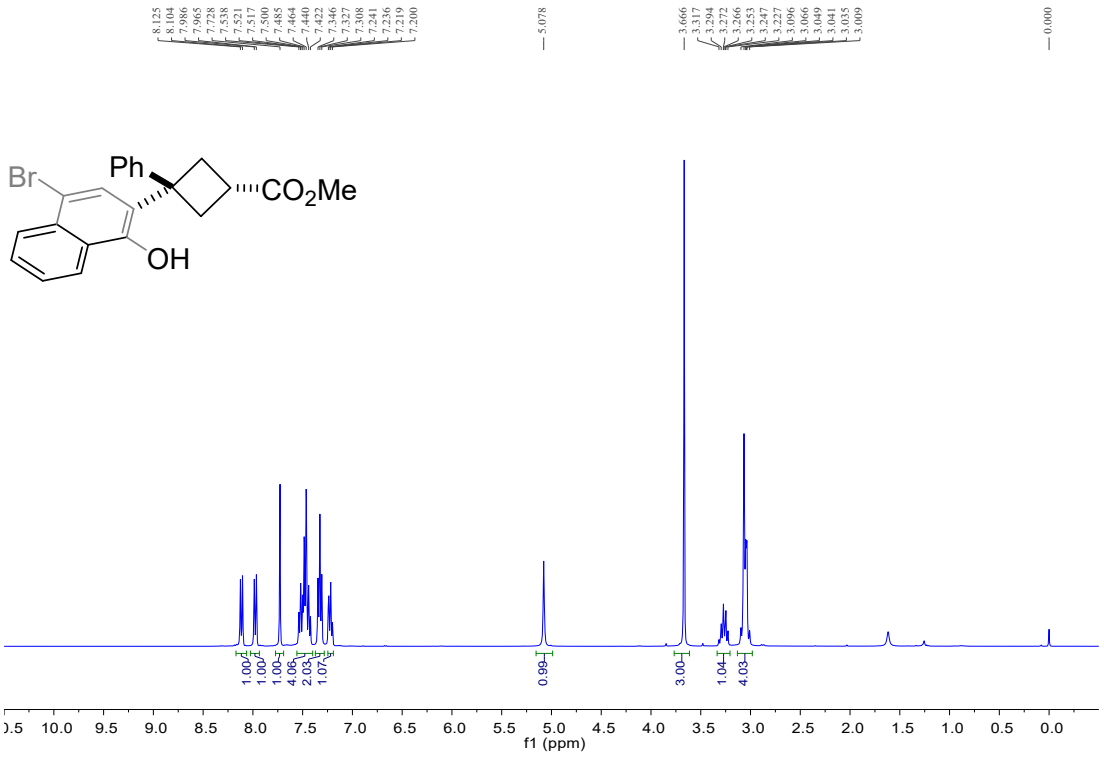


^{13}C NMR (100 MHz, $CDCl_3$)

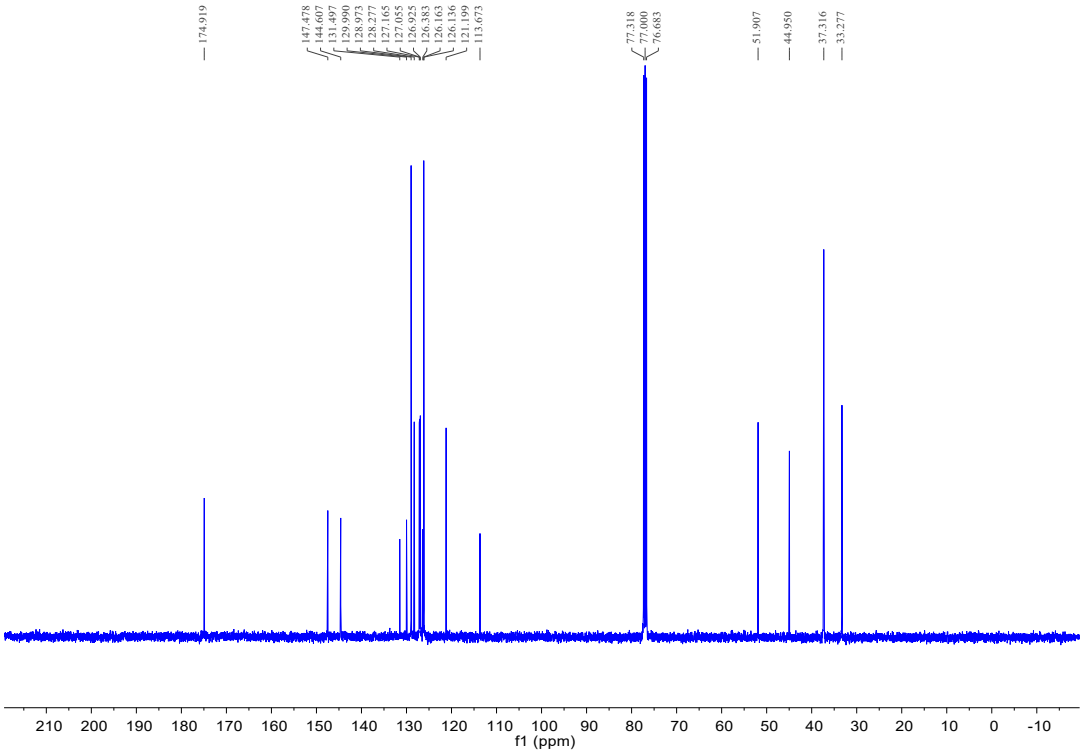


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3am

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

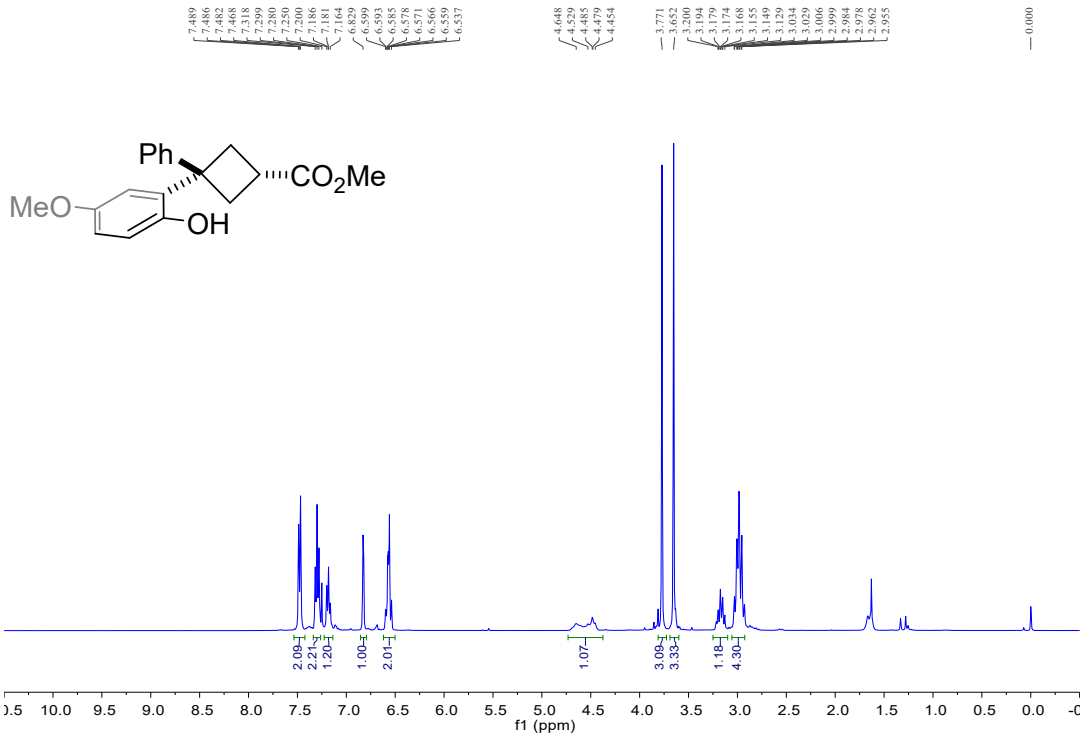


^{13}C NMR (100 MHz, $CDCl_3$)

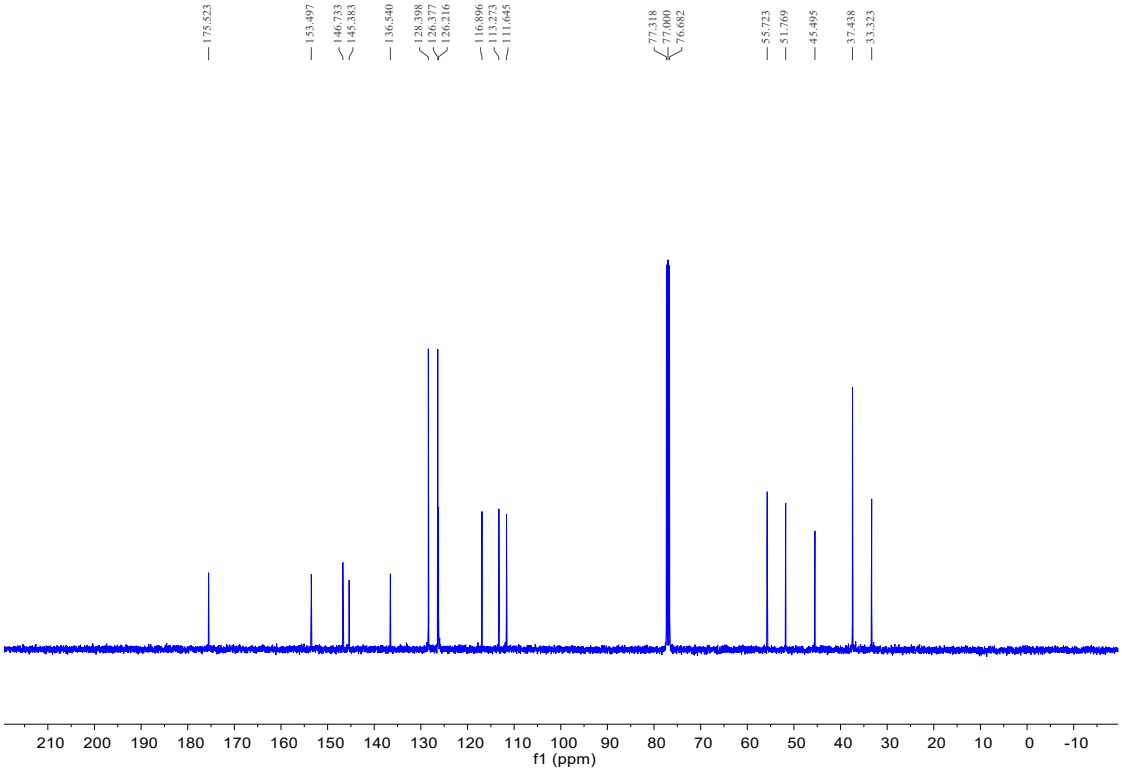


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3an

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

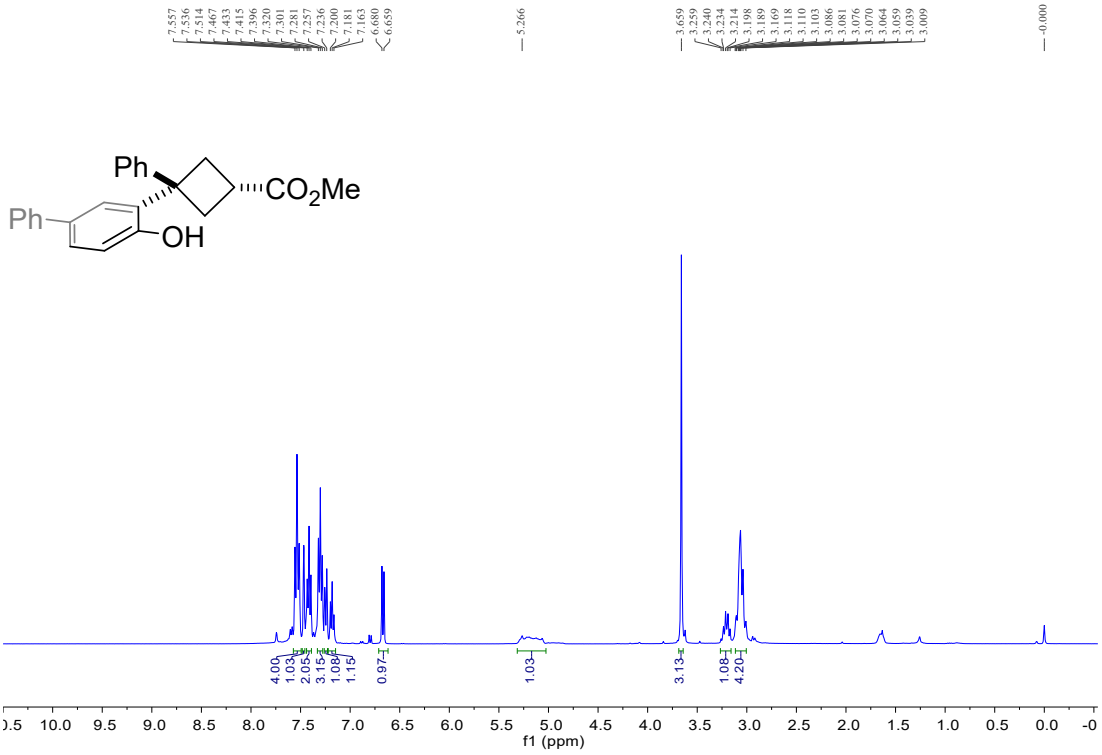


^{13}C NMR (100 MHz, $CDCl_3$)

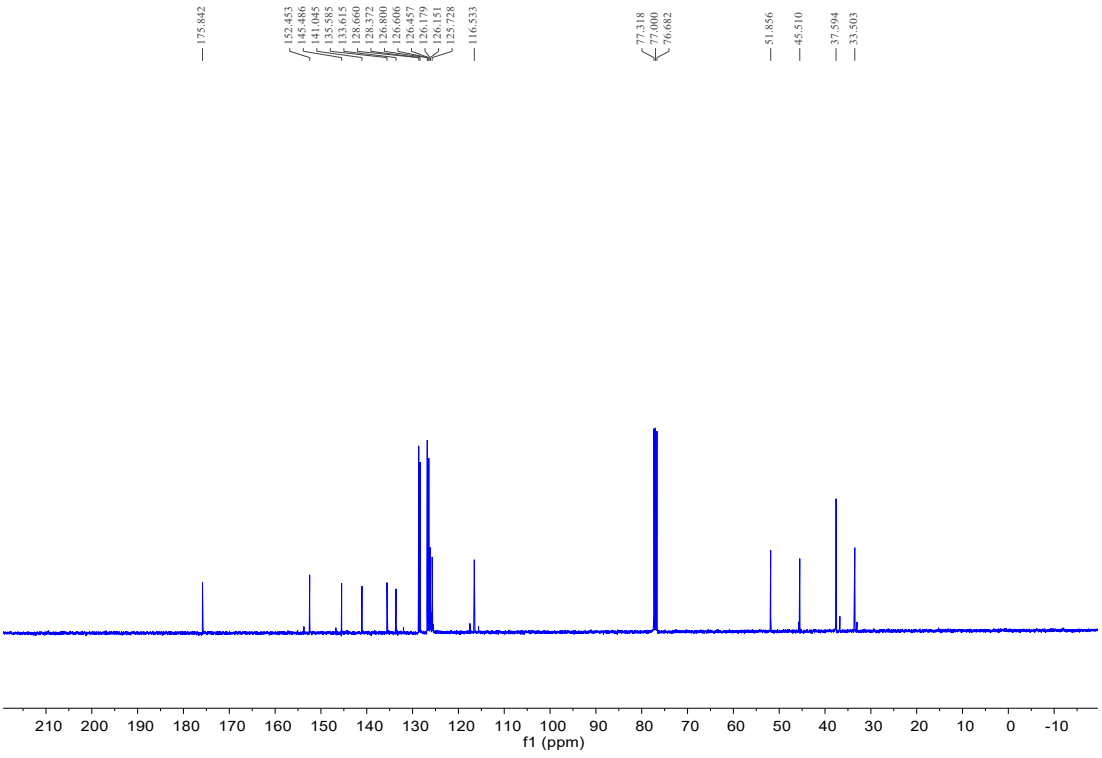


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ao

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

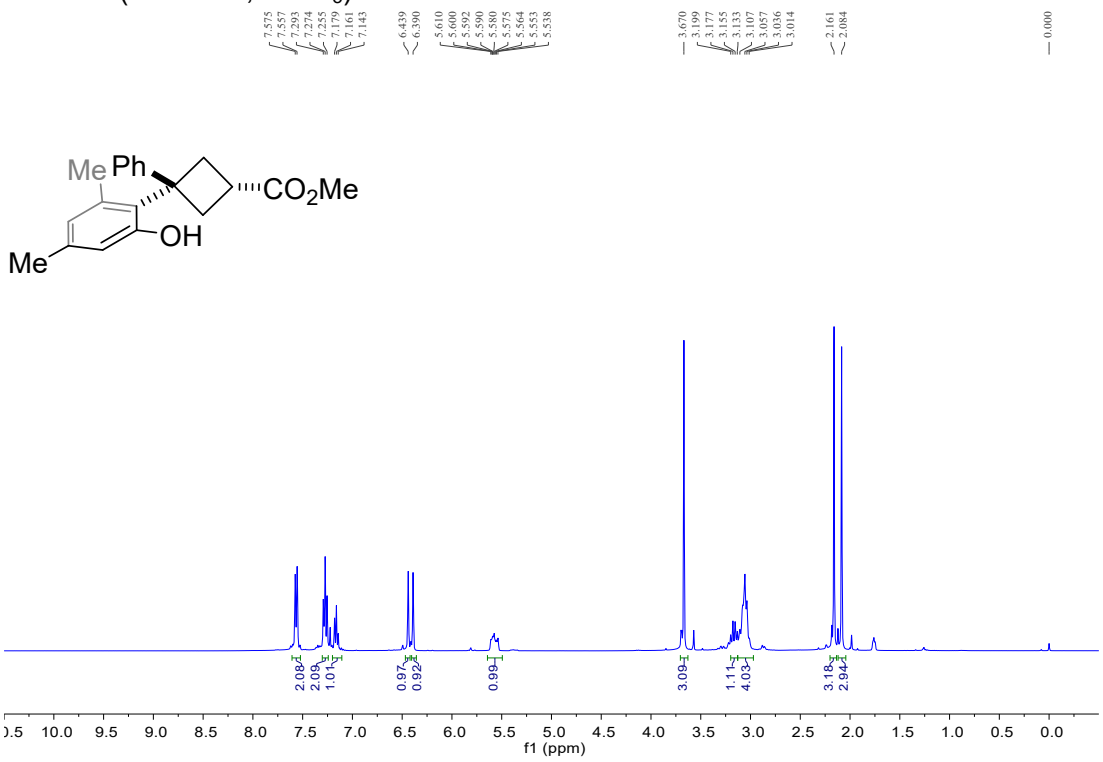


^{13}C NMR (100 MHz, $CDCl_3$)

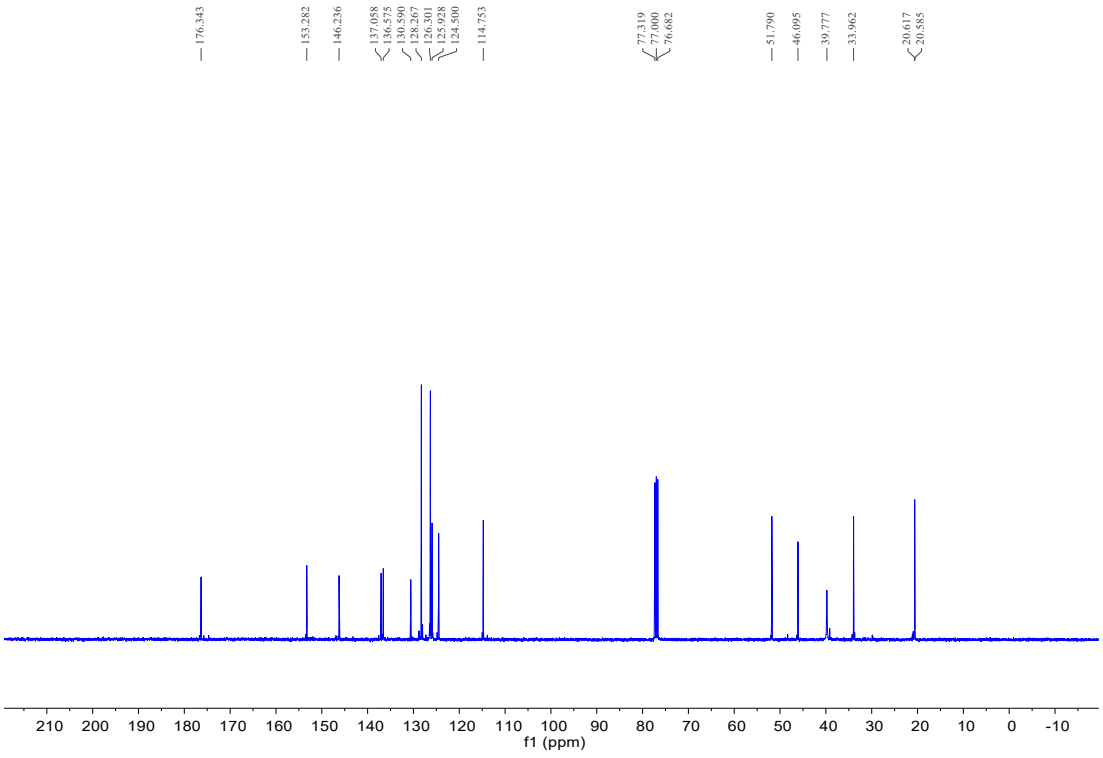


^{1}H and ^{13}C NMR Spectra for Compound *cis*-3ap

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

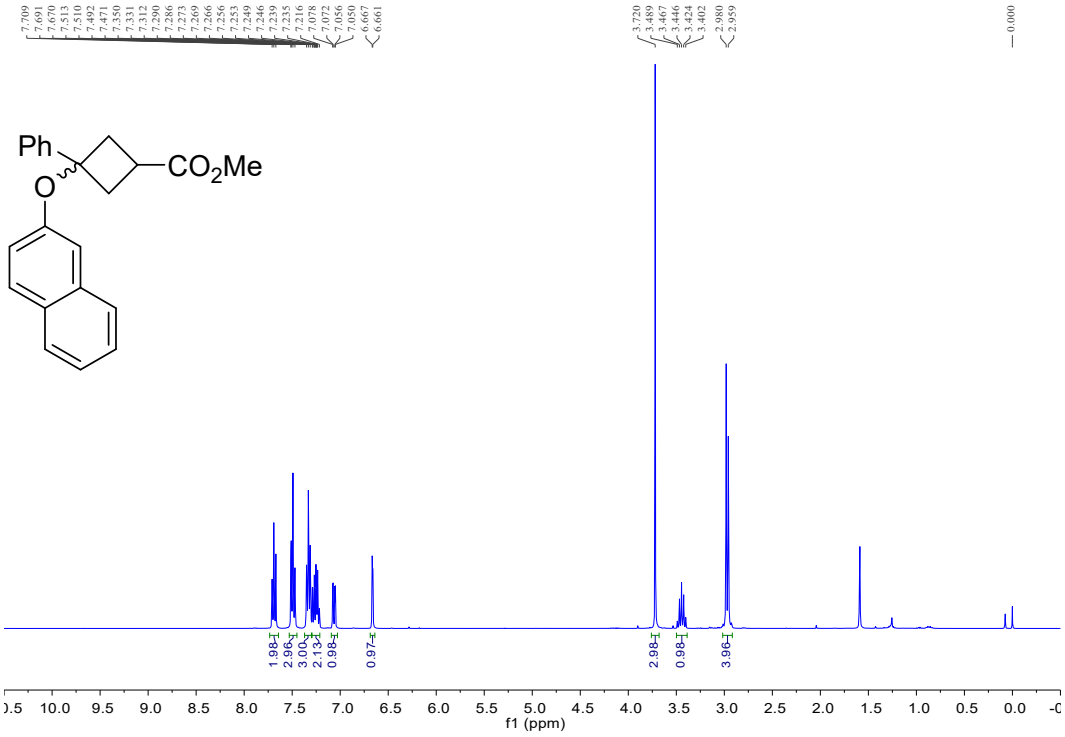


^{13}C NMR (100 MHz, $CDCl_3$)

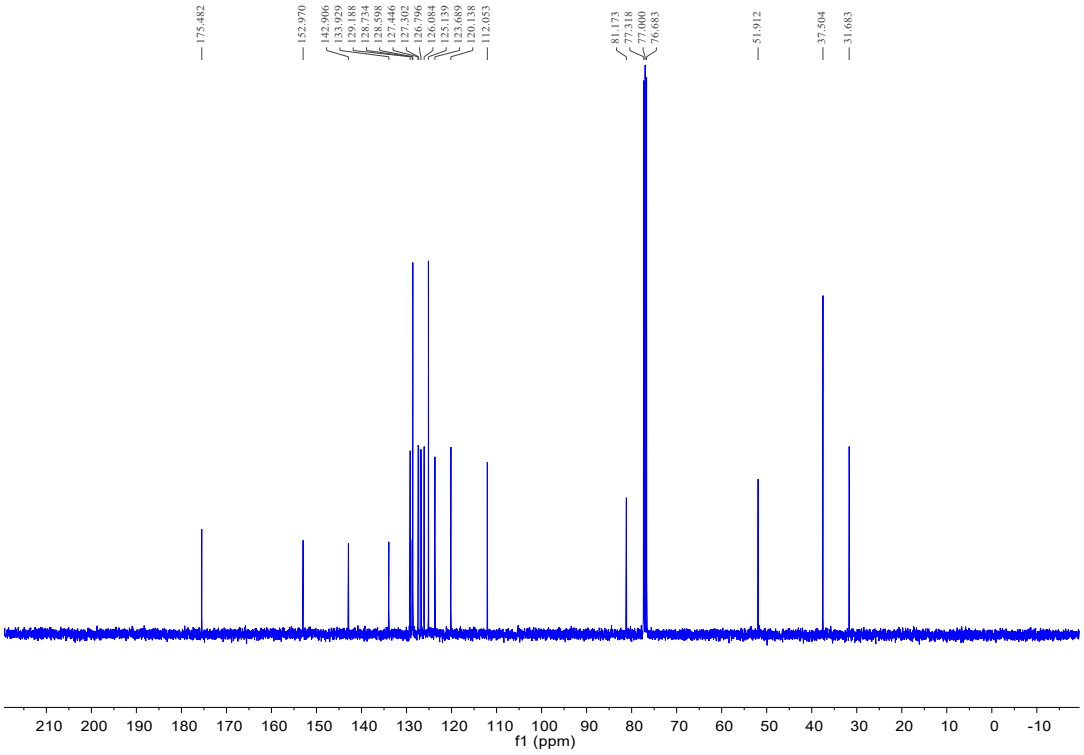


^{1}H and ^{13}C NMR Spectra for Compound 5aa

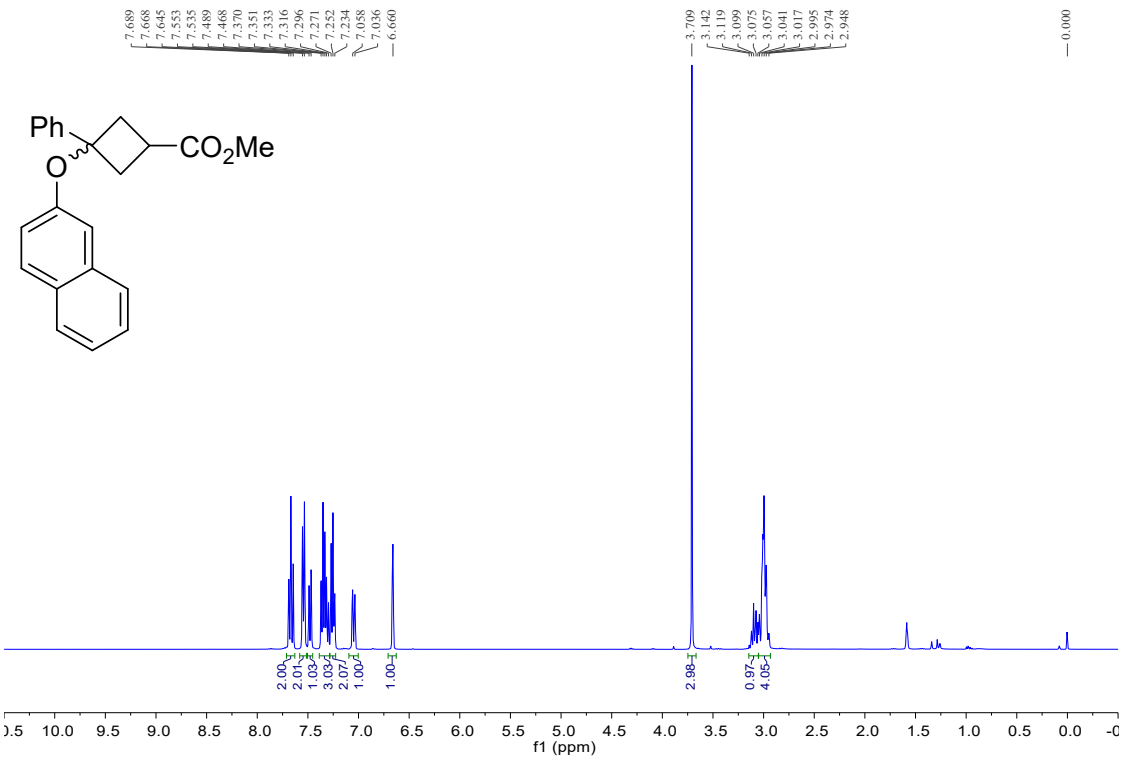
^{1}H NMR (400 MHz, $CDCl_3$) for **major isomer**:



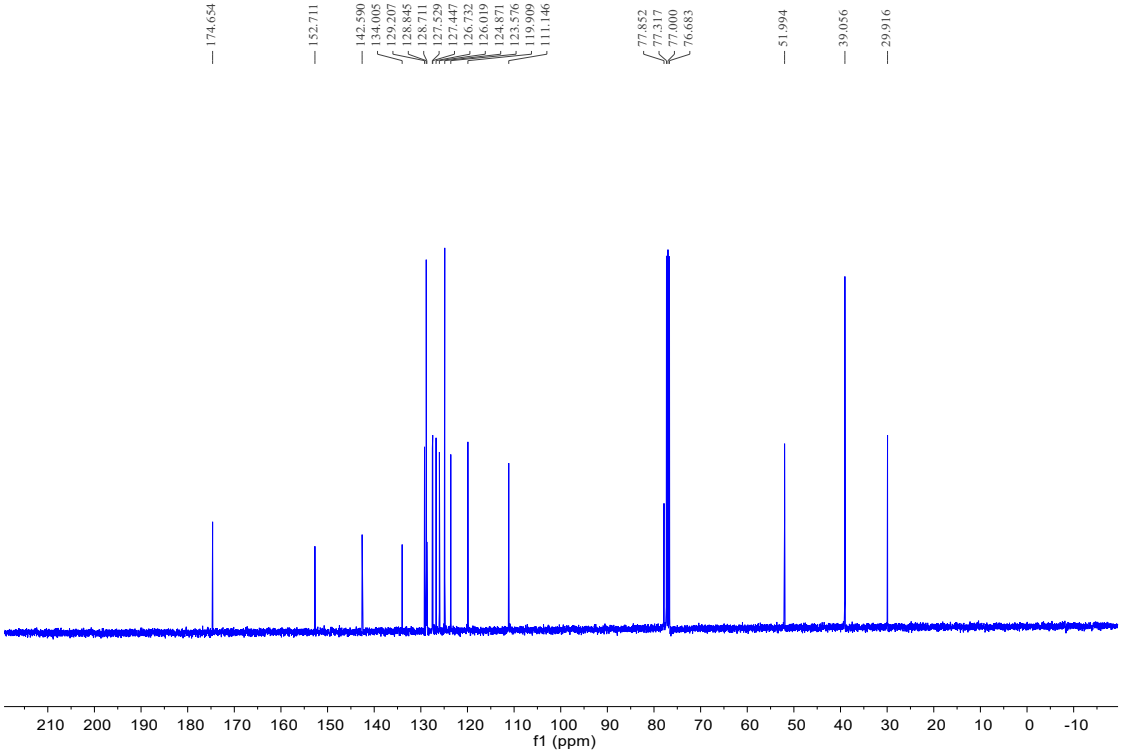
^{13}C NMR (100 MHz, $CDCl_3$) for **major isomer**:



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

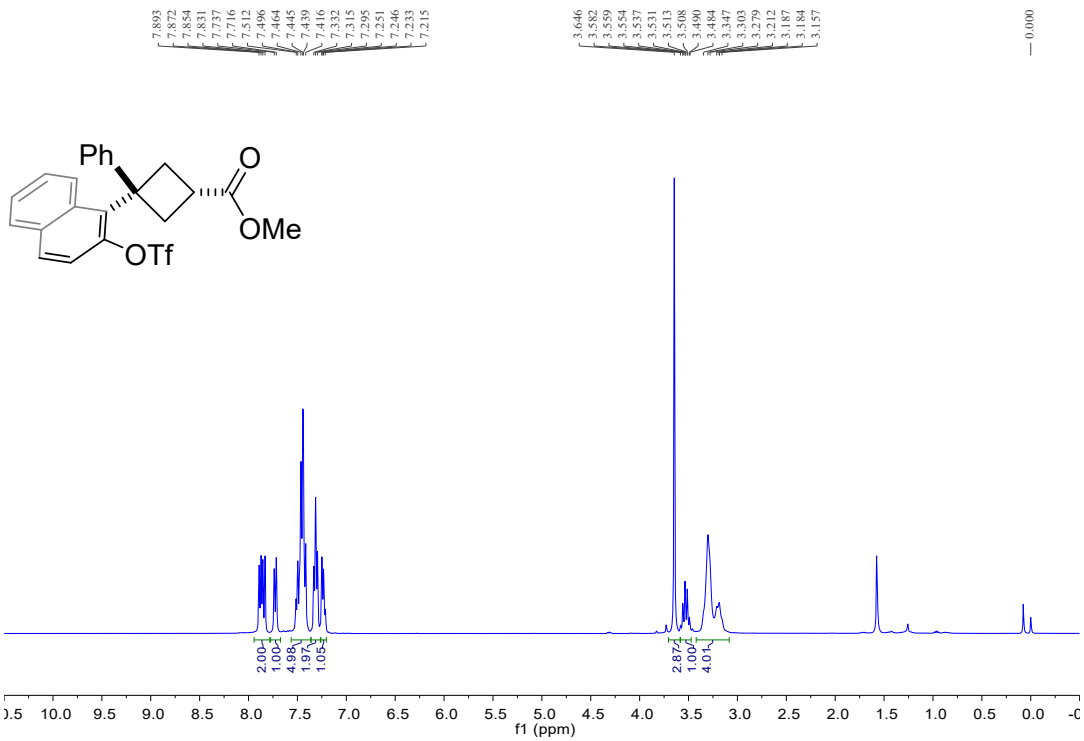


^{13}C NMR (100 MHz, $CDCl_3$) for **minor isomer**:

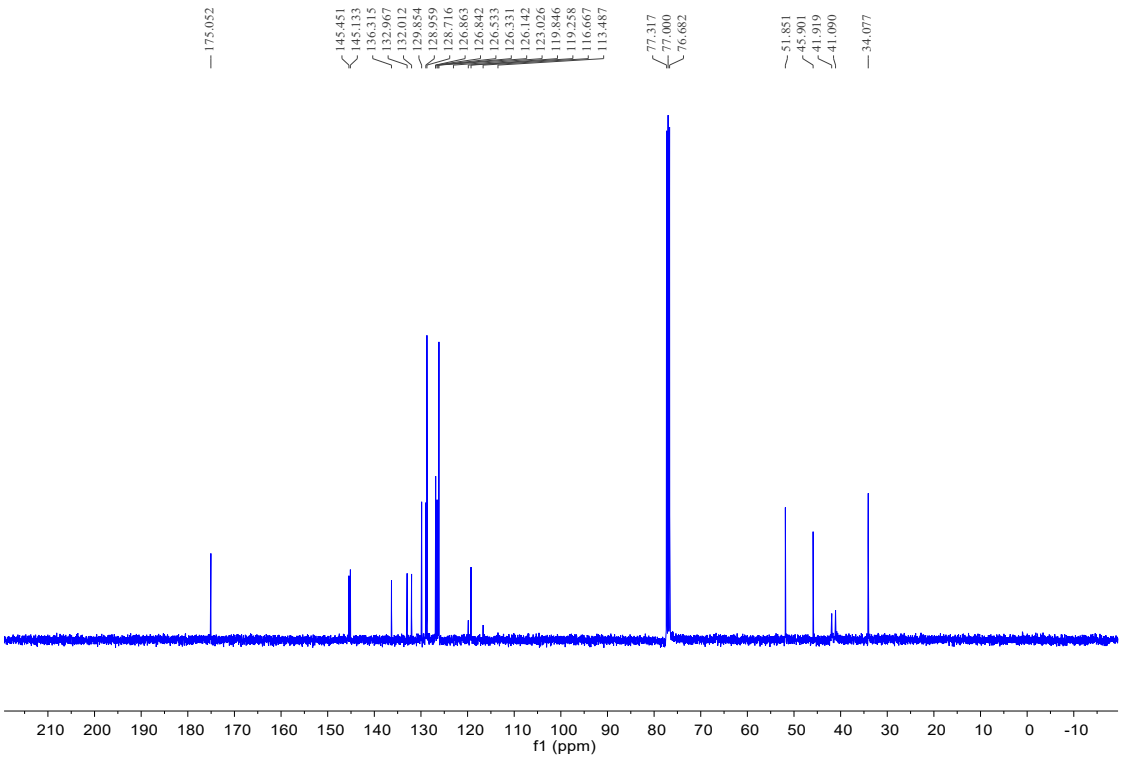


^{1}H ,^{13}C NMR and ^{19}F NMR Spectra for Compound 6

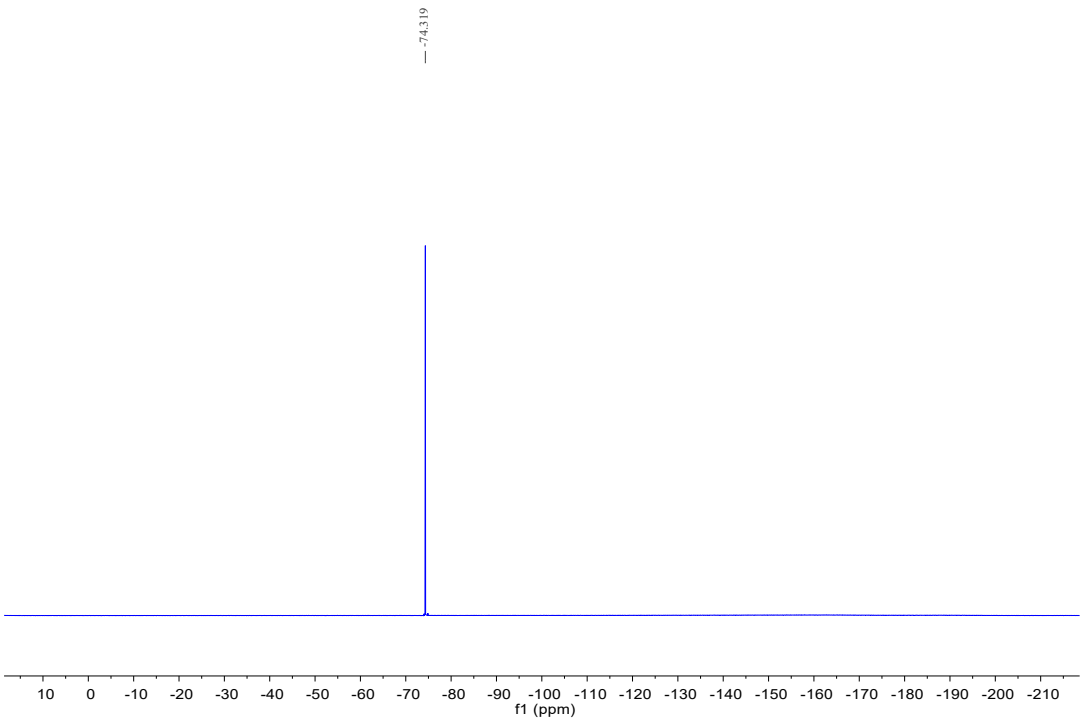
^{1}H NMR (400 MHz, $CDCl_3$)



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

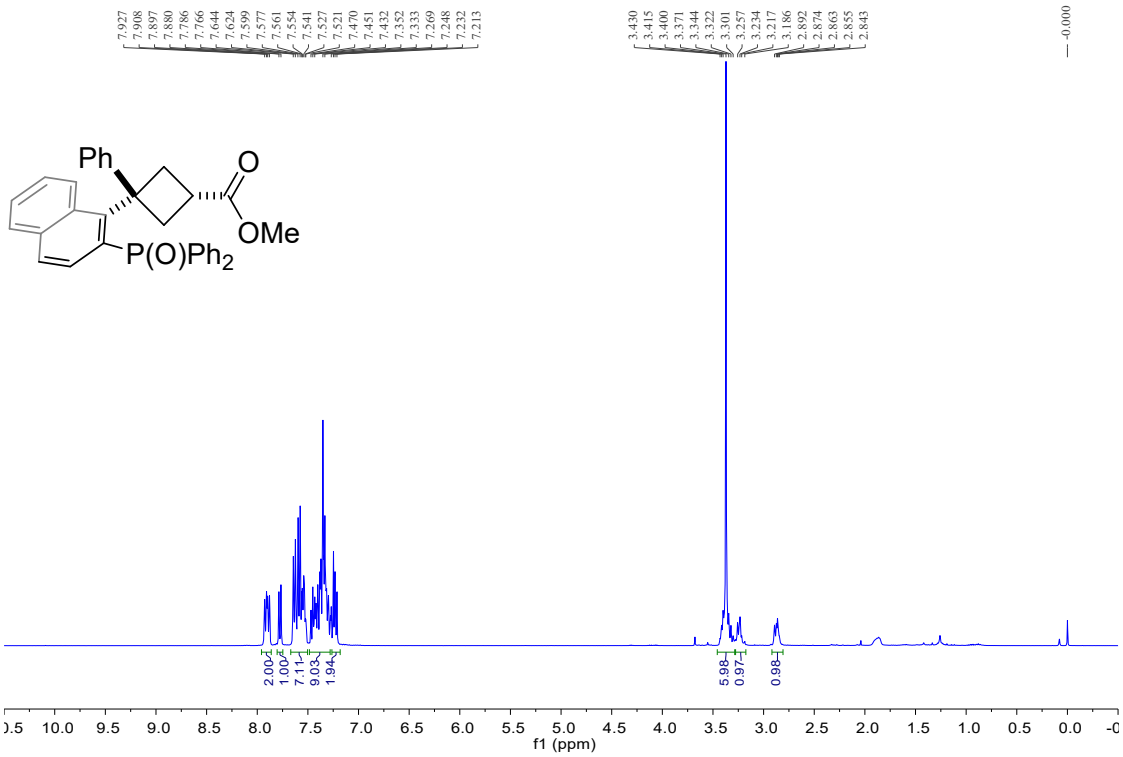


^{19}F NMR (376 MHz, $CDCl_3$)

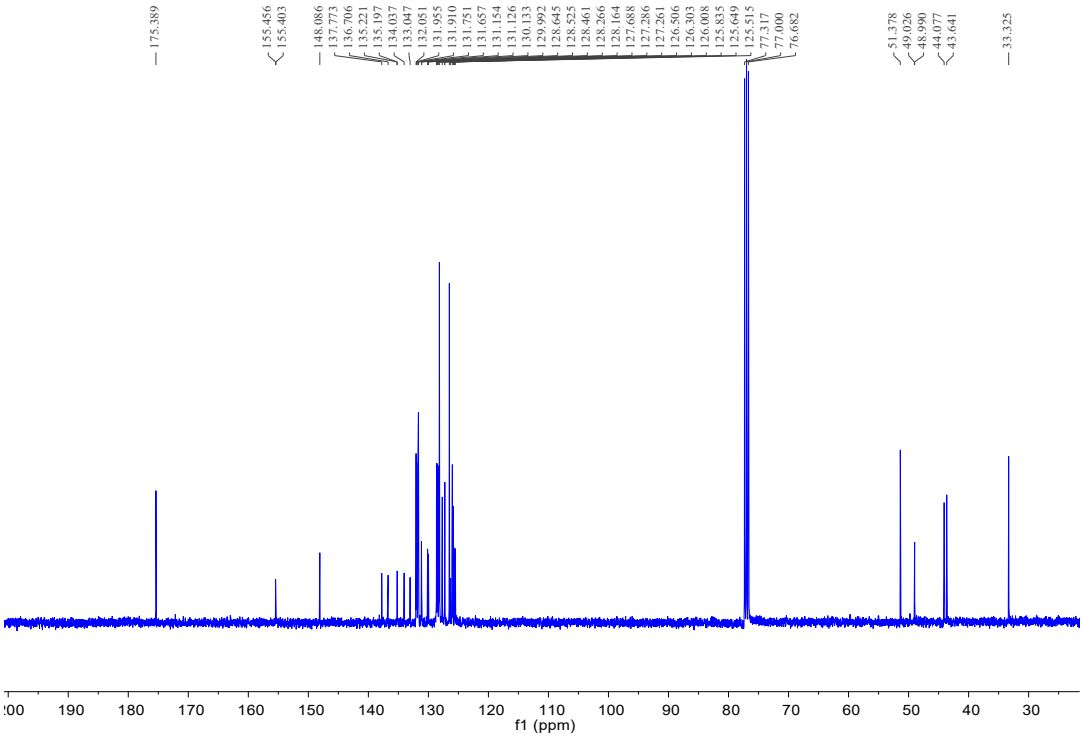


^{1}H ,^{13}C NMR and ^{31}P NMR Spectra for Compound 7

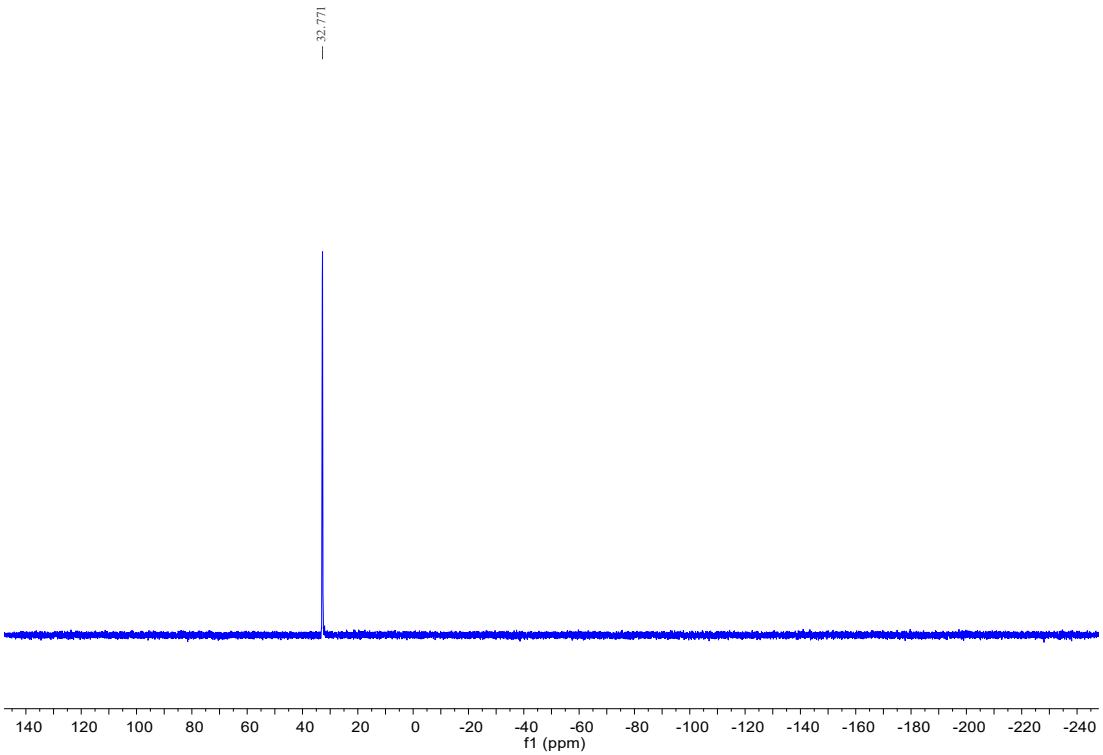
^{1}H NMR (400 MHz, $CDCl_3$)



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

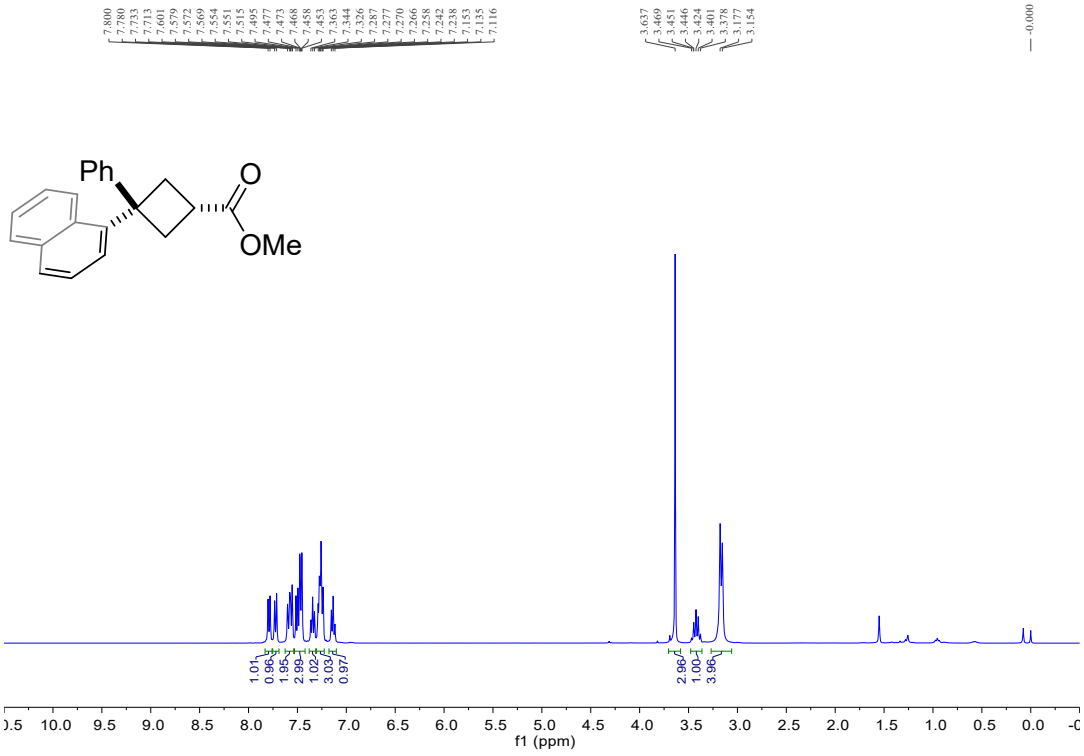


^{31}P NMR (162 MHz, $CDCl_3$)

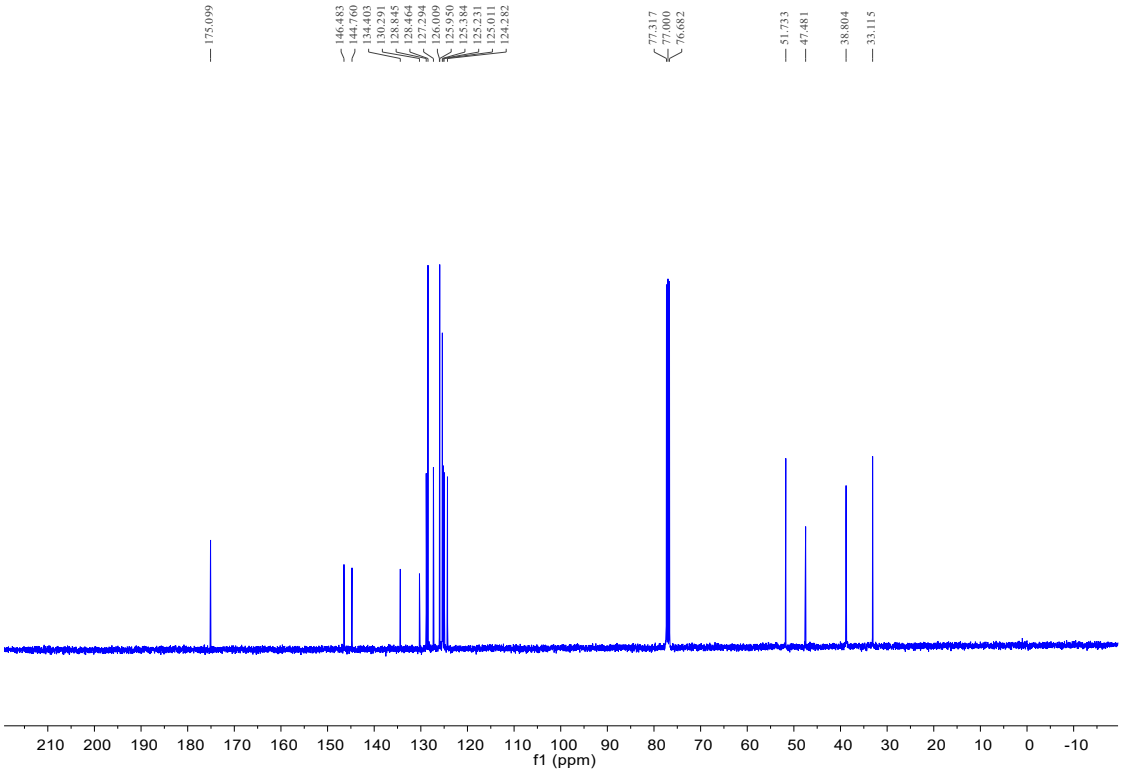


^{1}H and ^{13}C NMR Spectra for Compound 8

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

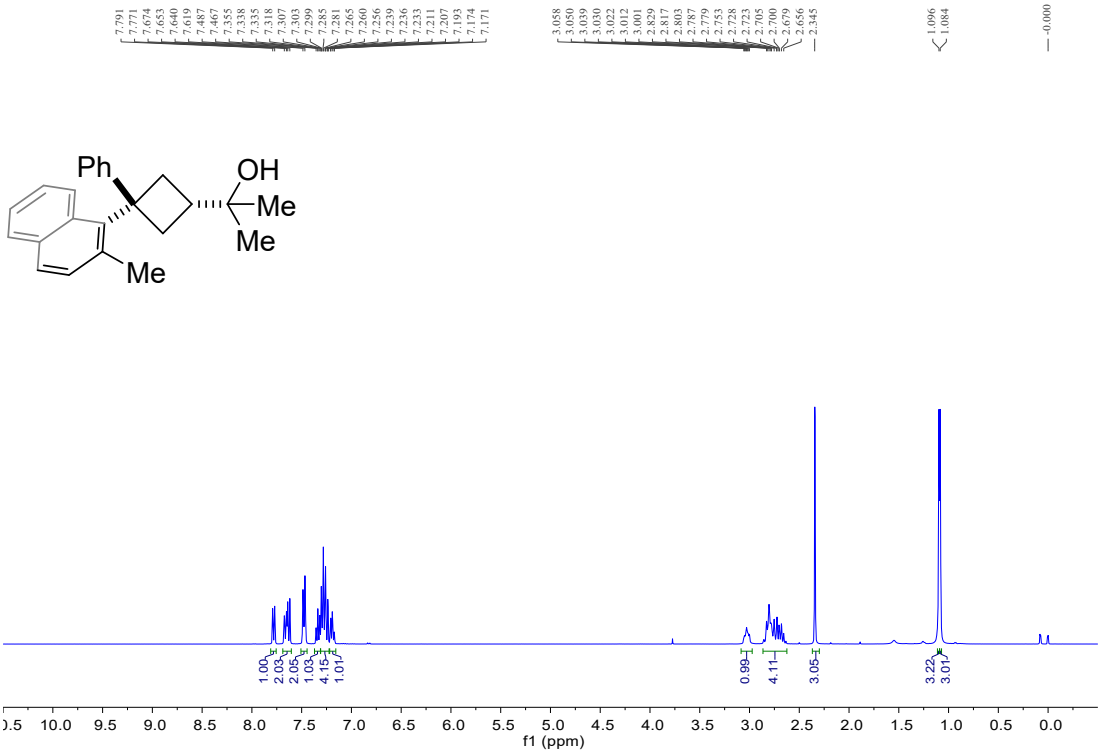


^{13}C NMR (100 MHz, $CDCl_3$)

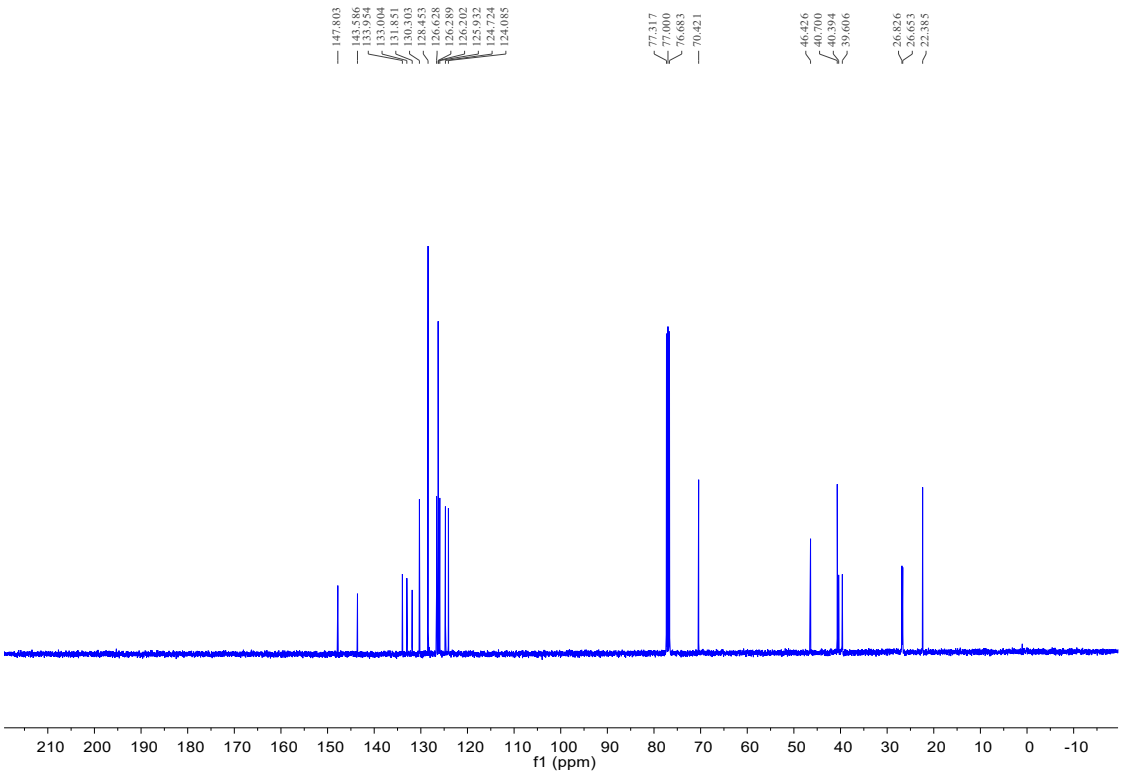


^{1}H and ^{13}C NMR Spectra for Compound 9

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

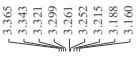


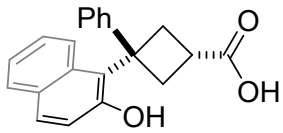
^{13}C NMR (100 MHz, $CDCl_3$)

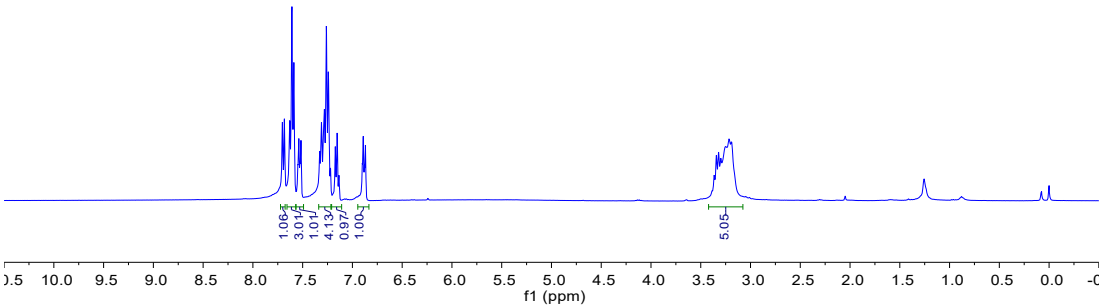


^{1}H and ^{13}C NMR Spectra for Compound 10

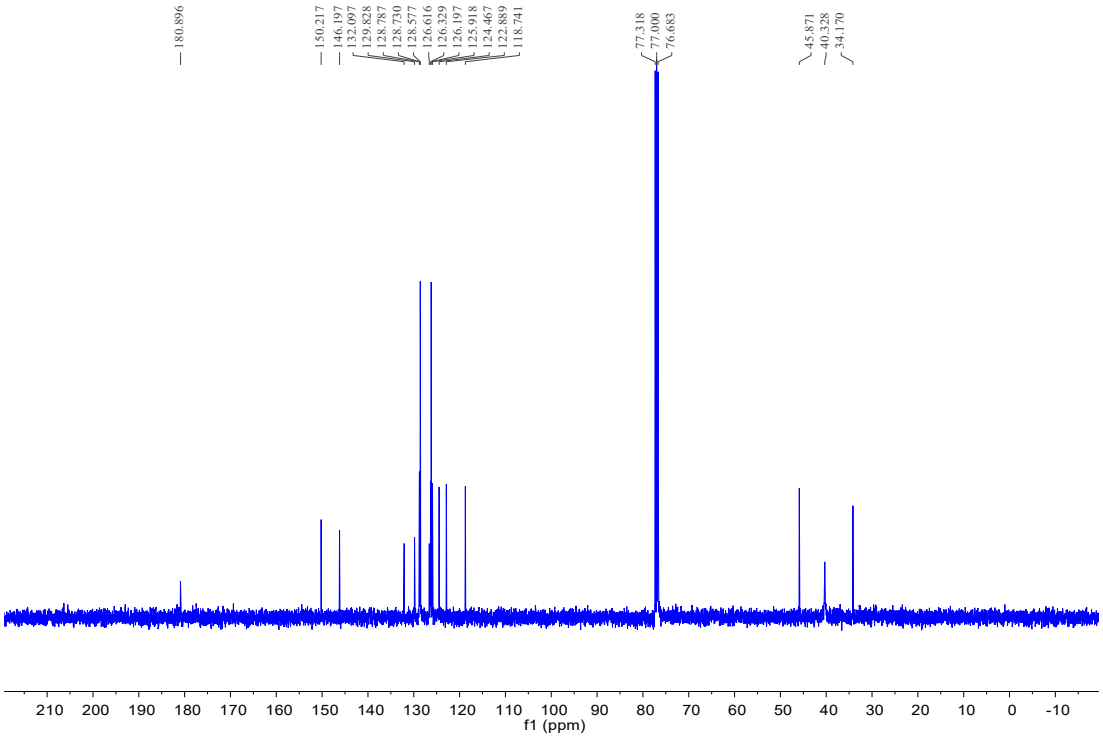
^{1}H NMR (400 MHz, $CDCl_3$)





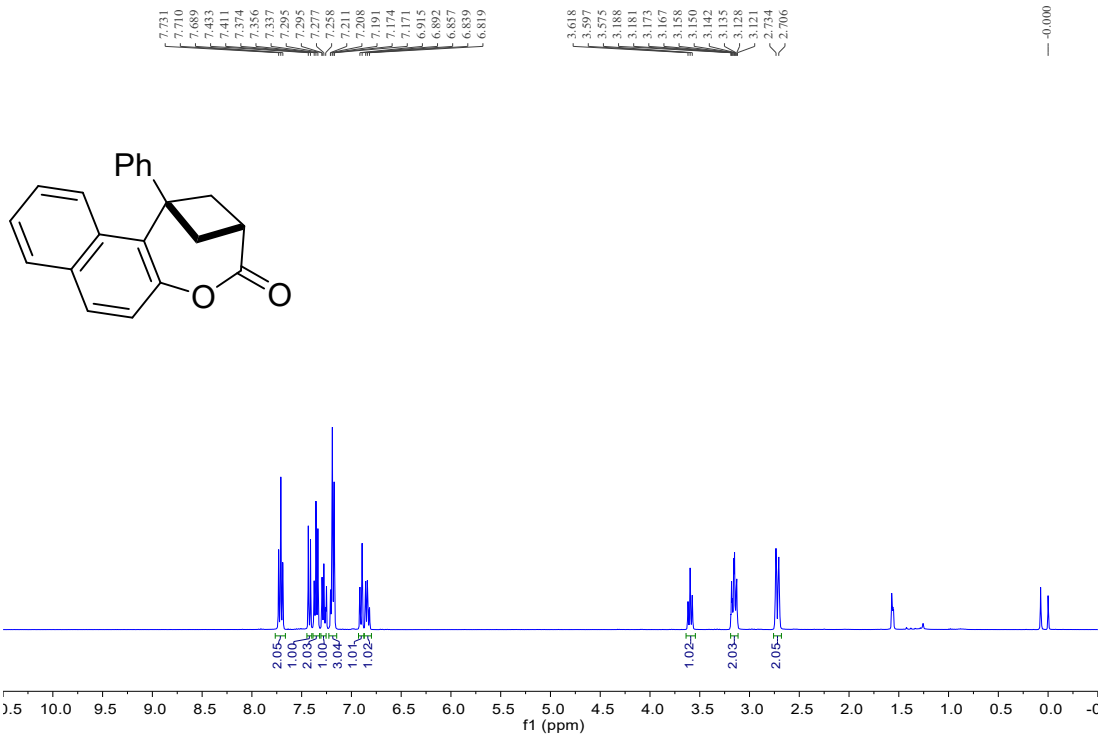


^{13}C NMR (100 MHz, $CDCl_3$)

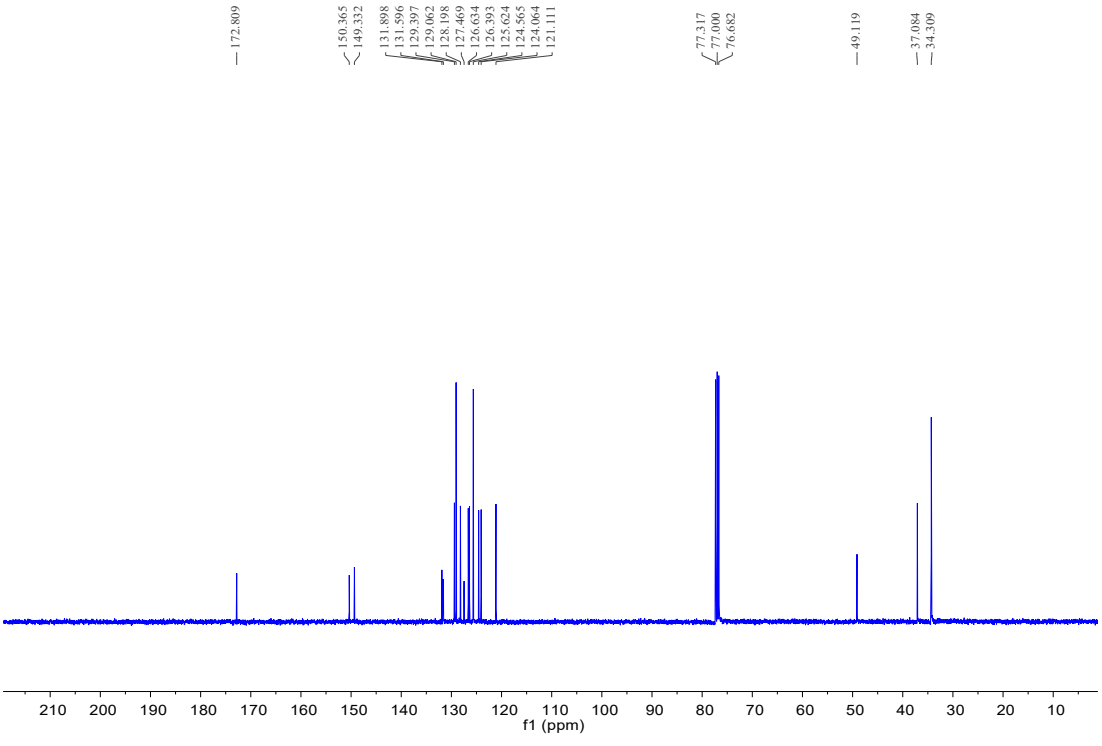


^{1}H and ^{13}C NMR Spectra for Compound 11

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

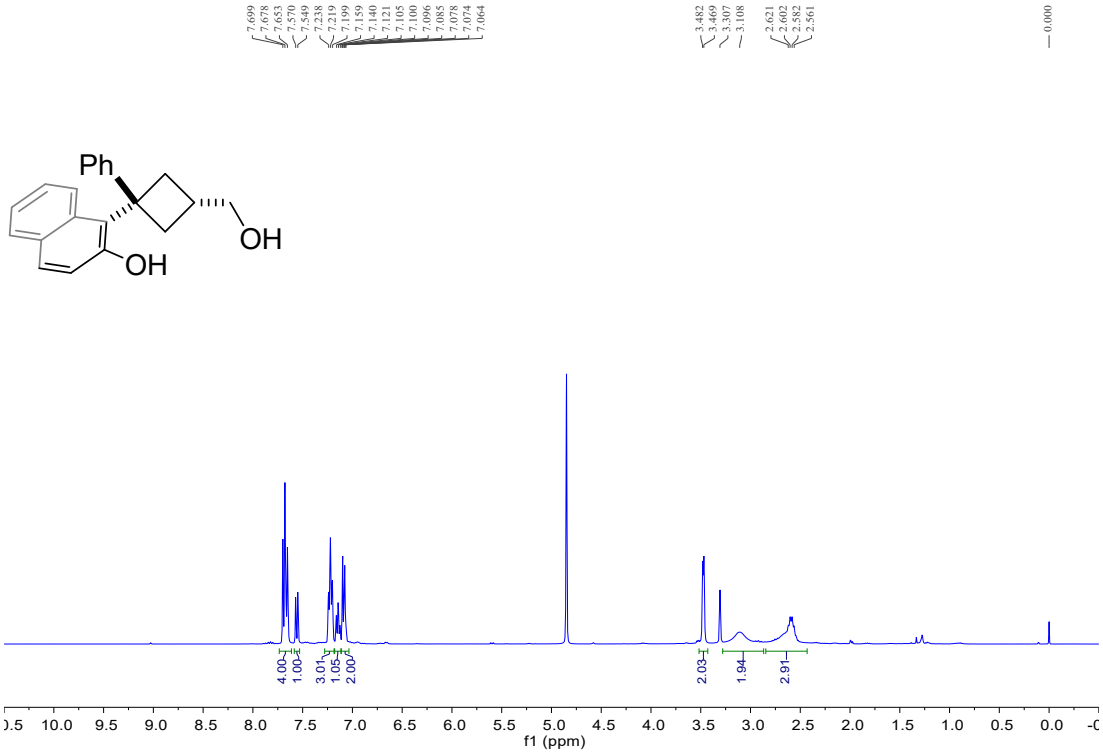


^{13}C NMR (100 MHz, $CDCl_3$)

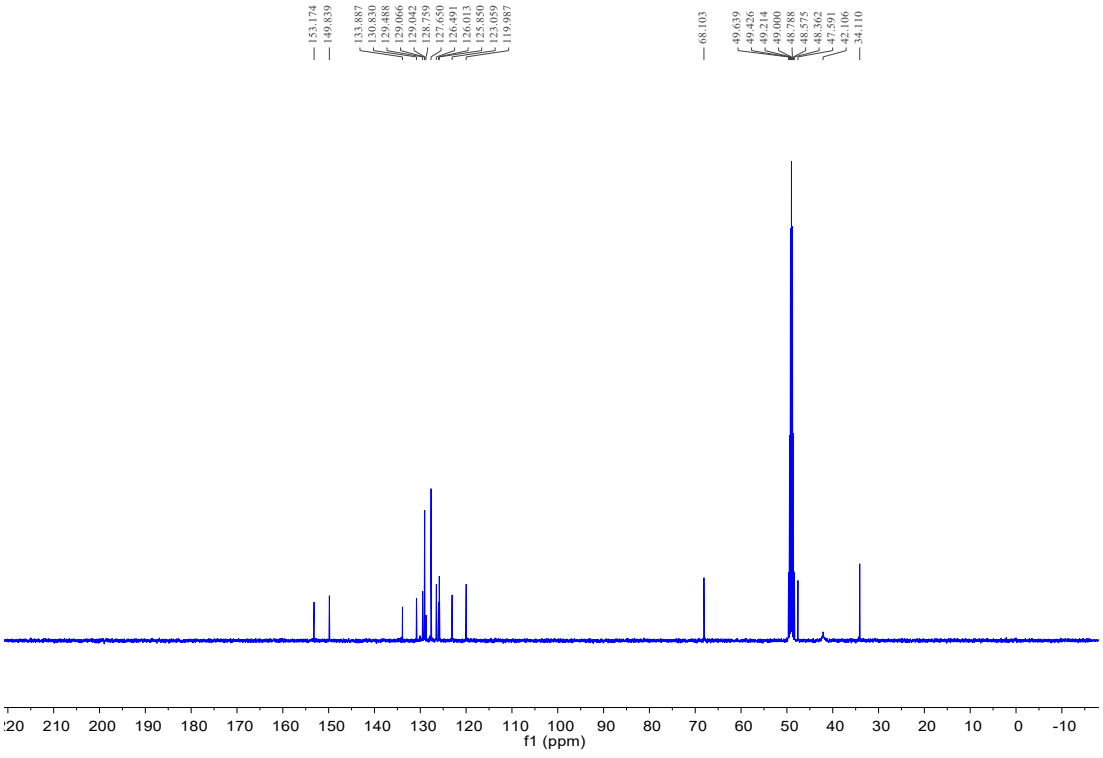


^{1}H and ^{13}C NMR Spectra for Compound 12

^{1}H NMR (400 MHz, Methanol-d_4)

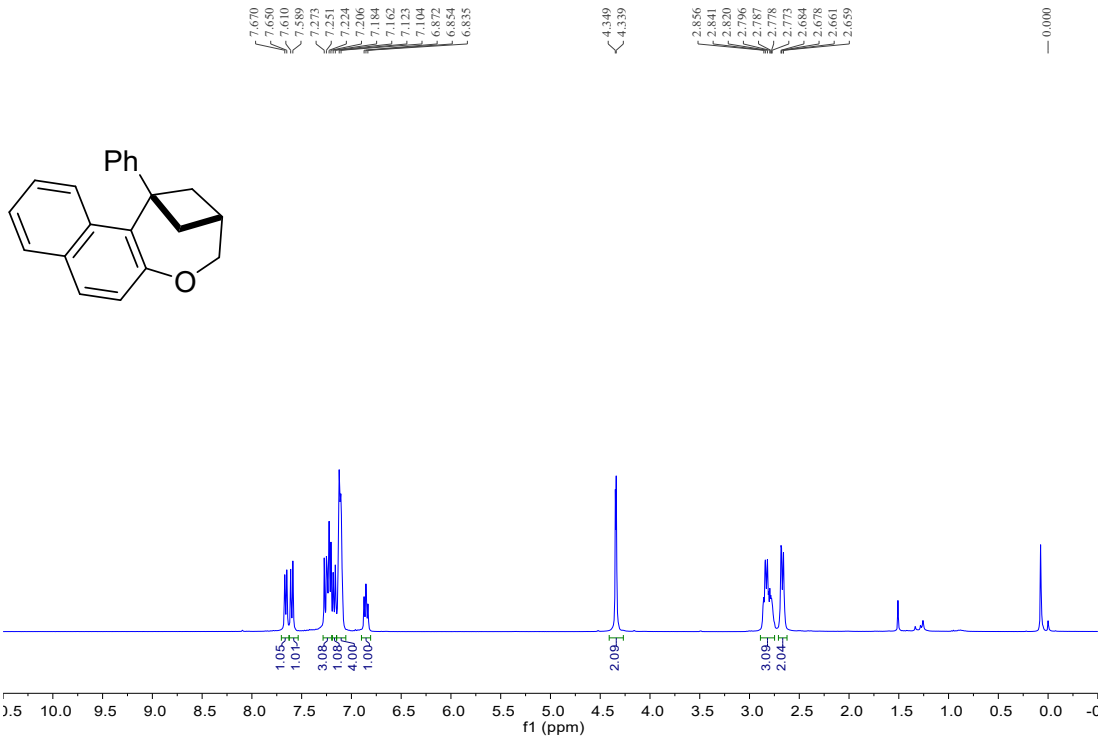


^{13}C NMR (100 MHz, $CDCl_3$)

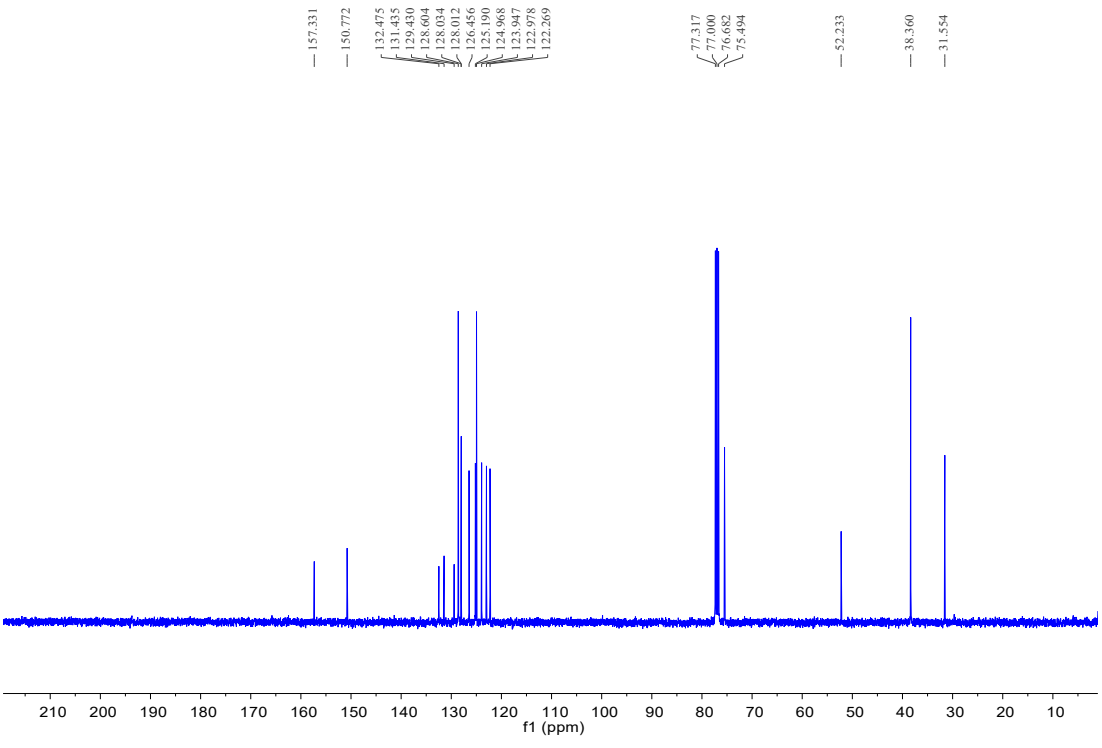


^{1}H and ^{13}C NMR Spectra for Compound 13

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



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



11 DFT Studies

All calculations were performed by using the Gaussian 16 package.[7] All

geometries were optimized in the gas phase at B3LYP-D3(BJ)[8]/BS1 level, where BS1 represents a basis set of SDD[9] for Ag atom, and 6-31G(d, p)[10] for all other elements. For all optimized structures, vibrational frequency calculations were performed at the same level of theory to ensure that every optimized structure has no imaginary frequency and that all the optimized transition state has only one imaginary frequency. The energies were improved by single-point energy calculations at the level of B3LYP-D3(BJ)/def2-TZVP[12] including solvation effects with the SMD[11]continuum solvation model for toluene. The thermodynamic quantities, such as concentration (1 mol/L) and temperature (373.15 K), were evaluated using the GoodVibes code[13]. All the energies discussed are Gibbs free energies at 373.15K with solvation effects considered. Quasi-rigid-rotor-harmonic-oscillator approximations were employed in GoodVibes, with a frequency cutoff of 100 cm^{-1}.[14,15] Molecular visualizations were conducted using CYLview [16] and PyMOL [17].

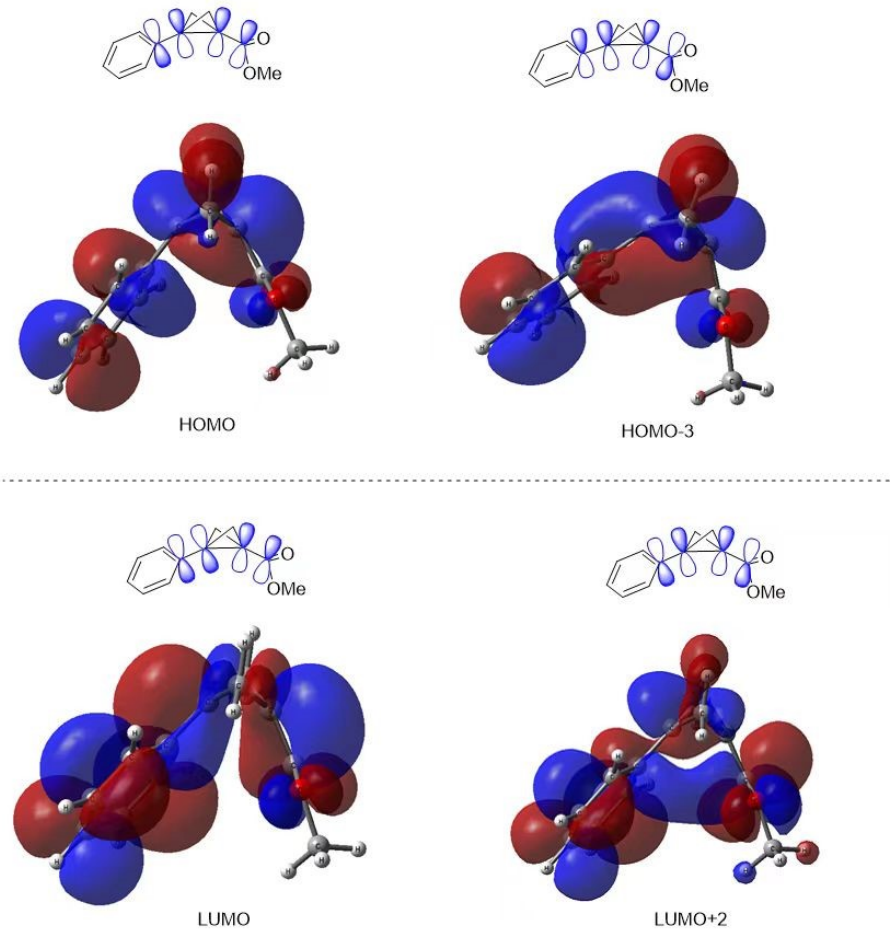


Figure S1. Molecular orbital analysis of **1a**.

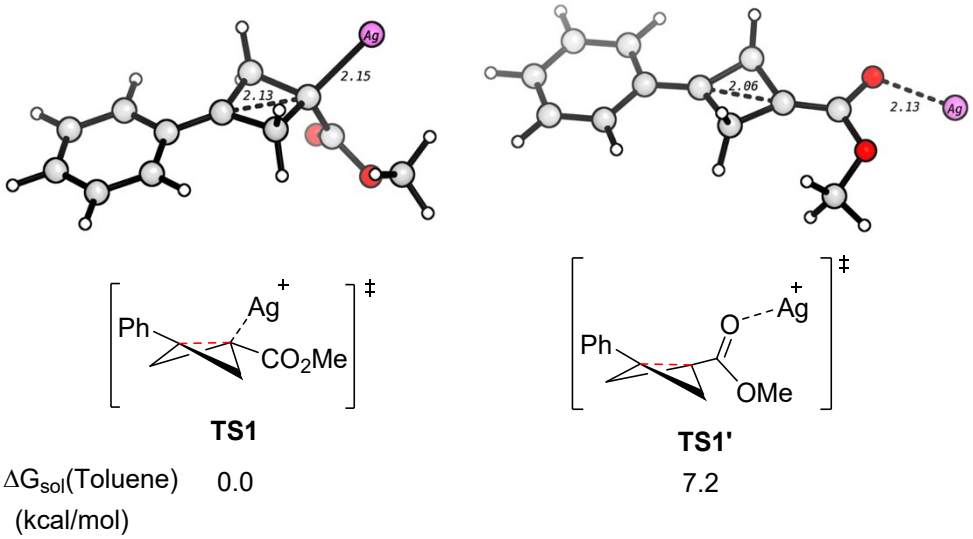


Figure S2. Comparison of two activation modes of the ring-opening step.

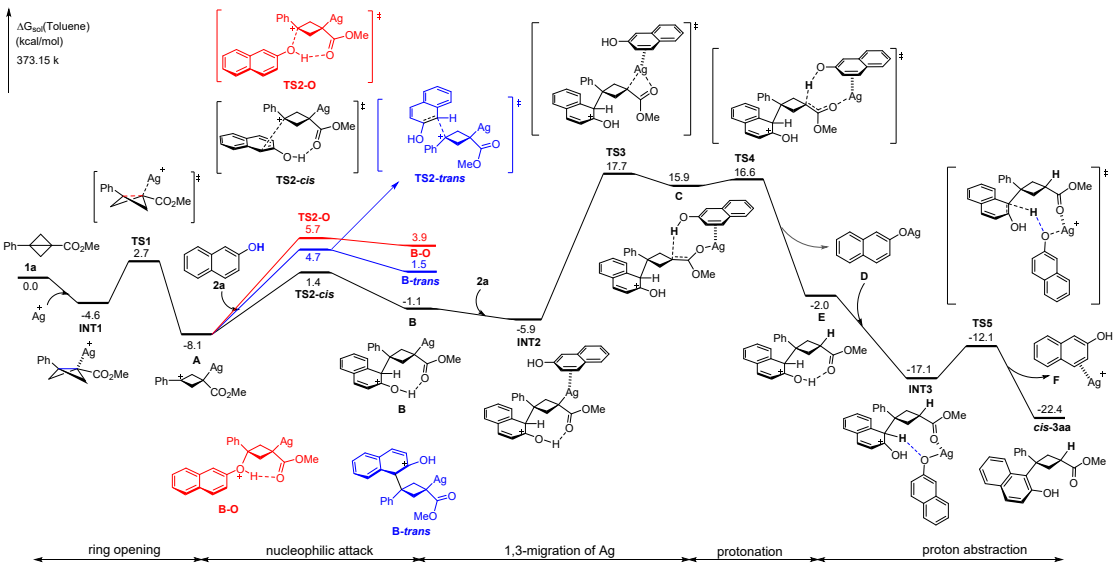


Figure S3. Calculated free energy profile of the catalytic cycle.

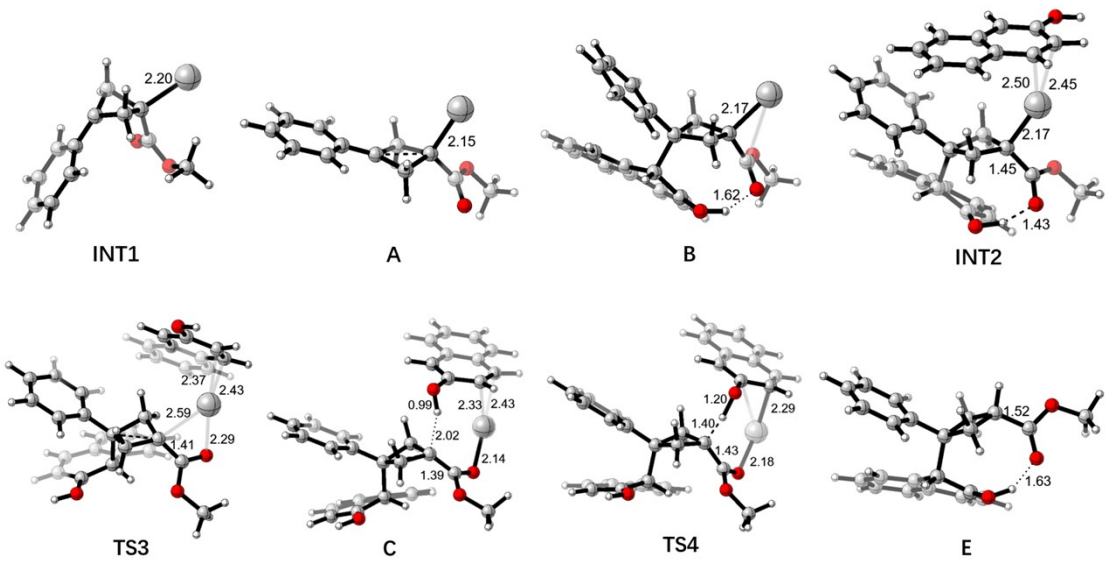
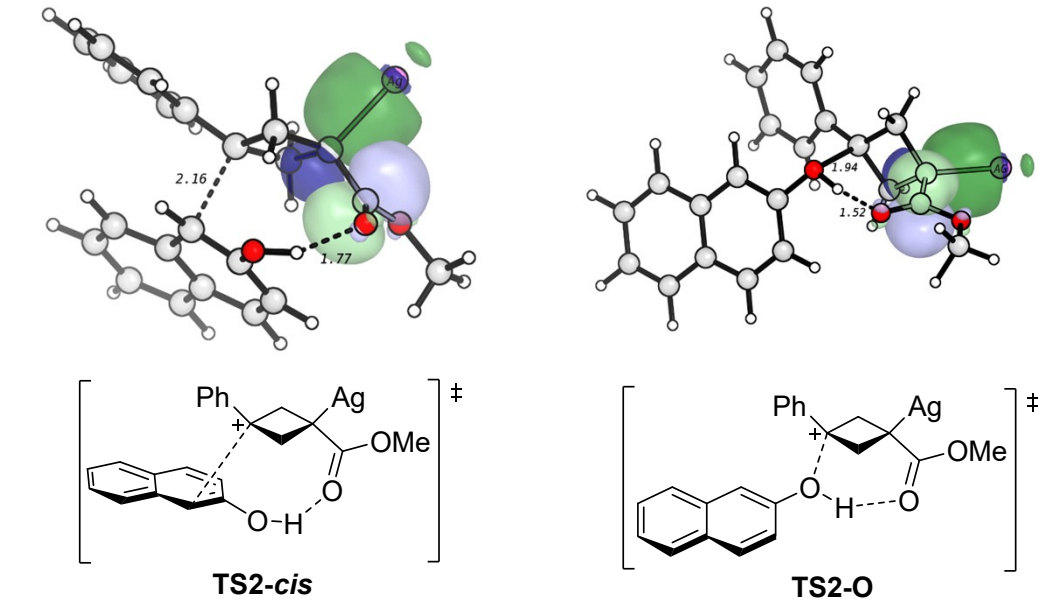


Figure S4. Optimized geometries of key stationary points in Figure S3.



ΔG_{sol}(Toluene) (kcal/mol)	0.0	4.3

Figure S5. NBO orbital analysis of two transition states of nucleophilic attack.

The analysis using the NBO module of the Gaussian software, based on second-order perturbation theory, reveals that the primary stabilizing factor for the stable C-Ag bond in TS2-*cis* is the C-Ag -> LP* C orbital interaction (Figure S4), where C-Ag bond acts as the donor and empty p orbital of C as the acceptor. This effect lower the energy by 36 kcal/mol. This suggests that the negative charge of the carbon-silver bond will be somewhat delocalized. However, in the transition state involving oxygen attack, the presence of strong hydrogen bonding leads to the orthogonality of the corresponding

orbitals, resulting in the loss of this stabilizing effect and consequently an unstable C-Ag bond.

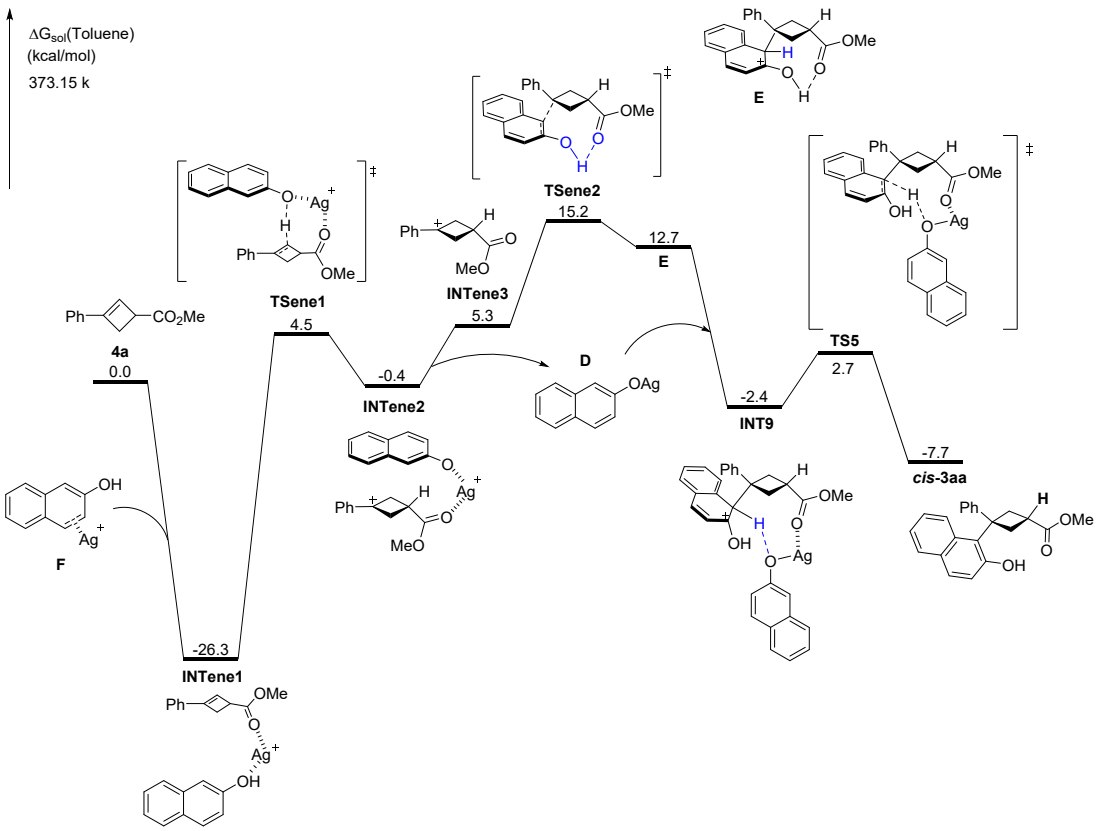


Figure S6. The reaction pathway for the conversion of a byproduct cyclobutene to the main product.

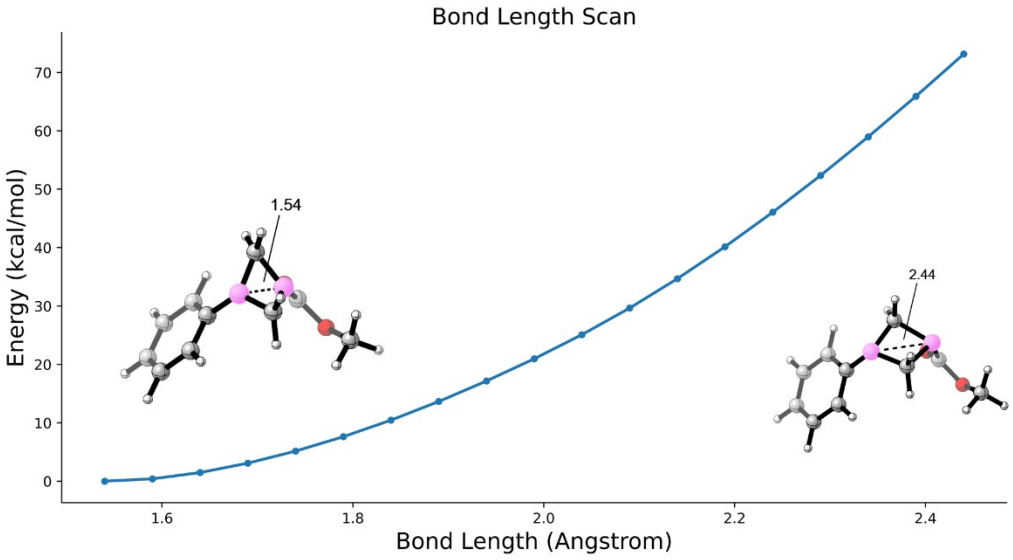


Figure S7. The calculated potential energy surface (PES) scanned by varying the bridging C-C bond of **1a**.

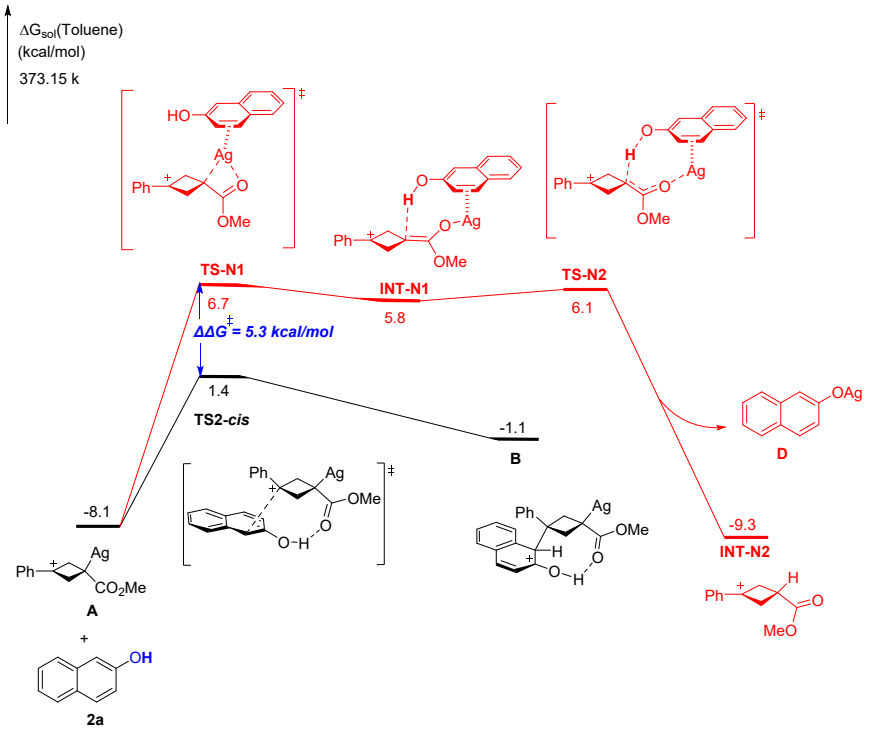


Figure S8. Calculated energy free profiles for the comparison of nucleophilic attack and protonation pathways.

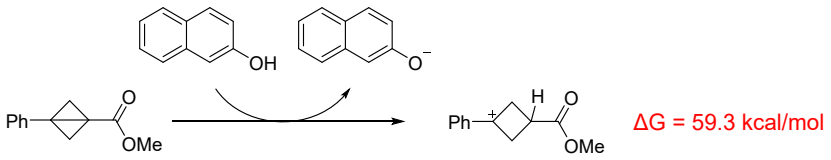


Figure S9. Calculated reaction energy of the direct protonation step.

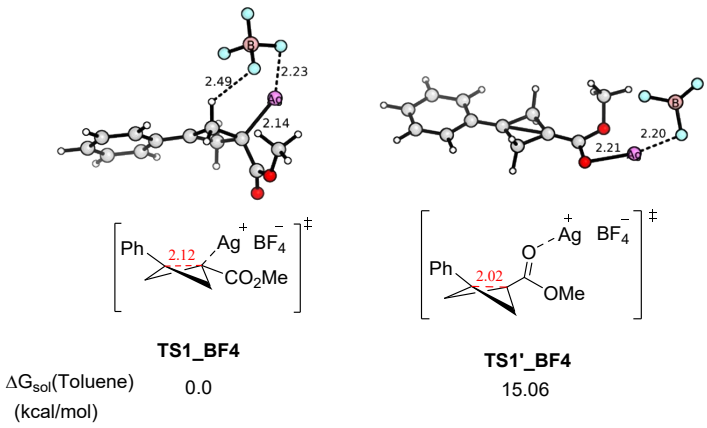


Figure S10. Comparison of two activation modes of the ring-opening step with BF_4^- included.

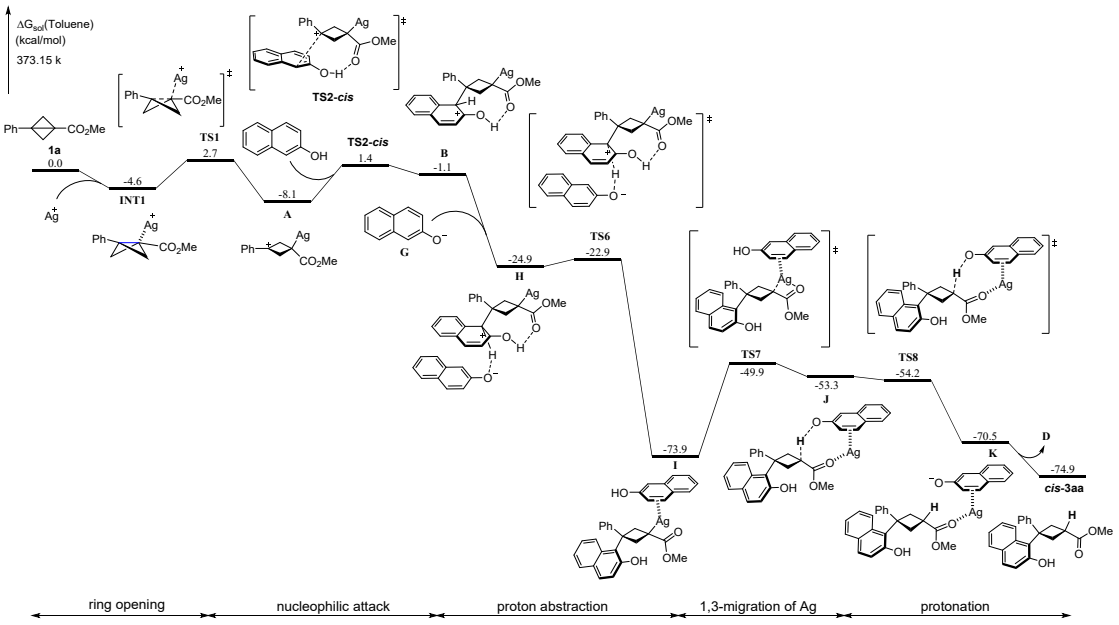


Figure S11. Calculated energy profile of another possible pathway with the proton abstraction step occurring prior to the protonation step.

We have performed calculations on another possible reaction pathway, in which the proton abstraction step occurs prior to the protonation step after the formation of **B** (see Figure S11). Thermodynamically, this appears to be a reasonable pathway, which drives the energy profile downhill significantly because of the charge neutralization and aromatization (from **B** to **I**). However, our system is acidic, which lacks additional base anion to facilitate the deprotonation process. The naphthol anion moiety **G** could only be generated in the protonation step (**TS4** in Figure S3 or **TS8** in Figure S11). Before the protonation step, the concentration of naphthol anion in the system could be neglected. As the reaction goes on, the concentration of naphthol anion **G** should still be very low when comparing to that of the substrate **2a**. Therefore, we don't think that the reaction pathway shown in Figure S11 is the major mechanism. Eventhough we could not completely exculde the reaction pathway of Figure S11, the samll amount of **G** formed during the reaction process would not change the major mechanism, because the key steps in Figure S3 and Figure S11 are similar to each other despite the exact suequnces. In addition, the energy barriers for the rate-determining step in

both scenarios are very close to each other (23.6 kcal/mol (**TS3**) in Figure S3 and 24.0 kcal/mol (**TS7**) in Figure S11, respectively).

Cartesian coordinates:

65

Name: TS5 Energy: -1057225.5621585

C	3.49627	0.06660	-0.14401
C	4.20779	-1.23870	0.08296
C	1.74630	2.51311	-0.62854
C	2.45214	0.54194	0.90368
C	1.53540	1.04424	-0.26309
C	2.36309	0.09736	-1.19803
C	1.53519	2.92439	-1.95311
C	1.65644	4.26381	-2.31541
C	1.99114	5.22190	-1.35661
C	2.19724	4.82684	-0.03649
C	2.07283	3.48373	0.32414
O	3.66826	-2.34661	0.24594
O	5.51770	-1.11703	0.08844
C	6.30530	-2.31896	0.29754
H	2.81532	1.26474	1.63336
H	1.89358	-0.88152	-1.31059
H	2.62428	0.47063	-2.18696
H	1.27191	2.19182	-2.70938
H	1.49422	4.55918	-3.34734
H	2.09030	6.26535	-1.63746
H	2.45503	5.56231	0.71898
H	2.22380	3.20802	1.36115

H	7.34024	-1.98636	0.26589
H	6.06261	-2.75641	1.26704
H	6.09948	-3.03833	-0.49638
Ag	1.50392	-2.60404	0.42706
H	1.99646	-0.29622	1.43849
C	-0.93478	2.45364	3.14007
C	-0.20674	1.79321	2.16200
C	-0.75022	1.54987	0.88860
C	-2.08549	1.98990	0.64737
C	-2.81316	2.66182	1.65826
C	-2.24654	2.89653	2.89303
H	-0.09636	-0.38639	0.34173
H	-0.48523	2.62404	4.11318
H	0.78942	1.45066	2.40076
C	-0.00549	0.78104	-0.14288
C	-2.69780	1.72007	-0.60554
H	-3.83009	2.97640	1.44462
H	-2.80521	3.40824	3.66899
C	-2.04712	1.01283	-1.58465
C	-0.72376	0.59139	-1.38404
H	-3.71732	2.05298	-0.77109
H	-2.54539	0.78051	-2.52112
O	-0.07820	-0.04585	-2.37436
H	-0.68837	-0.22454	-3.10512
H	4.24100	0.84039	-0.32895
C	-6.42214	-1.01194	-0.90695
C	-5.40706	-1.73693	-1.49218

C	-4.13283	-1.82676	-0.87696
C	-3.91928	-1.17068	0.38103
C	-4.98646	-0.42988	0.95787
C	-6.20738	-0.34923	0.32592
H	-3.21744	-3.05652	-2.40773
H	-7.39235	-0.94719	-1.38872
H	-5.57024	-2.24712	-2.43741
C	-3.04949	-2.53062	-1.47181
C	-2.64140	-1.22519	0.98069
H	-4.81906	0.07146	1.90684
H	-7.01600	0.21826	0.77590
C	-1.58742	-1.84655	0.33772
C	-1.80353	-2.52961	-0.89159
H	-2.45734	-0.71261	1.91868
H	-0.96299	-3.03512	-1.36177
O	-0.33587	-1.65324	0.82857

65

Name: TS4 Energy: -1057194.0253775

C	0.06163	-1.34645	-1.11358
C	-0.12024	-2.55978	-0.36932
C	2.44577	1.19727	-1.22314
C	0.35385	-0.06897	-0.30546
C	1.82039	-0.11294	-0.82810
C	1.34135	-1.11244	-1.93109
C	3.17046	1.32348	-2.41511
C	3.79899	2.52536	-2.74013
C	3.71197	3.61814	-1.87508

C	2.98147	3.50638	-0.69139
C	2.35078	2.30369	-0.36942
O	-0.84861	-2.67908	0.66519
O	0.50990	-3.64116	-0.84426
C	0.17619	-4.91429	-0.25440
H	0.16641	-0.07048	0.76878
H	1.12623	-0.56962	-2.85587
H	1.97069	-1.97178	-2.16009
H	3.23487	0.47978	-3.09568
H	4.34707	2.61325	-3.67311
H	4.19703	4.55481	-2.13021
H	2.89421	4.35745	-0.02304
H	1.77936	2.22377	0.55027
H	0.44859	-4.93218	0.80263
H	-0.89294	-5.11170	-0.35567
H	0.75426	-5.64862	-0.81310
Ag	-2.67048	-1.48161	0.53833
H	-0.13306	0.80885	-0.73312
C	-3.92445	-0.66160	-1.18957
C	-4.74314	0.00337	-0.26461
C	-4.50881	1.36345	0.07300
C	-3.42973	2.04827	-0.58348
C	-2.60045	1.35313	-1.49853
C	-2.79010	0.00663	-1.80772
H	-6.14136	1.53281	1.48208
H	-4.21810	-1.62915	-1.59276
H	-5.61998	-0.49931	0.13627

C	-5.32282	2.06167	1.00152
C	-3.21650	3.41832	-0.26993
H	-1.78618	1.88096	-1.98661
C	-4.02238	4.06806	0.63736
C	-5.08598	3.38810	1.28116
H	-2.40725	3.94667	-0.76558
H	-3.84861	5.11633	0.85986
H	-5.71531	3.91904	1.98754
O	-1.96986	-0.68632	-2.57904
H	-1.04926	-1.09594	-1.92484
C	5.10469	0.00231	0.03751
C	4.87550	0.74223	1.18077
C	3.73555	0.53811	2.01371
C	2.74706	-0.39351	1.60257
C	2.78992	-0.95332	0.21849
C	4.13163	-0.90322	-0.39211
H	4.39299	1.88748	3.56876
H	6.02400	0.12445	-0.52678
H	5.62265	1.46423	1.49801
C	3.63356	1.17058	3.27187
C	1.72349	-0.72808	2.48830
H	2.38605	-1.96879	0.18675
C	1.64591	-0.10819	3.73756
C	2.58744	0.85626	4.12410
H	0.99191	-1.48113	2.21183
H	0.84904	-0.38476	4.42058
H	2.50918	1.33504	5.09392

O	4.30085	-1.68344	-1.44524
H	5.15381	-1.51773	-1.87983

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Name: TS3 Energy: -1057196.0449226

C	-0.43105	1.84883	0.62772
C	-0.83013	2.69006	-0.43576
C	2.18238	-0.23134	1.62654
C	-0.03781	0.39021	0.40570
C	1.41820	0.77511	0.80918
C	0.80810	2.06043	1.48260
C	2.91536	0.14773	2.75725
C	3.65386	-0.79536	3.47262
C	3.66873	-2.13056	3.06448
C	2.93263	-2.51949	1.94395
C	2.19280	-1.57597	1.23094
O	-1.67978	2.35163	-1.32733
O	-0.28851	3.92723	-0.46294
C	-0.87670	4.86807	-1.37893
H	-0.23415	-0.08645	-0.55516
H	0.63828	1.85418	2.54476
H	1.34521	3.00448	1.38539
H	2.90270	1.18427	3.08109
H	4.21057	-0.49068	4.35349
H	4.24019	-2.86454	3.62353
H	2.93051	-3.55888	1.62913
H	1.61479	-1.88277	0.36497
H	-0.35907	5.80968	-1.19834

H	-0.73462	4.54613	-2.41258
H	-1.94626	4.97720	-1.18341
Ag	-2.84418	1.03360	0.13835
H	-0.40064	-0.27942	1.19135
C	-4.13521	-0.74731	1.02484
C	-3.94552	-1.08679	-0.32365
C	-2.85768	-1.92098	-0.72042
C	-1.99496	-2.44549	0.29651
C	-2.23067	-2.12757	1.66012
C	-3.26813	-1.29859	2.02762
H	-3.27456	-1.83848	-2.84130
H	-5.04519	-0.23372	1.32885
H	-4.68169	-0.78491	-1.06315
C	-2.60745	-2.23414	-2.08089
C	-0.89931	-3.25749	-0.09853
H	-1.58649	-2.53556	2.43171
C	-0.67185	-3.53244	-1.42878
C	-1.53381	-3.02224	-2.42964
H	-0.24281	-3.65548	0.66908
H	0.17238	-4.15111	-1.71612
H	-1.35038	-3.26269	-3.47160
O	-3.43629	-1.01175	3.34090
H	-4.22473	-0.46900	3.47349
C	4.67241	0.66057	-0.19989
C	4.49488	-0.44819	-1.00363
C	3.30321	-0.66357	-1.75874
C	2.22879	0.25199	-1.61589

C	2.25629	1.26457	-0.51763
C	3.61273	1.55383	-0.02259
H	4.04542	-2.40710	-2.79823
H	5.62004	0.83455	0.30088
H	5.31273	-1.15407	-1.11635
C	3.21871	-1.70938	-2.70415
C	1.13308	0.15122	-2.47382
H	1.73270	2.17946	-0.81510
C	1.07113	-0.87838	-3.41344
C	2.10287	-1.82266	-3.51711
H	0.32575	0.87507	-2.41428
H	0.21177	-0.94386	-4.07188
H	2.03875	-2.62119	-4.24840
O	3.72174	2.65326	0.70874
H	4.60254	2.72473	1.11121

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Name: TS2-trans Energy: -767693.8774292

C	-1.88013	0.35930	-0.30648
C	-3.03982	0.97790	-1.00707
C	1.39649	1.61946	-0.31962
C	-1.04488	1.24500	0.65931
C	0.21643	0.79997	-0.08137
C	-0.62138	0.14798	-1.17702
C	2.27294	1.31463	-1.37646
C	3.39779	2.10382	-1.60928
C	3.66043	3.20257	-0.79009
C	2.79727	3.51372	0.26758

C	1.67816	2.72569	0.50532
O	-3.27453	0.84650	-2.19338
O	-3.79909	1.71708	-0.16517
C	-4.95967	2.33010	-0.76143
H	-1.09562	1.07709	1.73513
H	-0.63998	0.79738	-2.06214
H	-0.35014	-0.84849	-1.52519
H	2.06392	0.46353	-2.01608
H	4.06227	1.86743	-2.43379
H	4.53047	3.82335	-0.97818
H	2.99644	4.37707	0.89409
H	1.00191	2.97206	1.31835
H	-5.43487	2.89583	0.03844
H	-4.66534	2.98928	-1.58054
H	-5.63675	1.56441	-1.14742
H	-1.22445	2.31407	0.48719
C	1.88147	-3.26367	-1.62448
C	1.08597	-2.59029	-0.70597
C	1.65092	-1.63325	0.15289
C	3.05279	-1.39270	0.08973
C	3.84299	-2.08292	-0.85679
C	3.26159	-3.00217	-1.71029
H	-0.16480	-1.17772	1.26813
H	1.43504	-4.00623	-2.27781
H	0.02696	-2.81911	-0.63041
C	0.84503	-0.83661	1.05613
C	3.62901	-0.48320	1.02398

H	4.91007	-1.88702	-0.89898
H	3.86787	-3.53455	-2.43486
C	2.89581	0.11134	2.02799
C	1.51086	-0.12166	2.09087
H	4.69544	-0.28672	0.96152
H	3.37589	0.75583	2.75759
O	0.74242	0.39525	3.05318
H	1.26533	0.92956	3.67076
Ag	-2.75639	-1.40868	0.55346

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Name: TS2-O Energy: -767693.1174775

C	2.45354	0.00199	0.05659
C	2.56746	-1.38568	0.63089
C	-0.56581	1.89356	0.19254
C	1.14837	0.13869	-0.81523
C	0.49007	0.92462	0.30152
C	1.78345	0.98843	1.09049
C	-0.78130	2.83640	1.21871
C	-1.86477	3.70036	1.14966
C	-2.74731	3.62907	0.06211
C	-2.54883	2.69484	-0.95568
C	-1.46524	1.82409	-0.88996
O	1.63378	-1.97863	1.19097
O	3.75246	-1.95984	0.50033
C	3.89894	-3.29782	1.04898
H	0.65095	-0.78069	-1.13755
H	2.20542	1.99599	1.07450

H	1.73053	0.65811	2.13190
H	-0.10145	2.87637	2.06396
H	-2.02992	4.43007	1.93506
H	-3.59269	4.30803	0.01252
H	-3.24134	2.63815	-1.78813
H	-1.31362	1.08422	-1.66883
H	4.93164	-3.57391	0.84890
H	3.69526	-3.28200	2.12032
H	3.20642	-3.97841	0.55199
H	1.27984	0.76975	-1.69773
C	-6.26860	-0.34590	-0.17632
C	-5.12566	0.06345	0.47208
C	-3.91141	-0.65341	0.31022
C	-3.88889	-1.80750	-0.54043
C	-5.08604	-2.20492	-1.18838
C	-6.24938	-1.48967	-1.01130
H	-2.71162	0.61806	1.60328
H	-7.19419	0.20563	-0.04667
H	-5.13627	0.93754	1.11644
C	-2.71671	-0.24836	0.95211
C	-2.66838	-2.51713	-0.70643
H	-5.07039	-3.08265	-1.82764
H	-7.16019	-1.80180	-1.51171
C	-1.51128	-2.10140	-0.09133
C	-1.55321	-0.95533	0.74220
H	-2.65978	-3.40353	-1.33336
H	-0.58504	-2.65523	-0.20327

O	-0.39483	-0.46910	1.32275
H	0.35066	-1.17073	1.32955
Ag	4.30809	0.60292	-0.82562

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Name: TS2-cis Energy: -767698.9670581

C	1.66645	0.28088	0.09878
C	2.39554	-0.97573	0.39020
C	-1.50135	1.66913	0.30223
C	0.37160	0.15013	-0.76435
C	-0.42133	0.70148	0.41584
C	0.84211	0.92181	1.24337
C	-1.84016	2.48543	1.40125
C	-2.87897	3.40113	1.30279
C	-3.59415	3.52157	0.10385
C	-3.27322	2.71644	-0.98979
C	-2.24262	1.78510	-0.88932
O	2.68147	-1.41042	1.50790
O	2.73682	-1.63461	-0.73464
C	3.52309	-2.82985	-0.56255
H	0.14493	-0.86596	-1.09859
H	1.01016	1.99029	1.39899
H	0.92063	0.43100	2.21492
H	-1.28305	2.39434	2.32914
H	-3.13177	4.02828	2.15117
H	-4.39990	4.24442	0.02663
H	-3.82983	2.80855	-1.91642
H	-2.00475	1.14855	-1.73473

H	3.72954	-3.18779	-1.56960
H	4.45070	-2.60095	-0.03410
H	2.96965	-3.58210	0.00382
H	0.29866	0.80273	-1.63670
C	-4.52550	-0.97936	-0.84840
C	-3.66827	-0.63885	0.18938
C	-2.44272	-1.30808	0.34149
C	-2.10118	-2.34755	-0.57224
C	-2.98557	-2.67023	-1.62606
C	-4.18233	-1.99058	-1.76399
H	-1.81179	-0.30544	2.17746
H	-5.47245	-0.45986	-0.95271
H	-3.94240	0.14035	0.89218
C	-1.48332	-0.93039	1.35435
C	-0.89215	-3.07651	-0.35933
H	-2.71857	-3.46428	-2.31685
H	-4.86294	-2.24374	-2.56966
C	-0.05946	-2.82916	0.70822
C	-0.38421	-1.79656	1.61783
H	-0.64926	-3.88229	-1.04661
H	0.81371	-3.44322	0.89232
O	0.33123	-1.56093	2.71111
H	1.28735	-1.76025	2.54153
Ag	3.20323	1.55518	-0.72741

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Name: TS1 Energy: -478180.8838067

C	-0.20799	0.40382	-0.96751

C	-1.26246	-0.23543	-0.11611
C	0.82683	0.04666	0.16699
C	-0.28429	-0.81451	0.84634
C	-2.65633	-0.17181	-0.12841
C	1.18504	1.20527	1.05770
O	0.92362	1.21011	2.24336
C	-3.40757	-0.81666	0.89976
C	-4.78746	-0.76409	0.87966
C	-5.43788	-0.07196	-0.15565
C	-4.71857	0.57191	-1.17733
C	-3.33859	0.52899	-1.16771
O	1.77317	2.30234	0.52060
C	2.40634	2.30753	-0.75949
H	-0.37859	1.46232	-1.19629
H	-0.07081	-0.12403	-1.91912
H	-0.46035	-0.58110	1.90468
H	-0.18984	-1.90195	0.74219
H	-2.88402	-1.33819	1.69392
H	-5.36834	-1.24751	1.65694
H	-6.52291	-0.03020	-0.16498
H	-5.24810	1.10024	-1.96203
H	-2.76481	1.02242	-1.94507
H	2.73495	3.33457	-0.91787
H	3.28388	1.64924	-0.76574
H	1.73397	2.01785	-1.57140
Ag	2.65230	-0.99152	-0.29652

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Name: INT3 Energy: -1057233.0071128

C	3.30765	1.00876	-0.56095
C	4.28606	-0.10470	-0.31443
C	0.64194	2.72791	-0.79930
C	2.34798	1.36021	0.61238
C	1.14016	1.35805	-0.37787
C	2.06749	0.65744	-1.42167
C	0.17137	2.93660	-2.10227
C	-0.36741	4.16576	-2.48075
C	-0.44833	5.20793	-1.55694
C	0.00933	5.00986	-0.25400
C	0.54796	3.77971	0.12093
O	3.99266	-1.26235	0.02505
O	5.53917	0.25381	-0.49053
C	6.56464	-0.75060	-0.26819
H	2.56692	2.28775	1.13989
H	1.89860	-0.41921	-1.47722
H	2.06696	1.06071	-2.43358
H	0.21973	2.13309	-2.83099
H	-0.71973	4.30928	-3.49737
H	-0.86195	6.16722	-1.85082
H	-0.05075	5.81359	0.47297
H	0.87985	3.63840	1.14370
H	7.50492	-0.24130	-0.46613
H	6.51852	-1.10430	0.76280
H	6.41817	-1.58597	-0.95434
Ag	2.07331	-2.14684	0.50099

H	2.29085	0.54421	1.33712
C	-0.96911	1.97475	3.50888
C	-0.28716	1.28452	2.50734
C	-0.84669	1.13350	1.23764
C	-2.13875	1.66741	0.99672
C	-2.81044	2.37762	2.01401
C	-2.22786	2.53822	3.25995
H	0.38109	-0.45152	0.51885
H	-0.52084	2.06928	4.49266
H	0.67776	0.84508	2.72959
C	-0.07709	0.46710	0.12718
C	-2.78374	1.41293	-0.25335
H	-3.79739	2.78173	1.80987
H	-2.74767	3.07943	4.04285
C	-2.21583	0.61040	-1.21996
C	-0.95503	0.06182	-1.00215
H	-3.75973	1.85063	-0.43266
H	-2.77183	0.35210	-2.11524
O	-0.39050	-0.75468	-1.88778
H	-1.06227	-1.15714	-2.46399
H	3.84764	1.88028	-0.92915
C	-5.52591	-1.50899	-1.28311
C	-4.50836	-2.34548	-1.71310
C	-3.33813	-2.52088	-0.94222
C	-3.21318	-1.83023	0.30644
C	-4.27540	-0.99480	0.73203
C	-5.40851	-0.83698	-0.05116

H	-2.36269	-3.91388	-2.29103
H	-6.41932	-1.38346	-1.88555
H	-4.60306	-2.88075	-2.65431
C	-2.24959	-3.34197	-1.37292
C	-1.99400	-1.90540	1.01904
H	-4.19216	-0.48763	1.68813
H	-6.21789	-0.19953	0.29184
C	-0.91259	-2.67743	0.56095
C	-1.08666	-3.42637	-0.65030
H	-1.88440	-1.37892	1.96097
H	-0.26285	-4.05018	-0.98497
O	0.21483	-2.69150	1.23531

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Name: INT2 Energy: -1057219.0594787

C	-0.09688	-1.37887	-0.47570
C	0.23757	-2.76909	-0.70900
C	1.15511	1.84039	-0.41118
C	0.70877	-0.55905	0.57133
C	1.23128	0.34505	-0.58641
C	0.16153	-0.28596	-1.53225
C	1.09375	2.66235	-1.54472
C	1.07808	4.04978	-1.41886
C	1.11156	4.63745	-0.15092
C	1.16108	3.82771	0.98370
C	1.18971	2.43806	0.85286
O	0.49834	-3.30883	-1.81461
O	0.25772	-3.51505	0.41580

C	0.50665	-4.92246	0.25444
H	1.44163	-1.11644	1.15823
H	-0.67314	0.41189	-1.63000
H	0.46240	-0.59524	-2.53199
H	1.06188	2.21243	-2.53361
H	1.03696	4.67256	-2.30706
H	1.10127	5.71814	-0.05055
H	1.19259	4.27613	1.97189
H	1.25931	1.81967	1.74155
H	0.51864	-5.33012	1.26413
H	-0.28718	-5.38491	-0.33647
H	1.46320	-5.10081	-0.24153
H	0.09229	0.01464	1.26365
C	4.97746	2.02450	1.25260
C	4.14982	1.68340	0.18244
C	3.73741	0.36318	0.00559
C	4.20002	-0.62760	0.90874
C	5.02456	-0.26633	1.99499
C	5.40496	1.05481	2.16933
H	2.90199	0.56613	-1.97610
H	5.29339	3.05565	1.37303
H	3.82463	2.44819	-0.51320
C	2.76959	-0.02611	-1.06820
C	3.90007	-2.00342	0.64381
H	5.36902	-1.03604	2.67907
H	6.04317	1.33485	3.00030
C	3.23824	-2.42612	-0.48368

C	2.77918	-1.46957	-1.41686
H	4.27923	-2.74703	1.34044
H	3.12726	-3.47960	-0.70985
O	2.27360	-1.80595	-2.56287
H	1.57436	-2.59766	-2.43149
Ag	-2.21390	-1.45805	0.00385
C	-4.36243	-0.76301	0.95889
C	-4.33389	-0.16105	-0.30395
C	-3.68292	1.08973	-0.50865
C	-3.06542	1.72933	0.61971
C	-3.13609	1.12044	1.89935
C	-3.77467	-0.09115	2.08064
H	-4.08131	1.20818	-2.63296
H	-4.94184	-1.67001	1.11454
H	-4.85544	-0.63111	-1.13282
C	-3.60595	1.69884	-1.78851
C	-2.38260	2.95649	0.41164
H	-2.69259	1.61132	2.75912
C	-2.32096	3.51943	-0.84199
C	-2.93680	2.88967	-1.95200
H	-1.90007	3.43971	1.25436
H	-1.78804	4.45214	-0.98447
H	-2.88156	3.35308	-2.93142
O	-3.80965	-0.62518	3.32667
H	-4.35583	-1.42228	3.33929

27

Name: INT1 Energy: -478188.7256532

C	0.06860	0.06586	-1.67357
C	-0.88345	-0.84548	-0.99482
C	0.67747	-0.26700	-0.26090
C	0.09361	-1.72919	-0.33267
C	-2.19500	-0.50552	-0.53759
C	0.23328	0.46894	0.99206
O	-0.14589	-0.14900	1.96219
C	-2.81414	-1.24728	0.49775
C	-4.09007	-0.91319	0.92389
C	-4.77056	0.15148	0.32193
C	-4.17843	0.88561	-0.71479
C	-2.90042	0.56542	-1.14131
O	0.30283	1.81215	1.05259
C	0.80627	2.65400	0.00902
H	-0.25690	1.07634	-1.89558
H	0.64978	-0.36810	-2.48529
H	-0.17797	-2.19620	0.60878
H	0.66780	-2.37455	-0.99391
H	-2.28896	-2.07076	0.96453
H	-4.55934	-1.47633	1.72273
H	-5.77056	0.40771	0.65701
H	-4.72089	1.69950	-1.18293
H	-2.44952	1.12064	-1.95628
H	1.11450	3.57680	0.49957
H	1.66785	2.21193	-0.50217
H	0.02179	2.88177	-0.71773
Ag	2.86306	-0.28714	-0.02917

20

Name: FEnergy: -381656.8889396

C	-0.99269	0.75347	1.10058
C	-0.05944	-0.30668	1.28115
C	1.21004	-0.28309	0.64194
C	1.53059	0.84999	-0.18752
C	0.59450	1.90565	-0.33657
C	-0.63807	1.88105	0.29114
H	1.93036	-2.15293	1.47518
H	-1.86187	0.81053	1.75476
H	-0.26322	-1.06402	2.03564
C	2.17312	-1.31130	0.83235
C	2.80410	0.89064	-0.81456
H	0.85091	2.77438	-0.93497
C	3.71222	-0.12688	-0.61755
C	3.40000	-1.23228	0.21465
H	3.05533	1.73991	-1.44238
H	4.68450	-0.08112	-1.09777
H	4.13688	-2.01414	0.36580
O	-1.47657	2.92558	0.10234
H	-2.21162	2.91311	0.73070
Ag	-1.72160	-0.94582	-0.38594

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Name: E Energy: -675811.0295162

C	-2.11415	-1.35248	-0.46920
C	-3.42403	-0.61349	-0.27820
C	1.21678	-1.61102	0.00252

C	-0.92191	-0.52909	-1.07360
C	-0.05772	-0.81096	0.19932
C	-1.24236	-1.66000	0.78194
C	1.69656	-2.40958	1.05415
C	2.86250	-3.15902	0.90912
C	3.57006	-3.12659	-0.29551
C	3.10686	-2.33462	-1.34530
C	1.94389	-1.57636	-1.19433
O	-3.67518	0.25741	0.55928
O	-4.32440	-0.99877	-1.17012
C	-5.62632	-0.36149	-1.12014
H	-1.13555	0.51685	-1.29489
H	-0.98313	-2.71731	0.84559
H	-1.65320	-1.35085	1.74003
H	1.15100	-2.45638	1.99354
H	3.21259	-3.77547	1.73112
H	4.47279	-3.71738	-0.41367
H	3.64901	-2.30368	-2.28524
H	1.61084	-0.95498	-2.01969
H	-6.20310	-0.83250	-1.91317
H	-6.08792	-0.53248	-0.14658
H	-5.52566	0.71087	-1.29541
H	-0.52970	-0.99038	-1.97947
C	3.73372	1.77402	-0.11557
C	2.76066	1.01337	0.53778
C	1.41403	1.36481	0.45231
C	1.06263	2.53186	-0.28241

C	2.05674	3.28071	-0.95334
C	3.38557	2.89950	-0.87454
H	0.66525	0.11998	2.05264
H	4.77679	1.48650	-0.02891
H	3.05942	0.14767	1.11760
C	0.33182	0.54711	1.10265
C	-0.28418	3.00167	-0.24049
H	1.76760	4.16723	-1.51001
H	4.15279	3.47568	-1.38016
C	-1.26520	2.41531	0.53289
C	-0.93585	1.29117	1.30824
H	-0.52680	3.90361	-0.79781
H	-2.25418	2.85229	0.61497
O	-1.77578	0.77522	2.16596
H	-2.70106	0.76973	1.76241
H	-2.33563	-2.23889	-1.06357

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Name: D Energy: -289169.7994639

C	-2.89453	0.41569	-0.00034
C	-1.80393	1.26882	-0.00044
C	-0.48011	0.78511	-0.00002
C	-0.23371	-0.64061	0.00034
C	-1.38647	-1.49044	0.00026
C	-2.66682	-0.98239	-0.00006
H	0.48685	2.72267	0.00060
H	-3.90835	0.80824	-0.00069
H	-1.95570	2.34847	-0.00066

C 0.65818 1.64476 0.00035

C 1.07849 -1.13162 0.00053

H -1.22760 -2.56750 0.00048

H -3.51631 -1.66409 -0.00007

C 2.23840 -0.28940 -0.00009

C 1.93134 1.14778 0.00055

H 1.24468 -2.20775 0.00068

H 2.79066 1.81657 0.00085

O 3.43009 -0.70286 -0.00096

45

Name: cis-3aa Energy: -675560.0476915

C 1.67270 -2.08338 -0.62466

C 2.94198 -1.33379 -0.31913

C 0.11384 0.39272 0.55200

C -1.65067 -1.34346 0.07860

H 1.95517 -3.00146 -1.14904

C 0.69772 -2.22662 0.55583

C -0.15758 -1.01880 0.01757

C 0.60465 -1.21519 -1.35154

C -0.44597 1.49086 -0.20477

C -0.27851 2.84134 0.24495

C 0.42422 3.08589 1.45259

C 0.94972 2.04353 2.16107

C 0.81048 0.70062 1.71546

C -1.19048 1.30132 -1.40411

C -1.70745 2.36362 -2.11270

C -1.52095 3.68958 -1.66756

C	-0.82171	3.91494	-0.50549
C	-2.45834	-0.77241	1.07020
C	-3.80425	-1.11507	1.18680
C	-4.37573	-2.03723	0.31077
C	-3.58167	-2.62134	-0.67521
C	-2.23357	-2.28154	-0.78386
O	1.39580	-0.23072	2.53900
O	3.33741	-0.99570	0.78700
O	3.63319	-1.06931	-1.43675
C	4.85122	-0.32227	-1.25660
H	0.10890	-3.13804	0.43765
H	1.07883	-2.18894	1.56969
H	0.04906	-1.79789	-2.08723
H	0.96584	-0.30479	-1.82963
H	0.54151	4.10918	1.79798
H	1.49898	2.19554	3.08366
H	-1.38344	0.30161	-1.76589
H	-2.27169	2.17437	-3.02095
H	-1.93304	4.51891	-2.23381
H	-0.67416	4.92614	-0.13586
H	-2.02735	-0.04779	1.75146
H	-4.40768	-0.65500	1.96362
H	-5.42576	-2.29926	0.39624
H	-4.00946	-3.34457	-1.36329
H	-1.63723	-2.76204	-1.55278
H	2.15519	-0.61915	2.05573
H	5.26065	-0.18750	-2.25659

H 4.63817 0.64262 -0.79179

H 5.54840 -0.87602 -0.62426

65

Name: C Energy: -1057197.2816433

C -0.19275 1.44624 -1.04131

C 0.12862 2.59365 -0.31639

C -2.53855 -1.11754 -1.25806

C -0.39272 0.09809 -0.36685

C -1.89226 0.16435 -0.80819

C -1.46346 1.25016 -1.85893

C -3.31621 -1.16996 -2.42156

C -3.96073 -2.35023 -2.79185

C -3.83649 -3.49447 -2.00128

C -3.05393 -3.45541 -0.84639

C -2.40764 -2.27458 -0.47914

O 0.89643 2.63749 0.72436

O -0.41773 3.75336 -0.74785

C 0.06783 4.96796 -0.15573

H -0.14680 -0.01211 0.69024

H -1.28425 0.75771 -2.82115

H -2.11540 2.10964 -2.01696

H -3.41142 -0.28457 -3.04295

H -4.55154 -2.38043 -3.70218

H -4.33480 -4.41383 -2.29158

H -2.93996 -4.34594 -0.23586

H -1.79711 -2.24956 0.41838

H -0.46665 5.76973 -0.66453

H	-0.13935	4.99341	0.91632
H	1.14442	5.07479	-0.31319
Ag	2.61082	1.39073	0.44396
H	0.06402	-0.73218	-0.91375
C	3.57805	0.57720	-1.51328
C	4.48511	0.18324	-0.51765
C	4.47380	-1.15609	-0.01273
C	3.52844	-2.08199	-0.56341
C	2.59371	-1.63908	-1.54007
C	2.57849	-0.33601	-1.98569
H	6.11162	-0.88930	1.37417
H	3.69096	1.52926	-2.02540
H	5.30735	0.84087	-0.24599
C	5.38934	-1.59550	0.97448
C	3.53403	-3.41873	-0.08845
H	1.85315	-2.33083	-1.92933
C	4.43190	-3.81701	0.87758
C	5.36866	-2.90136	1.41272
H	2.82107	-4.12455	-0.50387
H	4.42897	-4.84405	1.22828
H	6.07588	-3.23401	2.16520
O	1.63317	0.09208	-2.86297
H	1.13840	0.83651	-2.43018
C	-5.11667	-0.00405	0.28276
C	-4.81638	-0.78670	1.37969
C	-3.61831	-0.61989	2.13630
C	-2.65478	0.32133	1.69051

C	-2.78969	0.93780	0.33717
C	-4.16818	0.91089	-0.18217
H	-4.17320	-2.02121	3.68577
H	-6.07318	-0.10098	-0.22164
H	-5.54626	-1.51451	1.72275
C	-3.43151	-1.29780	3.36090
C	-1.56856	0.62167	2.51282
H	-2.37554	1.95151	0.32663
C	-1.40789	-0.04317	3.73015
C	-2.32608	-1.01796	4.14745
H	-0.85375	1.38174	2.21066
H	-0.56415	0.20671	4.36567
H	-2.18328	-1.53104	5.09215
O	-4.40377	1.72358	-1.19903
H	-5.28382	1.57029	-1.58039

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Name: B-trans Energy: -767698.6458171

C	-1.87724	0.36753	-0.31403
C	-3.08580	0.92621	-0.98060
C	1.38255	1.60982	-0.34137
C	-1.04234	1.25169	0.63657
C	0.25172	0.67323	-0.01068
C	-0.63096	0.17069	-1.18807
C	2.25286	1.32049	-1.39904
C	3.34718	2.14528	-1.66512
C	3.58198	3.27294	-0.87750
C	2.71076	3.57855	0.16992

C	1.61996	2.75127	0.43609
O	-3.35965	0.76160	-2.15404
O	-3.83876	1.65647	-0.12498
C	-5.03704	2.22241	-0.69126
H	-1.17270	1.16437	1.71437
H	-0.61084	0.91833	-1.98939
H	-0.42073	-0.79414	-1.64504
H	2.07253	0.44860	-2.02029
H	4.00835	1.91265	-2.49396
H	4.42763	3.91920	-1.08905
H	2.87403	4.46744	0.77126
H	0.94113	3.00169	1.24619
H	-5.50233	2.78840	0.11432
H	-4.79131	2.87513	-1.53136
H	-5.70311	1.42980	-1.04063
H	-1.14752	2.30864	0.36758
C	1.81914	-3.30379	-1.54727
C	1.03445	-2.50006	-0.71597
C	1.62773	-1.53408	0.09336
C	3.04363	-1.42401	0.09791
C	3.82458	-2.23005	-0.75922
C	3.21277	-3.15713	-1.58681
H	-0.10380	-1.06021	1.27552
H	1.34054	-4.05554	-2.16658
H	-0.04103	-2.64311	-0.68707
C	0.80986	-0.58125	0.90456
C	3.66033	-0.55388	1.04128

H 4.90508 -2.12501 -0.74850

H 3.80702 -3.78143 -2.24456

C 2.95205 0.12058 2.01749

C 1.55842 0.03662 2.01831

H 4.74344 -0.46688 1.02785

H 3.46724 0.70738 2.77141

O 0.81473 0.58958 2.95601

H 1.35180 1.06875 3.60947

Ag -2.66969 -1.42816 0.58109

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Name: B-O Energy: -767695.3504512

C 2.42259 -0.03023 0.07866

C 2.43782 -1.42369 0.63201

C -0.54503 1.93272 0.18654

C 1.15383 0.17271 -0.83749

C 0.40149 0.80024 0.35343

C 1.74171 0.95371 1.09658

C -0.75185 2.82733 1.24468

C -1.69725 3.84310 1.12500

C -2.43951 3.96981 -0.05280

C -2.23391 3.08319 -1.11085

C -1.28925 2.06524 -0.99105

O 1.47927 -1.92743 1.26561

O 3.52000 -2.13414 0.41709

C 3.54531 -3.49868 0.92752

H 0.70830 -0.70585 -1.30967

H 2.11394 1.97244 0.99325

H	1.75161	0.67991	2.15521
H	-0.18216	2.72105	2.16327
H	-1.85474	4.53581	1.94514
H	-3.17475	4.76259	-0.14569
H	-2.81096	3.18066	-2.02431
H	-1.14414	1.36337	-1.80636
H	4.51735	-3.88819	0.63527
H	3.43359	-3.48543	2.01203
H	2.73672	-4.07465	0.47631
H	1.32859	0.92492	-1.60624
C	-6.31911	-0.45753	-0.03738
C	-5.15710	0.02127	0.52226
C	-3.92365	-0.64195	0.29302
C	-3.90241	-1.81570	-0.53077
C	-5.12032	-2.28321	-1.08995
C	-6.30082	-1.61887	-0.84876
H	-2.70449	0.71401	1.47936
H	-7.25916	0.05390	0.14228
H	-5.16687	0.91119	1.14438
C	-2.71036	-0.17034	0.85399
C	-2.66684	-2.47655	-0.75794
H	-5.10471	-3.17376	-1.71108
H	-7.22711	-1.98363	-1.28044
C	-1.49286	-1.99827	-0.22087
C	-1.54573	-0.83705	0.57883
H	-2.65611	-3.37565	-1.36618
H	-0.55411	-2.51706	-0.37723

O -0.33560 -0.32753 1.13413

H 0.42939 -1.11964 1.27967

Ag 4.33766 0.49178 -0.71961

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Name: B Energy: -767702.6367334

C 1.60634 0.26440 0.10510

C 2.37086 -0.96698 0.38415

C -1.54319 1.63452 0.30583

C 0.32545 0.13250 -0.76450

C -0.52841 0.53364 0.47715

C 0.78599 0.93471 1.22374

C -1.91649 2.40308 1.41775

C -2.88158 3.40082 1.30018

C -3.48644 3.64583 0.06409

C -3.12108 2.88748 -1.04771

C -2.15966 1.88307 -0.92570

O 2.68828 -1.40917 1.49975

O 2.71751 -1.62235 -0.74096

C 3.54163 -2.79255 -0.57633

H 0.15712 -0.84958 -1.21009

H 0.87139 2.02158 1.22421

H 0.94625 0.58408 2.24163

H -1.44782 2.22101 2.38163

H -3.15809 3.99015 2.16849

H -4.23564 4.42519 -0.02968

H -3.58718 3.07190 -2.01034

H -1.90335 1.28295 -1.79259

H	3.71602	-3.16636	-1.58370
H	4.48458	-2.52750	-0.09356
H	3.03430	-3.54622	0.02986
H	0.23673	0.87596	-1.55509
C	-4.55159	-1.05255	-0.77150
C	-3.61767	-0.60779	0.16539
C	-2.38509	-1.24730	0.28297
C	-2.11167	-2.37234	-0.53974
C	-3.06088	-2.80100	-1.49419
C	-4.27134	-2.13897	-1.61269
H	-1.72289	-0.30113	2.11099
H	-5.50925	-0.54785	-0.84698
H	-3.85189	0.23698	0.80243
C	-1.31719	-0.74462	1.19961
C	-0.91372	-3.11712	-0.31765
H	-2.83657	-3.66142	-2.11722
H	-5.00576	-2.46745	-2.33978
C	-0.02846	-2.83875	0.70275
C	-0.28647	-1.74557	1.54740
H	-0.73144	-3.98545	-0.94594
H	0.81070	-3.49103	0.91226
O	0.41832	-1.49938	2.61935
H	1.39909	-1.68138	2.44463
Ag	3.17117	1.53182	-0.71432

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Name: Ag Energy: -92136.9129415

Ag	0.00000	0.00000	0.00000

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Name: A Energy: -478190.3030124

C	-0.89655	0.31389	0.16433
C	-2.06302	1.22091	0.39536
C	2.57701	0.37351	0.01026
C	0.13336	0.76957	-0.92768
C	1.19901	0.59797	0.10345
C	0.23080	0.47587	1.22452
C	3.34159	0.11617	1.18608
C	4.71055	-0.04934	1.09690
C	5.33782	0.03182	-0.15699
C	4.60432	0.28144	-1.32851
C	3.23503	0.44990	-1.25234
O	-2.33222	1.71487	1.47303
O	-2.76455	1.42946	-0.73527
C	-3.91948	2.28897	-0.60142
H	-0.01261	1.82837	-1.19010
H	0.43334	-0.29168	1.97560
H	0.07942	1.42598	1.76478
H	2.84072	0.05872	2.14655
H	5.29990	-0.24202	1.98627
H	6.41326	-0.10247	-0.22243
H	5.11311	0.34014	-2.28409
H	2.65349	0.64609	-2.14682
H	-4.34016	2.36727	-1.60219
H	-4.63986	1.84478	0.08858
H	-3.62082	3.26968	-0.22663

Ag -1.71593 -1.65407 -0.08112

H 0.26038 0.21786 -1.86248

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Name: 2a Energy: -289495.6685303

C 1.05330 -1.09288 -0.00000

C -0.28497 -0.62267 0.00000

C -0.52973 0.78854 0.00000

C 0.58471 1.66996 0.00000

C 1.87142 1.19399 -0.00000

C 2.10744 -0.20494 -0.00001

C -1.39726 -1.50496 -0.00000

C -2.68461 -1.01780 -0.00000

C -2.92554 0.37677 0.00000

C -1.86775 1.25751 0.00000

O 3.41750 -0.59182 -0.00002

H 0.40323 2.74110 0.00002

H 2.72671 1.86061 0.00000

H -1.21477 -2.57614 -0.00001

H -3.52401 -1.70660 -0.00001

H -3.94578 0.74720 -0.00000

H -2.04295 2.33002 -0.00000

H 3.45865 -1.55727 0.00013

H 1.23693 -2.16541 0.00006

26

Name: 1a Energy: -386036.4482026

C -1.05825 -1.69605 1.26863

C -0.12428 -1.55012 0.10848

C	-1.60260	-1.09979	0.00273
C	-1.01710	-2.07075	-0.97426
C	1.06255	-0.68874	0.01985
C	-1.90773	0.29667	-0.30653
O	-1.94671	0.75935	-1.43147
C	1.44530	-0.08962	-1.19129
C	2.55397	0.75018	-1.24229
C	3.30412	1.00193	-0.09149
C	2.93522	0.40564	1.11403
C	1.82445	-0.43419	1.16934
O	-2.08785	1.03018	0.81737
C	-2.27532	2.43530	0.59134
H	-0.91424	-1.01424	2.10238
H	-1.40693	-2.69098	1.54967
H	-0.85595	-1.70076	-1.98253
H	-1.34925	-3.10854	-0.91921
H	0.86285	-0.26504	-2.08866
H	2.83232	1.21205	-2.18461
H	4.17061	1.65424	-0.13631
H	3.51483	0.58998	2.01350
H	1.54641	-0.90638	2.10599
H	-2.40794	2.87682	1.57862
H	-1.40193	2.86307	0.09312
H	-3.15630	2.61101	-0.03036

46

Name: TSene2 Energy: -675807.4035532

C	-2.15357	-1.38503	-0.52975

C	-3.44602	-0.61950	-0.32441
C	1.19070	-1.67989	-0.03602
C	-0.94427	-0.56571	-1.11203
C	-0.10752	-1.03165	0.07948
C	-1.30921	-1.70091	0.74240
C	1.63650	-2.56317	0.97357
C	2.85152	-3.22323	0.84924
C	3.64604	-3.01943	-0.28655
C	3.22755	-2.14010	-1.28706
C	2.01757	-1.46330	-1.15863
O	-3.63895	0.23879	0.52916
O	-4.36444	-0.97548	-1.21569
C	-5.64527	-0.30075	-1.14143
H	-1.11798	0.50937	-1.18322
H	-1.16420	-2.76433	0.94543
H	-1.68267	-1.22269	1.64880
H	1.02029	-2.73556	1.85110
H	3.17919	-3.90589	1.62640
H	4.58869	-3.54781	-0.38852
H	3.84412	-1.98161	-2.16574
H	1.70144	-0.77849	-1.93858
H	-6.24611	-0.74079	-1.93451
H	-6.10175	-0.47230	-0.16534
H	-5.51464	0.77099	-1.30088
H	-0.58617	-0.91957	-2.08111
C	3.72112	1.77217	-0.16702
C	2.78913	1.07816	0.59583

C	1.43076	1.43649	0.55694
C	1.03083	2.52954	-0.26912
C	1.99493	3.21219	-1.04580
C	3.32564	2.83648	-0.99612
H	0.74010	0.07511	2.12246
H	4.76868	1.49256	-0.11628
H	3.11111	0.26685	1.24033
C	0.42038	0.72002	1.31043
C	-0.33216	2.95363	-0.23437
H	1.68012	4.04468	-1.66828
H	4.06543	3.36871	-1.58455
C	-1.26432	2.37070	0.59382
C	-0.87139	1.30366	1.43474
H	-0.62672	3.79539	-0.85581
H	-2.28044	2.74553	0.64621
O	-1.70296	0.77688	2.33167
H	-2.62206	0.82682	1.98291
H	-2.35935	-2.27065	-1.13080

46

Name: TSene1 Energy: -767704.9628232

C	2.38585	1.53709	-0.99334
C	3.60422	0.83343	-0.44931
C	-0.89256	2.59003	-0.28365
C	0.99585	0.87023	-0.88086
C	0.42748	2.10225	-0.42614
C	1.77817	2.74641	-0.20718
C	-1.11720	3.91395	0.17277

C	-2.41031	4.39555	0.29554
C	-3.49494	3.56799	-0.02735
C	-3.29129	2.25479	-0.47173
C	-2.00311	1.76435	-0.59920
O	3.78890	-0.38511	-0.45161
O	4.51079	1.68934	-0.01337
C	5.76367	1.14181	0.47381
H	0.96591	0.11265	0.08574
H	1.91648	3.73562	-0.65194
H	2.08064	2.79451	0.84398
H	-0.27111	4.54745	0.41883
H	-2.58468	5.40876	0.64067
H	-4.50629	3.94896	0.07474
H	-4.13601	1.61256	-0.69536
H	-1.83953	0.74062	-0.91537
H	6.35907	2.00612	0.75907
H	5.57625	0.49608	1.33326
H	6.25250	0.57334	-0.31864
Ag	2.33154	-2.13327	0.02314
H	0.53640	0.25005	-1.65391
C	-1.35288	-0.48624	1.93019
C	-2.72163	-0.47533	1.84932
C	-3.40304	-1.11075	0.77387
C	-2.63165	-1.80534	-0.21646
C	-1.21744	-1.80500	-0.10872
C	-0.58065	-1.14235	0.92926
H	-5.39385	-0.55121	1.40275

H	-0.82718	0.01039	2.73861
H	-3.30792	0.03320	2.60934
C	-4.81429	-1.07120	0.64507
C	-3.31055	-2.43726	-1.29291
H	-0.62221	-2.31700	-0.86336
C	-4.68208	-2.37584	-1.39179
C	-5.44236	-1.68542	-0.41679
H	-2.72861	-2.96889	-2.04071
H	-5.18842	-2.86163	-2.21972
H	-6.52333	-1.65025	-0.50537
O	0.76269	-0.98272	0.97308
H	2.62510	1.83113	-2.02166

27

Name: INTene3 Energy: -386300.5078706

C	-1.52565	-0.00009	-0.53364
C	-2.89401	-0.00048	0.12871
C	1.88132	0.00002	0.01132
C	-0.53854	1.07975	0.03093
C	0.48597	-0.00013	0.09370
C	-0.53837	-1.08011	0.03006
C	2.60130	-1.23326	-0.00772
C	3.98236	-1.22589	-0.03608
C	4.66847	0.00027	-0.05133
C	3.98216	1.22630	-0.03523
C	2.60110	1.23342	-0.00682
O	-3.01691	-0.00187	1.33651
O	-3.88185	0.00099	-0.76035

C	-5.22834	0.00090	-0.21621
H	-0.87136	1.34684	1.04615
H	-0.32157	-1.98833	-0.53654
H	-0.87127	-1.34819	1.04499
H	2.05761	-2.17198	0.00597
H	4.53694	-2.15758	-0.04787
H	5.75422	0.00036	-0.07721
H	4.53659	2.15809	-0.04637
H	2.05725	2.17204	0.00754
H	-5.88662	0.00273	-1.08231
H	-5.38368	-0.89166	0.39193
H	-5.38262	0.89160	0.39493
H	-0.32198	1.98854	-0.53484
H	-1.58006	0.00039	-1.62171

46

Name: INTene2 Energy: -767713.4671327

C	-0.89344	1.47616	0.53142
C	-2.21107	2.10228	0.18025
C	2.48890	1.33228	-0.44230
C	-0.10308	0.80556	-0.64560
C	1.14126	1.41645	-0.08465
C	0.37314	2.31923	0.85057
C	3.45972	2.15868	0.19410
C	4.77277	2.14942	-0.23573
C	5.15785	1.31365	-1.29810
C	4.23244	0.45999	-1.90593
C	2.91468	0.44576	-1.47175

O	-3.22401	1.43531	-0.07916
O	-2.21006	3.41491	0.14726
C	-3.45832	4.07779	-0.20390
H	-0.36029	1.20183	-1.63629
H	0.68886	2.37915	1.89446
H	0.30544	3.33968	0.45198
H	3.15108	2.81361	1.00223
H	5.50559	2.79323	0.23847
H	6.18774	1.32211	-1.64026
H	4.54530	-0.19669	-2.71041
H	2.19183	-0.21943	-1.93072
H	-3.23246	5.14071	-0.16554
H	-3.76538	3.77454	-1.20554
H	-4.22964	3.81182	0.51965
Ag	-3.16656	-0.76490	-0.20797
H	-0.16255	-0.28975	-0.68201
C	-0.05177	-3.33624	-0.94549
C	1.29329	-3.17087	-0.76423
C	1.81495	-2.29801	0.24350
C	0.88756	-1.65649	1.13352
C	-0.48745	-1.87839	0.96466
C	-1.00157	-2.62837	-0.12078
H	3.88302	-2.49616	-0.30996
H	-0.44667	-3.96790	-1.73375
H	1.99489	-3.68687	-1.41431
C	3.18227	-2.00883	0.36188
C	1.39614	-0.73502	2.09452

H	-1.19742	-1.43162	1.65751
C	2.75751	-0.49460	2.20473
C	3.65475	-1.11465	1.32617
H	0.70201	-0.27007	2.78964
H	3.12713	0.19310	2.95851
H	4.71687	-0.90883	1.39769
O	-2.26813	-2.66261	-0.41999
H	-1.08250	0.73237	1.30712

46

Name: INTene1 Energy: -767737.5241766

C	-3.64436	-0.06049	1.37028
C	-3.90403	-1.17462	0.38405
C	-0.89809	2.18646	0.90846
C	-2.19243	0.10721	1.78798
C	-2.02638	1.29225	1.14496
C	-3.47442	1.35060	0.66593
C	-0.98557	3.16516	-0.09779
C	0.13153	3.93537	-0.43028
C	1.33828	3.74566	0.25050
C	1.42535	2.78903	1.26762
C	0.31826	2.01317	1.59334
O	-3.13357	-1.49841	-0.53451
O	-5.05736	-1.77281	0.56272
C	-5.41843	-2.83685	-0.36085
H	0.49559	1.60265	-1.39608
H	-4.07939	2.13286	1.13116
H	-3.64573	1.36254	-0.41521

H	-1.92419	3.31605	-0.62261
H	0.05609	4.68919	-1.20734
H	2.20529	4.34566	-0.00520
H	2.36191	2.64081	1.79394
H	0.39362	1.26173	2.37280
H	-6.39339	-3.18129	-0.02445
H	-5.46930	-2.44136	-1.37615
H	-4.67845	-3.63644	-0.30773
Ag	-1.19573	-0.49974	-0.87931
H	-1.55208	-0.51733	2.40204
C	2.98367	1.05218	-1.34827
C	4.22448	0.65427	-0.90778
C	4.39994	-0.55678	-0.18707
C	3.25507	-1.37611	0.08149
C	1.98154	-0.93790	-0.36958
C	1.86723	0.24015	-1.05805
H	6.53927	-0.36106	0.06422
H	2.85462	1.96939	-1.91300
H	5.09455	1.26774	-1.12104
C	5.67329	-0.98251	0.27212
C	3.42782	-2.58764	0.79771
H	1.10181	-1.54597	-0.15860
C	4.67752	-2.97125	1.22949
C	5.80980	-2.16337	0.96542
H	2.56062	-3.21099	0.99749
H	4.80006	-3.90146	1.77488
H	6.78761	-2.48195	1.31113

O	0.59910	0.64197	-1.51480
H	-4.39483	-0.09312	2.16215

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Name: 4a Energy: -386050.5116913

C	-1.66876	0.27530	0.92448
C	-2.79770	0.29529	-0.08149
C	1.79651	-0.04639	0.14831
H	-2.08460	0.29340	1.93810
C	-0.62692	-0.81248	0.68039
C	0.37766	0.05964	0.45644
C	-0.50585	1.28610	0.65620
C	2.56217	1.11609	-0.03253
C	3.92103	1.03302	-0.32894
C	4.53601	-0.21321	-0.44911
C	3.78368	-1.37817	-0.27115
C	2.42795	-1.29672	0.02502
O	-2.84352	0.95944	-1.09417
O	-3.76310	-0.58187	0.27863
C	-4.85825	-0.69401	-0.64433
H	-0.71186	-1.89372	0.68852
H	-0.25298	1.91952	1.51296
H	-0.66541	1.90621	-0.22891
H	2.08342	2.08627	0.05834
H	4.49995	1.94110	-0.46696
H	5.59469	-0.27902	-0.68012
H	4.25838	-2.35030	-0.36391
H	1.84635	-2.20312	0.16366

H -5.53466 -1.43071 -0.21198

H -5.36215 0.26832 -0.76176

H -4.50333 -1.02521 -1.62327

27

Name: TS1' Energy: -478171.0520228

C 1.28096 1.23122 0.40805

C 2.18150 0.03032 0.30114

C 0.12912 0.23437 0.26737

C 1.06121 -0.96169 0.39064

C 3.55460 -0.10386 0.07568

C -1.22602 0.20554 0.18532

O -1.90039 -0.89760 0.21664

C 4.13327 -1.40147 -0.03728

C 5.49552 -1.53419 -0.22923

C 6.29669 -0.38420 -0.31434

C 5.74721 0.90410 -0.20797

C 4.38652 1.04962 -0.01626

O -2.03448 1.32123 0.06509

C -1.44316 2.58798 -0.23772

H 1.46187 1.99859 -0.35884

H 1.39165 1.73271 1.38664

H 1.05929 -1.73368 -0.39396

H 1.04819 -1.49806 1.35714

H 3.49432 -2.27547 0.03045

H 5.94633 -2.51642 -0.31521

H 7.36620 -0.49319 -0.46720

H 6.38990 1.77445 -0.27766

H	3.94132	2.03527	0.06771
H	-2.27057	3.27811	-0.40025
H	-0.83561	2.94976	0.59695
H	-0.83649	2.52145	-1.14603
Ag	-3.96302	-0.47466	-0.12438

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Name: TS1_BF4 Energy: -744780.5775394

C	0.61860	0.15359	0.75009
C	1.76746	0.20554	-0.18070
C	-0.08836	1.22404	-0.18887
C	1.08996	1.05113	-1.19425
C	3.10054	-0.24218	-0.05741
C	-0.13240	2.60836	0.32744
O	0.39365	3.55172	-0.24292
C	4.04962	0.05417	-1.06945
C	5.34539	-0.42068	-0.96050
C	5.70679	-1.19548	0.15104
C	4.78164	-1.49956	1.15948
C	3.48493	-1.02382	1.06272
O	-0.75517	2.85452	1.51571
C	-1.69292	1.93577	2.08306
H	0.86305	0.41408	1.78884
H	0.12476	-0.83118	0.75652
H	1.62807	1.98496	-1.42724
H	0.88039	0.53497	-2.13843
H	3.74722	0.65802	-1.91845
H	6.07845	-0.19697	-1.72764

H	6.72373	-1.56737	0.23222
H	5.08233	-2.10368	2.00827
H	2.75030	-1.25160	1.82776
H	-2.00636	2.38569	3.02644
H	-2.56692	1.81769	1.43188
H	-1.27440	0.94622	2.27596
Ag	-1.96669	0.37427	-0.77619
B	-2.31196	-2.21933	0.25105
F	-2.82470	-3.45629	0.48597
F	-1.03531	-2.26045	-0.36717
F	-2.20694	-1.42314	1.40604
F	-3.19214	-1.48682	-0.67913

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Name: TS1'_BF4Energy: -744766.1505884

C	-2.32932	0.92441	-0.63931
C	-3.35234	-0.04576	-0.09066
C	-1.35601	-0.20960	-0.32615
C	-2.40023	-1.18293	0.19954
C	-4.73696	0.07340	0.08203
C	-0.00171	-0.43446	-0.53827
O	0.54448	-1.56199	-0.33790
C	-5.48603	-1.00733	0.62681
C	-6.85390	-0.88536	0.79713
C	-7.49763	0.30624	0.43163
C	-6.77689	1.38286	-0.10661
C	-5.40868	1.27410	-0.28251
O	0.82158	0.54279	-1.01263

C	0.69329	1.89474	-0.53412
H	-2.23924	1.86935	-0.07638
H	-2.48067	1.20151	-1.69785
H	-2.33553	-1.48500	1.25870
H	-2.58269	-2.10264	-0.38311
H	-4.96914	-1.92006	0.90351
H	-7.42930	-1.70606	1.21181
H	-8.57087	0.39699	0.56779
H	-7.29359	2.29582	-0.38252
H	-4.83395	2.09568	-0.69670
H	1.69537	2.31453	-0.60916
H	-0.01561	2.45786	-1.14924
H	0.37510	1.89617	0.51159
Ag	2.70371	-1.13258	-0.17989
F	3.17719	0.83157	1.38564
F	3.90228	1.80923	-0.55694
F	4.70780	-0.26264	0.07093
F	5.34413	1.63543	1.24349
B	4.30669	1.08128	0.55908

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Name: TS-N1 Energy: -767686.2107067

C	1.58697	1.49551	0.00023
C	0.86230	2.63199	-0.45030
C	4.18579	-0.82668	-0.32573
C	1.79519	0.22428	-0.85026
C	3.21695	0.19059	-0.37970
C	3.08910	1.51943	0.28581

C	5.43432	-0.59946	0.32324
C	6.41508	-1.57563	0.31282
C	6.17659	-2.79751	-0.33487
C	4.95319	-3.04579	-0.97647
C	3.96493	-2.07737	-0.97252
O	-0.33771	2.58320	-0.86769
O	1.49317	3.81006	-0.35325
C	0.71235	5.00117	-0.59022
H	1.71525	0.41979	-1.93234
H	3.47675	1.57760	1.31090
H	3.58990	2.31944	-0.28542
H	5.61215	0.34861	0.82073
H	7.36577	-1.39958	0.80489
H	6.94782	-3.56181	-0.33783
H	4.78443	-3.99619	-1.47165
H	3.01673	-2.26296	-1.46707
H	1.38678	5.83181	-0.38626
H	0.36774	5.03293	-1.62534
H	-0.14973	5.03299	0.07998
Ag	-1.12368	1.00534	0.45858
H	1.23907	-0.70107	-0.65274
C	-2.10912	-0.51881	1.89004
C	-3.25348	0.01159	1.26650
C	-3.89156	-0.67305	0.19252
C	-3.34978	-1.93356	-0.22961
C	-2.20050	-2.46277	0.42138
C	-1.59383	-1.78994	1.45808

H	-5.46211	0.78870	-0.10709
H	-1.76671	-0.09696	2.83445
H	-3.72451	0.89869	1.68226
C	-5.05503	-0.16201	-0.44038
C	-3.99697	-2.62844	-1.28484
H	-1.80471	-3.42753	0.11975
C	-5.12224	-2.10448	-1.88332
C	-5.65872	-0.86394	-1.45917
H	-3.59547	-3.58397	-1.60944
H	-5.60898	-2.64909	-2.68650
H	-6.54943	-0.47130	-1.93871
O	-0.49589	-2.34083	2.04589
H	-0.27358	-1.86137	2.85519

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Name: INT-N1 Energy: -767689.3509712

C	1.19523	1.79068	0.02237
C	0.51873	2.97104	-0.36754
C	3.48104	-0.79886	-0.28117
C	1.29751	0.56124	-0.91083
C	2.67524	0.34413	-0.37918
C	2.71247	1.68710	0.27159
C	4.71307	-0.75375	0.42856
C	5.51821	-1.87686	0.49372
C	5.11183	-3.06148	-0.13780
C	3.89852	-3.12843	-0.84029
C	3.08614	-2.01179	-0.91295
O	-0.62731	2.99739	-0.92658

O	1.13047	4.12095	-0.06917
C	0.38490	5.34033	-0.26838
H	1.32408	0.85588	-1.97271
H	3.13351	1.72921	1.28202
H	3.27366	2.40860	-0.34535
H	5.01293	0.16750	0.91632
H	6.45796	-1.84560	1.03379
H	5.74465	-3.94154	-0.08018
H	3.60296	-4.05385	-1.32225
H	2.14571	-2.04849	-1.45253
H	1.04228	6.13663	0.07679
H	0.14231	5.47190	-1.32419
H	-0.53722	5.32323	0.31681
Ag	-1.87571	1.36621	-0.25714
H	0.61998	-0.29661	-0.82455
C	-1.71521	0.07430	1.67843
C	-2.92224	-0.38623	1.13282
C	-2.97648	-1.62868	0.42669
C	-1.77532	-2.40435	0.32034
C	-0.55722	-1.89361	0.84998
C	-0.50185	-0.67029	1.48563
H	-5.09012	-1.53991	-0.02238
H	-1.70104	0.91157	2.37184
H	-3.85285	0.11985	1.37866
C	-4.18280	-2.12893	-0.12067
C	-1.83434	-3.65588	-0.34357
H	0.35945	-2.46598	0.74303

C	-3.02109	-4.11504	-0.87265
C	-4.20500	-3.34891	-0.76067
H	-0.92933	-4.25075	-0.42343
H	-3.05313	-5.07645	-1.37488
H	-5.13241	-3.72922	-1.17531
O	0.67696	-0.15522	1.90686
H	0.74595	0.77287	1.50869

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Name: INT-N2 Energy: -386300.5995466

C	-1.52559	-0.00002	-0.54675
C	-2.88622	-0.00015	0.12366
C	1.87734	0.00001	0.01121
C	-0.53852	1.07904	0.01932
C	0.48425	-0.00003	0.08865
C	-0.53847	-1.07915	0.01906
C	2.59476	-1.23327	-0.00568
C	3.97517	-1.22598	-0.03087
C	4.66061	0.00007	-0.04484
C	3.97512	1.22609	-0.03063
C	2.59472	1.23333	-0.00545
O	-2.99894	-0.00053	1.33251
O	-3.88069	0.00028	-0.75644
C	-5.21960	0.00026	-0.19574
H	-0.87561	1.34659	1.03257
H	-0.31737	-1.98558	-0.54768
H	-0.87556	-1.34713	1.03218
H	2.04859	-2.17009	0.00707

H 4.53003 -2.15705 -0.04118

H 5.74603 0.00009 -0.06824

H 4.52995 2.15718 -0.04077

H 2.04851 2.17012 0.00748

H -5.88887 0.00019 -1.05302

H -5.36510 -0.89109 0.41635

H -5.36515 0.89168 0.41622

H -0.31753 1.98573 -0.54706

H -1.58221 0.00012 -1.63409

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Name: TS-N2 Energy: -767687.6244165

C 1.25747 1.75378 0.03474

C 0.67154 3.01294 -0.34627

C 3.32626 -0.97995 -0.27802

C 1.31852 0.58246 -0.99290

C 2.63715 0.23499 -0.39043

C 2.77576 1.56058 0.27815

C 4.50666 -1.06943 0.51027

C 5.18844 -2.26946 0.60374

C 4.70795 -3.39710 -0.07830

C 3.54442 -3.33038 -0.86028

C 2.85478 -2.13592 -0.96185

O -0.47278 3.12765 -0.86898

O 1.39119 4.09281 -0.06497

C 0.76941 5.38232 -0.27668

H 1.43411 0.94470 -2.02543

H 3.18163 1.57308 1.29341

H	3.37270	2.24810	-0.34083
H	4.86201	-0.19126	1.03823
H	6.08782	-2.34236	1.20499
H	5.24401	-4.33764	0.00150
H	3.19131	-4.21345	-1.38136
H	1.95478	-2.06860	-1.56339
H	1.50276	6.11099	0.06329
H	0.54460	5.52287	-1.33504
H	-0.15043	5.45687	0.30632
Ag	-1.80551	1.50560	-0.23989
H	0.56416	-0.21211	-0.98799
C	-1.71831	0.14736	1.62310
C	-2.93581	-0.35441	1.13863
C	-2.98835	-1.59497	0.43955
C	-1.77109	-2.34040	0.28578
C	-0.54739	-1.80451	0.76633
C	-0.48051	-0.56997	1.40192
H	-5.12055	-1.56001	0.07792
H	-1.70339	0.97325	2.33155
H	-3.86636	0.14372	1.40042
C	-4.20421	-2.12784	-0.05618
C	-1.83041	-3.59773	-0.37077
H	0.37173	-2.36896	0.64064
C	-3.02622	-4.08761	-0.84758
C	-4.22428	-3.35015	-0.69047
H	-0.91554	-4.17151	-0.48630
H	-3.05551	-5.05222	-1.34410

H -5.15811 -3.75497 -1.06547

O 0.67431 -0.02202 1.76827

H 0.78509 0.96144 1.17722

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Name: H Energy: -1056915.2710629

C 2.75590 -0.47597 0.12580

C 2.59831 -1.91827 0.41889

C 0.99849 2.45599 -0.00591

C 1.80500 0.13541 -0.93358

C 1.11615 0.96217 0.19981

C 2.27944 0.54872 1.17186

C 0.80491 3.27732 1.11511

C 0.63883 4.65269 0.97124

C 0.66542 5.23370 -0.29938

C 0.85411 4.42616 -1.41982

C 1.01534 3.04690 -1.27281

O 2.47931 -2.43853 1.52815

O 2.59700 -2.66829 -0.71372

C 2.49117 -4.08304 -0.52214

H 1.18344 -0.58385 -1.46856

H 2.96491 1.38647 1.30174

H 2.01451 0.15636 2.15093

H 0.75782 2.83051 2.10417

H 0.48268 5.27021 1.85059

H 0.53516 6.30569 -0.41296

H 0.86510 4.86526 -2.41316

H 1.12332 2.42838 -2.15725

H	2.53899	-4.51850	-1.51994
H	3.31191	-4.45216	0.09843
H	1.54477	-4.34270	-0.04140
H	2.29992	0.77027	-1.66694
C	-2.65849	1.85045	-2.03443
C	-1.85328	1.73968	-0.90410
C	-1.28661	0.51472	-0.54667
C	-1.57376	-0.62667	-1.34787
C	-2.36594	-0.49141	-2.50921
C	-2.89874	0.73773	-2.85261
H	-0.65563	1.03794	1.45530
H	-3.10130	2.81029	-2.28167
H	-1.68207	2.60557	-0.27687
C	-0.32890	0.40661	0.61438
C	-1.13917	-1.91726	-0.91424
H	-2.58396	-1.37508	-3.10062
H	-3.52266	0.83490	-3.73558
C	-0.51444	-2.08823	0.30564
C	-0.26515	-0.98685	1.12865
H	-1.34672	-2.77540	-1.54374
H	-0.29952	-3.08326	0.68184
O	0.26372	-1.12937	2.34958
H	0.86667	-1.90232	2.36329
Ag	4.86513	-0.37393	-0.33361
C	-4.40536	-3.05929	-0.61115
C	-3.64809	-2.59442	0.45628
C	-3.73673	-1.24520	0.88898

C	-4.66099	-0.38000	0.20827
C	-5.41378	-0.87830	-0.86047
C	-5.28113	-2.19779	-1.28616
H	-2.30609	-1.38031	2.51830
H	-4.31767	-4.09632	-0.92351
H	-2.98840	-3.26951	0.99133
C	-2.90120	-0.72172	1.89893
C	-4.76633	0.98637	0.64048
H	-6.10181	-0.20928	-1.37126
H	-5.86674	-2.56202	-2.12467
C	-3.95022	1.49167	1.59988
C	-2.91140	0.68216	2.23745
H	-5.50423	1.61870	0.15134
H	-4.00010	2.53322	1.90277
O	-2.04673	1.20710	2.98364

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Name: TS6 Energy: -1056911.2185315

C	-2.64753	-0.80364	-0.11643
C	-2.13078	-2.18733	-0.21238
C	-1.48067	2.42620	-0.29871
C	-1.98989	0.13127	0.92465
C	-1.30861	0.91940	-0.25222
C	-2.30164	0.19241	-1.23596
C	-1.10109	3.10642	-1.46614
C	-1.26569	4.48496	-1.57219
C	-1.81519	5.21331	-0.51442
C	-2.19411	4.54816	0.65019

C	-2.02865	3.16513	0.75504
O	-1.84566	-2.79837	-1.24407
O	-1.99446	-2.76376	1.00761
C	-1.51679	-4.11419	1.00882
H	-1.32114	-0.35216	1.63854
H	-3.12269	0.87529	-1.45606
H	-1.91859	-0.21127	-2.16794
H	-0.64291	2.55773	-2.28164
H	-0.95433	4.99204	-2.48034
H	-1.94010	6.28887	-0.59638
H	-2.61353	5.10292	1.48459
H	-2.30180	2.67341	1.68212
H	-1.51696	-4.42343	2.05374
H	-2.17216	-4.75746	0.41613
H	-0.50525	-4.16435	0.59954
H	-2.70465	0.73865	1.47700
C	1.75571	2.35132	2.59184
C	1.06427	2.08590	1.42040
C	0.97901	0.77858	0.90723
C	1.65333	-0.25961	1.60770
C	2.35714	0.03156	2.79851
C	2.40452	1.31953	3.29180
H	0.73053	1.23899	-1.17541
H	1.81520	3.37231	2.95675
H	0.61837	2.89986	0.86758
C	0.22246	0.50050	-0.35383
C	1.65659	-1.58425	1.07425

H	2.88029	-0.77513	3.30414
H	2.95295	1.53807	4.20281
C	1.10422	-1.85211	-0.15052
C	0.47417	-0.82894	-0.88587
H	2.17076	-2.36738	1.62266
H	1.20683	-2.83036	-0.60762
O	0.01900	-1.08912	-2.12588
H	-0.43612	-1.95918	-2.12533
Ag	-4.75815	-1.18248	0.14654
C	5.17444	-2.90773	-0.77090
C	4.23624	-2.16502	-1.45745
C	4.04276	-0.78574	-1.17967
C	4.84799	-0.17856	-0.16199
C	5.80584	-0.96256	0.52005
C	5.96972	-2.30283	0.22785
H	2.44308	-0.46524	-2.61235
H	5.30615	-3.96169	-0.99908
H	3.62431	-2.62838	-2.22725
C	3.04110	-0.02261	-1.82422
C	4.64826	1.20667	0.13143
H	6.41368	-0.49013	1.28789
H	6.70804	-2.89279	0.76277
C	3.66555	1.92304	-0.48612
C	2.79555	1.31873	-1.47157
H	5.27592	1.67050	0.88839
H	3.47624	2.96144	-0.23558
O	1.75254	1.95843	-1.90793

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Name: I Energy: -1056962.0737626

C	0.57908	1.94175	-0.47477
C	0.50106	3.39983	-0.59970
C	0.77218	-1.02446	-0.36796
C	1.33064	1.15358	-1.55977
C	1.77294	0.13173	-0.44809
C	1.49453	1.28682	0.57554
C	-0.01243	-1.28971	0.76353
C	-0.90914	-2.36161	0.78611
C	-1.04423	-3.18760	-0.32671
C	-0.27047	-2.93485	-1.46133
C	0.62697	-1.86923	-1.48029
O	0.44008	4.04140	-1.63804
O	0.49563	4.02182	0.62795
C	0.39324	5.44505	0.57649
H	2.18918	1.72157	-1.93218
H	1.08701	1.04739	1.55834
H	2.41309	1.86584	0.73116
H	0.07422	-0.66428	1.64501
H	-1.50619	-2.54189	1.67384
H	-1.74819	-4.01179	-0.31181
H	-0.36380	-3.57355	-2.33542
H	1.22819	-1.68101	-2.36322
H	0.45306	5.78764	1.61076
H	1.20483	5.87790	-0.01461
H	-0.55702	5.75554	0.12934

Ag	-1.45200	1.25171	-0.30562
H	0.79221	0.74615	-2.41501
C	-3.81294	1.32988	0.16748
C	-3.93257	0.38192	-0.84583
C	-4.11062	-0.99403	-0.54344
C	-4.18944	-1.38503	0.83303
C	-4.03641	-0.41068	1.85189
C	-3.84876	0.91660	1.53694
H	-4.18152	-1.66613	-2.59647
H	-3.84132	2.39119	-0.07075
H	-3.95279	0.70455	-1.88286
C	-4.25269	-1.97501	-1.55750
C	-4.42079	-2.75307	1.13481
H	-4.07231	-0.70464	2.89565
C	-4.57109	-3.67959	0.12796
C	-4.48401	-3.29108	-1.23114
H	-4.48269	-3.05513	2.17623
H	-4.75523	-4.72067	0.37545
H	-4.59729	-4.03575	-2.01227
O	-3.71337	1.81913	2.54551
H	-3.45305	2.67617	2.18251
C	5.18663	-1.00731	-1.83297
C	5.90370	-1.29613	-0.70268
C	5.29000	-1.20935	0.57064
C	3.92114	-0.78338	0.65998
C	3.19788	-0.41058	-0.52274
C	3.83709	-0.58525	-1.74369

H	7.04254	-1.86235	1.64678
H	5.64499	-1.09939	-2.81587
H	6.94086	-1.61091	-0.77243
C	6.00521	-1.55344	1.74685
C	3.33248	-0.77311	1.95584
C	4.04799	-1.12505	3.07827
C	5.40416	-1.51014	2.98243
H	2.29350	-0.50473	2.06210
H	3.56034	-1.11092	4.04871
H	5.95923	-1.77913	3.87581
O	3.14195	-0.35883	-2.90637
H	3.74977	-0.43519	-3.65203

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Name: TS7 Energy: -1056938.5662287

C	-0.05794	1.89009	-0.11702
C	-0.70506	3.01845	-0.60667
C	1.00802	-0.64384	1.27680
C	0.12654	0.54296	-0.82765
C	1.37413	0.27057	0.10766
C	1.32464	1.80167	0.49084
C	0.25182	-0.17611	2.36350
C	-0.05280	-1.00688	3.44207
C	0.37457	-2.33495	3.45405
C	1.10128	-2.82329	2.36677
C	1.41341	-1.98612	1.29460
O	-1.80199	3.01552	-1.29103
O	-0.13805	4.21831	-0.29838

C	-0.93137	5.37742	-0.55445
H	0.42126	0.66336	-1.87516
H	1.44120	2.02884	1.55621
H	2.08343	2.37867	-0.05332
H	-0.10957	0.84545	2.35946
H	-0.64082	-0.61734	4.26673
H	0.14322	-2.97995	4.29664
H	1.44337	-3.85477	2.35848
H	1.99916	-2.37410	0.46951
H	-0.33581	6.22391	-0.20796
H	-1.15186	5.48347	-1.61946
H	-1.87853	5.33656	-0.00534
Ag	-2.63931	1.29967	-0.14750
H	-0.62625	-0.24790	-0.79063
C	-4.08745	-0.32483	0.76252
C	-4.07158	-0.62521	-0.60727
C	-3.17840	-1.60875	-1.12403
C	-2.31707	-2.29472	-0.20629
C	-2.38053	-2.00821	1.18194
C	-3.24436	-1.05233	1.66336
H	-3.75856	-1.37499	-3.19380
H	-4.86890	0.31818	1.16374
H	-4.80235	-0.16921	-1.26859
C	-3.10151	-1.90281	-2.50827
C	-1.39048	-3.23742	-0.72168
H	-1.71903	-2.51960	1.86961
C	-1.33144	-3.49407	-2.07233

C	-2.19595	-2.82874	-2.97484
H	-0.71126	-3.72520	-0.03116
H	-0.61143	-4.21271	-2.45218
H	-2.13911	-3.04650	-4.03671
O	-3.27974	-0.80492	3.00142
H	-3.88755	-0.07626	3.18119
C	3.75464	-1.34259	-2.45590
C	4.98983	-0.93794	-2.02216
C	5.11816	-0.21252	-0.81165
C	3.93418	0.13339	-0.07821
C	2.63826	-0.19958	-0.59449
C	2.58720	-0.99707	-1.72998
H	7.27350	-0.11354	-0.88797
H	3.65478	-1.93602	-3.36290
H	5.88270	-1.19220	-2.58610
C	6.39386	0.14803	-0.30535
C	4.10934	0.77592	1.17996
C	5.36189	1.09572	1.65364
C	6.52036	0.79650	0.90048
H	3.24294	0.98738	1.79052
H	5.46054	1.57698	2.62226
H	7.50124	1.06276	1.28225
O	1.37470	-1.49096	-2.14179
H	1.48465	-1.92946	-2.99409

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Name: TS8 Energy: -1056940.9919921

C	-0.23006	1.60603	-0.45586

C	0.19983	2.91016	-0.10988
C	-1.30543	-1.27589	-0.89487
C	-0.34242	0.52447	0.63828
C	-1.63938	-0.02368	-0.08341
C	-1.66706	1.32093	-0.89926
C	-1.09748	-1.26898	-2.27768
C	-0.75970	-2.44052	-2.96121
C	-0.61816	-3.64323	-2.27314
C	-0.81598	-3.66294	-0.88933
C	-1.15525	-2.49436	-0.21166
O	1.16014	3.20391	0.68139
O	-0.45887	3.92366	-0.70301
C	0.06385	5.24329	-0.50884
H	-0.56595	0.94936	1.61926
H	-1.86339	1.26056	-1.97182
H	-2.39780	2.01659	-0.47388
H	-1.16021	-0.34368	-2.83522
H	-0.59543	-2.40260	-4.03389
H	-0.35339	-4.55279	-2.80378
H	-0.70980	-4.59286	-0.33709
H	-1.28948	-2.51722	0.86405
H	-0.57940	5.89921	-1.09587
H	0.03256	5.52602	0.54611
H	1.09625	5.30906	-0.86335
Ag	2.75449	1.75770	0.59076
H	0.45310	-0.21433	0.75506
C	3.71153	0.66088	-1.19639

C	4.60760	0.03682	-0.31864
C	4.33112	-1.25571	0.20574
C	3.12253	-1.90736	-0.21327
C	2.21853	-1.24954	-1.08228
C	2.45195	0.03784	-1.55437
H	6.12844	-1.41748	1.39846
H	3.99497	1.56724	-1.72812
H	5.56451	0.50541	-0.10089
C	5.21304	-1.91997	1.09621
C	2.84680	-3.20681	0.29584
H	1.29822	-1.74447	-1.36042
C	3.72070	-3.82330	1.16157
C	4.91698	-3.17915	1.56636
H	1.92669	-3.69368	-0.01187
H	3.49567	-4.81587	1.54077
H	5.59713	-3.68280	2.24600
O	1.55933	0.74435	-2.24281
H	0.74769	1.12328	-1.52578
C	-3.90649	-0.75082	2.96057
C	-5.16448	-0.56798	2.45146
C	-5.34117	-0.29579	1.07242
C	-4.18427	-0.17272	0.23214
C	-2.86507	-0.27233	0.79107
C	-2.76493	-0.62607	2.12953
H	-7.49647	-0.25343	1.17783
H	-3.76706	-0.99357	4.01248
H	-6.03692	-0.65232	3.09285

C	-6.63954	-0.16786	0.51464
C	-4.41049	0.01692	-1.16047
C	-5.68338	0.12030	-1.67529
C	-6.81521	0.04349	-0.83248
H	-3.56796	0.04626	-1.83528
H	-5.81777	0.25410	-2.74465
H	-7.81292	0.13463	-1.25066
O	-1.52770	-0.88920	2.66948
H	-1.63645	-1.08504	3.60829

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Name: K Energy: -1056959.2101168

C	-0.25527	1.59270	-0.39005
C	0.17601	2.91583	0.14544
C	-1.34215	-1.21891	-0.91557
C	-0.47778	0.52323	0.72639
C	-1.72894	-0.00523	-0.06960
C	-1.71212	1.36710	-0.83076
C	-0.90089	-1.11893	-2.23784
C	-0.49795	-2.25386	-2.94603
C	-0.52727	-3.50746	-2.34295
C	-0.95624	-3.61951	-1.01710
C	-1.35964	-2.48782	-0.31378
O	1.34274	3.20465	0.46362
O	-0.80327	3.78620	0.34349
C	-0.44478	5.05308	0.93464
H	-0.76758	0.99002	1.66751
H	-1.89924	1.37541	-1.90427

H	-2.39486	2.06900	-0.35155
H	-0.81003	-0.15687	-2.72374
H	-0.13389	-2.14075	-3.96171
H	-0.20631	-4.38799	-2.89100
H	-0.97659	-4.59060	-0.53068
H	-1.67968	-2.58288	0.71783
H	-1.37714	5.61085	1.00222
H	-0.01146	4.89703	1.92447
H	0.27569	5.57380	0.30131
Ag	2.96978	1.81859	-0.07943
H	0.33389	-0.18250	0.89629
C	4.03751	0.30721	-1.33324
C	4.87078	-0.25517	-0.34075
C	4.44170	-1.32345	0.46094
C	3.11711	-1.85649	0.22416
C	2.29332	-1.32681	-0.77354
C	2.69590	-0.26229	-1.64821
H	6.24734	-1.47256	1.64600
H	4.47309	0.96569	-2.08437
H	5.87746	0.13708	-0.20890
C	5.25411	-1.88663	1.48727
C	2.68341	-2.94277	1.05350
H	1.32526	-1.77746	-0.94970
C	3.49442	-3.45448	2.03161
C	4.79999	-2.92558	2.25786
H	1.69062	-3.34968	0.88184
H	3.14418	-4.27985	2.64584

H	5.42637	-3.35084	3.03573
O	1.97507	0.22302	-2.56455
H	0.46537	1.23980	-1.13855
C	-4.15244	-0.75875	2.83721
C	-5.37995	-0.57781	2.25689
C	-5.48109	-0.29874	0.87112
C	-4.27995	-0.17314	0.09660
C	-2.99717	-0.27072	0.73126
C	-2.96659	-0.62433	2.07207
H	-7.63915	-0.25463	0.85339
H	-4.07219	-1.00512	3.89420
H	-6.28682	-0.66821	2.84761
C	-6.74547	-0.16725	0.24104
C	-4.42421	0.01594	-1.30683
C	-5.66618	0.12325	-1.89195
C	-6.84344	0.04906	-1.11340
H	-3.54425	0.02955	-1.93398
H	-5.74075	0.25410	-2.96741
H	-7.81564	0.14256	-1.58720
O	-1.75533	-0.86878	2.67223
H	-1.90565	-1.10710	3.59535

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Name: J Energy: -1056941.6007955

C	0.22146	1.64722	0.37039
C	-0.29401	2.90031	0.05380
C	1.33011	-1.20409	0.95408
C	0.31732	0.50828	-0.64870

C	1.63385	0.01509	0.08325
C	1.64888	1.39613	0.83953
C	1.13600	-1.13787	2.33769
C	0.82452	-2.28161	3.07893
C	0.69824	-3.51761	2.44928
C	0.88484	-3.59804	1.06595
C	1.19485	-2.45636	0.33062
O	-1.27505	3.15325	-0.75013
O	0.29297	3.96010	0.66436
C	-0.34569	5.22935	0.51666
H	0.51518	0.86869	-1.66140
H	1.84530	1.37844	1.91471
H	2.38141	2.07821	0.39280
H	1.19696	-0.18778	2.85255
H	0.67159	-2.19654	4.15062
H	0.45617	-4.40621	3.02442
H	0.79319	-4.55506	0.55909
H	1.31900	-2.52717	-0.74413
H	0.25745	5.92822	1.09803
H	-0.37679	5.54022	-0.53071
H	-1.36818	5.20465	0.90682
Ag	-2.79944	1.67614	-0.64492
H	-0.46790	-0.25103	-0.70710
C	-3.73440	0.60718	1.18946
C	-4.56464	-0.04306	0.26995
C	-4.22083	-1.33314	-0.23285
C	-3.01931	-1.94848	0.24890

C	-2.17798	-1.25407	1.15859
C	-2.48254	0.02044	1.59516
H	-5.94923	-1.55367	-1.51422
H	-4.05590	1.51707	1.69096
H	-5.52760	0.38908	0.00932
C	-5.03599	-2.02628	-1.16223
C	-2.67686	-3.23870	-0.23525
H	-1.25299	-1.71172	1.48159
C	-3.48673	-3.88588	-1.14176
C	-4.67751	-3.27888	-1.60895
H	-1.75867	-3.69418	0.12111
H	-3.21296	-4.87231	-1.50390
H	-5.30719	-3.80468	-2.31976
O	-1.63488	0.77172	2.33382
H	-0.88692	1.10632	1.70284
C	3.87919	-0.82549	-2.94826
C	5.13943	-0.59477	-2.46502
C	5.32695	-0.25112	-1.10350
C	4.17766	-0.10531	-0.25644
C	2.85370	-0.25550	-0.79295
C	2.74521	-0.67964	-2.11027
H	7.47984	-0.17858	-1.23741
H	3.73199	-1.12387	-3.98471
H	6.00579	-0.69564	-3.11226
C	6.62927	-0.07422	-0.56874
C	4.41673	0.15830	1.12190
C	5.69343	0.30787	1.61546

C	6.81679	0.20688	0.76392
H	3.58135	0.21059	1.80414
H	5.83759	0.49836	2.67492
H	7.81753	0.33517	1.16478
O	1.50793	-0.99696	-2.62051
H	1.60825	-1.22169	-3.55378

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